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Thermal fluctuations and conformational effects on NMR parameters in b-O-4 lignin dimer from QM/MM and machine-learning approaches.

aSonia Milena Aguilera-Segura, bDominik Dragún, aRobin Gaumard, aFrancesco Di Renzo, cIrina Malkin Ondík ,aTzonka Mineva*

a.ICGM, Univ Montpellier, CNRS, ENSCM, Montpellier, France
b.FIIT STU in Bratislava, Ilkovičova 2, 842 16 Bratislava, Slovakia
c.MicroStep-MIS spol. s.r.o. Čavojského 1, 84104 Bratislava, Slovakia

* To whom correspondence should be addressed
Email: tzonka.mineva@enscm.fr

SUPPORTING FILE 5

Number of atoms, Chemical element, Cartesian coordinates in Å, and isotropic shielding in ppm in G-b-G in acetonitrile solvent.

55
name = lig-ACN-frame_1

C	3.519069	2.634426	0.151619	58.35
H	3.067533	3.573584	0.375403	25.26
C	3.909586	0.327943	0.739816	52.40
H	3.769428	-0.579660	1.337479	22.23
C	4.643621	0.136556	-0.467837	7.99
O	5.176094	-1.107569	-0.816178	184.41
C	5.405816	-2.083093	0.261318	122.98
H	5.859596	-1.671542	1.163570	26.87
H	6.055342	-2.748763	-0.213849	26.85
H	4.455441	-2.556956	0.544438	25.01
C	4.898547	1.259247	-1.319347	8.65
O	5.567664	1.143922	-2.530985	178.51
H	6.377406	0.686280	-2.490213	32.83
C	4.244735	2.486949	-1.033610	56.53
H	4.385762	3.418741	-1.599748	19.07
C	3.309245	1.583864	1.093298	-11.46
C	2.492161	1.761170	2.377224	98.10
H	2.770533	2.732199	2.691652	24.80
O	2.772856	0.849705	3.405519	331.36
H	2.168193	0.154300	3.416848	29.80
C	1.028615	1.950535	2.004337	72.72
H	0.982599	2.634106	1.058234	20.86
C	0.047262	2.500722	3.168582	96.41
O	0.391113	3.831212	3.681857	268.56
H	0.528214	4.545192	2.946871	29.30
H	0.243177	1.765331	4.047316	24.64
H	-1.026499	2.571501	2.783375	24.45
C	-2.482118	-1.129548	0.568002	64.62
H	-3.268458	-1.738709	1.071003	22.88
C	-1.949078	0.503724	-1.165462	80.37
H	-2.032242	0.803095	-2.205168	21.38
C	-0.828800	0.964011	-0.414806	20.61
O	-0.029074	2.021819	-0.794211	240.96
C	-0.692015	3.203846	-1.338293	90.30
H	0.135213	3.848925	-1.787390	25.33
H	-1.296330	2.833585	-2.280387	24.78
H	-1.449868	3.735520	-0.561092	23.55
C	-0.535256	0.368659	0.854314	21.60

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 O       0.492120     0.636970     1.690104     220.24
 C      -1.377624    -0.689831     1.307815      35.93
 H      -1.158421    -1.203844     2.281488      18.08
 C      -2.768509    -0.541860    -0.724632      68.68
 C      -3.842703    -1.153313    -1.703825      53.34
 H      -3.913858    -0.518185    -2.548570      30.50
 O      -3.409291    -2.521371    -2.000037     210.04
 H      -2.467564    -2.404492    -2.310174      25.55
 C      -5.252045    -1.228491    -1.024149      99.76
 H      -5.167012    -1.734837    -0.013043      27.29
 O      -5.781312     0.113031    -0.847709     306.57
 H      -5.409801     0.429859    -0.033429      31.36
 C      -6.344606    -1.973617    -1.866778     103.92
 O      -6.075179    -3.396686    -2.096233     249.79
 H      -5.142291    -3.422884    -2.222677      32.43
 H      -6.419926    -1.389711    -2.865025      28.19
 H      -7.222030    -1.809147    -1.258373      29.49
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name = lig-ACN-frame_2
 C       3.516840     2.617129     0.165723      52.32
 H       3.156720     3.651933     0.387986      23.76
 C       3.932183     0.292635     0.740835      89.55
 H       3.702590    -0.508143     1.390471      21.92
 C       4.638330     0.172536    -0.444504      -0.70
 O       5.178866    -1.069954    -0.821541     189.19
 C       5.419154    -2.092697     0.185414     125.02
 H       5.868359    -1.663534     1.100199      27.62
 H       6.157046    -2.734415    -0.229147      27.45
 H       4.541887    -2.701577     0.419755      26.44
 C       4.844901     1.261598    -1.341757       2.06
 O       5.587763     1.182230    -2.547906      68.25
 H       6.305366     0.491848    -2.365555      25.65
 C       4.279967     2.509490    -1.010080      28.33
 H       4.436781     3.357253    -1.722769      21.67
 C       3.364124     1.537699     1.056293      -8.20
 C       2.516030     1.816415     2.317792      86.22
 H       2.846893     2.731958     2.757035      25.30
 O       2.823773     0.875964     3.424543     256.89
 H       2.236127     0.065684     3.327879      25.78
 C       0.958054     2.013943     2.027055      72.05
 H       0.872884     2.736492     1.120001      19.89
 C       0.095556     2.507585     3.151524     103.60
 O       0.407145     3.789146     3.732809     257.58
 H       0.310098     4.415507     2.844021      27.58
 H       0.022923     1.760821     4.058064      24.88
 H      -0.973693     2.431302     2.754393      24.88
 C      -2.525068    -1.075924     0.551736      65.83
 H      -3.183203    -1.814148     0.972130      22.75
 C      -1.916188     0.503072    -1.207216      48.72
 H      -2.026565     0.940960    -2.190665      18.09
 C      -0.886557     0.989826    -0.373583      37.06
 O      -0.015024     2.049831    -0.822128     235.51
 C      -0.708915     3.171321    -1.406835     102.39
 H       0.098659     3.963289    -1.702341      24.97
 H      -1.410223     2.937544    -2.276271      26.28
 H      -1.303376     3.746149    -0.557312      23.75
 C      -0.587874     0.340437     0.856139      31.39
 O       0.535720     0.610207     1.685361     181.79
 C      -1.396970    -0.702718     1.309604      39.21
 H      -1.106736    -1.117051     2.290541      17.75
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 C      -2.764192    -0.544825    -0.727330      63.94
 C      -3.792025    -1.138429    -1.624038      61.98
 H      -3.807666    -0.601997    -2.531637      30.18
 O      -3.432418    -2.521483    -2.020594     179.61
 H      -2.486736    -2.586673    -2.484366      23.84
 C      -5.245659    -1.251030    -1.059758     101.23
 H      -5.128042    -1.809095    -0.077513      28.29
 O      -5.771983     0.098280    -0.837569     266.82
 H      -5.790256     0.279127     0.164288      28.04
 C      -6.332380    -1.952841    -1.850910     109.40
 O      -6.112886    -3.360990    -2.101252     230.12
 H      -5.154751    -3.463596    -2.373115      31.20
 H      -6.547409    -1.389344    -2.836959      28.57
 H      -7.288420    -1.948194    -1.342026      29.59
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name = lig-ACN-frame_3
 C       3.550926     2.664481     0.177681      64.26
 H       2.989846     3.619651     0.525836      22.94
 C       3.897825     0.293814     0.775026      74.57
 H       3.850387    -0.514386     1.460965      23.84
 C       4.672956     0.138867    -0.449913     -38.77
 O       5.223632    -1.041717    -0.876183     178.85
 C       5.455367    -2.102370     0.104841     116.57
 H       5.773681    -1.633650     1.060285      26.50
 H       6.231681    -2.765605    -0.283759      26.88
 H       4.515490    -2.631124     0.295389      25.47
 C       4.811659     1.259304    -1.374591       6.71
 O       5.608453     1.189096    -2.524843     112.49
 H       6.160863     0.309874    -2.528275      18.45
 C       4.307462     2.508755    -1.007441      42.92
 H       4.509117     3.356225    -1.714395      26.51
 C       3.347155     1.564088     1.040763       3.19
 C       2.543570     1.873419     2.345593      84.15
 H       2.842992     2.882562     2.659041      25.31
 O       2.842183     0.918547     3.389227     247.40
 H       2.411604    -0.020969     3.078692      23.31
 C       0.998014     1.973148     2.016425      78.64
 H       0.799225     2.623630     1.119689      22.60
 C       0.054744     2.458885     3.208058     100.92
 O       0.412173     3.758447     3.746624     280.35
 H       0.597445     4.444238     3.069556      31.99
 H       0.220682     1.697487     4.086279      24.76
 H      -0.986019     2.558216     2.797062      25.76
 C      -2.558246    -1.087259     0.567339      52.58
 H      -3.000287    -2.008341     0.769451      21.94
 C      -1.896183     0.491951    -1.190174      24.89
 H      -2.153670     0.902304    -2.169478      19.48
 C      -0.875559     1.052225    -0.362941      39.87
 O      -0.042585     2.027525    -0.840626     237.78
 C      -0.724967     3.219630    -1.429501      97.81
 H       0.186174     3.891879    -1.772977      24.93
 H      -1.244486     2.961584    -2.371662      25.82
 H      -1.408847     3.672206    -0.652880      25.05
 C      -0.575878     0.387233     0.894984      33.84
 O       0.555112     0.620435     1.645017     224.77
 C      -1.450179    -0.697104     1.319481      48.30
 H      -1.310446    -1.225300     2.254627      23.11
 C      -2.734820    -0.509994    -0.718715      50.16
 C      -3.800614    -1.158717    -1.668424      71.11
 H      -3.937437    -0.500505    -2.500899      27.63
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 O      -3.462103    -2.550998    -2.044645     249.16
 H      -2.462316    -2.527593    -2.131779      27.29
 C      -5.231230    -1.230712    -1.007756      91.65
 H      -5.219757    -1.785304    -0.025651      29.12
 O      -5.749397     0.087504    -0.811830     286.65
 H      -5.726457     0.283982     0.203968      28.26
 C      -6.355950    -1.954186    -1.906813     100.71
 O      -6.136383    -3.355269    -2.115187     216.43
 H      -5.173644    -3.458462    -2.465271      29.29
 H      -6.500886    -1.362507    -2.874378      28.95
 H      -7.236351    -1.842328    -1.270015      29.70
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name = lig-ACN-frame_4
 C       3.583880     2.677953     0.168340      45.19
 H       3.194865     3.775853     0.234284      24.74
 C       3.929251     0.341100     0.725571      64.09
 H       3.813973    -0.483125     1.444205      24.45
 C       4.629954     0.157055    -0.457829      16.88
 O       5.315385    -1.049002    -0.954450     178.32
 C       5.464001    -2.085177     0.044814     117.26
 H       5.860143    -1.764438     1.043521      26.33
 H       6.261902    -2.744671    -0.406850      25.88
 H       4.539508    -2.679997     0.161430      25.90
 C       4.838287     1.234020    -1.331323       8.21
 O       5.602783     1.169342    -2.496147     146.27
 H       6.002919     0.321163    -2.549398      27.25
 C       4.297964     2.527853    -1.015952      40.73
 H       4.500763     3.454128    -1.590259      18.34
 C       3.321410     1.630414     1.072469     -28.86
 C       2.523950     1.865345     2.330366      85.85
 H       2.804631     2.851182     2.808243      24.85
 O       2.845870     0.951436     3.332549     278.42
 H       2.447768     0.063404     3.122309      26.15
 C       1.000696     1.949291     2.031417      92.89
 H       0.981181     2.666059     1.215158      24.65
 C       0.079668     2.419213     3.224298     106.76
 O       0.441761     3.744085     3.779446     304.34
 H       0.700560     4.153122     3.009661      35.58
 H       0.153392     1.671627     4.094715      25.98
 H      -1.001065     2.330920     2.959115      27.38
 C      -2.510060    -1.158584     0.519901      65.07
 H      -3.156923    -1.879400     0.934203      25.79
 C      -1.936361     0.529821    -1.129670      55.93
 H      -1.885093     0.886029    -2.175423      20.76
 C      -0.883153     1.007960    -0.346255      11.44
 O      -0.065295     2.063191    -0.861506     237.63
 C      -0.690417     3.233086    -1.457307     109.68
 H       0.152438     4.030893    -1.563793      25.46
 H      -1.136053     2.987619    -2.391824      27.44
 H      -1.461377     3.726474    -0.855420      26.67
 C      -0.628300     0.424843     0.916085      25.15
 O       0.583633     0.616891     1.618356     222.56
 C      -1.463055    -0.623404     1.356473      42.80
 H      -1.102805    -1.130492     2.228209      17.92
 C      -2.795935    -0.568727    -0.753069      54.09
 C      -3.860538    -1.158144    -1.675523      68.01
 H      -3.883505    -0.634747    -2.621266      27.35
 O      -3.457058    -2.540076    -2.048365     231.38
 H      -2.535957    -2.670971    -2.047342      29.73
 C      -5.264868    -1.254357    -1.009539     100.86
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 H      -5.108483    -1.800650    -0.051291      28.31
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 H      -5.292150     0.456016     0.026162      30.02
 C      -6.325302    -1.912284    -1.896098     104.66
 O      -6.157442    -3.373131    -2.146713     239.37
 H      -5.237048    -3.442241    -2.389364      32.02
 H      -6.355997    -1.367656    -2.885355      28.12
 H      -7.347601    -1.801106    -1.476582      28.16
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name = lig-ACN-frame_5
 C       3.574954     2.737594     0.150102      63.51
 H       3.198948     3.725064     0.537531      24.82
 C       3.917324     0.401190     0.722079      44.44
 H       3.652080    -0.456186     1.416944      22.91
 C       4.647279     0.146788    -0.527038      -7.81
 O       5.349600    -0.978638    -0.947061     172.97
 C       5.497591    -2.129123    -0.038787     109.62
 H       5.846692    -1.669550     0.926164      24.55
 H       6.281640    -2.874491    -0.444334      24.53
 H       4.512403    -2.626610     0.136486      24.55
 C       4.878997     1.307104    -1.339229      15.74
 O       5.579894     1.140852    -2.486918     130.28
 H       6.061287     0.289477    -2.372013      28.28
 C       4.328236     2.521067    -1.032257      81.49
 H       4.574381     3.248070    -1.798410      20.47
 C       3.387053     1.654237     1.010538      15.31
 C       2.485440     1.870686     2.310598      75.98
 H       2.766886     2.933086     2.665540      24.29
 O       2.862865     0.895419     3.349420     277.39
 H       2.310092     0.160865     3.278771      29.95
 C       0.957406     1.986360     2.051129      87.35
 H       0.689160     2.642049     1.283225      25.01
 C       0.144800     2.360941     3.279860     112.21
 O       0.476059     3.683420     3.756817     266.06
 H       0.541544     4.436304     3.052649      30.76
 H       0.312990     1.674527     4.113841      26.81
 H      -0.875127     2.411982     2.877780      27.12
 C      -2.463330    -1.153169     0.529895      65.71
 H      -3.061167    -1.943286     0.988275      24.46
 C      -2.018607     0.507344    -1.137947      47.50
 H      -2.223015     0.938795    -2.148577      20.61
 C      -0.925035     1.048569    -0.366713      30.67
 O      -0.068761     2.062856    -0.832166     230.75
 C      -0.688454     3.258001    -1.483847     113.75
 H       0.153969     4.013545    -1.442249      25.84
 H      -0.950363     3.170807    -2.498118      27.64
 H      -1.461432     3.525048    -0.838827      27.69
 C      -0.615143     0.455035     0.919073      47.02
 O       0.577354     0.611952     1.592736     201.41
 C      -1.464449    -0.616545     1.342668      41.48
 H      -1.311463    -1.027302     2.328215      17.16
 C      -2.783690    -0.585244    -0.735872      66.95
 C      -3.847605    -1.192436    -1.685738      49.28
 H      -4.015375    -0.489179    -2.528483      27.73
 O      -3.476761    -2.555400    -2.033553     223.10
 H      -2.490494    -2.474117    -2.261202      25.27
 C      -5.274113    -1.233019    -1.006452      95.97
 H      -5.265311    -1.837179    -0.085152      27.71
 O      -5.719061     0.122388    -0.710380     313.67
 H      -5.159295     0.443869     0.008115      29.57
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 C      -6.323487    -1.911382    -1.947098     104.37
 O      -6.175204    -3.338122    -2.158427     245.65
 H      -5.228108    -3.557364    -2.225360      31.55
 H      -6.254134    -1.369179    -2.911438      28.64
 H      -7.359725    -1.765100    -1.525682      27.68
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name = lig-ACN-frame_6
 C       3.604554     2.793175     0.130942      52.17
 H       3.172410     3.761869     0.275830      25.02
 C       3.913099     0.350167     0.655342      71.58
 H       3.746211    -0.523965     1.372051      21.98
 C       4.675498     0.209541    -0.455910      -1.69
 O       5.363785    -0.945150    -0.937876     180.18
 C       5.499883    -2.096716    -0.071027     112.88
 H       5.948585    -1.952679     0.960057      26.39
 H       6.239893    -2.765370    -0.680688      25.27
 H       4.507186    -2.648120     0.034492      24.96
 C       4.866756     1.288213    -1.338719     -11.18
 O       5.595744     1.111502    -2.546308     102.76
 H       6.353635     0.383263    -2.472910      20.46
 C       4.345049     2.626499    -1.065303      35.98
 H       4.443161     3.496820    -1.683151      23.65
 C       3.364860     1.671617     1.003864     -47.79
 C       2.540245     1.865746     2.266561      72.97
 H       2.842747     2.855901     2.799112      23.71
 O       2.852003     0.880480     3.341218     240.85
 H       2.162140     0.110248     3.294561      23.77
 C       0.971505     1.946019     2.014031      88.43
 H       0.870967     2.673938     1.286910      26.04
 C       0.154943     2.345307     3.314106     117.90
 O       0.536750     3.662595     3.766856     252.50
 H       0.258932     4.234973     2.896591      28.95
 H       0.384255     1.704253     4.103368      27.96
 H      -0.922514     2.205937     3.216463      27.42
 C      -2.489636    -1.148589     0.570018      57.47
 H      -2.950964    -2.152913     0.811936      20.72
 C      -2.049685     0.554001    -1.164542      39.75
 H      -2.403904     1.063530    -2.080104      19.27
 C      -0.989175     1.078786    -0.387583      54.85
 O      -0.096654     2.056520    -0.824623     259.13
 C      -0.666703     3.271094    -1.437224     130.80
 H       0.055443     4.052600    -1.297280      26.79
 H      -0.821496     3.046102    -2.447450      28.03
 H      -1.588521     3.577991    -1.104007      29.64
 C      -0.632881     0.427341     0.833223      35.51
 O       0.546755     0.648044     1.589421     229.82
 C      -1.435124    -0.610064     1.345472      49.01
 H      -1.281591    -1.016148     2.355691      20.83
 C      -2.758497    -0.600789    -0.704692      58.01
 C      -3.847929    -1.192136    -1.597759      57.06
 H      -3.843586    -0.628500    -2.568145      27.18
 O      -3.484252    -2.562836    -2.039433     227.22
 H      -2.495811    -2.640948    -2.412393      23.52
 C      -5.278334    -1.245098    -1.001299      95.84
 H      -5.239348    -1.824984    -0.081504      30.35
 O      -5.693563     0.107272    -0.718002     288.60
 H      -5.533525     0.325107     0.290753      27.28
 C      -6.326358    -1.860478    -2.034080     103.34
 O      -6.192734    -3.311872    -2.140341     223.60
 H      -5.153070    -3.417577    -2.176809      28.53
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 H      -6.343162    -1.375767    -3.010496      29.52
 H      -7.321952    -1.660316    -1.539119      28.67
55
name = lig-ACN-frame_7
 C       3.623457     2.750333     0.118552      75.45
 H       3.161014     3.652271     0.311639      25.31
 C       3.862395     0.392209     0.694521      61.21
 H       3.724534    -0.446276     1.423216      21.86
 C       4.756662     0.269235    -0.481310     -34.17
 O       5.368908    -0.898054    -0.892962     162.53
 C       5.490348    -2.103960    -0.116696     109.59
 H       5.979135    -1.842859     0.875065      25.76
 H       6.197438    -2.806835    -0.700879      25.06
 H       4.467739    -2.625078     0.030735      24.82
 C       4.899173     1.386553    -1.424374      -0.84
 O       5.586381     1.117353    -2.595136     109.79
 H       6.398996     0.613387    -2.333023      23.15
 C       4.369188     2.622945    -1.081685      59.74
 H       4.611790     3.415068    -1.764202      22.73
 C       3.353464     1.648309     0.970521      16.56
 C       2.544269     1.815919     2.309807      87.42
 H       2.812801     2.893599     2.677733      24.15
 O       2.833030     0.887562     3.293316     286.93
 H       2.314755    -0.022603     3.058099      22.86
 C       1.005077     1.964934     2.012644      81.53
 H       0.826608     2.666085     1.252973      25.13
 C       0.217119     2.287607     3.347339     117.08
 O       0.555480     3.674688     3.751192     286.83
 H       0.488276     4.313007     3.060002      33.86
 H       0.572646     1.668655     4.077087      28.19
 H      -0.829471     2.209120     3.159913      28.68
 C      -2.468296    -1.167584     0.565882      67.30
 H      -3.106359    -2.010806     1.038937      24.10
 C      -2.103835     0.593305    -1.127841      46.80
 H      -2.179605     0.954181    -2.158045      19.86
 C      -0.992965     1.067859    -0.398553      22.78
 O      -0.143686     2.090253    -0.802438     256.47
 C      -0.660316     3.270671    -1.432572     128.52
 H      -0.019848     4.041436    -1.162331      28.27
 H      -0.666946     3.262509    -2.496710      28.20
 H      -1.551617     3.480720    -0.972977      29.33
 C      -0.648200     0.409049     0.814909      19.55
 O       0.499240     0.651017     1.542510     227.25
 C      -1.441418    -0.643113     1.347362      50.99
 H      -0.912481    -1.091443     2.221181      16.63
 C      -2.777961    -0.569550    -0.682259      51.18
 C      -3.798742    -1.207202    -1.592381      59.37
 H      -3.934706    -0.476776    -2.469322      26.19
 O      -3.507295    -2.597448    -2.027180     240.18
 H      -2.521302    -2.617057    -2.124074      26.57
 C      -5.284979    -1.258539    -1.051284     100.06
 H      -5.364082    -1.925463    -0.208178      28.81
 O      -5.689739     0.111839    -0.724704     267.96
 H      -5.711374     0.202158     0.279824      27.85
 C      -6.327961    -1.806129    -2.027022     105.58
 O      -6.189751    -3.270884    -2.118464     229.31
 H      -5.261713    -3.470655    -2.358756      31.71
 H      -6.149744    -1.330032    -2.973454      30.80
 H      -7.405856    -1.618793    -1.756986      28.57
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name = lig-ACN-frame_8
 C       3.593062     2.730454     0.103501      51.71
 H       3.277636     3.679525     0.422630      26.61
 C       3.969545     0.414060     0.631850      74.24
 H       3.796018    -0.464301     1.213090      21.95
 C       4.722760     0.306374    -0.478419      -1.40
 O       5.401854    -0.846611    -0.909471     186.96
 C       5.467115    -2.082576    -0.104554     110.30
 H       5.933265    -1.916243     0.920771      26.07
 H       6.130013    -2.795539    -0.677851      25.26
 H       4.406551    -2.537938     0.096288      24.50
 C       4.941956     1.347879    -1.388504       1.33
 O       5.589207     1.170033    -2.642315     130.62
 H       6.330010     0.586084    -2.623951      27.09
 C       4.395988     2.606692    -1.098218      43.96
 H       4.501311     3.515670    -1.699826      24.10
 C       3.330187     1.658028     0.977828     -23.72
 C       2.491717     1.855922     2.217360      78.74
 H       2.834463     2.807342     2.791542      23.56
 O       2.827105     0.837574     3.271020     240.39
 H       2.552811    -0.047552     2.990515      24.11
 C       0.975665     1.961135     2.021509      94.49
 H       0.767953     2.780080     1.328222      22.85
 C       0.315036     2.322711     3.312296     122.48
 O       0.560135     3.678937     3.769851     303.96
 H       0.714879     4.130215     2.966273      35.19
 H       0.549889     1.695691     4.113848      26.91
 H      -0.721058     2.184969     3.150931      27.48
 C      -2.482398    -1.168857     0.577287      81.97
 H      -3.156552    -2.008153     0.974674      19.34
 C      -2.097280     0.568157    -1.107815      68.92
 H      -2.320265     0.893323    -2.111619      19.02
 C      -0.999178     1.072492    -0.374267      22.84
 O      -0.141019     2.091430    -0.787109     243.61
 C      -0.688283     3.340511    -1.397120     121.20
 H      -0.038097     4.043460    -1.096901      28.42
 H      -0.699126     3.238954    -2.481377      27.15
 H      -1.697835     3.510658    -1.183801      29.73
 C      -0.661763     0.434650     0.859776      63.86
 O       0.542600     0.641589     1.515184     234.72
 C      -1.370373    -0.695648     1.299246       1.34
 H      -1.232638    -1.264721     2.249456      21.59
 C      -2.839710    -0.561093    -0.653372      62.59
 C      -3.873646    -1.215325    -1.643944      35.24
 H      -3.822060    -0.644612    -2.650189      25.93
 O      -3.489147    -2.595209    -1.989422     252.06
 H      -2.567395    -2.730931    -2.013345      27.88
 C      -5.302181    -1.227684    -1.025645      99.68
 H      -5.274722    -1.806446    -0.120265      28.98
 O      -5.708329     0.115008    -0.727733     295.82
 H      -5.341154     0.376021     0.107437      31.11
 C      -6.282688    -1.804703    -2.086436     108.34
 O      -6.218344    -3.234090    -2.117147     259.07
 H      -5.341841    -3.391026    -2.428261      33.07
 H      -6.141419    -1.381388    -3.058699      30.34
 H      -7.279679    -1.496200    -1.699966      28.61
55
name = lig-ACN-frame_9
 C       3.595782     2.759078     0.076052      66.24
 H       3.172410     3.774614     0.189336      23.90
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 C       3.990110     0.414976     0.665484      63.15
 H       3.853146    -0.401690     1.302786      21.15
 C       4.780630     0.250129    -0.566017      -5.63
 O       5.461787    -0.878900    -0.930759     194.48
 C       5.421348    -2.009915    -0.068982     114.31
 H       5.937375    -1.856236     0.927167      25.74
 H       5.997280    -2.751955    -0.641495      25.60
 H       4.327354    -2.425147    -0.000761      24.75
 C       4.974773     1.386215    -1.431244       9.31
 O       5.587588     1.253146    -2.672828      91.07
 H       6.139052     0.398668    -2.544815      23.89
 C       4.362750     2.611779    -1.046706      54.73
 H       4.579298     3.441287    -1.768961      19.31
 C       3.363295     1.653918     0.930295       4.80
 C       2.521327     1.809708     2.223207      82.09
 H       2.782361     2.855399     2.623281      23.95
 O       2.827603     0.822145     3.206166     299.55
 H       2.350916     0.042965     2.996183      27.92
 C       0.989992     1.958252     1.969201      79.95
 H       0.764504     2.671361     1.129883      21.29
 C       0.250048     2.333030     3.358892     112.56
 O       0.594040     3.696510     3.762522     259.02
 H       0.725977     4.397654     2.963438      28.61
 H       0.693612     1.646005     4.090232      26.21
 H      -0.785754     2.233798     3.268041      28.84
 C      -2.539317    -1.164060     0.550029      71.48
 H      -2.946511    -2.124816     0.897927      21.45
 C      -2.088686     0.525676    -1.110948      38.10
 H      -2.321513     1.106739    -1.978188      20.47
 C      -1.023715     1.083915    -0.320752      19.25
 O      -0.156755     2.113263    -0.783624     246.08
 C      -0.711299     3.354521    -1.379455     118.00
 H      -0.205074     4.178507    -1.061742      27.69
 H      -0.611720     3.250607    -2.469834      25.78
 H      -1.700273     3.561957    -0.973250      27.15
 C      -0.637900     0.413834     0.895903      36.73
 O       0.622593     0.658415     1.524353     213.89
 C      -1.388276    -0.755942     1.273721      50.48
 H      -1.015697    -1.102685     2.252599      21.74
 C      -2.880666    -0.570632    -0.697925      44.84
 C      -3.854923    -1.197597    -1.617858      72.60
 H      -3.988794    -0.545018    -2.576518      25.81
 O      -3.488125    -2.605985    -1.928255     225.54
 H      -2.494470    -2.505682    -2.149912      25.48
 C      -5.282348    -1.194987    -1.056739     103.16
 H      -5.342920    -1.859960    -0.206003      29.35
 O      -5.736685     0.158213    -0.728291     321.62
 H      -5.046447     0.572381    -0.147445      29.32
 C      -6.293546    -1.769273    -2.084189     105.38
 O      -6.259394    -3.237747    -2.144826     214.49
 H      -5.287946    -3.548141    -2.277481      30.55
 H      -6.088518    -1.317294    -3.038802      30.22
 H      -7.342837    -1.555535    -1.873547      28.28
55
name = lig-ACN-frame_10
 C       3.574082     2.774052     0.075001      42.11
 H       2.862643     3.654230     0.299339      21.07
 C       4.045375     0.412007     0.596932      70.79
 H       3.982648    -0.306512     1.369982      20.18
 C       4.801419     0.285722    -0.555137      -0.84
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 O       5.522844    -0.905379    -0.982973     191.76
 C       5.388439    -2.023344    -0.045087     113.36
 H       5.755340    -1.648738     0.951950      25.44
 H       5.953198    -2.882286    -0.337344      25.69
 H       4.271682    -2.251109     0.201545      24.29
 C       4.919992     1.400463    -1.440622      19.40
 O       5.595128     1.316795    -2.669922     143.05
 H       6.230868     0.486188    -2.746498      21.40
 C       4.400266     2.634769    -1.125925      59.42
 H       4.544318     3.543845    -1.773692      24.16
 C       3.400968     1.652576     0.902746     -16.56
 C       2.564670     1.837335     2.207056      82.03
 H       2.934410     2.751032     2.745375      24.15
 O       2.831619     0.814989     3.154502     276.37
 H       2.166239     0.013375     3.079778      21.01
 C       1.000895     1.979504     1.991336      72.84
 H       0.841397     2.810505     1.197523      20.95
 C       0.237152     2.366998     3.304670     113.21
 O       0.634316     3.723492     3.764848     248.80
 H       0.443197     4.289846     2.891075      29.75
 H       0.559870     1.720428     4.191410      25.74
 H      -0.805464     2.254476     3.251275      27.61
 C      -2.495970    -1.205734     0.537031      62.57
 H      -3.139678    -1.980548     0.849502      23.57
 C      -2.076180     0.604942    -1.080270      29.59
 H      -2.236094     0.954809    -2.092927      17.03
 C      -1.013132     1.091923    -0.294583      33.45
 O      -0.200595     2.124720    -0.758532     242.58
 C      -0.747779     3.335183    -1.337458     109.17
 H      -0.051131     4.043017    -1.001417      25.15
 H      -0.834706     3.395744    -2.449375      25.94
 H      -1.832625     3.409731    -1.039839      26.08
 C      -0.585228     0.368417     0.856405      30.92
 O       0.591221     0.590037     1.514199     230.02
 C      -1.400981    -0.706284     1.290794      51.01
 H      -1.108024    -1.455813     2.007416      16.51
 C      -2.797612    -0.553804    -0.677905      34.65
 C      -3.870863    -1.182871    -1.615180      41.97
 H      -3.809351    -0.588344    -2.604507      22.82
 O      -3.483953    -2.571382    -1.875939     216.39
 H      -2.490760    -2.698266    -2.235768      22.80
 C      -5.348612    -1.185931    -1.056835      97.11
 H      -5.366205    -1.755407    -0.126571      28.67
 O      -5.744878     0.189040    -0.777040     274.17
 H      -5.165897     0.526059     0.028850      25.42
 C      -6.324400    -1.761759    -2.114831     105.30
 O      -6.297121    -3.240238    -2.173212     240.21
 H      -5.297608    -3.402756    -2.120207      31.23
 H      -6.078073    -1.369950    -3.090833      30.14
 H      -7.293945    -1.429601    -1.800171      28.47
55
name = lig-ACN-frame_11
 C       3.565479     2.736217    -0.014813      56.14
 H       3.126417     3.791571     0.204712      24.24
 C       4.087923     0.445890     0.600686      54.17
 H       4.013293    -0.444319     1.253827      19.73
 C       4.865524     0.276668    -0.613408       0.18
 O       5.510159    -0.897846    -0.995087     187.05
 C       5.353681    -1.989015     0.047812     111.61
 H       5.815098    -1.757511     1.028241      26.44
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 H       5.916572    -2.778583    -0.404370      26.00
 H       4.268067    -2.325443     0.030854      25.23
 C       4.921260     1.408864    -1.486747       1.70
 O       5.612614     1.362869    -2.680888     148.42
 H       6.336409     0.726718    -2.548637      23.76
 C       4.334178     2.704122    -1.126271      51.67
 H       4.496876     3.523741    -1.848321      21.90
 C       3.413855     1.663112     0.901752      23.19
 C       2.570453     1.843945     2.183991      88.15
 H       2.846627     2.809713     2.618516      24.55
 O       2.855892     0.790596     3.163097     264.31
 H       2.320578    -0.072007     2.830841      22.35
 C       1.041023     1.958037     2.016081      75.04
 H       0.700543     2.658359     1.142797      19.56
 C       0.274677     2.406327     3.274377     108.62
 O       0.633487     3.730012     3.714153     311.65
 H       0.501021     4.382248     3.091721      34.62
 H       0.434058     1.620264     4.137926      25.02
 H      -0.725197     2.419054     2.931144      27.57
 C      -2.450611    -1.173677     0.519685      76.45
 H      -2.979494    -1.968456     0.920703      25.00
 C      -2.092983     0.635227    -1.063387      39.32
 H      -2.216238     1.089292    -2.062225      16.02
 C      -0.986925     1.090814    -0.325091      39.91
 O      -0.193036     2.121893    -0.729137     259.75
 C      -0.821454     3.315165    -1.292737     104.77
 H      -0.266415     4.237862    -1.020157      26.09
 H      -0.769815     3.118248    -2.382485      25.14
 H      -1.827443     3.615344    -0.815921      26.67
 C      -0.607331     0.335715     0.827827      37.25
 O       0.593591     0.584229     1.547019     205.27
 C      -1.380569    -0.764012     1.305196      31.05
 H      -1.035415    -1.115522     2.258495      14.64
 C      -2.790338    -0.518004    -0.690134      61.13
 C      -3.824699    -1.152794    -1.585691      44.88
 H      -3.955324    -0.590509    -2.574239      25.83
 O      -3.519014    -2.570284    -1.840899     229.89
 H      -2.539563    -2.559480    -1.983775      25.33
 C      -5.340379    -1.151660    -1.073863      92.46
 H      -5.461094    -1.781186    -0.172593      28.58
 O      -5.746424     0.215915    -0.824677     276.66
 H      -5.628937     0.382715     0.126590      28.65
 C      -6.367084    -1.765114    -2.132893     106.90
 O      -6.315418    -3.204441    -2.177859     261.39
 H      -5.423240    -3.470916    -2.186473      35.20
 H      -6.198742    -1.305962    -3.121981      30.19
 H      -7.390531    -1.538166    -1.921488      28.76
55
name = lig-ACN-frame_12
 C       3.520897     2.768325    -0.003536      44.44
 H       3.095974     3.770491     0.280020      21.56
 C       4.132321     0.479511     0.568190      61.28
 H       3.937138    -0.363894     1.318015      16.11
 C       4.829353     0.353160    -0.617817      12.54
 O       5.452904    -0.894214    -0.911525     199.79
 C       5.364832    -1.966462     0.003840     112.11
 H       5.707390    -1.651844     1.002350      27.48
 H       5.999584    -2.769196    -0.361465      25.88
 H       4.317908    -2.291077     0.214204      27.52
 C       4.952150     1.464554    -1.526497      25.66
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 O       5.681250     1.390018    -2.718827     124.79
 H       6.462060     0.827360    -2.653535      24.21
 C       4.309668     2.613503    -1.220052      49.63
 H       4.438972     3.489587    -1.815617      23.66
 C       3.422482     1.664396     0.868728     -10.93
 C       2.588497     1.790852     2.192070      93.83
 H       2.867401     2.699271     2.674465      24.03
 O       2.885646     0.803525     3.160885     313.01
 H       2.629145    -0.070505     2.879102      26.40
 C       1.059423     1.901369     1.929119      84.56
 H       0.995282     2.699101     1.090563      17.74
 C       0.246396     2.424732     3.184703     106.15
 O       0.646634     3.745554     3.705982     293.77
 H       0.743674     4.257554     2.873926      31.18
 H       0.396422     1.757441     4.149445      23.64
 H      -0.819918     2.392300     3.003872      25.15
 C      -2.448663    -1.177875     0.544244      60.23
 H      -3.010380    -2.057226     0.749057      17.04
 C      -2.100819     0.642606    -1.102338      61.14
 H      -2.501422     1.274286    -1.931828      18.77
 C      -0.969099     1.038159    -0.323341      14.34
 O      -0.142662     2.170538    -0.680210     236.36
 C      -0.875112     3.299344    -1.271507      90.64
 H      -0.115202     4.168678    -1.124917      22.53
 H      -1.176061     3.291937    -2.352220      24.48
 H      -1.918385     3.268070    -0.748045      23.98
 C      -0.554386     0.373497     0.880676      45.66
 O       0.589187     0.598647     1.603930     233.81
 C      -1.297067    -0.739830     1.297766      39.08
 H      -1.222688    -1.140246     2.294942      24.55
 C      -2.829735    -0.513081    -0.667919      40.10
 C      -3.898684    -1.141680    -1.586730      62.70
 H      -3.769802    -0.563226    -2.547621      26.72
 O      -3.535136    -2.560489    -1.813443     265.16
 H      -2.617795    -2.690576    -1.888254      28.17
 C      -5.355765    -1.129835    -1.111668      95.63
 H      -5.376722    -1.735689    -0.167220      27.89
 O      -5.767529     0.253479    -0.857398     289.34
 H      -5.704437     0.448806     0.077105      29.48
 C      -6.366945    -1.726093    -2.136902     103.54
 O      -6.335488    -3.202366    -2.179784     229.57
 H      -5.370849    -3.387201    -2.389990      31.79
 H      -6.164708    -1.299739    -3.140459      29.76
 H      -7.331775    -1.449442    -1.754759      29.02
55
name = lig-ACN-frame_13
 C       3.533718     2.768389    -0.042209      58.46
 H       2.884460     3.609445     0.076668      21.63
 C       4.074458     0.539386     0.576772      58.30
 H       4.173863    -0.365528     1.270539      17.82
 C       4.820301     0.341417    -0.615681      18.26
 O       5.408162    -0.831180    -0.920079     227.34
 C       5.370969    -1.952307     0.044438     110.97
 H       5.841209    -1.681539     0.980868      26.75
 H       6.020297    -2.741963    -0.404980      25.20
 H       4.376266    -2.364901     0.117683      26.99
 C       5.008951     1.407060    -1.550322       2.48
 O       5.770790     1.412986    -2.771241     143.56
 H       6.452541     0.617563    -2.668623      22.59
 C       4.228453     2.648755    -1.243648      61.21
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 H       4.345400     3.442807    -1.923129      24.74
 C       3.405878     1.698951     0.888375      25.47
 C       2.616818     1.772559     2.185549      96.13
 H       2.876119     2.684794     2.626351      23.95
 O       2.955488     0.784046     3.193335     338.18
 H       2.502781    -0.022175     3.017551      28.30
 C       1.084071     1.960841     1.917950      70.09
 H       0.881145     2.550435     0.996502      19.80
 C       0.237711     2.436660     3.135833      99.16
 O       0.653842     3.747310     3.633538     272.54
 H       0.956435     4.448358     2.853542      27.14
 H       0.484385     1.611747     3.908284      24.61
 H      -0.839986     2.436296     2.851667      25.84
 C      -2.420355    -1.168441     0.524516      86.98
 H      -2.931319    -2.025609     1.004260      27.34
 C      -2.090153     0.626862    -1.018157      45.83
 H      -2.393062     1.154833    -1.954798      18.06
 C      -0.905610     1.071869    -0.345656      11.28
 O      -0.150636     2.170903    -0.679798     265.34
 C      -0.937751     3.258875    -1.233003      87.87
 H      -0.316692     4.306956    -1.102403      22.77
 H      -1.102849     3.000426    -2.304719      23.17
 H      -1.823222     3.588012    -0.563079      24.34
 C      -0.550131     0.368469     0.872610      31.75
 O       0.599458     0.593656     1.642362     216.11
 C      -1.361619    -0.733023     1.289127      37.70
 H      -0.907975    -1.381652     2.048550      14.12
 C      -2.844168    -0.497025    -0.632319      54.37
 C      -3.880712    -1.130473    -1.608710      44.97
 H      -3.932070    -0.638682    -2.599041      25.63
 O      -3.580112    -2.561241    -1.794890     219.41
 H      -2.589610    -2.492355    -2.047774      24.46
 C      -5.374737    -1.091379    -1.110768      96.69
 H      -5.493981    -1.674591    -0.137698      27.13
 O      -5.803218     0.290495    -0.892750     261.95
 H      -5.258703     0.579786    -0.051203      24.73
 C      -6.365731    -1.708072    -2.111970     104.72
 O      -6.337397    -3.172845    -2.190952     217.31
 H      -5.376827    -3.421563    -2.459865      31.21
 H      -6.245453    -1.263056    -3.140566      28.90
 H      -7.401875    -1.433707    -1.869386      28.02
55
name = lig-ACN-frame_14
 C       3.463315     2.768189    -0.103728      52.11
 H       2.918048     3.650935    -0.073545      24.00
 C       4.080269     0.505268     0.572858      51.64
 H       3.945952    -0.235259     1.397182      15.91
 C       4.813211     0.392250    -0.636607       3.67
 O       5.422733    -0.864056    -0.961930     190.74
 C       5.403850    -1.933354     0.045741     104.43
 H       5.785461    -1.682828     1.023365      26.65
 H       6.063899    -2.682268    -0.470840      24.32
 H       4.428371    -2.285394     0.223323      27.78
 C       4.973914     1.487293    -1.583526      19.27
 O       5.800572     1.395352    -2.722524     118.90
 H       6.452221     0.585964    -2.625676      21.75
 C       4.276912     2.605417    -1.297160      62.90
 H       4.203773     3.388205    -2.009985      23.24
 C       3.405568     1.728613     0.882571     -15.23
 C       2.621363     1.875340     2.231090      84.22
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 H       2.904528     2.752374     2.698022      24.66
 O       3.002054     0.781095     3.193917     266.74
 H       2.345657    -0.020041     3.018857      20.76
 C       1.095807     1.957563     1.926806      82.81
 H       0.998033     2.648191     1.114087      20.86
 C       0.289425     2.468414     3.086608     108.37
 O       0.658193     3.737606     3.585391     280.18
 H       0.677106     4.346049     2.693602      27.77
 H       0.267216     1.847933     4.012681      23.77
 H      -0.797832     2.497822     2.715702      22.94
 C      -2.470903    -1.196281     0.553884      75.45
 H      -3.082615    -2.137276     0.813175      19.86
 C      -2.054183     0.639490    -0.983307     131.63
 H      -2.138901     1.054735    -1.999301      16.27
 C      -0.922859     1.057356    -0.264669      31.47
 O      -0.172653     2.174002    -0.704663     249.62
 C      -0.962890     3.271358    -1.208612      73.28
 H      -0.112237     4.183952    -1.370967      22.17
 H      -1.397368     3.115127    -2.244829      25.80
 H      -1.925560     3.332236    -0.596789      25.88
 C      -0.539644     0.352739     0.862830      25.57
 O       0.594167     0.565112     1.636608     223.95
 C      -1.309384    -0.742191     1.260458      24.64
 H      -0.946710    -1.287387     2.171432      17.51
 C      -2.844630    -0.497997    -0.643310     120.38
 C      -3.903863    -1.112533    -1.572053      40.69
 H      -3.808695    -0.534529    -2.491284      31.42
 O      -3.591121    -2.538867    -1.805594     204.80
 H      -2.594578    -2.719541    -2.131798      22.91
 C      -5.390488    -1.050030    -1.082609      91.69
 H      -5.442129    -1.642589    -0.096564      28.45
 O      -5.808476     0.321706    -0.900568     283.69
 H      -5.129465     0.837519    -0.370598      29.34
 C      -6.401235    -1.696526    -2.138008      97.75
 O      -6.330048    -3.133807    -2.201409     257.35
 H      -5.410417    -3.332132    -2.311603      34.71
 H      -6.142017    -1.210892    -3.125852      29.28
 H      -7.444542    -1.481723    -1.793646      27.53
55
name = lig-ACN-frame_15
 C       3.417119     2.749873    -0.188304      59.55
 H       2.928804     3.643097     0.063239      26.80
 C       4.080889     0.548561     0.553534      58.07
 H       4.034545    -0.346826     1.118783      16.38
 C       4.822214     0.343935    -0.627516      14.50
 O       5.439893    -0.857178    -0.996257     247.43
 C       5.436426    -1.904705     0.011452     122.13
 H       5.925029    -1.462662     0.856563      29.36
 H       6.039334    -2.812345    -0.250040      25.02
 H       4.479546    -2.251127     0.199537      28.66
 C       4.973596     1.415702    -1.546479       8.76
 O       5.793373     1.368259    -2.653040     151.70
 H       6.450632     0.682003    -2.512380      23.91
 C       4.225794     2.670850    -1.327355      60.27
 H       4.381150     3.500552    -2.041349      20.26
 C       3.421734     1.763126     0.838373      19.63
 C       2.659174     1.875665     2.249713      91.53
 H       2.829019     2.783632     2.743906      21.71
 O       2.995681     0.855303     3.137599     296.51
 H       2.476421    -0.031021     2.942573      22.53
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 C       1.137509     1.905944     1.952783      78.36
 H       0.981238     2.463023     1.091673      20.05
 C       0.206328     2.463402     3.109548     102.33
 O       0.666837     3.783831     3.549660     315.18
 H       0.692641     4.437640     2.855687      31.14
 H       0.290758     1.751651     3.912022      24.99
 H      -0.900764     2.500482     2.725625      24.11
 C      -2.471179    -1.174144     0.569634      67.60
 H      -3.025384    -2.120027     0.940307      19.51
 C      -2.053690     0.598546    -1.040272      25.02
 H      -2.313582     1.104142    -1.961072      16.83
 C      -0.973370     1.095893    -0.245687      26.54
 O      -0.190096     2.141403    -0.729516     248.34
 C      -1.000485     3.259953    -1.247510      95.86
 H      -0.255461     4.300808    -1.169728      22.02
 H      -1.420129     3.083781    -2.280765      23.89
 H      -1.663329     3.649252    -0.444517      24.23
 C      -0.518126     0.324499     0.915790      40.43
 O       0.652040     0.579150     1.626051     232.24
 C      -1.315298    -0.843978     1.266073      67.91
 H      -1.208468    -1.258414     2.301330      22.30
 C      -2.814047    -0.509349    -0.605835      38.17
 C      -3.886795    -1.074467    -1.556597      70.24
 H      -3.897290    -0.581779    -2.505320      26.64
 O      -3.614802    -2.522412    -1.834222     251.00
 H      -2.642160    -2.497134    -1.948765      26.53
 C      -5.399356    -1.036211    -1.076400      92.85
 H      -5.515654    -1.574256    -0.061012      26.62
 O      -5.812386     0.359611    -0.923925     299.25
 H      -5.208280     0.688255    -0.281932      29.96
 C      -6.389789    -1.634407    -2.115044      99.79
 O      -6.313441    -3.111915    -2.209976     243.45
 H      -5.353921    -3.266333    -2.146124      31.97
 H      -6.274295    -1.193670    -3.160659      27.88
 H      -7.449988    -1.313834    -1.849555      26.66
55
name = lig-ACN-frame_16
 C       3.405592     2.788572    -0.175116      54.09
 H       2.800452     3.713135    -0.159754      19.63
 C       4.090171     0.527452     0.540238      66.68
 H       3.998603    -0.105670     1.353698      19.60
 C       4.814510     0.322653    -0.650555      16.26
 O       5.454643    -0.852503    -1.039088     219.55
 C       5.485323    -1.865883     0.025270     105.36
 H       5.934253    -1.600293     0.973195      27.63
 H       6.077250    -2.594906    -0.531982      25.26
 H       4.518438    -2.164969     0.271939      29.46
 C       4.929512     1.452293    -1.512674      19.03
 O       5.791347     1.338181    -2.612380     149.00
 H       6.463457     0.661413    -2.483403      22.89
 C       4.219348     2.606108    -1.345629      62.12
 H       4.465335     3.505697    -2.006383      24.61
 C       3.408878     1.750676     0.811017      13.36
 C       2.633129     1.878807     2.127179      93.40
 H       2.980357     2.810632     2.528774      24.65
 O       3.009223     0.881699     3.130826     300.84
 H       2.692524     0.074843     2.798958      27.93
 C       1.060215     1.953228     1.940918      86.33
 H       0.939076     2.615516     1.141921      21.74
 C       0.202952     2.469951     3.112465     106.31
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 O       0.635237     3.791025     3.581391     316.73
 H       0.869489     4.228356     2.819041      34.57
 H       0.238061     1.900484     3.983018      26.05
 H      -0.940391     2.504438     2.763371      23.58
 C      -2.441500    -1.197942     0.586958     101.92
 H      -3.150368    -1.954135     1.029599      28.39
 C      -2.072083     0.571742    -1.027293      18.65
 H      -2.352748     1.098449    -1.916740      17.20
 C      -0.977343     1.031834    -0.255069      36.11
 O      -0.229650     2.126357    -0.752892     257.13
 C      -0.968928     3.293276    -1.204782      87.55
 H      -0.067711     4.115858    -1.557242      20.91
 H      -1.439127     3.026455    -2.216286      22.96
 H      -1.844199     3.464229    -0.593045      24.47
 C      -0.560156     0.306622     0.901981      29.68
 O       0.712538     0.518984     1.621134     220.63
 C      -1.300316    -0.807189     1.351931      18.62
 H      -0.885628    -1.454211     2.153647      14.84
 C      -2.840872    -0.528289    -0.635831      67.38
 C      -3.928317    -1.081917    -1.560821      52.50
 H      -3.858249    -0.463528    -2.424557      28.15
 O      -3.606044    -2.469603    -1.853696     255.69
 H      -2.697039    -2.644079    -1.924704      30.15
 C      -5.399251    -0.992570    -1.092205      98.91
 H      -5.548601    -1.594662    -0.125450      27.20
 O      -5.788018     0.396715    -0.927606     268.32
 H      -5.631436     0.696557     0.018516      26.30
 C      -6.372584    -1.608746    -2.110554      99.74
 O      -6.304502    -3.052504    -2.196512     222.26
 H      -5.306562    -3.332676    -2.181746      30.18
 H      -6.118928    -1.086736    -3.096259      28.92
 H      -7.438427    -1.438543    -1.763296      27.19
55
name = lig-ACN-frame_17
 C       3.429163     2.788918    -0.182925      47.58
 H       2.726156     3.682850    -0.022119      20.41
 C       4.077485     0.521978     0.574110      62.57
 H       4.201979    -0.275959     1.256142      16.81
 C       4.767149     0.354775    -0.642226      15.29
 O       5.456821    -0.813050    -1.002041     236.13
 C       5.543223    -1.879287    -0.012502     117.64
 H       6.123361    -1.455511     0.807700      27.46
 H       6.070041    -2.756343    -0.319738      25.46
 H       4.571268    -2.237222     0.252695      27.69
 C       4.948915     1.411885    -1.553552      17.42
 O       5.794787     1.335823    -2.624579     153.47
 H       6.418139     0.511670    -2.458528      21.12
 C       4.222299     2.612807    -1.301747      67.51
 H       4.234539     3.411233    -2.141547      24.12
 C       3.339664     1.721427     0.739548      24.46
 C       2.576688     1.919773     2.063388      89.13
 H       2.828605     2.873168     2.575216      24.84
 O       3.016650     0.915859     3.100102     249.51
 H       2.630546     0.032364     2.953853      24.81
 C       1.040209     1.956055     1.897937      70.56
 H       0.703904     2.504616     1.046010      20.18
 C       0.225488     2.468077     3.164993     103.84
 O       0.594639     3.768171     3.609773     299.71
 H       0.838004     4.419789     2.866624      30.17
 H       0.290205     1.762982     3.912589      26.73
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 H      -0.910738     2.511373     2.774046      23.38
 C      -2.461187    -1.208981     0.621482      42.50
 H      -2.973918    -2.103174     0.936173      22.70
 C      -2.105145     0.572802    -0.982836      84.49
 H      -2.246586     1.021846    -1.954287      16.99
 C      -0.957241     0.985039    -0.295512      32.65
 O      -0.232496     2.091572    -0.727707     240.57
 C      -0.960495     3.226735    -1.261393      94.71
 H      -0.154957     4.198468    -1.219776      22.45
 H      -1.461808     3.118847    -2.275732      25.37
 H      -1.553079     3.676588    -0.491267      25.85
 C      -0.490865     0.311908     0.916538      30.28
 O       0.661565     0.519584     1.556058     214.78
 C      -1.307116    -0.764928     1.337386      46.45
 H      -0.902839    -1.352581     2.160413      15.31
 C      -2.850571    -0.564682    -0.562214      66.78
 C      -3.907600    -1.046237    -1.558772      45.89
 H      -3.881997    -0.517782    -2.475566      30.28
 O      -3.622075    -2.466412    -1.889432     230.84
 H      -2.590434    -2.373644    -1.995199      22.63
 C      -5.403099    -0.968674    -1.056451      90.54
 H      -5.454107    -1.487312    -0.048123      27.42
 O      -5.765478     0.442193    -0.906005     243.58
 H      -5.767043     0.614729     0.107471      26.77
 C      -6.367892    -1.585568    -2.123695     103.70
 O      -6.287234    -3.022875    -2.181489     244.72
 H      -5.332495    -3.159096    -2.363491      32.28
 H      -6.249175    -1.147227    -3.177612      29.01
 H      -7.419549    -1.266466    -1.869217      28.18
55
name = lig-ACN-frame_18
 C       3.411534     2.713360    -0.184279      56.93
 H       2.899997     3.746012    -0.033240      23.57
 C       4.052635     0.527838     0.551775      57.76
 H       3.893997    -0.231520     1.349904      13.48
 C       4.786471     0.341143    -0.623510      21.62
 O       5.465746    -0.804411    -0.976074     222.88
 C       5.599385    -1.882861    -0.003274     112.26
 H       6.152454    -1.604432     0.913255      27.84
 H       6.129941    -2.562810    -0.601121      25.35
 H       4.620447    -2.201929     0.392053      28.37
 C       4.922223     1.429252    -1.566823      12.60
 O       5.804428     1.327395    -2.683623     156.40
 H       6.392548     0.486668    -2.594366      22.86
 C       4.250897     2.648577    -1.356775      55.39
 H       4.324655     3.489875    -2.130676      18.79
 C       3.282881     1.699465     0.787806      18.37
 C       2.533186     1.899735     2.102872      98.52
 H       2.798488     2.962858     2.417426      23.40
 O       2.984546     0.995412     3.042505     270.59
 H       2.367029     0.138716     2.868214      22.58
 C       1.008958     1.919650     1.872937      93.31
 H       0.933051     2.662819     1.038990      18.57
 C       0.225586     2.393300     3.127417     105.03
 O       0.593964     3.753078     3.665048     233.07
 H       0.525330     4.355644     2.747655      26.86
 H       0.479671     1.811118     3.960264      25.62
 H      -0.958187     2.329048     2.969403      23.11
 C      -2.467090    -1.229157     0.658134      77.77
 H      -2.875541    -2.118819     0.995575      19.68
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 C      -2.107344     0.550263    -0.946531      64.39
 H      -2.435722     1.009113    -1.890045      16.51
 C      -0.943795     0.995057    -0.288905      24.19
 O      -0.191566     2.057114    -0.743508     257.58
 C      -0.925972     3.232019    -1.232642      89.27
 H      -0.005222     3.975177    -1.492832      22.30
 H      -1.379355     2.986524    -2.253199      23.52
 H      -1.769101     3.441213    -0.606288      25.93
 C      -0.558968     0.293986     0.834055      47.59
 O       0.656708     0.589333     1.544483     233.14
 C      -1.324884    -0.790955     1.314852      50.28
 H      -1.175443    -1.145134     2.309503      21.64
 C      -2.864667    -0.529272    -0.529394      55.78
 C      -3.911873    -1.041037    -1.516866      46.89
 H      -3.823252    -0.377312    -2.346664      28.92
 O      -3.610185    -2.452640    -1.927423     206.12
 H      -2.582051    -2.605623    -2.172565      22.24
 C      -5.388915    -0.936918    -1.066879      98.56
 H      -5.596574    -1.536054    -0.150554      27.30
 O      -5.756802     0.468505    -0.860302     300.17
 H      -5.398419     0.779408    -0.021695      28.38
 C      -6.390547    -1.529722    -2.114503      98.36
 O      -6.273062    -3.013727    -2.172068     244.49
 H      -5.386480    -3.203426    -2.445638      33.82
 H      -6.072500    -1.054260    -3.099129      29.37
 H      -7.446640    -1.351229    -1.860167      27.90
55
name = lig-ACN-frame_19
 C       3.411286     2.734869    -0.237610      52.20
 H       2.869895     3.707524    -0.042015      22.81
 C       3.971728     0.501189     0.541377      55.07
 H       3.973621    -0.411092     1.234233      17.85
 C       4.808522     0.386860    -0.625747       9.03
 O       5.488057    -0.808972    -0.951312     220.84
 C       5.645289    -1.887023     0.006497     113.86
 H       6.318664    -1.614749     0.837753      26.82
 H       6.121007    -2.719173    -0.461073      25.00
 H       4.642616    -2.335977     0.280539      25.47
 C       4.956116     1.436265    -1.610098      16.37
 O       5.764047     1.316285    -2.718156     167.80
 H       6.380683     0.627089    -2.524885      24.54
 C       4.235821     2.602731    -1.354529      68.85
 H       4.512647     3.536353    -1.868975      23.51
 C       3.313330     1.719493     0.751010      28.97
 C       2.518779     1.972415     2.052318      85.35
 H       2.815025     2.969095     2.591604      22.18
 O       2.922531     0.995473     3.083638     267.18
 H       2.472346     0.118723     2.995062      24.39
 C       0.994813     2.007041     1.887913      79.87
 H       0.648568     2.710986     1.041301      19.14
 C       0.248071     2.351754     3.182986     103.18
 O       0.567441     3.683448     3.630269     277.98
 H       0.567224     4.419672     2.941973      30.84
 H       0.523268     1.609759     3.944999      25.48
 H      -0.910595     2.217526     2.989360      24.76
 C      -2.494627    -1.259362     0.648859      49.00
 H      -3.227152    -1.905280     1.036319      23.75
 C      -2.131128     0.584318    -0.968981      37.73
 H      -2.454142     1.177511    -1.863069      18.59
 C      -0.983307     1.016109    -0.316626      18.02
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 O      -0.128150     2.047483    -0.774631     255.36
 C      -0.879038     3.168547    -1.282868     112.23
 H      -0.251907     4.162592    -1.290944      23.92
 H      -1.295461     2.953423    -2.301221      24.57
 H      -1.614321     3.528353    -0.559715      25.96
 C      -0.544377     0.283725     0.867135      12.96
 O       0.600338     0.585447     1.514037     218.54
 C      -1.331755    -0.790761     1.378127      50.01
 H      -0.933512    -1.263841     2.263632      16.81
 C      -2.884397    -0.559406    -0.507478      62.49
 C      -3.907478    -1.059133    -1.502115      50.61
 H      -3.850906    -0.460238    -2.401534      27.81
 O      -3.610954    -2.420205    -1.959551     244.63
 H      -2.644434    -2.389350    -2.044991      27.54
 C      -5.428669    -0.939724    -1.040084      98.20
 H      -5.517428    -1.488847    -0.092114      27.92
 O      -5.739925     0.472935    -0.814857     287.98
 H      -5.044232     0.789209    -0.226849      28.50
 C      -6.354566    -1.522947    -2.120699     111.13
 O      -6.287961    -2.967101    -2.172707     232.07
 H      -5.286874    -3.142739    -2.324734      29.90
 H      -6.264860    -1.069051    -3.151315      28.47
 H      -7.363655    -1.261466    -1.829283      28.00
55
name = lig-ACN-frame_20
 C       3.409328     2.777689    -0.228242      56.24
 H       2.854026     3.699419    -0.152154      24.88
 C       3.973823     0.497951     0.449877      60.44
 H       3.887477    -0.308366     1.247210      19.27
 C       4.810692     0.339820    -0.632417      25.42
 O       5.526617    -0.799826    -0.954799     232.70
 C       5.661659    -1.918070     0.011589     107.95
 H       6.185505    -1.523025     0.906330      25.83
 H       6.237866    -2.662228    -0.537584      23.31
 H       4.650555    -2.199441     0.477975      23.74
 C       4.960765     1.394945    -1.570435      15.87
 O       5.741295     1.296406    -2.742619     171.40
 H       6.477936     0.656676    -2.634240      24.13
 C       4.259754     2.631344    -1.362271      62.27
 H       4.392341     3.377538    -2.127106      19.36
 C       3.306982     1.743615     0.723910      26.91
 C       2.531744     1.974878     2.035202      80.42
 H       2.865019     3.054234     2.409927      22.27
 O       2.849276     0.999679     3.145011     277.37
 H       2.548933     0.215056     2.761852      26.34
 C       0.951134     2.026259     1.891307      78.37
 H       0.584344     2.737308     1.039978      17.65
 C       0.247758     2.308732     3.218778     107.30
 O       0.544642     3.641634     3.637271     306.05
 H       0.673840     4.051138     2.851395      35.53
 H       0.598987     1.651692     4.089631      23.63
 H      -0.901757     2.206041     3.045417      23.60
 C      -2.507526    -1.193652     0.698037      61.74
 H      -2.972086    -2.101898     1.110406      19.31
 C      -2.173372     0.608747    -0.973908     103.55
 H      -2.479338     1.026415    -1.974505      15.40
 C      -0.966901     0.986503    -0.292669      28.41
 O      -0.111120     2.016080    -0.800304     240.23
 C      -0.848079     3.188779    -1.329978      92.89
 H      -0.031436     3.938473    -1.358784      25.53
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 H      -1.243107     3.089733    -2.363892      25.40
 H      -1.734557     3.327334    -0.677629      27.21
 C      -0.598559     0.306476     0.875833      22.80
 O       0.617455     0.596780     1.522631     219.68
 C      -1.364743    -0.802882     1.371624      39.45
 H      -0.993278    -1.421590     2.198983      17.07
 C      -2.862092    -0.522429    -0.559451      71.30
 C      -3.970296    -1.034696    -1.526598      42.35
 H      -3.960103    -0.337228    -2.378890      25.89
 O      -3.592585    -2.396813    -1.962619     256.37
 H      -2.662261    -2.523309    -1.980870      24.40
 C      -5.389807    -0.953712    -1.016292     101.26
 H      -5.612643    -1.537905    -0.135878      29.24
 O      -5.715861     0.444893    -0.809187     290.81
 H      -5.149844     0.848930    -0.026082      29.57
 C      -6.398362    -1.492172    -2.103070     105.03
 O      -6.297184    -2.935868    -2.181080     237.98
 H      -5.321966    -3.176458    -2.162504      31.02
 H      -6.077856    -1.016982    -3.059305      30.20
 H      -7.423643    -1.273378    -1.882167      28.30
55
name = lig-ACN-frame_21
 C       3.445603     2.816207    -0.249121      53.31
 H       2.903885     3.690387    -0.101756      22.87
 C       3.964186     0.534100     0.467811      56.58
 H       3.821440    -0.279541     1.189966      16.99
 C       4.815755     0.299440    -0.685285      15.01
 O       5.578401    -0.848843    -0.968466     222.34
 C       5.650201    -1.854468     0.051202     110.71
 H       6.299301    -1.625789     0.914642      27.23
 H       6.182539    -2.720481    -0.463768      24.52
 H       4.626369    -2.348910     0.230175      25.90
 C       4.971237     1.413850    -1.574810      18.50
 O       5.719762     1.275062    -2.738518     148.80
 H       6.460679     0.547877    -2.547401      21.04
 C       4.282456     2.611287    -1.386880      44.73
 H       4.234222     3.307781    -2.190380      22.49
 C       3.284838     1.736182     0.703024      21.91
 C       2.500962     1.938384     2.071476      87.12
 H       2.853309     2.983662     2.518511      23.26
 O       2.784100     1.052647     3.108031     258.89
 H       2.567913     0.059242     2.894370      23.28
 C       0.962664     1.918312     1.914872      93.19
 H       0.734816     2.732142     1.137142      19.97
 C       0.216652     2.260482     3.239718      96.32
 O       0.532890     3.660021     3.653721     256.62
 H       0.777742     4.304872     2.892164      29.97
 H       0.640322     1.487024     4.038645      23.40
 H      -0.900419     2.076504     3.183497      24.55
 C      -2.549010    -1.133422     0.632681      57.64
 H      -3.048734    -2.148050     0.805282      21.05
 C      -2.129456     0.604029    -0.968252      58.08
 H      -2.278979     1.090244    -1.955915      16.82
 C      -0.990243     0.999892    -0.316867      18.35
 O      -0.168763     1.959438    -0.829814     252.81
 C      -0.787608     3.184140    -1.373913     109.97
 H      -0.142345     4.025328    -1.280385      26.39
 H      -0.990135     2.963423    -2.405934      24.94
 H      -1.680350     3.587258    -0.817870      25.90
 C      -0.590790     0.339789     0.919509      34.65
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 O       0.631281     0.605653     1.525073     228.06
 C      -1.344207    -0.756753     1.335518      46.80
 H      -1.092731    -1.225780     2.320936      22.59
 C      -2.923911    -0.504660    -0.537282      40.02
 C      -3.916228    -1.008388    -1.525917      64.15
 H      -3.916718    -0.387540    -2.454600      26.67
 O      -3.603979    -2.391314    -1.958775     225.11
 H      -2.553033    -2.375586    -1.986151      23.53
 C      -5.444367    -0.978900    -0.987976      97.64
 H      -5.447118    -1.541142    -0.083802      29.99
 O      -5.699590     0.436220    -0.802081     285.66
 H      -5.589171     0.617326     0.186097      28.14
 C      -6.391421    -1.460253    -2.082848     109.87
 O      -6.323294    -2.936606    -2.186242     250.57
 H      -5.397309    -3.084143    -2.202657      33.88
 H      -6.149361    -0.983415    -3.045996      30.19
 H      -7.415161    -1.188268    -1.874723      28.62
55
name = lig-ACN-frame_22
 C       3.470642     2.782903    -0.236206      56.44
 H       3.022257     3.725669    -0.169574      21.44
 C       3.993772     0.500589     0.473710      55.80
 H       3.928894    -0.314351     1.129428      18.39
 C       4.790299     0.351065    -0.654672       9.18
 O       5.591818    -0.841962    -0.973570     232.97
 C       5.641109    -1.901921     0.050885      95.51
 H       6.030181    -1.433181     0.980287      26.84
 H       6.297550    -2.774665    -0.330323      23.32
 H       4.581332    -2.131800     0.419702      26.51
 C       4.971292     1.386652    -1.618467      11.57
 O       5.741452     1.238457    -2.735877     169.39
 H       6.381907     0.475712    -2.597041      22.62
 C       4.238511     2.602639    -1.402974      69.57
 H       4.541317     3.448071    -2.027565      25.31
 C       3.290733     1.755206     0.713342      27.76
 C       2.461412     1.938373     2.037071      91.65
 H       2.670485     3.008739     2.480366      23.34
 O       2.826437     1.016083     3.128484     246.26
 H       2.410692     0.094261     2.832592      23.12
 C       0.948332     1.944539     1.931249      81.35
 H       0.547622     2.574083     1.106461      21.22
 C       0.248295     2.297286     3.245187     103.77
 O       0.507449     3.643583     3.694249     229.22
 H       0.625891     4.165332     2.736949      28.09
 H       0.607035     1.674245     4.197477      23.44
 H      -0.832459     2.179944     3.071936      25.69
 C      -2.520847    -1.153762     0.594219      83.10
 H      -3.206859    -1.948213     1.104245      25.17
 C      -2.127510     0.593043    -1.013412      22.23
 H      -2.389870     1.078126    -1.948937      20.35
 C      -0.999339     1.020145    -0.265552      27.93
 O      -0.183072     1.989423    -0.851042     244.99
 C      -0.721867     3.179741    -1.440784     115.67
 H       0.032084     3.835458    -1.272222      26.19
 H      -0.931835     3.172194    -2.487644      26.12
 H      -1.701506     3.361608    -0.909496      24.73
 C      -0.583212     0.368309     0.886698      21.94
 O       0.625331     0.534586     1.509181     230.73
 C      -1.421964    -0.705613     1.333110      42.43
 H      -1.077561    -1.251324     2.256975      17.68
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 C      -2.933329    -0.412372    -0.562846      62.47
 C      -3.963742    -1.031636    -1.528884      56.73
 H      -3.925977    -0.343142    -2.433150      26.05
 O      -3.591460    -2.384728    -1.935659     205.77
 H      -2.546613    -2.452221    -2.137479      24.36
 C      -5.381805    -0.954456    -1.013407     109.88
 H      -5.607642    -1.525845    -0.152113      29.37
 O      -5.734198     0.441049    -0.763080     288.43
 H      -5.627367     0.697681     0.137903      29.53
 C      -6.406155    -1.497602    -2.070915     107.40
 O      -6.362361    -2.919278    -2.191840     232.13
 H      -5.423967    -3.180471    -2.420910      32.22
 H      -6.210803    -1.005453    -3.016824      30.59
 H      -7.426689    -1.250980    -1.753565      28.64
55
name = lig-ACN-frame_23
 C       3.470015     2.750496    -0.224970      51.53
 H       3.012654     3.709271     0.036095      23.65
 C       3.997150     0.502791     0.504221      58.59
 H       3.906415    -0.192278     1.270874      19.82
 C       4.840947     0.314048    -0.659021      16.79
 O       5.547674    -0.798050    -0.950956     199.65
 C       5.581071    -1.852450     0.106387     109.58
 H       6.128654    -1.530636     1.023405      26.23
 H       6.261776    -2.668788    -0.377105      23.12
 H       4.592049    -2.374863     0.212303      25.16
 C       4.903443     1.364787    -1.638832      15.86
 O       5.794263     1.203482    -2.750634     174.92
 H       6.323312     0.452088    -2.558279      27.68
 C       4.282120     2.588394    -1.404473      63.81
 H       4.507445     3.496853    -2.033907      20.16
 C       3.319678     1.704530     0.751852      21.36
 C       2.502301     1.966138     2.027125      84.20
 H       2.864504     2.987170     2.402038      23.77
 O       2.889790     0.968875     3.105331     263.49
 H       2.457117     0.173867     2.894053      27.22
 C       0.928664     1.923053     1.891447      86.44
 H       0.658342     2.677266     1.162229      22.67
 C       0.217376     2.313269     3.269989     101.90
 O       0.498752     3.671272     3.687336     290.42
 H       0.461928     4.325082     2.984500      33.12
 H       0.534551     1.513551     4.089695      24.92
 H      -0.847808     2.163489     3.148345      26.70
 C      -2.573612    -1.106181     0.615804      71.38
 H      -3.179578    -1.987703     1.050007      22.84
 C      -2.145895     0.658143    -1.043184      42.03
 H      -2.321866     1.110184    -1.995966      17.28
 C      -1.017566     1.086156    -0.340749      42.63
 O      -0.123480     2.007620    -0.854099     241.43
 C      -0.693422     3.216176    -1.485771     126.80
 H      -0.099828     3.989031    -1.311732      28.19
 H      -0.751600     3.028500    -2.518631      26.89
 H      -1.659710     3.589067    -1.072133      27.93
 C      -0.638318     0.310094     0.853566      29.61
 O       0.615108     0.509896     1.530856     207.04
 C      -1.446854    -0.682036     1.356781      36.82
 H      -1.164442    -1.284274     2.240675      16.61
 C      -2.920242    -0.487646    -0.593295      54.32
 C      -3.948584    -0.989575    -1.549416      38.29
 H      -4.006510    -0.383034    -2.516826      26.98
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 O      -3.591928    -2.395768    -1.908437     213.57
 H      -2.635141    -2.341092    -2.043005      25.20
 C      -5.435772    -0.954372    -1.014409      97.76
 H      -5.395824    -1.553842    -0.133088      29.35
 O      -5.797028     0.445481    -0.760284     280.02
 H      -5.154686     0.750536    -0.065285      27.60
 C      -6.429321    -1.486000    -2.063582     107.74
 O      -6.397051    -2.956248    -2.202238     204.43
 H      -5.443734    -3.144268    -2.543410      30.52
 H      -6.331526    -1.006647    -3.014615      29.48
 H      -7.461523    -1.279737    -1.679912      27.68
55
name = lig-ACN-frame_24
 C       3.490876     2.728129    -0.210081      57.03
 H       2.979562     3.739749    -0.078740      24.24
 C       4.037944     0.482032     0.531550      63.03
 H       4.082006    -0.366224     1.196760      18.61
 C       4.770725     0.350552    -0.634176      12.56
 O       5.523921    -0.824364    -0.884507     235.97
 C       5.565163    -1.842193     0.075995     110.88
 H       5.877474    -1.475858     1.098486      27.03
 H       6.292939    -2.623067    -0.335144      24.01
 H       4.530799    -2.215213     0.280237      26.90
 C       4.929724     1.333647    -1.661954      15.65
 O       5.786648     1.182367    -2.723058     185.98
 H       6.507434     0.483155    -2.530608      24.09
 C       4.296967     2.583957    -1.346906      72.29
 H       4.298850     3.372734    -2.171845      19.99
 C       3.340708     1.705098     0.714154      29.08
 C       2.557769     1.888593     2.082354      98.21
 H       2.738371     2.875263     2.566450      23.56
 O       2.944398     0.981109     3.043905     283.04
 H       2.556997     0.103425     2.826320      26.75
 C       0.982185     1.923537     1.918691      83.83
 H       0.703758     2.504099     1.077489      21.56
 C       0.173658     2.296304     3.204165     108.78
 O       0.501427     3.698229     3.704519     273.66
 H       0.455004     4.186076     2.922718      33.74
 H       0.652143     1.731404     4.078336      24.58
 H      -0.872774     2.154272     3.142103      27.12
 C      -2.664751    -1.074221     0.638589      48.01
 H      -3.193225    -2.033861     0.792980      22.62
 C      -2.184589     0.675319    -1.048539      59.26
 H      -2.416513     1.081604    -2.008040      19.55
 C      -0.986572     1.050392    -0.359523      15.53
 O      -0.089964     2.077336    -0.825726     229.02
 C      -0.653231     3.262595    -1.540278     121.80
 H      -0.036373     3.971798    -1.373596      29.56
 H      -0.739719     3.074020    -2.580761      27.50
 H      -1.667958     3.395288    -1.163490      27.99
 C      -0.609505     0.369382     0.826790      15.73
 O       0.544158     0.559653     1.526042     224.09
 C      -1.480975    -0.710012     1.350464      49.92
 H      -1.176845    -1.070980     2.325819      21.24
 C      -2.879549    -0.443966    -0.640674      33.70
 C      -3.968119    -1.002961    -1.600701      67.55
 H      -3.843622    -0.354466    -2.538718      24.25
 O      -3.610535    -2.389653    -1.889321     257.25
 H      -2.675583    -2.504113    -1.925919      27.55
 C      -5.442443    -0.951462    -1.021745      98.78
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 H      -5.585575    -1.508783    -0.112598      29.11
 O      -5.844260     0.415121    -0.776735     288.71
 H      -5.141356     0.901221    -0.184176      29.30
 C      -6.503449    -1.513669    -2.038912     104.31
 O      -6.411657    -2.971524    -2.222763     224.75
 H      -5.502062    -3.139811    -2.418699      33.47
 H      -6.328054    -0.993950    -2.951909      29.43
 H      -7.568806    -1.261527    -1.722761      27.36
55
name = lig-ACN-frame_25
 C       3.500461     2.736615    -0.209371      52.84
 H       2.866894     3.714743    -0.138207      19.86
 C       4.047886     0.507424     0.532956      58.71
 H       3.926585    -0.262405     1.354027      18.08
 C       4.781266     0.292038    -0.654096      20.48
 O       5.533051    -0.811430    -0.896689     221.68
 C       5.516707    -1.887629     0.132425     103.73
 H       5.921763    -1.452693     1.090230      26.86
 H       6.242954    -2.668411    -0.173658      25.48
 H       4.538066    -2.367417     0.225939      28.45
 C       4.970856     1.360090    -1.564389      21.86
 O       5.762075     1.161014    -2.710884     156.64
 H       6.591248     0.584240    -2.410270      21.63
 C       4.282097     2.549920    -1.393543      53.53
 H       4.478050     3.424632    -2.082298      26.32
 C       3.333943     1.705146     0.794431      19.30
 C       2.527986     1.894706     2.054283      99.39
 H       2.847599     2.861827     2.396034      25.69
 O       3.013513     0.907289     3.065094     223.13
 H       2.724439    -0.059836     2.702692      22.46
 C       0.999899     1.944556     1.908453      90.95
 H       0.854898     2.748977     1.225427      22.84
 C       0.252561     2.342199     3.213594     111.83
 O       0.472062     3.667937     3.655201     267.49
 H       0.702981     4.360434     2.872231      29.00
 H       0.386381     1.589024     4.004140      26.12
 H      -0.759758     2.237378     2.913162      26.91
 C      -2.634057    -1.062271     0.571276      70.46
 H      -3.248019    -1.754443     1.084868      23.23
 C      -2.116080     0.700123    -1.068317      70.42
 H      -2.374461     1.230598    -1.981348      22.22
 C      -0.941326     1.082734    -0.397464       9.94
 O      -0.112683     2.123924    -0.794688     233.65
 C      -0.640560     3.236683    -1.559054     131.54
 H      -0.066729     3.968485    -1.365669      29.42
 H      -0.649066     3.126771    -2.628346      27.12
 H      -1.595743     3.567898    -1.226272      28.32
 C      -0.684285     0.369286     0.835190      29.72
 O       0.524896     0.599553     1.550023     197.16
 C      -1.508220    -0.628474     1.286062      20.96
 H      -1.325625    -1.165852     2.186084      19.24
 C      -2.976663    -0.398224    -0.627093      70.58
 C      -3.973296    -1.013691    -1.580799      44.08
 H      -4.110956    -0.471583    -2.572004      27.80
 O      -3.657622    -2.419284    -1.887181     177.96
 H      -2.608778    -2.428540    -1.948974      25.09
 C      -5.459603    -0.964205    -1.048356      99.31
 H      -5.403003    -1.565489    -0.139726      29.08
 O      -5.880971     0.407428    -0.836541     273.82
 H      -5.533144     0.699869     0.047209      27.40
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 C      -6.526057    -1.537512    -2.047373     108.10
 O      -6.428296    -2.959157    -2.225962     234.84
 H      -5.472180    -3.145093    -2.212856      33.11
 H      -6.479286    -1.051316    -2.998578      29.53
 H      -7.565816    -1.378445    -1.602719      27.33
55
name = lig-ACN-frame_26
 C       3.456150     2.737803    -0.219889      57.40
 H       2.925989     3.737040    -0.010101      21.89
 C       4.017547     0.518167     0.542143      59.12
 H       4.007036    -0.365811     1.270171      18.29
 C       4.816408     0.283976    -0.594276      10.60
 O       5.564117    -0.903291    -0.905092     204.41
 C       5.503404    -1.918035     0.169538     112.26
 H       5.792884    -1.574169     1.205075      27.91
 H       6.195328    -2.634159    -0.206758      26.29
 H       4.491588    -2.309401     0.239254      28.03
 C       5.003655     1.352538    -1.536243      19.84
 O       5.755501     1.153600    -2.677544     136.02
 H       6.532867     0.586133    -2.527402      21.74
 C       4.263055     2.565320    -1.361551      62.65
 H       4.512873     3.401714    -2.019086      26.40
 C       3.372290     1.741977     0.722229      41.22
 C       2.588235     1.876357     2.084693      93.00
 H       2.797762     2.749204     2.623908      25.00
 O       3.026614     0.856632     3.077067     239.15
 H       2.698398    -0.052907     2.816256      24.73
 C       1.029716     1.973790     1.923595      80.41
 H       0.715569     2.582048     1.090560      22.18
 C       0.229400     2.343041     3.162180     115.06
 O       0.487518     3.698145     3.637485     259.46
 H       0.866449     4.205115     2.785415      28.88
 H       0.472168     1.747254     3.985546      26.70
 H      -0.804541     2.250450     2.916512      27.50
 C      -2.645019    -1.002484     0.518321      74.29
 H      -3.281027    -1.747519     0.870094      25.55
 C      -2.120272     0.676678    -1.122364      52.50
 H      -2.309943     1.189071    -2.092930      22.10
 C      -0.990275     1.111246    -0.380848      27.86
 O      -0.131220     2.140389    -0.764411     241.24
 C      -0.640259     3.268714    -1.557948     128.01
 H      -0.021267     3.993343    -1.400555      29.00
 H      -0.604970     2.887437    -2.568880      26.70
 H      -1.625518     3.491972    -1.304137      28.81
 C      -0.622206     0.477097     0.825823      20.65
 O       0.514282     0.631381     1.559656     207.18
 C      -1.528029    -0.598657     1.276848      38.37
 H      -1.189885    -1.072760     2.185200      18.81
 C      -2.989504    -0.325212    -0.675709      46.52
 C      -4.067872    -0.980598    -1.602198      59.31
 H      -3.892019    -0.398315    -2.547143      28.20
 O      -3.686333    -2.439496    -1.872773     171.69
 H      -2.642276    -2.462159    -2.082246      25.20
 C      -5.494494    -0.997441    -1.080086     106.00
 H      -5.647019    -1.527428    -0.125461      28.64
 O      -5.898578     0.407875    -0.870833     257.80
 H      -5.907524     0.602440     0.051249      29.71
 C      -6.539200    -1.548393    -2.032604     110.58
 O      -6.430341    -2.995927    -2.222629     195.28
 H      -5.410909    -3.222835    -2.190135      30.10
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 H      -6.540605    -0.962985    -2.945735      29.65
 H      -7.525510    -1.325160    -1.541292      28.53
55
name = lig-ACN-frame_27
 C       3.427610     2.776749    -0.234322      56.08
 H       2.994229     3.796953    -0.133214      24.78
 C       4.051584     0.458852     0.512091      56.66
 H       3.893439    -0.260207     1.331509      18.35
 C       4.904213     0.280060    -0.578607      19.40
 O       5.546305    -0.940110    -0.836509     243.09
 C       5.493876    -1.975240     0.155802     118.97
 H       5.816246    -1.485683     1.103007      26.26
 H       6.138360    -2.780112    -0.024161      25.87
 H       4.473070    -2.321244     0.281119      27.46
 C       4.978770     1.328895    -1.533511      19.92
 O       5.770440     1.178666    -2.668164     208.39
 H       6.402440     0.495505    -2.436560      25.83
 C       4.318247     2.570275    -1.329789      53.08
 H       4.343799     3.273558    -2.115432      19.92
 C       3.353035     1.707643     0.773511       5.44
 C       2.641121     1.855093     2.152333      97.15
 H       2.963136     2.771253     2.501001      24.99
 O       2.979614     0.842497     3.055301     311.94
 H       2.511370     0.088999     2.822934      29.19
 C       1.039413     1.952950     1.898994      86.61
 H       1.041525     2.724534     1.106442      21.55
 C       0.195404     2.372686     3.170479     111.58
 O       0.533790     3.757273     3.604149     299.17
 H       0.660704     4.306153     2.872886      33.64
 H       0.486933     1.727621     3.896164      27.80
 H      -0.877337     2.206031     3.049826      26.49
 C      -2.667657    -0.917496     0.534598      51.06
 H      -3.056692    -1.876933     0.740469      23.71
 C      -2.145001     0.719905    -1.201302      45.01
 H      -2.261731     1.071894    -2.267883      19.48
 C      -1.042612     1.167054    -0.363240      20.45
 O      -0.143081     2.175904    -0.745356     213.97
 C      -0.649802     3.253182    -1.576767     130.23
 H      -0.052298     4.039586    -1.431450      28.69
 H      -0.701788     3.171819    -2.674609      27.41
 H      -1.597863     3.532139    -1.257919      29.47
 C      -0.680625     0.462983     0.840348      22.35
 O       0.549816     0.631898     1.562395     209.11
 C      -1.481843    -0.545253     1.254825      56.38
 H      -1.300502    -1.099390     2.189497      22.52
 C      -2.974967    -0.347881    -0.741263      43.60
 C      -4.032466    -0.976240    -1.639931      66.48
 H      -4.256883    -0.494221    -2.612921      29.04
 O      -3.718289    -2.397748    -1.852661     229.83
 H      -2.785000    -2.463257    -2.062817      27.72
 C      -5.550506    -0.947354    -1.055364      90.70
 H      -5.484747    -1.559607    -0.112916      29.00
 O      -5.933243     0.415381    -0.909462     265.33
 H      -5.663407     0.724579     0.041431      27.58
 C      -6.593623    -1.593382    -2.039258     107.01
 O      -6.431268    -3.034311    -2.220698     200.35
 H      -5.461505    -3.140467    -2.356673      31.44
 H      -6.477038    -1.130824    -3.032651      28.81
 H      -7.622064    -1.475549    -1.674365      28.73
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name = lig-ACN-frame_28
 C       3.494843     2.704833    -0.175101      51.55
 H       2.864428     3.555380    -0.062996      22.25
 C       4.049938     0.496098     0.555772      60.96
 H       4.048929    -0.307630     1.219001      19.73
 C       4.899009     0.262009    -0.556117      25.86
 O       5.557950    -0.937912    -0.836869     195.30
 C       5.463415    -2.005835     0.225051     118.48
 H       5.876293    -1.733769     1.204123      27.77
 H       6.107070    -2.692609    -0.253080      25.78
 H       4.471614    -2.431400     0.309916      26.70
 C       5.001491     1.309890    -1.532037      19.37
 O       5.785455     1.197716    -2.669087      81.22
 H       6.563426     0.494804    -2.598650      22.11
 C       4.308204     2.533646    -1.325964      62.43
 H       4.483463     3.278781    -2.044388      25.32
 C       3.363345     1.681239     0.764961      39.51
 C       2.574496     1.877522     2.095349      97.80
 H       2.818434     2.753157     2.593677      25.74
 O       2.920763     0.825764     3.078957     241.45
 H       2.489008    -0.052840     2.794887      23.38
 C       1.073459     1.998606     1.943709      77.00
 H       0.726395     2.650869     1.090686      21.63
 C       0.272701     2.446479     3.184423     117.18
 O       0.556121     3.778463     3.578983     296.45
 H       0.439768     4.325843     2.813066      33.11
 H       0.415569     1.892517     3.999161      28.18
 H      -0.793839     2.429872     2.855270      25.95
 C      -2.644447    -0.921641     0.487396      73.11
 H      -3.295975    -1.683112     0.950502      24.55
 C      -2.128130     0.762873    -1.191516      54.39
 H      -2.219438     1.245924    -2.200998      19.32
 C      -1.058382     1.209929    -0.401402      28.76
 O      -0.175157     2.203015    -0.778973     235.19
 C      -0.689902     3.310053    -1.574339     123.63
 H      -0.006505     4.072091    -1.386644      26.69
 H      -0.650400     2.905454    -2.592781      25.88
 H      -1.650294     3.584521    -1.264059      28.78
 C      -0.681795     0.523616     0.824072      29.71
 O       0.556246     0.625842     1.494341     169.55
 C      -1.557823    -0.570727     1.267761      44.17
 H      -1.229362    -1.174161     2.160064      18.09
 C      -2.940483    -0.339062    -0.777008      47.44
 C      -4.083819    -0.981966    -1.661052      55.03
 H      -3.924409    -0.430509    -2.598497      27.52
 O      -3.742453    -2.373116    -1.852761     228.58
 H      -2.804868    -2.430170    -1.952600      28.55
 C      -5.538698    -0.945652    -1.057817      91.22
 H      -5.603561    -1.388569    -0.012032      26.85
 O      -5.977730     0.458876    -0.903438     274.90
 H      -5.313358     0.893360    -0.258075      27.96
 C      -6.610261    -1.647155    -2.066268     106.58
 O      -6.422844    -3.076593    -2.209464     215.55
 H      -5.527518    -3.187824    -2.461560      33.28
 H      -6.556624    -1.069907    -3.031401      28.21
 H      -7.600103    -1.442777    -1.698123      28.66
55
name = lig-ACN-frame_29
 C       3.526545     2.671810    -0.163214      53.60
 H       3.047556     3.596546    -0.075482      22.58
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 C       4.110708     0.440998     0.619256      63.41
 H       4.010549    -0.262867     1.358165      20.96
 C       4.837260     0.266736    -0.568449      15.47
 O       5.552864    -0.937369    -0.770901     226.61
 C       5.484833    -2.029311     0.188596     113.98
 H       5.870407    -1.717194     1.146853      28.61
 H       6.067584    -2.884245    -0.135514      26.64
 H       4.424605    -2.279729     0.355152      28.55
 C       5.056790     1.305818    -1.522675      25.93
 O       5.796053     1.203918    -2.686995     149.49
 H       6.680544     0.694659    -2.435658      21.25
 C       4.311364     2.478603    -1.320683      55.84
 H       4.494320     3.370584    -1.899247      27.00
 C       3.372323     1.650512     0.818520      17.96
 C       2.534608     1.845315     2.077578     101.55
 H       2.858724     2.774683     2.469627      25.59
 O       2.835518     0.855642     3.088542     243.50
 H       2.592286    -0.118272     2.690460      21.99
 C       1.005070     1.985750     1.903098      83.32
 H       0.899001     2.819891     1.128946      21.20
 C       0.275006     2.465350     3.183697     108.18
 O       0.592174     3.850359     3.582551     243.43
 H       0.687482     4.498024     2.704979      26.86
 H       0.456118     1.861301     3.991519      27.42
 H      -0.827009     2.326436     2.954768      25.84
 C      -2.669760    -0.969282     0.453622      59.05
 H      -3.515675    -1.662132     0.788787      21.77
 C      -2.142584     0.771330    -1.163180      42.76
 H      -2.431619     1.282451    -2.091815      21.54
 C      -1.022978     1.197688    -0.369823      16.89
 O      -0.196325     2.248714    -0.802063     220.33
 C      -0.718171     3.345885    -1.590637     122.67
 H      -0.036776     4.194025    -1.505358      25.76
 H      -0.798262     3.232368    -2.681110      26.58
 H      -1.703322     3.663716    -1.299686      27.54
 C      -0.700875     0.502823     0.817318      25.79
 O       0.528242     0.663327     1.428209     206.32
 C      -1.538551    -0.510868     1.232580      41.75
 H      -1.301015    -1.012782     2.210745      21.11
 C      -2.958660    -0.306298    -0.761583      60.83
 C      -4.055718    -0.916950    -1.635405      56.37
 H      -4.233978    -0.453148    -2.599622      28.54
 O      -3.753961    -2.395972    -1.876990     155.11
 H      -2.707444    -2.468409    -1.912316      26.53
 C      -5.551413    -0.900485    -1.128613      95.59
 H      -5.560133    -1.549419    -0.176517      28.04
 O      -6.003035     0.476446    -0.929978     278.73
 H      -5.418275     0.891108    -0.317518      30.39
 C      -6.560293    -1.619337    -2.030760     106.28
 O      -6.427767    -3.101755    -2.200475     165.62
 H      -5.424731    -3.252288    -2.371590      30.17
 H      -6.552660    -1.178627    -3.078354      28.08
 H      -7.515971    -1.542608    -1.580531      29.29
55
name = lig-ACN-frame_30
 C       3.510460     2.657575    -0.148448      58.19
 H       3.133964     3.623114     0.061892      25.80
 C       4.120775     0.426902     0.656455      60.91
 H       4.171475    -0.373970     1.373068      18.92
 C       4.870181     0.190708    -0.540784      23.81
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 O       5.582297    -0.944080    -0.762641     195.71
 C       5.461807    -2.001025     0.193257     125.99
 H       5.984574    -1.740641     1.093616      28.99
 H       6.051672    -2.820137    -0.303507      25.44
 H       4.428370    -2.370297     0.355972      26.72
 C       5.024566     1.276010    -1.503587      26.77
 O       5.833447     1.184885    -2.674831     111.83
 H       6.709974     0.782185    -2.522454      19.14
 C       4.351557     2.497873    -1.276161      48.49
 H       4.475057     3.240989    -2.108084      19.90
 C       3.391430     1.615546     0.836224      19.22
 C       2.529038     1.830350     2.108512      95.04
 H       2.789143     2.788718     2.570613      23.61
 O       2.756841     0.889552     3.111663     262.98
 H       2.455692    -0.034210     2.805631      23.91
 C       0.973500     2.017909     1.821792      71.41
 H       0.784484     2.719450     0.958517      19.13
 C       0.229476     2.481280     3.175019     104.50
 O       0.615774     3.871134     3.594291     234.28
 H       0.903190     4.383887     2.666958      26.54
 H       0.677056     1.862865     3.926199      25.16
 H      -0.902192     2.461488     3.209313      24.99
 C      -2.681932    -0.937273     0.479770      67.35
 H      -2.995476    -1.978506     0.889586      21.54
 C      -2.191643     0.802263    -1.138863      52.94
 H      -2.320229     1.303870    -2.082824      20.08
 C      -1.049872     1.233224    -0.448480      23.87
 O      -0.202012     2.288427    -0.823624     219.82
 C      -0.782120     3.408047    -1.627362     108.77
 H      -0.027162     4.215738    -1.361994      24.77
 H      -0.819176     3.081003    -2.655673      26.20
 H      -1.721918     3.673217    -1.127575      27.11
 C      -0.696295     0.507132     0.747788      27.49
 O       0.505684     0.719268     1.417523     196.72
 C      -1.588845    -0.542865     1.216080      48.22
 H      -1.394522    -0.989486     2.206953      19.98
 C      -3.003924    -0.306067    -0.737594      51.29
 C      -4.059591    -0.913735    -1.693356      62.54
 H      -3.891465    -0.372122    -2.605954      29.72
 O      -3.753935    -2.357444    -1.895394     203.02
 H      -2.703526    -2.452860    -2.052379      24.21
 C      -5.504268    -0.898689    -1.115151      95.17
 H      -5.530315    -1.337907    -0.051997      27.82
 O      -6.011974     0.458653    -0.986984     261.55
 H      -5.832680     0.713183    -0.046415      28.63
 C      -6.554829    -1.632789    -2.051662     108.03
 O      -6.403667    -3.072015    -2.168120     196.75
 H      -5.392847    -3.243162    -2.155099      30.49
 H      -6.598290    -1.095151    -3.073101      28.24
 H      -7.504025    -1.395954    -1.622567      29.60
55
name = lig-ACN-frame_31
 C       3.528252     2.647545    -0.106363      44.35
 H       2.892484     3.535653     0.008690      22.86
 C       4.126807     0.407834     0.634220      60.91
 H       4.055152    -0.328375     1.491244      19.00
 C       4.920897     0.234978    -0.504049      23.57
 O       5.623804    -0.961698    -0.804677     215.39
 C       5.495637    -2.034338     0.203349     111.83
 H       5.932661    -1.849053     1.174189      26.24
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 H       6.033558    -2.917351    -0.283291      24.09
 H       4.401103    -2.251622     0.398311      24.48
 C       5.014831     1.232760    -1.492642      22.32
 O       5.814367     1.164383    -2.627981     127.82
 H       6.587577     0.631557    -2.380260      25.56
 C       4.370122     2.464374    -1.240064      68.41
 H       4.497600     3.348643    -1.966096      20.68
 C       3.396021     1.625059     0.837345      18.79
 C       2.479632     1.911311     2.084414      79.62
 H       2.825400     2.878135     2.564125      24.19
 O       2.688861     0.885245     3.184323     251.54
 H       2.310070     0.091675     2.894072      26.25
 C       0.939180     2.097486     1.812644      83.73
 H       0.759327     2.842857     1.019495      21.78
 C       0.282468     2.527656     3.152302     107.02
 O       0.632770     3.813396     3.604859     278.33
 H       0.585725     4.454686     2.832982      30.87
 H       0.509322     1.786607     3.971225      25.26
 H      -0.829363     2.348344     2.937015      25.02
 C      -2.667923    -0.963920     0.496015      56.09
 H      -3.326494    -1.903539     0.659158      20.53
 C      -2.278614     0.830855    -1.174155      47.63
 H      -2.549485     1.171648    -2.154910      19.85
 C      -1.086154     1.250443    -0.465111      17.02
 O      -0.236480     2.305324    -0.869520     234.00
 C      -0.819023     3.411175    -1.579955     116.70
 H      -0.103604     4.353854    -1.667745      24.01
 H      -0.936706     3.223247    -2.638488      26.69
 H      -1.871022     3.744430    -1.323518      26.75
 C      -0.714516     0.544408     0.706594      21.63
 O       0.457464     0.712115     1.425276     204.43
 C      -1.514601    -0.487383     1.218397      45.69
 H      -1.100891    -1.082755     2.013019      19.69
 C      -3.022256    -0.299697    -0.725931      43.52
 C      -4.014344    -0.916103    -1.712596      62.93
 H      -4.098222    -0.425323    -2.661039      28.52
 O      -3.737018    -2.307910    -1.928064     253.33
 H      -2.784329    -2.400423    -2.113522      27.11
 C      -5.504281    -0.905502    -1.145965      89.26
 H      -5.397491    -1.472199    -0.151443      28.81
 O      -5.994840     0.463460    -1.025752     215.71
 H      -6.168543     0.696346    -0.033202      27.19
 C      -6.553418    -1.605414    -2.038414     110.14
 O      -6.369714    -3.037604    -2.122354     211.05
 H      -5.439030    -3.148996    -2.097298      32.72
 H      -6.383554    -1.146375    -3.085607      28.68
 H      -7.578746    -1.484554    -1.697247      29.62
55
name = lig-ACN-frame_32
 C       3.534682     2.642191    -0.105977      53.81
 H       2.970269     3.625121    -0.132113      21.22
 C       4.105877     0.433485     0.666890      53.94
 H       4.017745    -0.449570     1.407865      17.89
 C       4.959067     0.213515    -0.481118      23.23
 O       5.654339    -0.975381    -0.787205     202.57
 C       5.523870    -2.064379     0.178474     112.06
 H       6.056476    -1.709895     1.064911      27.40
 H       6.038163    -3.024650    -0.179080      24.47
 H       4.411320    -2.296551     0.330014      24.60
 C       5.031816     1.284105    -1.444065      22.00
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 O       5.775822     1.117174    -2.589886      35.59
 H       6.613315     0.513087    -2.462677      20.39
 C       4.339763     2.466623    -1.212076      59.33
 H       4.610374     3.341985    -1.898068      25.88
 C       3.361688     1.628712     0.880263      32.45
 C       2.483023     1.888941     2.096155      93.51
 H       2.822232     2.934704     2.488276      23.57
 O       2.608157     0.968714     3.186691     269.60
 H       2.331803     0.087909     2.838640      26.07
 C       1.000328     2.092215     1.839771      91.58
 H       0.797220     2.801800     1.061712      23.08
 C       0.225521     2.473926     3.088812     103.75
 O       0.641107     3.790953     3.640061     264.23
 H       0.449428     4.403616     3.007368      34.49
 H       0.462703     1.702058     3.964808      23.72
 H      -0.874165     2.610079     2.905142      24.80
 C      -2.627349    -0.942660     0.443902      84.10
 H      -3.201829    -1.703947     1.024392      21.86
 C      -2.298556     0.840313    -1.191050      47.25
 H      -2.547602     1.387337    -2.095287      19.51
 C      -1.169562     1.295714    -0.494166      25.68
 O      -0.300783     2.313100    -0.908269     226.11
 C      -0.895008     3.426639    -1.655246     100.40
 H      -0.080464     4.275292    -1.316264      22.28
 H      -1.030584     3.141894    -2.681330      25.42
 H      -1.786312     3.692196    -0.986938      24.97
 C      -0.754002     0.598242     0.715850      33.93
 O       0.443551     0.781965     1.434484     185.05
 C      -1.497302    -0.539861     1.143784      41.59
 H      -1.132314    -1.007149     2.023707      18.74
 C      -3.004958    -0.274867    -0.740289      53.47
 C      -4.079119    -0.877834    -1.677058      45.35
 H      -4.005834    -0.281333    -2.564803      29.71
 O      -3.698456    -2.310123    -1.984183     219.37
 H      -2.770225    -2.400135    -2.004136      27.58
 C      -5.521285    -0.894692    -1.149113     102.39
 H      -5.637156    -1.393526    -0.130290      27.64
 O      -5.966602     0.482455    -1.046726     273.97
 H      -5.830909     0.717098    -0.115120      29.01
 C      -6.514173    -1.590074    -2.075472     109.26
 O      -6.339636    -3.043578    -2.067652     185.24
 H      -5.380153    -3.170966    -2.244217      31.73
 H      -6.530388    -1.160329    -3.143631      29.06
 H      -7.515179    -1.306057    -1.669216      29.40
55
name = lig-ACN-frame_33
 C       3.483193     2.666742    -0.088657      52.73
 H       3.044871     3.669959     0.266760      24.00
 C       4.111343     0.411947     0.690701      60.06
 H       3.985390    -0.415479     1.451997      17.32
 C       4.915553     0.205135    -0.425330      31.18
 O       5.652681    -0.957752    -0.755603     191.55
 C       5.557153    -2.050961     0.177037     113.83
 H       6.000167    -1.931847     1.208662      28.16
 H       6.163307    -2.803969    -0.411899      24.62
 H       4.491715    -2.426942     0.416983      26.22
 C       5.089461     1.257258    -1.367165      36.86
 O       5.741992     1.078278    -2.602487      45.96
 H       6.679601     0.635158    -2.392679      15.98
 C       4.368676     2.490869    -1.221574      47.22
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 H       4.456937     3.268712    -2.008238      23.27
 C       3.370177     1.619295     0.852857      13.64
 C       2.494162     1.906670     2.121655      83.54
 H       2.803243     2.929623     2.628913      23.23
 O       2.579697     1.014917     3.200075     236.22
 H       2.348756     0.008868     2.898795      21.64
 C       0.965466     2.092353     1.785102      92.38
 H       0.934612     2.822558     1.011854      22.40
 C       0.135186     2.516606     3.090856      95.65
 O       0.631754     3.746881     3.683425     237.18
 H       0.706536     4.411206     2.886181      29.31
 H       0.274891     1.614146     3.914807      23.47
 H      -0.945148     2.434503     2.783957      24.96
 C      -2.620652    -0.930030     0.423508      50.72
 H      -3.164587    -1.813905     0.681515      20.40
 C      -2.288683     0.871624    -1.187943      49.45
 H      -2.557566     1.343379    -2.156899      19.40
 C      -1.169563     1.320334    -0.433668      20.53
 O      -0.362284     2.304732    -0.958137     249.69
 C      -0.958080     3.441734    -1.615221     107.35
 H      -0.137352     4.389934    -1.766695      23.17
 H      -1.130936     3.310169    -2.696497      25.96
 H      -2.008471     3.833881    -1.321777      26.07
 C      -0.747813     0.643687     0.719711      41.58
 O       0.426702     0.832162     1.400365     221.42
 C      -1.444738    -0.531139     1.094195      49.15
 H      -1.306222    -1.006810     2.035985      22.69
 C      -3.047425    -0.288635    -0.772376      38.96
 C      -4.072348    -0.896812    -1.647860      74.38
 H      -4.177929    -0.356343    -2.580338      27.65
 O      -3.706738    -2.276886    -2.041024     225.59
 H      -2.707895    -2.339084    -1.982044      24.64
 C      -5.547517    -0.858787    -1.143496      93.69
 H      -5.593485    -1.370620    -0.144759      27.74
 O      -5.940644     0.540628    -1.032770     298.17
 H      -5.389858     0.939762    -0.365562      31.77
 C      -6.518107    -1.607795    -2.116796     104.12
 O      -6.325348    -3.043568    -2.028244     165.75
 H      -5.323295    -3.196458    -2.285227      28.83
 H      -6.392369    -1.196174    -3.174142      28.59
 H      -7.588303    -1.498534    -1.745100      28.00
55
name = lig-ACN-frame_34
 C       3.537902     2.658789    -0.080078      56.35
 H       3.002744     3.673085    -0.047137      22.55
 C       4.074577     0.382750     0.742223      51.08
 H       4.005400    -0.338041     1.542479      20.23
 C       4.917374     0.227779    -0.408635      22.84
 O       5.613212    -0.902817    -0.677388     178.82
 C       5.612748    -2.101359     0.171950     101.88
 H       6.103584    -1.776080     1.157233      24.64
 H       6.203842    -2.932812    -0.250587      24.37
 H       4.504342    -2.422918     0.199301      24.81
 C       5.055758     1.290219    -1.379297      27.59
 O       5.726461     1.045929    -2.584692      12.79
 H       6.652100     0.723354    -2.437143      17.69
 C       4.365384     2.477033    -1.170146      54.79
 H       4.545769     3.220336    -1.907824      24.65
 C       3.370547     1.636237     0.884439      10.57
 C       2.439015     1.944619     2.103263      70.65
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 H       2.869374     2.986769     2.472010      23.16
 O       2.619845     0.972210     3.262561     207.00
 H       2.179546     0.103044     2.860179      22.21
 C       0.905882     2.186643     1.789070      85.99
 H       0.671102     2.883841     1.010984      23.18
 C       0.104939     2.541572     3.022371     104.02
 O       0.587414     3.712126     3.689870     210.72
 H       0.837934     4.451179     2.915780      28.97
 H       0.187349     1.663901     3.902055      23.70
 H      -0.946032     2.810722     2.801774      25.19
 C      -2.615600    -0.967394     0.364908      82.28
 H      -3.012805    -1.885200     0.612925      24.31
 C      -2.321851     0.859284    -1.155208      37.84
 H      -2.442395     1.268265    -2.192625      18.85
 C      -1.202798     1.347365    -0.458336      29.61
 O      -0.384222     2.375258    -0.984906     223.52
 C      -1.036237     3.479513    -1.705961      86.54
 H      -0.170103     4.400268    -1.477124      21.86
 H      -1.226748     3.084858    -2.723418      24.57
 H      -1.911676     3.775243    -1.016721      25.10
 C      -0.753513     0.619798     0.712262      35.10
 O       0.462123     0.829201     1.353868     195.25
 C      -1.497674    -0.507275     1.123116      49.39
 H      -0.927277    -1.083473     1.861686      16.45
 C      -3.019944    -0.246543    -0.774562      34.11
 C      -4.094091    -0.901902    -1.746149      48.73
 H      -4.082299    -0.265143    -2.639183      26.97
 O      -3.749628    -2.250756    -2.074423     228.57
 H      -2.690060    -2.403519    -2.209219      22.48
 C      -5.571142    -0.842923    -1.118744      95.77
 H      -5.647640    -1.319911    -0.124687      28.62
 O      -5.919395     0.589058    -1.046405     265.63
 H      -5.307308     0.961712    -0.295361      26.84
 C      -6.525694    -1.612446    -2.093818     107.38
 O      -6.307834    -3.055175    -2.019072     191.55
 H      -5.327740    -3.157186    -2.112197      30.32
 H      -6.290666    -1.287755    -3.153844      28.81
 H      -7.640834    -1.352087    -1.973348      27.91
55
name = lig-ACN-frame_35
 C       3.558375     2.652678    -0.033888      42.43
 H       2.888801     3.548687    -0.009337      21.06
 C       4.042403     0.456304     0.771958      57.82
 H       3.999471    -0.354540     1.416996      18.67
 C       4.879892     0.255205    -0.338851      23.66
 O       5.652582    -0.917682    -0.663889     210.98
 C       5.611254    -2.076665     0.189907     113.71
 H       5.989312    -1.931224     1.295815      24.94
 H       6.305175    -2.697536    -0.353497      23.97
 H       4.606683    -2.579860     0.420918      24.96
 C       5.013178     1.226107    -1.385998      23.57
 O       5.721609     1.041385    -2.570737     136.67
 H       6.535474     0.598344    -2.335433      25.92
 C       4.407334     2.484663    -1.193091      50.90
 H       4.560214     3.319927    -1.786298      25.95
 C       3.319270     1.657532     0.942768      26.79
 C       2.417643     1.951379     2.148076      81.87
 H       2.720905     2.942914     2.715715      23.85
 O       2.622211     0.996791     3.207436     259.16
 H       2.198877     0.178256     3.034170      26.32
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 C       0.898989     2.162639     1.777290      91.68
 H       0.881599     2.917522     0.979086      22.97
 C       0.022446     2.590594     2.992890      99.26
 O       0.585833     3.749360     3.695638     256.55
 H       0.574564     4.461489     3.022430      32.18
 H       0.008424     1.604930     3.748943      24.52
 H      -1.011151     2.637596     2.593375      25.60
 C      -2.578330    -1.026871     0.366428      72.50
 H      -3.037838    -1.905600     0.687598      23.48
 C      -2.321816     0.913042    -1.194956      49.63
 H      -2.616920     1.405599    -2.157301      18.79
 C      -1.184602     1.383888    -0.487901      13.98
 O      -0.394947     2.421743    -0.962665     236.46
 C      -1.091983     3.473177    -1.699434     101.50
 H      -0.299706     4.480387    -1.901618      21.65
 H      -1.388410     3.363075    -2.803698      24.50
 H      -2.083902     3.820296    -1.258997      25.60
 C      -0.776377     0.646801     0.663545      38.58
 O       0.493699     0.835066     1.294208     202.47
 C      -1.510883    -0.509870     1.109238      26.37
 H      -1.169776    -1.230092     1.912788      14.82
 C      -3.062131    -0.320641    -0.800625      55.08
 C      -4.098367    -0.817336    -1.747639      42.73
 H      -4.129914    -0.256404    -2.702354      27.83
 O      -3.815595    -2.267732    -2.122287     204.46
 H      -2.746090    -2.339624    -2.165373      22.66
 C      -5.545441    -0.813298    -1.168135      99.88
 H      -5.536383    -1.240262    -0.174609      28.48
 O      -5.900256     0.593684    -1.071445     266.60
 H      -5.782932     0.835895    -0.081280      26.19
 C      -6.502470    -1.586868    -2.109810     107.02
 O      -6.321678    -3.051528    -1.996898     203.16
 H      -5.382384    -3.147204    -1.981894      31.68
 H      -6.309879    -1.205937    -3.147022      30.25
 H      -7.582982    -1.390135    -1.778675      28.80
55
name = lig-ACN-frame_36
 C       3.519592     2.695502    -0.032440      60.28
 H       3.175669     3.701174     0.169719      24.62
 C       4.054853     0.456657     0.804626      57.06
 H       3.831844    -0.236580     1.557004      19.58
 C       4.876827     0.219680    -0.363643      12.53
 O       5.642583    -0.887926    -0.620692     200.75
 C       5.636629    -2.063697     0.244593     106.54
 H       6.092943    -1.769815     1.284644      25.09
 H       6.236363    -2.867121    -0.159838      25.08
 H       4.559098    -2.371289     0.169027      26.17
 C       4.976861     1.234326    -1.371088      13.63
 O       5.732197     1.017777    -2.541762      92.01
 H       6.528946     0.403209    -2.361959      23.21
 C       4.381836     2.490486    -1.125750      54.35
 H       4.624892     3.183743    -1.883592      21.15
 C       3.316158     1.709991     0.946219       3.09
 C       2.391977     1.964155     2.206058      88.36
 H       2.699709     3.016339     2.582027      22.91
 O       2.601621     0.998748     3.191490     271.47
 H       2.237009     0.201522     2.781951      26.53
 C       0.945028     2.107236     1.766108      93.33
 H       0.903930     2.878115     0.951131      21.11
 C      -0.018472     2.591071     2.941657     105.92
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 O       0.529649     3.780226     3.643875     256.88
 H       0.407340     4.503899     3.099583      34.04
 H      -0.066312     1.819902     3.875165      24.20
 H      -1.024295     2.930017     2.663527      24.82
 C      -2.609194    -1.009466     0.313160      76.87
 H      -3.136712    -1.910387     0.620068      21.71
 C      -2.366567     0.872967    -1.192008      45.40
 H      -2.779903     1.433555    -2.025445      19.12
 C      -1.213483     1.357212    -0.520872      16.54
 O      -0.433296     2.497008    -0.949534     228.64
 C      -1.153065     3.505297    -1.745189      84.46
 H      -0.292824     4.457541    -1.712583      21.95
 H      -1.289728     2.869831    -2.686898      23.17
 H      -2.033820     3.854164    -1.155730      25.45
 C      -0.749102     0.642780     0.652652      58.23
 O       0.467430     0.850421     1.218723     216.01
 C      -1.468765    -0.516229     1.041682      66.06
 H      -1.175592    -0.778814     2.114073      20.34
 C      -2.964888    -0.284329    -0.829825      21.02
 C      -4.089600    -0.848477    -1.754707      64.30
 H      -4.066473    -0.183346    -2.668152      24.84
 O      -3.873592    -2.232022    -2.163916     249.43
 H      -2.927753    -2.454069    -2.080102      26.73
 C      -5.485744    -0.787601    -1.217824     100.77
 H      -5.527129    -1.321351    -0.290059      30.04
 O      -5.923081     0.599596    -1.077157     268.43
 H      -6.142256     0.736489    -0.179166      30.29
 C      -6.499670    -1.577776    -2.099675     109.21
 O      -6.360887    -3.007879    -1.976931     186.30
 H      -5.368816    -3.188391    -2.091520      29.68
 H      -6.538786    -1.288283    -3.166338      30.40
 H      -7.541834    -1.353735    -1.707262      29.80
55
name = lig-ACN-frame_37
 C       3.526650     2.790375    -0.007503      49.55
 H       3.193727     3.785041     0.097118      23.43
 C       4.036511     0.474656     0.791864      66.74
 H       4.107054    -0.314303     1.545625      19.05
 C       4.825272     0.217800    -0.332524      12.76
 O       5.680594    -0.885201    -0.606361     177.23
 C       5.592840    -2.015069     0.300163     118.83
 H       5.945676    -1.735036     1.376761      25.82
 H       6.258800    -2.754295    -0.143380      24.09
 H       4.590278    -2.395990     0.581341      25.39
 C       4.976284     1.230879    -1.325228      13.27
 O       5.712974     1.009578    -2.495350      13.61
 H       6.557566     0.448726    -2.234330      21.21
 C       4.349821     2.472610    -1.130563      49.96
 H       4.539719     3.346188    -1.774358      24.02
 C       3.362243     1.721432     0.942849       7.81
 C       2.433454     1.992425     2.121364      65.19
 H       2.683101     2.927611     2.693708      24.43
 O       2.569856     0.948355     3.230922     178.68
 H       2.175582    -0.000416     2.925275      19.99
 C       0.869593     2.159948     1.767640      77.01
 H       0.788913     2.961588     0.953565      20.99
 C      -0.008101     2.629387     2.919751     105.74
 O       0.466756     3.810576     3.575424     253.62
 H       0.428184     4.554512     2.796012      28.38
 H      -0.161248     1.743163     3.651688      25.73
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 H      -0.964803     2.708890     2.369764      25.48
 C      -2.550053    -0.959669     0.321830      74.74
 H      -3.098691    -1.881818     0.706423      22.92
 C      -2.343313     0.935740    -1.211685      81.62
 H      -2.639805     1.423360    -2.111530      17.99
 C      -1.201572     1.398644    -0.557395      21.04
 O      -0.515540     2.516678    -0.868360     240.36
 C      -1.163541     3.459426    -1.751854     113.06
 H      -0.420772     4.434734    -2.014311      23.23
 H      -1.480820     3.276966    -2.860332      25.97
 H      -2.113826     3.834263    -1.349629      27.91
 C      -0.760084     0.626074     0.533506      41.28
 O       0.495080     0.841083     1.195534     211.51
 C      -1.473475    -0.483439     1.029562      23.65
 H      -1.119141    -1.122966     1.899213      16.07
 C      -2.985463    -0.348519    -0.880302      70.95
 C      -4.021537    -0.827626    -1.820887      40.20
 H      -3.968952    -0.223429    -2.786581      25.71
 O      -3.880492    -2.221052    -2.199572     270.82
 H      -2.974224    -2.413770    -2.241149      26.75
 C      -5.522359    -0.798916    -1.212025      84.70
 H      -5.483750    -1.208218    -0.222988      29.70
 O      -5.969269     0.582687    -1.104587     259.82
 H      -5.831292     0.800650    -0.123927      27.91
 C      -6.565025    -1.549781    -2.083869     110.75
 O      -6.415287    -2.996009    -1.966498     183.07
 H      -5.429064    -3.111981    -2.253400      28.97
 H      -6.443118    -1.188283    -3.108762      31.41
 H      -7.557778    -1.254752    -1.701013      30.57
55
name = lig-ACN-frame_38
 C       3.599684     2.756764     0.019440      65.69
 H       2.963049     3.584488     0.124628      23.45
 C       4.032768     0.495681     0.789037      54.92
 H       3.826947    -0.188973     1.684071      18.19
 C       4.854154     0.240288    -0.350072      14.00
 O       5.645128    -0.880565    -0.561951     207.04
 C       5.564611    -1.963579     0.421725     105.71
 H       6.111089    -1.671096     1.365787      25.73
 H       6.161252    -2.808338    -0.020405      24.58
 H       4.545404    -2.300488     0.421617      28.00
 C       4.950055     1.262099    -1.311586      14.81
 O       5.701906     1.015838    -2.445160     131.50
 H       6.563932     0.613858    -2.226326      23.70
 C       4.332363     2.524730    -1.159129      51.20
 H       4.656623     3.247594    -1.985894      23.13
 C       3.370444     1.752260     0.961386       2.40
 C       2.400983     1.918976     2.175870      91.52
 H       2.754576     2.849480     2.612603      23.59
 O       2.533752     0.946218     3.203849     259.98
 H       1.977925     0.101659     2.870855      21.72
 C       0.933695     2.190856     1.690580      69.44
 H       0.892517     2.984106     0.859520      20.93
 C      -0.061138     2.581268     2.861834     109.29
 O       0.395741     3.858750     3.480507     237.29
 H       0.542655     4.596102     2.672444      28.04
 H       0.002396     1.909942     3.714395      26.25
 H      -1.122218     2.767096     2.621609      25.58
 C      -2.582639    -0.965094     0.280387      84.55
 H      -3.044109    -1.971422     0.653650      21.52
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 C      -2.350032     0.906098    -1.295908      31.47
 H      -2.605905     1.341785    -2.228785      17.72
 C      -1.240981     1.385773    -0.537749      21.99
 O      -0.571100     2.591568    -0.852970     228.59
 C      -1.206720     3.500730    -1.801593      91.63
 H      -0.357720     4.341377    -1.765447      22.63
 H      -1.245796     2.801003    -2.717738      23.73
 H      -2.107657     3.909474    -1.352115      26.59
 C      -0.665693     0.625113     0.556510      24.95
 O       0.505630     0.866311     1.181171     225.42
 C      -1.435934    -0.474994     1.004256      70.86
 H      -0.909740    -1.088551     1.755771      14.79
 C      -2.961632    -0.265909    -0.908682      35.85
 C      -4.099240    -0.829768    -1.873994      38.56
 H      -4.170930    -0.163836    -2.803510      25.08
 O      -3.833883    -2.260700    -2.249654     236.92
 H      -2.823205    -2.395104    -2.364259      23.65
 C      -5.519081    -0.777431    -1.216495      98.68
 H      -5.445250    -1.306809    -0.275650      28.67
 O      -6.002383     0.579102    -1.103203     273.84
 H      -5.403856     1.053346    -0.393208      27.68
 C      -6.603371    -1.514706    -2.061187     110.19
 O      -6.484379    -2.978042    -1.989884     223.43
 H      -5.578374    -3.179701    -2.180705      32.79
 H      -6.520818    -1.201870    -3.097783      30.39
 H      -7.630703    -1.361644    -1.780997      29.06
55
name = lig-ACN-frame_39
 C       3.566943     2.760631     0.005969      46.17
 H       3.156998     3.759365     0.074760      22.94
 C       4.038603     0.496978     0.824616      68.94
 H       3.840220    -0.443447     1.463427      17.22
 C       4.853152     0.288363    -0.272181       8.03
 O       5.596508    -0.876691    -0.517693     196.01
 C       5.546120    -1.923271     0.491170     114.82
 H       5.878280    -1.582565     1.481213      27.48
 H       6.125509    -2.824370     0.125094      24.12
 H       4.553242    -2.158902     0.791465      28.19
 C       4.970297     1.282716    -1.320508      13.75
 O       5.725568     1.039959    -2.468313      68.07
 H       6.550755     0.640200    -2.177732      24.46
 C       4.362205     2.534484    -1.149383      39.69
 H       4.421814     3.373581    -1.925146      22.31
 C       3.376066     1.708513     0.982981       6.29
 C       2.399860     1.980493     2.187946      77.74
 H       2.593548     2.870354     2.733899      25.41
 O       2.466860     0.907596     3.154084     263.96
 H       1.983294     0.139197     2.875450      25.63
 C       0.941866     2.162776     1.681250      87.37
 H       1.023800     2.924497     0.832996      21.27
 C      -0.030934     2.617423     2.835515     113.40
 O       0.333694     3.892501     3.378094     298.24
 H       0.316358     4.533147     2.599548      29.96
 H       0.117382     1.874289     3.556431      27.21
 H      -1.047011     2.505229     2.424714      26.38
 C      -2.554869    -0.924911     0.217021      81.66
 H      -3.118534    -1.907902     0.466862      20.66
 C      -2.289919     0.887449    -1.337442      60.29
 H      -2.580363     1.448402    -2.223308      19.84
 C      -1.233514     1.431221    -0.538127      16.10
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 O      -0.617297     2.636517    -0.797641     239.75
 C      -1.183190     3.506902    -1.820014     118.71
 H      -0.560343     4.418940    -2.069388      24.71
 H      -1.307133     3.111042    -2.897874      25.59
 H      -2.192460     3.826662    -1.606353      27.36
 C      -0.725966     0.659338     0.550545      48.68
 O       0.559515     0.895566     1.160177     209.32
 C      -1.390448    -0.547632     0.911889      21.90
 H      -1.176515    -0.990259     1.855912      20.56
 C      -3.055088    -0.287632    -0.953169      51.37
 C      -4.132101    -0.871128    -1.858829      63.26
 H      -4.133933    -0.275418    -2.829769      27.41
 O      -3.816168    -2.245507    -2.299641     225.95
 H      -2.737337    -2.353859    -2.184538      22.09
 C      -5.551664    -0.811679    -1.229699      98.02
 H      -5.569966    -1.201056    -0.204529      28.10
 O      -5.995982     0.595328    -1.112706     295.39
 H      -5.444804     0.989246    -0.426302      30.29
 C      -6.627851    -1.525087    -2.087178     118.45
 O      -6.553101    -2.962275    -2.018959     233.90
 H      -5.602750    -3.141740    -2.110996      31.97
 H      -6.634648    -1.153888    -3.098335      30.61
 H      -7.491038    -1.176685    -1.607905      30.30
55
name = lig-ACN-frame_40
 C       3.530113     2.743754     0.019355      65.70
 H       3.158971     3.767732     0.273028      24.58
 C       4.014660     0.493832     0.860942      37.64
 H       3.884185    -0.301085     1.653274      18.40
 C       4.893684     0.316529    -0.284578       3.31
 O       5.548904    -0.886722    -0.480508     193.83
 C       5.487403    -1.858662     0.616381     116.67
 H       6.069776    -1.484873     1.409390      26.05
 H       6.142804    -2.669468     0.177280      24.01
 H       4.540688    -2.291834     0.754384      26.97
 C       5.033842     1.293245    -1.302037      10.37
 O       5.764434     1.064942    -2.501255      29.06
 H       6.614634     0.494554    -2.332758      23.46
 C       4.363197     2.507667    -1.089746      50.27
 H       4.684892     3.345790    -1.764434      22.25
 C       3.350279     1.777514     1.009135       1.32
 C       2.402428     1.994445     2.156622      86.02
 H       2.720466     2.838804     2.669283      25.64
 O       2.415496     0.861190     3.128532     261.23
 H       2.004256     0.140932     2.688381      26.09
 C       0.955160     2.206158     1.676759      90.05
 H       0.819916     3.005350     0.900642      20.76
 C       0.035925     2.579787     2.784703     122.01
 O       0.253300     3.926394     3.288417     320.29
 H       0.166237     4.569259     2.653906      34.47
 H       0.022432     1.995029     3.601864      27.57
 H      -0.991095     2.620468     2.412206      25.62
 C      -2.561540    -0.964311     0.134412      96.17
 H      -3.080814    -1.807217     0.656489      21.76
 C      -2.291496     0.900346    -1.340761      28.23
 H      -2.583104     1.411238    -2.293975      18.19
 C      -1.246686     1.438394    -0.569288      25.98
 O      -0.646781     2.702288    -0.787109     226.98
 C      -1.197086     3.537837    -1.891559     107.17
 H      -0.547594     4.342542    -1.745119      25.12
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 H      -1.087088     2.934036    -2.823113      25.50
 H      -2.201672     3.837289    -1.567776      26.43
 C      -0.728163     0.670339     0.547277      64.00
 O       0.523648     0.863758     1.099396     191.13
 C      -1.410463    -0.544366     0.844312      24.95
 H      -1.073732    -1.165527     1.626544      17.48
 C      -3.002433    -0.259631    -0.994105      75.16
 C      -4.115084    -0.870981    -1.861515      36.82
 H      -4.250218    -0.190738    -2.757525      27.27
 O      -3.838705    -2.225277    -2.312106     214.62
 H      -2.818563    -2.493855    -2.222906      24.86
 C      -5.587020    -0.822775    -1.244978      98.24
 H      -5.572557    -1.366460    -0.265851      28.32
 O      -5.946145     0.590763    -1.163681     282.26
 H      -5.913919     0.759368    -0.221467      28.96
 C      -6.680215    -1.493198    -2.087080     112.57
 O      -6.593787    -2.965035    -2.050857     206.88
 H      -5.594105    -3.218396    -2.174091      31.68
 H      -6.628185    -1.129608    -3.096667      31.68
 H      -7.678785    -1.408593    -1.741660      29.70
55
name = lig-ACN-frame_41
 C       3.554809     2.765473     0.045534      50.45
 H       2.969633     3.749807     0.025316      22.93
 C       4.046836     0.587214     0.823673      93.46
 H       3.966142    -0.080410     1.659940      21.82
 C       4.860573     0.286971    -0.248187      13.24
 O       5.503539    -0.914267    -0.448988     212.13
 C       5.527479    -1.836901     0.670347     115.57
 H       5.791872    -1.416662     1.577236      28.29
 H       6.112881    -2.732328     0.414543      24.51
 H       4.516374    -2.041718     0.919306      28.76
 C       5.081064     1.282024    -1.268823       3.88
 O       5.775562     1.103531    -2.490997      -4.32
 H       6.641531     0.557242    -2.242574      22.39
 C       4.417684     2.540026    -1.063223      33.74
 H       4.643060     3.339674    -1.748126      22.25
 C       3.353608     1.736692     0.991317      13.54
 C       2.385488     1.924083     2.172421      90.89
 H       2.592723     2.773198     2.723060      26.33
 O       2.391957     0.873228     3.074392     277.87
 H       1.869245     0.027826     2.744986      22.52
 C       0.943137     2.202026     1.618295      72.34
 H       1.007316     2.915218     0.793380      23.21
 C      -0.070602     2.593302     2.797109     111.16
 O       0.202795     3.952108     3.278177     305.72
 H       0.256855     4.451501     2.428249      30.47
 H       0.160466     1.964179     3.547029      28.01
 H      -1.053281     2.428057     2.380673      26.99
 C      -2.559414    -1.008882     0.129995      49.75
 H      -3.096234    -1.916753     0.317022      22.23
 C      -2.334448     0.957589    -1.374700      61.06
 H      -2.624229     1.466637    -2.352600      18.16
 C      -1.254965     1.469035    -0.577734      27.04
 O      -0.689914     2.714862    -0.798628     237.10
 C      -1.164399     3.556643    -1.866899     128.07
 H      -0.667535     4.409125    -1.951532      28.05
 H      -1.000718     3.087637    -2.842464      27.77
 H      -2.245471     3.776741    -1.894665      27.93
 C      -0.735422     0.651991     0.457053      32.37
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 O       0.507846     0.876638     1.071298     209.63
 C      -1.414304    -0.526140     0.825406      41.06
 H      -0.839248    -1.130350     1.490612      16.36
 C      -2.962263    -0.289327    -1.023870      56.91
 C      -4.146894    -0.811249    -1.912178      39.30
 H      -4.156572    -0.224314    -2.861503      27.09
 O      -3.883957    -2.234099    -2.309045     275.77
 H      -2.933823    -2.294243    -2.399751      25.39
 C      -5.577358    -0.827569    -1.256553      89.30
 H      -5.572138    -1.237398    -0.192174      28.55
 O      -5.894176     0.579376    -1.163850     210.01
 H      -6.223674     0.816444    -0.218793      27.20
 C      -6.725213    -1.537614    -2.132674     106.56
 O      -6.596467    -2.983686    -2.095521     233.20
 H      -5.648443    -3.082637    -2.353409      31.25
 H      -6.661260    -1.162026    -3.138423      32.10
 H      -7.639970    -1.117117    -1.741056      31.07
55
name = lig-ACN-frame_42
 C       3.587901     2.810216    -0.002195      56.95
 H       2.952262     3.762215     0.004245      23.06
 C       4.109254     0.561157     0.888204      26.46
 H       3.965154    -0.239871     1.532475      18.45
 C       4.882878     0.279115    -0.307744      -2.03
 O       5.517382    -0.971264    -0.434906     184.61
 C       5.488123    -1.812390     0.764720     120.96
 H       5.991352    -1.307472     1.488799      29.58
 H       6.153117    -2.613864     0.508983      25.70
 H       4.546237    -2.292149     0.970718      27.40
 C       5.060680     1.327303    -1.246071      22.41
 O       5.782753     1.126910    -2.417306     177.76
 H       6.676188     0.747898    -2.237627      23.08
 C       4.495415     2.571560    -1.047466      70.57
 H       4.546244     3.260389    -1.816554      24.87
 C       3.333073     1.813495     0.964107     -26.58
 C       2.304286     1.931507     2.122614      80.69
 H       2.584891     2.774104     2.662588      25.51
 O       2.391433     0.808536     3.079852     233.06
 H       1.758284     0.016176     2.724901      20.30
 C       0.851781     2.157432     1.604552      92.05
 H       0.880408     2.944204     0.882035      22.46
 C      -0.101055     2.600163     2.752563     118.99
 O       0.148245     3.918216     3.271375     275.99
 H       0.265570     4.727621     2.547218      26.73
 H      -0.012758     1.955569     3.569106      27.08
 H      -1.151417     2.536990     2.555013      26.79
 C      -2.523534    -1.003820     0.070928      68.96
 H      -2.792771    -1.981570     0.306181      20.40
 C      -2.385348     0.956301    -1.371864      45.32
 H      -2.775358     1.576683    -2.236383      18.24
 C      -1.325517     1.497566    -0.649606      26.63
 O      -0.710023     2.741596    -0.796088     244.06
 C      -1.141346     3.567338    -1.936334     126.07
 H      -0.692789     4.378073    -1.720508      28.12
 H      -0.875686     3.124024    -2.854249      28.13
 H      -2.230971     3.726244    -1.751096      26.60
 C      -0.739000     0.661630     0.389265      54.42
 O       0.498272     0.900307     1.040850     207.92
 C      -1.380288    -0.562567     0.793297      54.76
 H      -1.133304    -1.105496     1.733845      20.23
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 C      -3.016454    -0.281069    -1.073495      45.01
 C      -4.135816    -0.835722    -1.952025      56.17
 H      -4.254392    -0.201160    -2.841276      28.34
 O      -3.931934    -2.222682    -2.304706     266.03
 H      -3.042284    -2.410602    -2.526061      28.43
 C      -5.554764    -0.792834    -1.313179      90.16
 H      -5.453403    -1.378747    -0.321897      28.18
 O      -5.908486     0.618738    -1.180284     284.69
 H      -5.779156     0.791334    -0.170556      26.28
 C      -6.655816    -1.524344    -2.153796     108.11
 O      -6.596325    -2.989744    -2.150779     237.81
 H      -5.726080    -3.216439    -2.405354      34.93
 H      -6.682999    -1.160533    -3.171907      31.36
 H      -7.665291    -1.457412    -1.696079      28.79
55
name = lig-ACN-frame_43
 C       3.572370     2.829034     0.000486      38.55
 H       3.106030     3.844005     0.092840      22.67
 C       4.090358     0.593308     0.859314      78.73
 H       3.809734    -0.052002     1.640899      20.13
 C       4.897158     0.279769    -0.231720       7.67
 O       5.504270    -0.977044    -0.441214     188.20
 C       5.542062    -1.819186     0.794646     110.79
 H       5.804844    -1.299610     1.645051      28.61
 H       6.179695    -2.610437     0.558118      25.19
 H       4.509342    -2.099584     1.055882      27.27
 C       5.092407     1.310468    -1.226013      -1.05
 O       5.819484     1.141845    -2.396840       8.68
 H       6.638466     0.722041    -2.111838      22.61
 C       4.489789     2.631916    -1.072600      38.77
 H       4.844372     3.339338    -1.761090      22.62
 C       3.380382     1.774840     0.959623      -0.14
 C       2.271600     1.939437     2.094902      73.22
 H       2.459762     2.803318     2.700713      25.56
 O       2.377965     0.780042     3.044062     238.46
 H       1.896960     0.007204     2.692281      24.71
 C       0.790215     2.190512     1.618553      84.56
 H       0.719800     2.933322     0.873424      22.79
 C      -0.176605     2.582465     2.751897     110.81
 O       0.141863     3.902176     3.298107     254.69
 H       0.051580     4.523415     2.433914      28.19
 H      -0.099262     1.913676     3.593071      26.65
 H      -1.087892     2.588414     2.176197      26.13
 C      -2.465493    -1.025944    -0.035814      63.18
 H      -3.019348    -1.857916     0.294619      25.06
 C      -2.486686     0.982025    -1.389660      56.38
 H      -2.931926     1.520314    -2.243741      20.65
 C      -1.317388     1.453913    -0.630087      15.09
 O      -0.732138     2.730414    -0.832042     227.23
 C      -1.131993     3.601219    -1.934250     126.99
 H      -0.683147     4.435677    -1.835757      28.96
 H      -0.820923     3.187863    -2.840265      28.81
 H      -2.226949     3.798001    -2.049043      26.73
 C      -0.756083     0.653649     0.388924      27.17
 O       0.439097     0.887040     0.973292     211.41
 C      -1.399207    -0.520670     0.714572      40.82
 H      -0.969181    -1.052581     1.633818      15.50
 C      -3.027371    -0.280388    -1.070133      66.41
 C      -4.136889    -0.848764    -2.006125      40.88
 H      -4.072844    -0.298727    -2.936671      28.42
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 O      -3.960887    -2.261196    -2.325834     253.49
 H      -2.920506    -2.376596    -2.404182      26.59
 C      -5.529589    -0.780012    -1.371155      91.75
 H      -5.546520    -1.211701    -0.298322      25.65
 O      -5.943768     0.634714    -1.158531     257.68
 H      -5.342060     0.970625    -0.517488      29.71
 C      -6.619643    -1.516226    -2.171923     104.79
 O      -6.565146    -2.999216    -2.212564     224.32
 H      -5.578285    -3.209896    -2.414978      30.31
 H      -6.655673    -1.077416    -3.178100      30.20
 H      -7.555317    -1.117864    -1.686715      28.63
55
name = lig-ACN-frame_44
 C       3.598451     2.837115     0.014673      75.19
 H       3.111290     3.793096     0.159504      28.13
 C       4.011546     0.590016     0.861533      26.36
 H       3.996468    -0.217034     1.610811      18.86
 C       4.925927     0.316762    -0.213889      -6.67
 O       5.500181    -0.935448    -0.396558     186.67
 C       5.559717    -1.792609     0.766883     117.49
 H       5.984985    -1.243277     1.557831      26.11
 H       6.196360    -2.613794     0.604419      24.90
 H       4.556587    -2.248951     0.940888      25.87
 C       5.101989     1.342266    -1.203062      10.05
 O       5.865378     1.136254    -2.384000      67.34
 H       6.687550     0.567814    -2.273429      23.67
 C       4.486856     2.579633    -1.044880      67.28
 H       4.763178     3.472787    -1.589656      23.55
 C       3.312370     1.847288     0.953980      -4.97
 C       2.297664     1.906566     2.100366      80.03
 H       2.579908     2.776896     2.720921      26.09
 O       2.348263     0.823520     2.973513     274.52
 H       1.911436     0.077952     2.635266      27.53
 C       0.831113     2.166927     1.591960      84.21
 H       0.907069     2.968735     0.895755      26.03
 C      -0.261191     2.566704     2.726217     106.37
 O       0.134220     3.868922     3.289456     284.46
 H       0.117602     4.526188     2.634798      32.92
 H      -0.331838     1.769585     3.553304      26.03
 H      -1.305947     2.616358     2.449244      26.18
 C      -2.508756    -1.075789    -0.068926      68.45
 H      -2.934893    -2.053886     0.212392      21.69
 C      -2.491594     1.032910    -1.356176      63.84
 H      -2.727155     1.586750    -2.239669      21.12
 C      -1.394020     1.501808    -0.709294      27.33
 O      -0.770928     2.702934    -0.864893     239.28
 C      -1.111895     3.603346    -1.977180     129.96
 H      -0.631915     4.435385    -1.762503      29.00
 H      -0.810665     3.197135    -2.887635      29.98
 H      -2.205152     3.794601    -1.936959      28.43
 C      -0.823643     0.689632     0.330508      41.60
 O       0.440039     0.909937     0.965058     193.07
 C      -1.420710    -0.564381     0.680902      42.14
 H      -0.879988    -1.275705     1.397880      17.05
 C      -3.028514    -0.289461    -1.154664      55.76
 C      -4.111324    -0.845607    -2.035372      55.56
 H      -4.182050    -0.313212    -2.961058      26.07
 O      -3.916080    -2.313822    -2.340685     218.41
 H      -2.870838    -2.575299    -2.406579      24.34
 C      -5.530290    -0.746199    -1.355152      83.93
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 H      -5.371142    -1.325615    -0.367689      27.75
 O      -5.962894     0.617929    -1.214682     266.27
 H      -5.415435     1.011881    -0.478306      28.87
 C      -6.639640    -1.474245    -2.229416      98.00
 O      -6.526249    -2.937953    -2.253581     226.31
 H      -5.511016    -3.064439    -2.383268      29.96
 H      -6.574013    -1.134293    -3.292970      29.56
 H      -7.681979    -1.347475    -1.823616      27.25
55
name = lig-ACN-frame_45
 C       3.588797     2.848960     0.061887      51.01
 H       3.158264     3.809886    -0.007797      22.54
 C       3.994472     0.600403     0.827873      77.06
 H       3.653250    -0.159164     1.608180      18.45
 C       4.878598     0.372337    -0.217827      15.05
 O       5.531147    -0.851011    -0.387232     211.70
 C       5.584898    -1.783243     0.732386     110.78
 H       5.981333    -1.330624     1.636255      26.75
 H       6.280369    -2.476569     0.308747      24.14
 H       4.599408    -2.201167     1.055868      26.93
 C       5.153671     1.335637    -1.219122       8.94
 O       5.868522     1.141255    -2.376406      52.21
 H       6.698885     0.599198    -2.006090      21.46
 C       4.503029     2.592523    -0.998772      23.76
 H       4.653557     3.254238    -1.907341      21.79
 C       3.270314     1.773972     0.966320      -0.49
 C       2.255631     1.981386     2.106838      80.68
 H       2.499057     2.913670     2.708911      24.36
 O       2.335410     0.809161     2.976281     245.25
 H       1.728824     0.077609     2.544418      22.30
 C       0.782861     2.176856     1.586808      90.48
 H       0.776766     2.964620     0.831137      23.49
 C      -0.237313     2.581713     2.657116     109.68
 O       0.130219     3.809873     3.310858     270.66
 H       0.188611     4.453041     2.582629      31.48
 H      -0.098968     1.854052     3.567817      24.53
 H      -1.188370     2.624582     2.107269      25.50
 C      -2.553169    -1.053687    -0.101385      51.35
 H      -2.804025    -2.161515    -0.075994      17.45
 C      -2.542213     1.008888    -1.455768      38.81
 H      -2.977601     1.517686    -2.274184      19.22
 C      -1.411238     1.519780    -0.646095       5.27
 O      -0.765303     2.736113    -0.913249     222.31
 C      -1.111322     3.590652    -2.004326     123.48
 H      -0.526029     4.422460    -1.808285      26.94
 H      -0.861493     3.200276    -2.954645      28.24
 H      -2.165226     3.902438    -1.959538      26.87
 C      -0.844954     0.658800     0.352103      38.06
 O       0.420981     0.922808     0.924225     209.09
 C      -1.417529    -0.607029     0.584909      65.06
 H      -0.964516    -1.175694     1.431988      22.41
 C      -3.008936    -0.297018    -1.189488      32.63
 C      -4.123261    -0.899094    -2.090257      74.96
 H      -4.154926    -0.364398    -3.024570      24.97
 O      -3.854569    -2.320702    -2.335375     288.20
 H      -2.876420    -2.376562    -2.552709      26.14
 C      -5.569421    -0.798789    -1.399681      87.17
 H      -5.635189    -1.232388    -0.348837      28.11
 O      -5.952627     0.615436    -1.278113     246.42
 H      -5.889259     0.829993    -0.254554      26.57
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 C      -6.644910    -1.451442    -2.287886     100.20
 O      -6.467597    -2.868273    -2.284528     271.28
 H      -5.561270    -3.065708    -2.434409      34.27
 H      -6.589018    -0.903783    -3.290034      29.81
 H      -7.671860    -1.170855    -1.939333      28.04
55
name = lig-ACN-frame_46
 C       3.591561     2.836044     0.040490      86.75
 H       3.009430     3.695920     0.182775      28.31
 C       3.933035     0.579337     0.823759      30.81
 H       3.769204    -0.359449     1.449221      19.17
 C       4.855025     0.354945    -0.218283      -6.39
 O       5.580463    -0.772970    -0.394965     179.50
 C       5.641039    -1.766572     0.670949     108.91
 H       6.047769    -1.311674     1.613369      25.86
 H       6.243730    -2.668895     0.429890      24.47
 H       4.607888    -2.152577     0.777366      26.31
 C       5.103073     1.397313    -1.171254       2.92
 O       5.884819     1.129289    -2.353323      99.54
 H       6.793169     0.695548    -2.193099      22.48
 C       4.494988     2.619356    -1.026677      61.70
 H       4.601618     3.505769    -1.763899      24.08
 C       3.262393     1.851332     0.952018     -25.85
 C       2.184332     1.971007     2.073228      63.30
 H       2.428264     2.874815     2.769499      24.78
 O       2.294593     0.828069     3.014325     198.96
 H       1.643858     0.017670     2.755125      21.69
 C       0.774408     2.221709     1.512793      86.51
 H       0.762351     3.029911     0.734095      24.51
 C      -0.189641     2.552700     2.629999     109.61
 O       0.138285     3.801859     3.309786     217.35
 H       0.242325     4.606317     2.574546      27.32
 H      -0.399704     1.625264     3.359162      25.47
 H      -1.238708     2.665224     2.259365      26.39
 C      -2.505107    -1.044149    -0.197597      67.54
 H      -3.110077    -1.994991     0.115415      23.74
 C      -2.499618     0.993921    -1.479845      61.01
 H      -2.884410     1.633471    -2.252688      22.05
 C      -1.485024     1.492351    -0.693742      19.47
 O      -0.744353     2.729292    -0.907305     222.73
 C      -1.126872     3.616006    -2.043629     121.27
 H      -0.480372     4.481315    -2.087751      26.63
 H      -1.002060     3.032073    -2.948176      27.31
 H      -2.157350     3.931459    -2.015111      27.32
 C      -0.857493     0.675759     0.329700      45.27
 O       0.395752     0.903893     0.896222     184.02
 C      -1.403626    -0.610518     0.582940      24.45
 H      -1.011413    -1.261484     1.341172      19.27
 C      -3.086677    -0.291393    -1.235232      63.90
 C      -4.158813    -0.923700    -2.072475      55.89
 H      -4.221070    -0.423492    -3.038834      28.52
 O      -3.794569    -2.317641    -2.335691     255.96
 H      -2.933256    -2.387060    -2.643218      31.93
 C      -5.594250    -0.791496    -1.475532     103.32
 H      -5.551568    -1.362067    -0.513953      27.94
 O      -5.931009     0.623900    -1.314775     264.22
 H      -5.994458     0.797129    -0.362246      28.46
 C      -6.641455    -1.396290    -2.352747     102.46
 O      -6.458930    -2.854002    -2.344265     241.13
 H      -5.518700    -2.942433    -2.588352      33.03
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 H      -6.585824    -1.073018    -3.450651      29.50
 H      -7.623467    -1.209472    -1.902075      28.44
55
name = lig-ACN-frame_47
 C       3.524930     2.876849     0.034129      38.66
 H       3.128387     3.877858     0.010629      22.72
 C       3.882906     0.554345     0.814263      79.44
 H       3.635421    -0.140681     1.636882      21.27
 C       4.851011     0.399863    -0.224574      -4.53
 O       5.691209    -0.767308    -0.428993     177.88
 C       5.630641    -1.750819     0.610258     107.19
 H       6.050183    -1.298794     1.588087      25.04
 H       6.415705    -2.463722     0.187701      23.88
 H       4.651875    -2.203892     0.868238      26.62
 C       5.100992     1.422607    -1.208007      -2.84
 O       5.874691     1.151694    -2.308803      84.49
 H       6.631162     0.677969    -1.965517      26.10
 C       4.438932     2.696805    -1.055733      23.06
 H       4.874304     3.573370    -1.671530      17.86
 C       3.272293     1.784319     0.978796       6.17
 C       2.198140     1.904607     2.047018      85.33
 H       2.412770     2.929868     2.614634      24.38
 O       2.219265     0.895997     3.043857     262.28
 H       1.760674     0.126973     2.699530      27.91
 C       0.774073     2.167875     1.443173      77.98
 H       0.874565     3.018734     0.662368      24.12
 C      -0.278428     2.573795     2.599586      93.90
 O       0.170423     3.795367     3.310012     216.05
 H       0.158165     4.514360     2.546417      28.69
 H      -0.054402     1.810817     3.481541      24.83
 H      -1.322166     2.694310     2.149739      25.27
 C      -2.506197    -1.044831    -0.208158      76.60
 H      -2.993128    -1.992900     0.186178      24.72
 C      -2.513224     1.015634    -1.514369      45.94
 H      -2.805441     1.562833    -2.437086      20.52
 C      -1.391023     1.522792    -0.736050      18.34
 O      -0.787168     2.720094    -0.914599     219.16
 C      -1.156374     3.544404    -2.084554     112.11
 H      -0.350168     4.342512    -2.011922      25.27
 H      -1.112323     3.010472    -3.058407      26.82
 H      -2.096712     3.989533    -1.843099      26.84
 C      -0.865185     0.662660     0.267903      30.70
 O       0.377551     0.924110     0.882114     205.91
 C      -1.441950    -0.585487     0.564366      30.04
 H      -0.952710    -1.167732     1.278295      19.07
 C      -3.072518    -0.242337    -1.234720      52.87
 C      -4.155822    -0.874987    -2.136276      43.11
 H      -4.166759    -0.324270    -3.101521      26.28
 O      -3.810046    -2.335229    -2.334844     238.84
 H      -2.845685    -2.328764    -2.505111      28.53
 C      -5.575098    -0.760272    -1.511219      97.90
 H      -5.663097    -1.252348    -0.538820      27.89
 O      -5.910090     0.635158    -1.334984     274.97
 H      -5.509881     0.906974    -0.509678      28.91
 C      -6.682987    -1.442084    -2.443496      95.36
 O      -6.477563    -2.865367    -2.426613     237.70
 H      -5.499367    -3.097934    -2.687293      30.86
 H      -6.655437    -0.883325    -3.463591      28.98
 H      -7.693336    -1.274804    -2.105192      28.00
55
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name = lig-ACN-frame_48
 C       3.503266     2.871465     0.021721      67.25
 H       3.004674     3.799964     0.352057      25.12
 C       3.953226     0.539218     0.774854      57.46
 H       3.818475    -0.280386     1.431734      21.01
 C       4.883908     0.387079    -0.252943       0.70
 O       5.699995    -0.675123    -0.453266     182.22
 C       5.695710    -1.755672     0.572805      97.27
 H       5.988557    -1.348252     1.647787      23.63
 H       6.392603    -2.642655     0.304518      23.44
 H       4.669991    -2.164134     0.555591      26.23
 C       5.017261     1.442267    -1.193258       8.14
 O       5.900750     1.203164    -2.270099     139.35
 H       6.524595     0.485621    -2.074459      22.25
 C       4.420868     2.693830    -1.011024      57.18
 H       4.618438     3.507430    -1.752066      26.48
 C       3.225147     1.805988     0.887709      -6.07
 C       2.187835     1.971931     2.031742      70.07
 H       2.439331     2.971398     2.646773      24.74
 O       2.144778     0.938449     3.079689     245.81
 H       1.833851     0.120268     2.734786      27.58
 C       0.725909     2.161557     1.489534      87.18
 H       0.757819     2.952879     0.624912      22.97
 C      -0.218427     2.607342     2.568885     111.20
 O       0.173943     3.812358     3.242125     282.47
 H       0.210029     4.525205     2.682205      33.24
 H      -0.393622     1.727388     3.340684      25.45
 H      -1.308085     2.649166     2.161692      25.58
 C      -2.589696    -1.024134    -0.155321      33.74
 H      -2.915696    -2.045409    -0.194334      17.91
 C      -2.480109     1.048383    -1.533372      43.07
 H      -2.864192     1.552168    -2.468661      19.77
 C      -1.386946     1.474745    -0.810334      17.74
 O      -0.801637     2.732613    -0.964309     240.07
 C      -1.168725     3.499830    -2.057941     120.54
 H      -0.348718     4.326644    -2.280814      25.14
 H      -1.209296     2.859793    -3.014384      27.43
 H      -2.131020     3.984130    -2.021160      27.84
 C      -0.826007     0.680535     0.217515      37.14
 O       0.365672     0.889746     0.850117     210.61
 C      -1.433927    -0.543612     0.543334      55.17
 H      -1.079793    -1.091892     1.372226      23.60
 C      -3.027229    -0.244372    -1.244447      47.49
 C      -4.106893    -0.862674    -2.173983      72.64
 H      -4.081423    -0.418957    -3.210500      24.12
 O      -3.863750    -2.286384    -2.336018     256.06
 H      -2.832795    -2.503997    -2.580861      23.94
 C      -5.625464    -0.766684    -1.568378      87.91
 H      -5.546152    -1.271761    -0.624699      28.89
 O      -5.895289     0.675611    -1.352562     267.59
 H      -5.148343     0.969146    -0.707696      28.39
 C      -6.659774    -1.440395    -2.478799      98.41
 O      -6.519089    -2.904581    -2.536004     253.35
 H      -5.542808    -2.986868    -2.695775      31.57
 H      -6.565086    -1.081933    -3.566838      28.59
 H      -7.629255    -1.225959    -2.066045      27.47
55
name = lig-ACN-frame_49
 C       3.473088     2.841081     0.073824      26.10
 H       2.970039     3.856328     0.059971      23.74
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 C       3.954608     0.580904     0.782951      94.59
 H       3.757842    -0.196492     1.443009      27.79
 C       4.885661     0.422639    -0.279460       6.26
 O       5.757565    -0.673315    -0.453878     175.43
 C       5.700391    -1.739324     0.497580     101.33
 H       5.950382    -1.321159     1.607741      23.46
 H       6.561748    -2.398907     0.135869      23.60
 H       4.712227    -2.280771     0.560050      25.94
 C       5.034448     1.447587    -1.231204      21.29
 O       5.911943     1.295276    -2.263771     120.52
 H       6.479776     0.458258    -2.007392      20.06
 C       4.388470     2.685553    -1.030576      38.02
 H       4.497090     3.471690    -1.752724      26.19
 C       3.177810     1.715517     0.903069     -15.79
 C       2.136854     1.991435     2.029078      75.46
 H       2.469786     2.987052     2.582431      22.94
 O       2.124758     0.995150     3.093077     214.24
 H       1.702635     0.111265     2.677169      25.17
 C       0.754170     2.204242     1.464160      82.39
 H       0.696496     3.070039     0.685886      23.49
 C      -0.274304     2.593356     2.554492     101.42
 O       0.178718     3.851519     3.194343     240.68
 H       0.268570     4.433858     2.397094      30.91
 H      -0.319869     1.872659     3.419267      26.30
 H      -1.241498     2.899368     1.985679      25.33
 C      -2.584690    -0.966405    -0.174516      70.47
 H      -3.027286    -1.844846     0.158245      25.04
 C      -2.491606     0.987309    -1.575187      53.76
 H      -2.898182     1.705090    -2.335780      20.65
 C      -1.372368     1.492802    -0.843448      24.69
 O      -0.769301     2.725600    -0.967280     212.95
 C      -1.202029     3.508874    -2.186161      99.57
 H      -0.351661     4.397203    -2.270847      24.52
 H      -1.157701     2.764803    -3.092714      26.25
 H      -2.177080     3.928270    -1.906918      26.29
 C      -0.832373     0.643640     0.194474      33.78
 O       0.414630     0.870642     0.860801     173.47
 C      -1.492334    -0.555387     0.567954      50.14
 H      -1.014163    -1.129976     1.374440      18.11
 C      -3.064335    -0.258307    -1.309178      36.40
 C      -4.109817    -0.859468    -2.180206      62.00
 H      -4.081649    -0.272642    -3.156137      26.69
 O      -3.905229    -2.285991    -2.342806     226.24
 H      -2.966844    -2.347916    -2.846971      25.08
 C      -5.514239    -0.726352    -1.633131      99.02
 H      -5.607305    -1.245138    -0.710153      29.09
 O      -5.894757     0.663047    -1.412808     266.34
 H      -5.383417     1.002518    -0.599117      27.73
 C      -6.643010    -1.424032    -2.526395      95.18
 O      -6.544977    -2.897655    -2.604358     249.35
 H      -5.638763    -3.142226    -2.649542      35.09
 H      -6.602448    -0.914998    -3.547106      29.04
 H      -7.653956    -1.223403    -2.167467      27.61
55
name = lig-ACN-frame_50
 C       3.450298     2.789268     0.020559      68.42
 H       2.819448     3.716423     0.135023      24.75
 C       3.923035     0.536787     0.817169      60.39
 H       3.826709    -0.230751     1.550384      23.61
 C       4.884973     0.435376    -0.264838      -1.59
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 O       5.771979    -0.633364    -0.474455     184.91
 C       5.737742    -1.742288     0.453636     103.28
 H       5.937273    -1.374281     1.600389      23.66
 H       6.585500    -2.425151     0.195339      24.66
 H       4.775597    -2.351236     0.369912      25.86
 C       5.070239     1.486523    -1.230188       2.74
 O       5.956621     1.370398    -2.315616     115.01
 H       6.663991     0.694809    -2.105693      24.99
 C       4.300466     2.674755    -1.050040      54.01
 H       4.591894     3.493990    -1.620638      19.85
 C       3.159692     1.771332     0.955060     -20.88
 C       2.148308     1.963696     2.046772      84.38
 H       2.405606     2.994947     2.528887      23.60
 O       2.126282     1.029088     3.086860     256.53
 H       1.568225     0.186075     2.801770      24.27
 C       0.708566     2.192733     1.432194      77.93
 H       0.863180     2.910328     0.574105      23.49
 C      -0.329638     2.663822     2.521683     107.62
 O       0.171221     3.882221     3.133083     242.04
 H       0.429436     4.671455     2.404945      25.99
 H      -0.380554     1.896543     3.293967      26.90
 H      -1.424846     2.597598     2.141246      26.13
 C      -2.621900    -0.989948    -0.175866      50.32
 H      -3.250771    -1.723054     0.195214      24.63
 C      -2.457145     1.003837    -1.605128      55.47
 H      -2.931278     1.504127    -2.452435      22.35
 C      -1.360330     1.452441    -0.801725      13.33
 O      -0.745049     2.747509    -1.057089     202.10
 C      -1.195221     3.471008    -2.219192      98.30
 H      -0.425348     4.481740    -2.317235      23.54
 H      -1.181417     2.926916    -3.282942      24.80
 H      -2.247497     3.880457    -2.145131      25.28
 C      -0.778157     0.635402     0.225207      26.38
 O       0.421693     0.895931     0.850551     223.25
 C      -1.488109    -0.513558     0.579931      53.46
 H      -1.179997    -1.190276     1.450734      18.07
 C      -3.048357    -0.255184    -1.298587      57.22
 C      -4.137869    -0.840501    -2.235939      45.05
 H      -4.109045    -0.422035    -3.291716      26.13
 O      -3.900203    -2.309195    -2.399521     253.59
 H      -3.051418    -2.436523    -2.770226      30.00
 C      -5.555317    -0.740460    -1.627114     101.79
 H      -5.451194    -1.199846    -0.673822      28.71
 O      -5.896897     0.660488    -1.487292     276.72
 H      -5.904446     0.801870    -0.560801      30.19
 C      -6.590995    -1.385253    -2.584460      99.43
 O      -6.572176    -2.827006    -2.625957     246.26
 H      -5.571106    -3.012834    -2.716714      31.15
 H      -6.561922    -0.934669    -3.596286      30.59
 H      -7.539094    -1.108959    -2.073229      27.88
55
name = lig-ACN-frame_51
 C       3.330358     2.781025    -0.016385      18.94
 H       2.857615     3.761726     0.155909      23.94
 C       3.946385     0.539515     0.798079      97.74
 H       3.819290    -0.313941     1.497959      22.44
 C       4.881876     0.440894    -0.233838     -36.64
 O       5.762907    -0.590215    -0.482123     154.35
 C       5.783509    -1.763862     0.424855     100.58
 H       5.808567    -1.425659     1.592753      23.19
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 H       6.613273    -2.385109     0.151826      25.52
 H       4.763183    -2.284368     0.268751      25.46
 C       5.072910     1.505108    -1.201456      -4.20
 O       5.993664     1.445725    -2.335711     118.04
 H       6.747544     0.945893    -2.081286      25.02
 C       4.314845     2.662518    -1.100057      53.68
 H       4.401833     3.494647    -1.736015      28.81
 C       3.244105     1.732071     0.951275      -4.07
 C       2.104739     2.033788     2.050524      81.69
 H       2.343494     2.969976     2.627792      25.61
 O       2.141676     0.990365     3.119646     245.19
 H       1.700849     0.230974     2.825926      29.48
 C       0.692513     2.198138     1.417139      93.41
 H       0.644554     2.981806     0.657782      23.86
 C      -0.304340     2.680421     2.470627     112.83
 O       0.120380     3.906840     3.096199     234.76
 H       0.245912     4.602897     2.255724      26.96
 H      -0.328453     2.013570     3.275999      27.76
 H      -1.321657     2.982663     2.044175      25.06
 C      -2.653381    -0.959166    -0.130729      49.76
 H      -3.000598    -1.962142     0.022702      21.70
 C      -2.394394     0.973903    -1.578624      56.58
 H      -2.511536     1.528889    -2.469195      20.89
 C      -1.329932     1.507501    -0.849222      22.67
 O      -0.735409     2.679861    -1.152989     223.50
 C      -1.185894     3.465759    -2.260667      92.29
 H      -0.434305     4.533266    -2.259536      23.39
 H      -0.925931     2.787306    -3.203752      25.31
 H      -2.279817     3.761682    -2.040026      25.42
 C      -0.816587     0.672986     0.209544      31.47
 O       0.409032     0.889824     0.849703     203.18
 C      -1.525985    -0.543168     0.585127      58.91
 H      -1.133987    -1.004636     1.576258      21.10
 C      -3.042238    -0.256130    -1.327794      40.09
 C      -4.088381    -0.873287    -2.251708      64.14
 H      -4.092164    -0.278727    -3.207430      26.07
 O      -3.884766    -2.323662    -2.465405     286.29
 H      -2.951863    -2.398524    -2.615840      29.73
 C      -5.565138    -0.753489    -1.664201      94.18
 H      -5.721408    -1.275383    -0.729314      28.74
 O      -5.921546     0.678878    -1.538439     241.80
 H      -6.077095     0.927079    -0.579201      28.83
 C      -6.625749    -1.323247    -2.568027     103.48
 O      -6.559780    -2.751809    -2.619966     250.56
 H      -5.621374    -3.051067    -2.853925      31.90
 H      -6.395023    -0.878201    -3.539249      31.31
 H      -7.689998    -1.041805    -2.379022      27.98
55
name = lig-ACN-frame_52
 C       3.351339     2.765030    -0.067670      71.19
 H       2.741233     3.648080    -0.069954      25.15
 C       3.982915     0.574241     0.795777      35.83
 H       3.745857    -0.300748     1.503930      23.29
 C       4.948702     0.480443    -0.300765       3.77
 O       5.796229    -0.615699    -0.456672     192.44
 C       5.749040    -1.738391     0.378553     113.81
 H       5.964873    -1.451135     1.513460      24.10
 H       6.633632    -2.237104     0.062791      25.98
 H       4.871661    -2.494476     0.301631      25.48
 C       5.090285     1.533588    -1.233352      16.56
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 O       5.980983     1.494599    -2.261612     124.73
 H       6.738353     0.873528    -2.006029      25.05
 C       4.241754     2.684504    -1.087444      43.77
 H       4.364112     3.357681    -1.929398      23.45
 C       3.163033     1.778297     0.945458     -34.67
 C       2.158277     1.990210     2.054799      85.85
 H       2.386872     2.950560     2.502008      26.16
 O       2.149236     0.983382     3.117259     252.28
 H       1.856760     0.152439     2.696265      27.88
 C       0.737203     2.219392     1.418933      84.67
 H       0.862006     2.892364     0.619190      24.85
 C      -0.340706     2.682911     2.466401     108.81
 O       0.078992     3.944747     3.085184     287.44
 H       0.296397     4.631664     2.408154      30.06
 H      -0.583017     1.996390     3.191395      28.80
 H      -1.254933     2.706757     1.792249      26.40
 C      -2.626679    -0.963297    -0.150185      63.63
 H      -3.066704    -1.967584     0.114882      23.71
 C      -2.383268     0.931076    -1.658441      55.38
 H      -2.719144     1.303627    -2.578289      20.14
 C      -1.321757     1.445994    -0.863564      21.41
 O      -0.636330     2.643856    -1.186702     197.45
 C      -1.157629     3.426455    -2.304746      93.58
 H      -0.480203     4.568208    -2.200513      22.60
 H      -1.055019     3.056276    -3.422321      24.95
 H      -2.277242     3.692652    -2.210973      25.64
 C      -0.884784     0.683739     0.236678      40.89
 O       0.361625     0.882982     0.856096     198.48
 C      -1.539200    -0.456080     0.597167      39.66
 H      -1.087066    -1.152059     1.375906      17.66
 C      -3.024468    -0.285971    -1.285711      67.84
 C      -4.106191    -0.882147    -2.203827      39.78
 H      -4.049688    -0.388150    -3.191734      27.50
 O      -3.835753    -2.301876    -2.523015     241.18
 H      -2.811526    -2.404040    -2.838540      24.01
 C      -5.577292    -0.680637    -1.659129      91.56
 H      -5.541745    -1.110940    -0.634390      27.59
 O      -5.941121     0.709717    -1.573935     252.79
 H      -5.600677     0.966023    -0.619582      25.60
 C      -6.631783    -1.272485    -2.678755     100.65
 O      -6.570662    -2.737617    -2.609102     268.41
 H      -5.675033    -2.890774    -2.859065      34.53
 H      -6.523133    -0.858484    -3.659177      31.47
 H      -7.618097    -0.969236    -2.230846      27.79
55
name = lig-ACN-frame_53
 C       3.300711     2.811124    -0.064285      54.71
 H       2.581800     3.592580    -0.057301      22.67
 C       4.011881     0.666473     0.747886     102.04
 H       3.988332    -0.202789     1.498107      25.94
 C       4.925823     0.500410    -0.239421      11.89
 O       5.817693    -0.577454    -0.501232     181.16
 C       5.795022    -1.779823     0.398566     107.62
 H       5.833951    -1.476665     1.508131      24.57
 H       6.581666    -2.489301     0.155609      25.70
 H       4.746920    -2.204754     0.205497      25.49
 C       5.059325     1.551507    -1.201141      17.56
 O       6.018958     1.501841    -2.228620     134.56
 H       6.615382     0.666424    -2.084353      22.75
 C       4.236099     2.649363    -1.166641      56.63
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 H       4.281852     3.569747    -1.802657      21.20
 C       3.183652     1.748690     0.865197      15.75
 C       2.178146     1.938872     2.053106     101.03
 H       2.459256     2.795010     2.577450      26.29
 O       2.172430     0.982388     3.071680     261.27
 H       1.799808     0.010492     2.797271      24.01
 C       0.769503     2.171520     1.467334      95.10
 H       0.840067     2.887245     0.722919      24.58
 C      -0.356462     2.711973     2.386332     116.79
 O       0.008374     3.933087     3.098301     310.94
 H       0.352307     4.463781     2.461500      35.00
 H      -0.432936     2.014376     3.165519      27.86
 H      -1.349080     2.939048     1.969143      26.46
 C      -2.586641    -1.007199    -0.138446      59.68
 H      -3.230521    -1.887385     0.269896      24.38
 C      -2.402332     0.868646    -1.731762      47.47
 H      -2.700028     1.423223    -2.598975      20.58
 C      -1.334311     1.428341    -0.957639      10.21
 O      -0.561394     2.583896    -1.253307     202.34
 C      -1.123987     3.418624    -2.313072      90.88
 H      -0.498309     4.610049    -2.273378      22.42
 H      -0.828079     2.865252    -3.279581      24.63
 H      -2.236221     3.577776    -2.095998      25.47
 C      -0.872558     0.742939     0.262809      32.08
 O       0.338177     0.917173     0.890266     208.71
 C      -1.556326    -0.488152     0.646106      44.73
 H      -1.119396    -1.035588     1.492353      19.33
 C      -3.049168    -0.306191    -1.301554      46.87
 C      -4.100758    -0.839265    -2.224059      67.31
 H      -4.075335    -0.226199    -3.124587      29.14
 O      -3.815243    -2.277520    -2.541735     203.63
 H      -2.832798    -2.207366    -3.013097      23.95
 C      -5.576182    -0.647388    -1.727983      99.08
 H      -5.852739    -1.210341    -0.785405      26.48
 O      -5.910837     0.781849    -1.551932     259.52
 H      -5.256746     1.205496    -1.010399      30.37
 C      -6.612729    -1.270549    -2.649559     108.50
 O      -6.583194    -2.710177    -2.630076     263.64
 H      -5.655743    -3.040653    -2.739412      32.61
 H      -6.494453    -0.879082    -3.627217      31.25
 H      -7.641154    -1.006532    -2.323281      28.03
55
name = lig-ACN-frame_54
 C       3.248966     2.805794    -0.137087      68.01
 H       2.772642     3.769304    -0.028623      24.98
 C       4.033202     0.614039     0.822458      45.80
 H       3.896777    -0.065676     1.711497      23.52
 C       4.999220     0.509190    -0.294508       6.80
 O       5.862070    -0.552920    -0.495528     172.56
 C       5.739130    -1.740843     0.402240     108.87
 H       5.943329    -1.454777     1.441736      25.39
 H       6.577297    -2.385395     0.030246      25.92
 H       4.744970    -2.290105     0.340842      25.84
 C       5.074549     1.564430    -1.239693      12.86
 O       6.064059     1.478943    -2.205780     127.39
 H       6.553095     0.677292    -2.056659      23.56
 C       4.176220     2.708946    -1.155195      36.64
 H       4.485693     3.448936    -1.956476      20.14
 C       3.165914     1.782839     0.848023     -13.50
 C       2.160701     1.953866     2.015762      90.72
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 H       2.407790     2.839040     2.469381      26.83
 O       2.221983     0.894940     3.073289     250.24
 H       1.690786     0.112293     2.669722      25.77
 C       0.710129     2.238298     1.433773      91.05
 H       0.841393     2.912979     0.644448      24.37
 C      -0.350142     2.704391     2.441743     113.18
 O      -0.017949     3.914309     3.100222     297.71
 H       0.284502     4.626944     2.481816      30.35
 H      -0.621700     1.969868     3.164531      27.92
 H      -1.182003     2.755535     1.715875      26.11
 C      -2.622905    -0.985850    -0.118896      51.45
 H      -3.083476    -2.021415     0.182060      20.55
 C      -2.344610     0.886545    -1.700376      67.29
 H      -2.641508     1.262853    -2.702057      20.71
 C      -1.270653     1.401480    -0.961478      14.67
 O      -0.541551     2.504259    -1.320667     221.95
 C      -1.063678     3.360881    -2.313366      99.53
 H      -0.372842     4.542123    -2.215515      22.54
 H      -0.957958     3.023148    -3.383473      26.34
 H      -2.166959     3.601432    -2.219923      26.05
 C      -0.918372     0.687441     0.202444      43.23
 O       0.334696     0.929835     0.922965     187.72
 C      -1.531893    -0.468778     0.653722      34.81
 H      -1.313834    -0.815509     1.614142      22.49
 C      -3.025162    -0.317801    -1.310258      49.72
 C      -4.130290    -0.818894    -2.278764      58.03
 H      -4.054748    -0.290594    -3.214416      28.00
 O      -3.847120    -2.206831    -2.561537     277.22
 H      -2.883717    -2.318257    -2.798349      26.77
 C      -5.588830    -0.635698    -1.710278      86.51
 H      -5.517362    -1.059254    -0.645229      27.10
 O      -5.857325     0.824536    -1.574389     262.57
 H      -5.167978     1.076900    -0.929041      30.07
 C      -6.623127    -1.253544    -2.678959     108.51
 O      -6.596042    -2.714396    -2.637564     253.85
 H      -5.581703    -2.917664    -2.704869      30.09
 H      -6.413256    -0.859379    -3.647572      31.26
 H      -7.614023    -0.925850    -2.395446      28.50
55
name = lig-ACN-frame_55
 C       3.258986     2.773809    -0.170012      44.25
 H       2.624660     3.686618    -0.059382      24.53
 C       4.049725     0.660370     0.799721      98.42
 H       4.003198    -0.169753     1.482479      24.48
 C       4.943682     0.536676    -0.227811     -24.69
 O       5.888527    -0.552215    -0.455942     188.43
 C       5.731403    -1.662674     0.385990     117.22
 H       5.998102    -1.423344     1.393437      25.54
 H       6.484039    -2.479801     0.053257      24.89
 H       4.696750    -2.067321     0.315866      25.63
 C       5.076300     1.557646    -1.247798       6.37
 O       6.087184     1.478618    -2.208666     136.85
 H       6.737940     0.819585    -1.906128      20.87
 C       4.263380     2.691099    -1.206333      47.39
 H       4.226179     3.568885    -1.890849      24.87
 C       3.162607     1.774246     0.860482       2.51
 C       2.143497     1.990357     2.014661      96.41
 H       2.396604     2.804963     2.594120      26.77
 O       2.235439     0.875485     2.986229     256.01
 H       1.816542     0.097202     2.736620      28.81
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 C       0.724352     2.231839     1.432310      86.29
 H       0.706488     2.986812     0.663275      23.15
 C      -0.391421     2.684619     2.417473     106.53
 O      -0.014520     3.918551     3.126232     243.83
 H       0.201628     4.612175     2.293250      27.92
 H      -0.521032     1.934841     3.236655      26.38
 H      -1.369088     2.885790     2.008799      25.88
 C      -2.659531    -0.957026    -0.136076      68.89
 H      -3.129865    -1.959102     0.128391      22.78
 C      -2.326963     0.856760    -1.683532      37.73
 H      -2.483065     1.355774    -2.691836      19.02
 C      -1.229341     1.332183    -0.955074      31.00
 O      -0.483781     2.433956    -1.365420     210.64
 C      -1.039467     3.353366    -2.378541      91.03
 H      -0.214136     4.415317    -2.099962      22.22
 H      -0.838886     2.991528    -3.385346      26.30
 H      -2.070512     3.649077    -2.084229      26.61
 C      -0.793841     0.659996     0.221833      32.16
 O       0.283703     0.916457     0.910134     207.77
 C      -1.619588    -0.452056     0.638286      55.79
 H      -1.248771    -1.012997     1.424688      19.08
 C      -3.002694    -0.282335    -1.326251      46.44
 C      -4.090066    -0.775664    -2.286216      59.90
 H      -4.090865    -0.184325    -3.185962      28.07
 O      -3.920563    -2.202843    -2.579321     319.25
 H      -3.024233    -2.303751    -2.701102      30.94
 C      -5.534619    -0.587223    -1.690588      86.92
 H      -5.704456    -1.126739    -0.676076      26.22
 O      -5.776852     0.815102    -1.611476     255.49
 H      -5.638056     1.147262    -0.622175      25.70
 C      -6.626627    -1.227046    -2.676282     101.99
 O      -6.595017    -2.698122    -2.637492     277.19
 H      -5.686056    -2.963908    -2.777394      31.98
 H      -6.391615    -0.862779    -3.672998      31.50
 H      -7.622149    -0.949605    -2.413157      28.76
55
name = lig-ACN-frame_56
 C       3.318875     2.729036    -0.167306      66.10
 H       2.520614     3.510145    -0.343561      21.77
 C       4.003630     0.688275     0.802748      77.21
 H       3.877156    -0.052791     1.536049      26.23
 C       4.993510     0.557142    -0.286521       6.63
 O       5.871437    -0.448710    -0.430451     182.47
 C       5.726986    -1.663980     0.443098     113.41
 H       5.932472    -1.467077     1.444509      26.61
 H       6.373069    -2.513858    -0.001187      25.25
 H       4.672485    -1.954671     0.446669      25.81
 C       5.127144     1.566373    -1.241189      23.51
 O       6.105150     1.477192    -2.211476      90.30
 H       6.939753     0.928629    -1.902514      23.07
 C       4.256191     2.664018    -1.194577      56.99
 H       4.470424     3.400675    -1.958269      23.60
 C       3.170721     1.801440     0.842894       7.71
 C       2.139378     1.957612     2.008183     102.14
 H       2.396693     2.869415     2.503804      26.12
 O       2.220659     0.915523     2.907355     284.00
 H       1.902218     0.107518     2.428475      27.54
 C       0.641631     2.205028     1.439245      88.87
 H       0.848180     2.878143     0.576353      23.42
 C      -0.407275     2.701448     2.475600     106.32
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 O       0.008682     3.920140     3.117547     280.17
 H       0.327494     4.665880     2.455454      28.43
 H      -0.342847     1.888171     3.298453      25.81
 H      -1.356901     2.669862     1.978755      27.15
 C      -2.700187    -0.937693    -0.176558      61.94
 H      -3.305394    -1.755420     0.182714      24.10
 C      -2.269954     0.869401    -1.726486      48.51
 H      -2.613355     1.431609    -2.647586      21.12
 C      -1.184328     1.322043    -0.986432      18.01
 O      -0.399971     2.387981    -1.408862     225.39
 C      -0.957298     3.330563    -2.351728     102.44
 H      -0.251155     4.514199    -2.465093      22.18
 H      -0.898127     2.935404    -3.336907      26.74
 H      -2.012101     3.596570    -2.228177      26.85
 C      -0.854052     0.603964     0.211763      31.64
 O       0.380550     0.888029     0.953933     191.93
 C      -1.613309    -0.487833     0.636095      41.11
 H      -1.262846    -1.059310     1.466473      18.53
 C      -3.047643    -0.275900    -1.360866      60.07
 C      -4.107655    -0.771705    -2.247099      55.30
 H      -4.016307    -0.212271    -3.172053      30.33
 O      -3.978248    -2.212178    -2.591638     236.18
 H      -3.062718    -2.393806    -2.961715      27.21
 C      -5.532388    -0.602112    -1.743931      96.68
 H      -5.618474    -1.086078    -0.691719      26.73
 O      -5.725739     0.861656    -1.612763     241.42
 H      -5.952760     0.981900    -0.664810      27.19
 C      -6.563534    -1.218474    -2.642462     111.83
 O      -6.612479    -2.657087    -2.631967     281.91
 H      -5.716862    -2.922145    -2.849226      33.09
 H      -6.481643    -0.766797    -3.661822      31.33
 H      -7.516122    -0.886948    -2.289840      29.93
55
name = lig-ACN-frame_57
 C       3.274335     2.803775    -0.233230      38.80
 H       2.632768     3.743382    -0.213292      23.09
 C       4.032958     0.657928     0.766028      94.28
 H       3.999070    -0.060864     1.545724      23.67
 C       4.962221     0.585644    -0.228198      -5.29
 O       5.915694    -0.482184    -0.362081     199.58
 C       5.673652    -1.618424     0.483831     125.86
 H       6.131089    -1.447152     1.399724      27.30
 H       6.404039    -2.343154    -0.000290      25.55
 H       4.683359    -2.045325     0.464620      26.74
 C       5.212247     1.576542    -1.222635      21.32
 O       6.146363     1.495157    -2.244247      49.42
 H       6.871324     0.861061    -1.930671      23.34
 C       4.285475     2.657964    -1.221121      47.53
 H       4.319962     3.430420    -1.942289      23.73
 C       3.148285     1.825526     0.818220     -21.85
 C       2.114051     2.042115     1.910023      99.25
 H       2.392835     2.931784     2.533797      24.38
 O       2.188935     0.915952     2.896822     204.58
 H       1.780450    -0.012414     2.499645      21.33
 C       0.693380     2.185597     1.435602      92.83
 H       0.437420     2.959489     0.623905      20.08
 C      -0.327156     2.656892     2.523806     107.54
 O       0.028680     3.944705     3.111303     296.96
 H       0.369230     4.421309     2.424331      35.29
 H      -0.562696     1.943685     3.453553      24.47
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 H      -1.300310     2.826112     2.125891      25.76
 C      -2.721695    -0.924086    -0.141911      52.50
 H      -3.285705    -1.745259     0.139674      21.90
 C      -2.276327     0.869848    -1.792979      52.86
 H      -2.564790     1.361298    -2.736912      20.31
 C      -1.147525     1.319019    -1.017187       7.43
 O      -0.295644     2.385411    -1.416888     197.83
 C      -0.904972     3.267367    -2.398144      96.58
 H      -0.056394     4.329030    -2.154306      21.71
 H      -0.874382     2.892495    -3.388704      26.56
 H      -1.867476     3.552737    -2.003200      26.47
 C      -0.801753     0.609479     0.230660      37.83
 O       0.355365     0.787724     0.931622     187.59
 C      -1.580563    -0.554841     0.596603      47.92
 H      -1.444680    -0.965696     1.630953      21.32
 C      -3.003450    -0.234901    -1.349890      13.48
 C      -4.136671    -0.809422    -2.338863      65.97
 H      -4.128995    -0.265442    -3.297921      25.93
 O      -4.005671    -2.227885    -2.597823     240.11
 H      -2.977643    -2.291113    -2.977125      23.47
 C      -5.500875    -0.568046    -1.717376      92.20
 H      -5.534801    -1.031684    -0.672471      27.03
 O      -5.731768     0.882154    -1.625182     266.72
 H      -5.648890     1.137077    -0.714630      29.97
 C      -6.620161    -1.177162    -2.632592      99.20
 O      -6.633919    -2.626566    -2.630671     253.97
 H      -5.666244    -2.946124    -2.819014      29.41
 H      -6.437728    -0.761338    -3.681289      29.68
 H      -7.584867    -0.877681    -2.252828      28.53
55
name = lig-ACN-frame_58
 C       3.285422     2.828113    -0.262510      66.00
 H       2.724697     3.778828    -0.186102      23.68
 C       3.989202     0.738638     0.761613      63.96
 H       3.860667    -0.059240     1.514288      23.03
 C       5.073961     0.571623    -0.227857      -0.56
 O       5.912803    -0.492497    -0.298651     205.57
 C       5.733251    -1.651788     0.529009     124.02
 H       5.847002    -1.459760     1.560378      27.04
 H       6.271080    -2.528075     0.168827      26.47
 H       4.664778    -1.825482     0.549547      26.09
 C       5.190977     1.621784    -1.218665      12.30
 O       6.177927     1.505126    -2.235859      83.87
 H       6.836271     0.850312    -2.082892      23.13
 C       4.293749     2.721350    -1.254388      52.38
 H       4.455038     3.435920    -2.019942      23.45
 C       3.150606     1.841239     0.716120      30.99
 C       2.134880     2.003630     1.895944      98.92
 H       2.363964     3.017415     2.439420      23.46
 O       2.156626     0.982182     2.895847     261.45
 H       1.682618     0.148293     2.529468      24.05
 C       0.644644     2.125582     1.433349      81.78
 H       0.727174     2.823790     0.500588      19.46
 C      -0.314032     2.629134     2.570912      97.66
 O       0.090848     3.951568     3.099412     280.68
 H       0.412812     4.562036     2.399385      30.49
 H      -0.236265     1.803823     3.463577      23.99
 H      -1.253908     2.630363     2.055294      25.62
 C      -2.702855    -0.914444    -0.167969      53.68
 H      -3.214970    -1.768277     0.126433      23.74
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 C      -2.219601     0.874798    -1.779220      89.85
 H      -2.302115     1.258464    -2.767947      19.06
 C      -1.102108     1.278395    -1.021469      19.28
 O      -0.242474     2.312433    -1.406820     221.23
 C      -0.814994     3.251678    -2.354620     101.99
 H      -0.064282     4.390925    -2.540394      22.29
 H      -0.803730     2.836077    -3.358563      27.06
 H      -1.825130     3.577174    -2.158073      27.77
 C      -0.803637     0.558152     0.142174      31.65
 O       0.331404     0.777620     0.933535     196.78
 C      -1.588971    -0.501793     0.583786      34.71
 H      -1.160378    -1.126123     1.477031      16.89
 C      -3.030429    -0.275015    -1.437084      65.12
 C      -4.085689    -0.774023    -2.347537      39.40
 H      -4.026970    -0.214033    -3.315634      26.79
 O      -3.969996    -2.242366    -2.608688     247.53
 H      -2.973773    -2.531771    -2.742382      23.92
 C      -5.543269    -0.522560    -1.708322      85.00
 H      -5.631034    -1.009013    -0.693131      26.82
 O      -5.761054     0.896559    -1.626460     250.41
 H      -5.069192     1.209432    -0.934057      28.78
 C      -6.680827    -1.137358    -2.594951      96.20
 O      -6.668738    -2.602105    -2.628636     283.65
 H      -5.705150    -2.837602    -2.743934      30.27
 H      -6.554547    -0.688384    -3.656933      28.99
 H      -7.712263    -0.836180    -2.321528      27.66
55
name = lig-ACN-frame_59
 C       3.333738     2.882428    -0.296709      48.71
 H       2.618259     3.676110    -0.417068      19.71
 C       4.044018     0.749640     0.693306      77.07
 H       3.773076     0.011220     1.496241      23.08
 C       5.054240     0.644729    -0.200440      22.92
 O       5.984088    -0.498804    -0.281688     177.95
 C       5.658998    -1.681556     0.645297     116.99
 H       6.087964    -1.480373     1.608509      26.31
 H       6.369158    -2.359686     0.265185      27.01
 H       4.673095    -2.113484     0.471303      26.70
 C       5.202706     1.596342    -1.238369      14.29
 O       6.153109     1.543749    -2.201812     115.60
 H       6.856875     0.954523    -1.813341      21.31
 C       4.350114     2.740303    -1.272191      52.36
 H       4.553709     3.542592    -1.978226      25.64
 C       3.116567     1.855677     0.696285     -12.96
 C       2.098970     1.985678     1.859635     105.12
 H       2.417453     3.019063     2.360144      24.09
 O       2.168224     1.034467     2.926727     275.28
 H       1.828224     0.224927     2.633829      29.56
 C       0.669544     2.126511     1.390405      89.29
 H       0.518564     2.925586     0.551826      21.48
 C      -0.260389     2.624071     2.525881     104.57
 O       0.139865     3.903242     3.081962     231.53
 H       0.375621     4.566415     2.227032      28.17
 H      -0.100093     1.942373     3.509317      24.62
 H      -1.353276     2.603121     2.469091      25.82
 C      -2.688446    -0.938822    -0.262471      68.53
 H      -3.280256    -1.786226     0.051311      23.10
 C      -2.174118     0.808385    -1.819738      42.34
 H      -2.390839     1.268341    -2.740941      21.00
 C      -1.078325     1.252199    -1.046242      26.76
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 O      -0.219651     2.270258    -1.404760     208.59
 C      -0.736227     3.227322    -2.376509      92.45
 H       0.147985     4.256988    -2.136961      20.70
 H      -0.695672     2.790191    -3.416176      24.93
 H      -1.733163     3.528730    -2.053488      26.69
 C      -0.763893     0.550606     0.150921      32.70
 O       0.319781     0.792775     0.952146     210.80
 C      -1.622271    -0.503446     0.533757      59.14
 H      -1.267364    -1.160689     1.451068      17.96
 C      -2.952894    -0.265693    -1.418969      45.02
 C      -4.115639    -0.794999    -2.333238      43.92
 H      -4.049319    -0.264447    -3.337880      25.60
 O      -3.935493    -2.231185    -2.596631     295.65
 H      -3.016785    -2.335477    -2.713734      30.30
 C      -5.583399    -0.524450    -1.758662      92.70
 H      -5.566320    -0.953667    -0.737780      26.33
 O      -5.782478     0.927938    -1.639772     255.84
 H      -5.056693     1.253275    -0.994028      26.35
 C      -6.715308    -1.108299    -2.597790      96.59
 O      -6.705302    -2.545713    -2.615866     310.31
 H      -5.819073    -2.822269    -2.718623      32.98
 H      -6.658187    -0.651138    -3.662601      27.58
 H      -7.648156    -0.789409    -2.040169      26.56
55
name = lig-ACN-frame_60
 C       3.323855     2.875809    -0.323647      66.61
 H       2.700969     3.725110    -0.362623      26.05
 C       3.996067     0.762335     0.714670      49.92
 H       4.035549    -0.073918     1.450897      19.91
 C       5.087958     0.591837    -0.237936       3.13
 O       5.959451    -0.486808    -0.206136     215.58
 C       5.705635    -1.641309     0.653040     121.04
 H       5.692166    -1.365444     1.739250      25.35
 H       6.372299    -2.379778     0.379341      26.55
 H       4.654534    -1.983848     0.637183      25.59
 C       5.210151     1.624836    -1.227318      16.52
 O       6.191452     1.556214    -2.198286      87.58
 H       7.087412     1.025908    -2.026272      19.13
 C       4.382677     2.749424    -1.223947      47.21
 H       4.563127     3.514704    -2.024266      20.49
 C       3.144914     1.874523     0.670135      32.53
 C       2.112209     2.078093     1.796066      89.66
 H       2.323468     3.062294     2.405137      22.24
 O       2.218178     1.062179     2.958985     201.23
 H       1.988250     0.144348     2.624159      24.03
 C       0.624462     2.198799     1.353765      89.18
 H       0.560837     2.878042     0.439256      19.28
 C      -0.218932     2.588111     2.591723     103.64
 O       0.191947     3.890261     3.037914     258.48
 H       0.402697     4.549880     2.250136      29.05
 H      -0.008575     1.739846     3.385632      23.25
 H      -1.223683     2.603633     2.109811      24.13
 C      -2.658454    -1.002860    -0.272534      53.56
 H      -3.291978    -1.897235     0.014514      20.79
 C      -2.135988     0.792971    -1.910191      45.73
 H      -2.416500     1.375741    -2.771907      19.63
 C      -1.050905     1.204466    -1.071715      13.09
 O      -0.190408     2.239802    -1.418991     218.98
 C      -0.638208     3.203262    -2.342667      99.74
 H       0.185990     4.310895    -2.238423      21.69
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 H      -0.504492     2.957502    -3.478779      23.99
 H      -1.670788     3.604641    -2.187555      25.03
 C      -0.804159     0.551257     0.187880      34.04
 O       0.318898     0.793261     0.967679     189.13
 C      -1.587700    -0.585448     0.525655      36.01
 H      -1.528088    -0.961997     1.602560      19.44
 C      -3.005195    -0.280536    -1.498728      47.74
 C      -4.134300    -0.781433    -2.357782      70.26
 H      -4.141577    -0.210259    -3.350424      25.98
 O      -3.930105    -2.205702    -2.558439     270.77
 H      -3.064084    -2.370769    -2.878512      29.32
 C      -5.522699    -0.502291    -1.763015     101.87
 H      -5.687524    -0.974470    -0.801246      27.46
 O      -5.790367     0.941077    -1.691591     276.09
 H      -5.595684     1.195011    -0.795434      28.90
 C      -6.739394    -1.062805    -2.580208      92.12
 O      -6.755894    -2.507927    -2.604013     282.13
 H      -5.811664    -2.806741    -2.821513      30.92
 H      -6.818096    -0.582978    -3.631893      27.74
 H      -7.757635    -0.786817    -2.127290      27.21
55
name = lig-ACN-frame_61
 C       3.303510     2.846979    -0.302386      65.55
 H       2.769792     3.768871    -0.263856      25.87
 C       4.018487     0.742260     0.713377      88.74
 H       3.732975     0.152175     1.571001      22.08
 C       5.018257     0.567723    -0.228563      14.89
 O       5.948282    -0.461677    -0.165329     211.96
 C       5.677019    -1.556891     0.698785     121.76
 H       5.875967    -1.268134     1.778834      26.13
 H       6.439679    -2.284870     0.550832      26.14
 H       4.733880    -2.001620     0.332603      26.33
 C       5.302972     1.607107    -1.197112      17.57
 O       6.240561     1.589909    -2.255825     -11.06
 H       6.966098     0.956966    -1.881884      19.32
 C       4.410921     2.736954    -1.216597      64.16
 H       4.605918     3.551876    -1.998769      20.19
 C       3.165027     1.871660     0.697272      16.56
 C       2.152762     2.108994     1.838000     100.38
 H       2.430276     3.139187     2.220424      22.55
 O       2.277389     1.157307     2.893909     232.48
 H       1.972222     0.224008     2.421538      22.58
 C       0.679562     2.155661     1.369726      95.92
 H       0.497536     2.897311     0.575567      20.04
 C      -0.215334     2.588756     2.512702     107.08
 O       0.224413     3.900202     3.046185     277.78
 H       0.494858     4.372796     2.331718      34.55
 H      -0.138530     1.918936     3.431166      24.88
 H      -1.354960     2.583958     2.416700      24.03
 C      -2.651401    -1.000577    -0.346124      67.12
 H      -3.248868    -1.936398    -0.027070      20.42
 C      -2.149346     0.774416    -1.904382      59.69
 H      -2.238163     1.251190    -2.906372      19.86
 C      -1.067882     1.152325    -1.107885      15.61
 O      -0.146486     2.189275    -1.423060     196.81
 C      -0.550789     3.264831    -2.373007      82.29
 H       0.244352     4.308133    -2.015308      21.30
 H      -0.356144     2.772437    -3.428191      23.49
 H      -1.665621     3.493218    -2.222651      24.82
 C      -0.843317     0.510599     0.164552      30.44
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 O       0.284347     0.821446     0.969032     198.05
 C      -1.601562    -0.612009     0.551496      41.20
 H      -1.248452    -1.190515     1.412479      17.56
 C      -2.954689    -0.295114    -1.511135      40.84
 C      -4.120061    -0.737508    -2.412529      30.43
 H      -4.044877    -0.266890    -3.449251      26.32
 O      -4.000976    -2.208497    -2.545884     233.82
 H      -2.969859    -2.391639    -2.756379      24.71
 C      -5.592406    -0.484322    -1.753425      91.13
 H      -5.441869    -0.829758    -0.755251      27.66
 O      -5.771574     0.958267    -1.711649     230.48
 H      -5.996204     1.177621    -0.782699      27.47
 C      -6.745743    -1.044596    -2.575548      92.85
 O      -6.798648    -2.489752    -2.611057     282.58
 H      -5.850602    -2.776539    -2.898830      31.14
 H      -6.597583    -0.587697    -3.612029      29.34
 H      -7.688972    -0.643727    -2.059906      27.88
55
name = lig-ACN-frame_62
 C       3.404133     2.848715    -0.307142      52.50
 H       2.680620     3.670117    -0.419823      20.90
 C       3.978559     0.733958     0.746339      54.95
 H       4.004427    -0.092521     1.396785      20.46
 C       5.030788     0.619761    -0.240151       6.72
 O       5.979733    -0.419319    -0.185895     191.49
 C       5.665904    -1.540676     0.749289     114.57
 H       5.534556    -1.187786     1.841229      25.89
 H       6.556469    -2.149185     0.568931      24.98
 H       4.703518    -2.093541     0.681594      26.23
 C       5.293829     1.623339    -1.213522      23.82
 O       6.251740     1.585053    -2.228856     113.25
 H       7.056361     1.083940    -2.085247      19.21
 C       4.417792     2.703286    -1.206683      62.90
 H       4.649084     3.567077    -1.900952      26.50
 C       3.145896     1.889445     0.709578      22.74
 C       2.183007     2.132396     1.810521     118.23
 H       2.345959     3.079041     2.320250      25.55
 O       2.351906     1.205059     2.855107     247.74
 H       1.862243     0.335824     2.696469      25.06
 C       0.672431     2.156197     1.373026      84.14
 H       0.674294     2.793015     0.532104      22.94
 C      -0.239975     2.647941     2.562213     108.73
 O       0.225723     3.905159     3.054947     273.33
 H       0.586712     4.512434     2.359947      30.89
 H      -0.080576     1.888818     3.336878      26.05
 H      -1.283014     2.730983     2.076427      24.09
 C      -2.651769    -1.013405    -0.333816      72.68
 H      -3.260096    -1.971100    -0.189894      21.67
 C      -2.128896     0.778246    -1.913733      59.47
 H      -2.297228     1.150378    -2.979153      19.09
 C      -1.043592     1.195531    -1.087178      30.60
 O      -0.123806     2.144804    -1.432047     213.64
 C      -0.486588     3.192305    -2.352976      96.76
 H       0.238137     4.257441    -1.946107      21.05
 H      -0.165899     3.160432    -3.501300      23.21
 H      -1.608784     3.570279    -2.283537      24.86
 C      -0.796236     0.519293     0.144522      33.76
 O       0.252609     0.793274     0.949071     201.57
 C      -1.607691    -0.626390     0.479206      28.97
 H      -1.299984    -1.294415     1.209128      19.58
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 C      -2.958308    -0.298407    -1.531428      61.74
 C      -4.133373    -0.766918    -2.400757      49.56
 H      -4.089450    -0.237080    -3.397670      25.95
 O      -4.097437    -2.212276    -2.566809     273.46
 H      -3.049256    -2.537065    -2.610211      25.52
 C      -5.508930    -0.437984    -1.759451      93.35
 H      -5.641463    -0.904077    -0.805863      27.75
 O      -5.773239     1.006359    -1.732783     224.64
 H      -5.793915     1.297930    -0.724142      25.26
 C      -6.721267    -1.050701    -2.573036      95.88
 O      -6.837184    -2.475762    -2.630415     308.85
 H      -5.974715    -2.832095    -2.772959      32.82
 H      -6.696897    -0.607082    -3.609217      29.27
 H      -7.753173    -0.730794    -2.219567      27.88
55
name = lig-ACN-frame_63
 C       3.404488     2.869062    -0.274782      67.43
 H       2.774915     3.799913    -0.381864      23.78
 C       4.016635     0.746662     0.673988      73.18
 H       3.702084     0.079364     1.442279      18.98
 C       5.095348     0.635281    -0.207692      21.22
 O       5.950382    -0.437172    -0.183471     228.55
 C       5.704401    -1.491139     0.789160     104.19
 H       5.728553    -1.010637     1.824028      24.54
 H       6.510869    -2.315358     0.864923      23.25
 H       4.796402    -1.943399     0.369100      25.76
 C       5.270029     1.620128    -1.244314      17.67
 O       6.251212     1.577637    -2.201862     109.11
 H       6.948101     1.048332    -1.829431      21.65
 C       4.469440     2.757275    -1.267445      60.46
 H       4.608082     3.504867    -2.068912      18.45
 C       3.200698     1.869143     0.674193      20.76
 C       2.110891     2.133936     1.785342     100.23
 H       2.333688     3.104656     2.093197      25.08
 O       2.416780     1.177479     2.939335     250.34
 H       2.016957     0.399611     2.660554      28.00
 C       0.654701     2.190816     1.342359      96.25
 H       0.468140     2.824300     0.553600      22.07
 C      -0.229006     2.683583     2.500526     108.48
 O       0.217041     3.951758     3.099901     219.05
 H       0.504305     4.557412     2.215224      27.16
 H      -0.401368     2.030789     3.298604      26.20
 H      -1.336550     2.816597     2.173673      23.86
 C      -2.689194    -1.026993    -0.371381      56.71
 H      -3.199451    -1.933344    -0.006980      20.02
 C      -2.110692     0.768147    -1.924230      39.12
 H      -2.244053     1.409378    -2.850336      18.13
 C      -1.072669     1.204968    -1.093374      21.27
 O      -0.079802     2.126281    -1.479696     219.38
 C      -0.418371     3.210709    -2.323519      86.09
 H       0.229318     4.254002    -1.828084      21.15
 H      -0.074351     2.803731    -3.371831      22.59
 H      -1.621478     3.361417    -2.329781      23.57
 C      -0.817538     0.506687     0.120474      24.56
 O       0.309864     0.769925     0.997440     184.52
 C      -1.542033    -0.643100     0.412502      39.71
 H      -1.372722    -0.997415     1.359223      19.90
 C      -2.986038    -0.299846    -1.542907      37.05
 C      -4.135930    -0.773855    -2.368891      69.05
 H      -4.096980    -0.305895    -3.374788      24.66
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 O      -4.177707    -2.237329    -2.591566     260.87
 H      -3.259876    -2.539684    -2.750840      28.41
 C      -5.544707    -0.428758    -1.778418      90.29
 H      -5.487753    -0.731327    -0.744773      26.91
 O      -5.758267     1.044433    -1.728454     274.56
 H      -5.219329     1.307181    -0.955832      27.83
 C      -6.700981    -1.018617    -2.634524     101.09
 O      -6.859302    -2.490231    -2.636783     304.34
 H      -5.939958    -2.834820    -2.678581      30.30
 H      -6.619617    -0.601478    -3.639167      29.12
 H      -7.558198    -0.599786    -2.070821      27.21
55
name = lig-ACN-frame_64
 C       3.432666     2.949145    -0.343572      45.12
 H       2.839960     3.870169    -0.184065      23.16
 C       4.022621     0.757359     0.653307      48.26
 H       3.930695    -0.085968     1.365997      19.06
 C       5.110965     0.634047    -0.215185      14.26
 O       6.012686    -0.480412    -0.212980     220.54
 C       5.713246    -1.441740     0.810617     114.83
 H       5.610155    -1.036944     1.861053      26.15
 H       6.678496    -2.078216     0.617924      22.76
 H       4.750228    -2.011115     0.819247      25.31
 C       5.278566     1.627887    -1.229617      11.88
 O       6.278098     1.536917    -2.191296     103.19
 H       7.049021     0.884799    -2.025008      21.45
 C       4.417260     2.807798    -1.270247      51.38
 H       4.604706     3.519691    -2.036494      22.72
 C       3.168397     1.934455     0.624070      14.08
 C       2.200418     2.089175     1.802593     107.76
 H       2.370408     2.968490     2.292311      24.23
 O       2.390362     1.221454     2.955614     235.60
 H       2.288544     0.244137     2.706849      24.63
 C       0.640510     2.140310     1.355394      88.85
 H       0.676653     2.726281     0.501063      23.38
 C      -0.318813     2.742147     2.481007     105.39
 O       0.203253     3.989271     3.092148     242.94
 H       0.478718     4.731995     2.422642      29.11
 H      -0.236848     2.051906     3.219349      27.14
 H      -1.338068     2.932308     2.002729      24.44
 C      -2.626556    -1.019298    -0.361249      53.05
 H      -3.324779    -1.768583    -0.105081      21.79
 C      -2.162331     0.783570    -1.915932      64.18
 H      -2.412667     1.225138    -2.900990      20.60
 C      -1.018741     1.180972    -1.107011      25.32
 O      -0.044927     2.078435    -1.462885     204.39
 C      -0.386589     3.201718    -2.358368      97.55
 H       0.236053     4.286995    -1.980586      22.29
 H      -0.046376     3.124794    -3.460828      24.36
 H      -1.573529     3.531539    -2.358442      24.32
 C      -0.735746     0.509131     0.135003      30.27
 O       0.292074     0.776276     0.998071     200.23
 C      -1.554471    -0.640970     0.442480      44.23
 H      -1.302498    -1.267657     1.275484      20.07
 C      -2.956602    -0.318238    -1.536787      57.94
 C      -4.185567    -0.767285    -2.446838      36.83
 H      -4.085379    -0.276009    -3.417189      26.13
 O      -4.208572    -2.251718    -2.595670     288.80
 H      -3.380023    -2.513484    -2.861335      31.55
 C      -5.554343    -0.406226    -1.783774      95.44
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 H      -5.711248    -0.910185    -0.821083      26.01
 O      -5.715762     1.038762    -1.739685     260.74
 H      -5.072896     1.379962    -1.132540      29.72
 C      -6.716397    -0.998596    -2.633182     107.40
 O      -6.858363    -2.440060    -2.629990     283.35
 H      -5.908324    -2.843451    -2.714420      28.19
 H      -6.550922    -0.638170    -3.629563      30.12
 H      -7.711633    -0.646016    -2.404303      27.87
55
name = lig-ACN-frame_65
 C       3.401250     2.982437    -0.312038      70.99
 H       2.854091     3.888798    -0.555540      19.59
 C       4.013833     0.806485     0.625024      69.14
 H       3.793612     0.052153     1.432939      19.25
 C       5.094692     0.631787    -0.285902      12.81
 O       5.992991    -0.442135    -0.247163     216.09
 C       5.788678    -1.454461     0.866291      94.45
 H       5.968671    -0.879573     1.783032      26.59
 H       6.579395    -2.327928     0.916844      23.60
 H       4.805667    -1.925748     0.625246      26.04
 C       5.339474     1.673823    -1.246364      16.14
 O       6.289149     1.514768    -2.219938     122.76
 H       6.993172     0.832227    -1.820215      19.08
 C       4.476545     2.761525    -1.303502      64.19
 H       4.730386     3.566786    -1.921469      27.48
 C       3.190424     1.912103     0.648370      19.45
 C       2.187248     2.116349     1.860094     110.54
 H       2.385069     3.094628     2.122510      26.20
 O       2.371351     1.220024     2.952251     264.04
 H       2.211178     0.225463     2.549856      22.39
 C       0.733331     2.162773     1.374759      77.58
 H       0.663655     2.776015     0.490342      21.29
 C      -0.297117     2.786359     2.439158     113.93
 O       0.165181     4.008101     3.052586     303.00
 H       0.452609     4.496445     2.363341      34.92
 H      -0.555651     2.152843     3.197450      27.43
 H      -1.336007     2.900270     2.021659      24.80
 C      -2.623470    -1.022283    -0.350269      58.17
 H      -3.062415    -1.929918    -0.070683      21.52
 C      -2.150848     0.805151    -1.890588      78.47
 H      -2.230589     1.298423    -2.837259      19.57
 C      -0.998689     1.116019    -1.132579      16.48
 O      -0.023085     2.102678    -1.512754     211.83
 C      -0.371936     3.208889    -2.383021      88.71
 H       0.342346     4.064964    -1.795293      20.84
 H      -0.082670     2.880349    -3.413838      23.87
 H      -1.572019     3.429672    -2.279771      23.64
 C      -0.756048     0.449400     0.119583      24.56
 O       0.277589     0.780807     1.015380     203.73
 C      -1.541844    -0.633926     0.495943      36.62
 H      -1.191638    -1.272191     1.365952      17.25
 C      -2.983538    -0.330583    -1.580627      45.59
 C      -4.167684    -0.790464    -2.425966      49.30
 H      -4.183320    -0.327935    -3.396575      24.80
 O      -4.197375    -2.223444    -2.604501     253.08
 H      -3.214547    -2.572229    -2.788712      24.57
 C      -5.590506    -0.422343    -1.807843      87.23
 H      -5.537618    -0.771772    -0.755696      27.28
 O      -5.681002     1.021476    -1.780450     249.97
 H      -5.253831     1.279592    -0.856212      25.05
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 C      -6.755065    -0.960519    -2.725424     109.03
 O      -6.850085    -2.387258    -2.595435     317.10
 H      -5.960356    -2.703389    -2.804180      32.43
 H      -6.533173    -0.649697    -3.709968      31.15
 H      -7.658803    -0.533257    -2.380028      28.54
55
name = lig-ACN-frame_66
 C       3.453168     2.891206    -0.356390      59.56
 H       2.734360     3.660365    -0.367213      26.00
 C       4.032839     0.808760     0.615763      43.47
 H       3.919496     0.037504     1.404206      19.18
 C       5.060063     0.629679    -0.301635      15.40
 O       5.976395    -0.445391    -0.256866     220.71
 C       5.859274    -1.386886     0.859251     110.74
 H       5.926740    -0.982110     1.874214      27.78
 H       6.641452    -2.143674     0.562563      23.90
 H       4.804262    -1.791510     0.965649      25.50
 C       5.357456     1.630779    -1.262818      13.19
 O       6.340537     1.495168    -2.255586     128.14
 H       7.121696     0.940529    -1.968931      20.59
 C       4.503307     2.804497    -1.246954      54.54
 H       4.655404     3.513731    -2.023861      21.25
 C       3.191118     2.003319     0.666725      19.53
 C       2.176431     2.181734     1.824170      96.79
 H       2.376801     3.061680     2.417738      21.49
 O       2.369507     1.185725     2.944727     244.17
 H       1.929542     0.338204     2.663262      23.33
 C       0.694590     2.209723     1.375034      87.28
 H       0.687198     2.877056     0.467063      20.26
 C      -0.286387     2.751435     2.382123     112.29
 O       0.128259     4.038901     2.974482     277.08
 H       0.609356     4.608386     2.317610      31.13
 H      -0.453655     2.078814     3.155793      26.07
 H      -1.103354     2.992017     1.712235      24.23
 C      -2.630944    -1.064900    -0.358462      50.39
 H      -3.155005    -1.985683    -0.202535      20.39
 C      -2.116660     0.767571    -1.915640      53.19
 H      -2.332933     1.355643    -2.761448      19.34
 C      -0.961124     1.120899    -1.136540      15.91
 O      -0.040403     2.048401    -1.518971     234.79
 C      -0.376114     3.165237    -2.361018     110.87
 H       0.250670     4.138281    -2.185233      24.51
 H      -0.222083     2.928440    -3.423975      25.36
 H      -1.515223     3.567766    -2.298062      24.25
 C      -0.737054     0.490884     0.130273      34.27
 O       0.301730     0.786267     1.047401     191.83
 C      -1.550492    -0.654810     0.453113      48.43
 H      -1.422635    -1.076965     1.543863      18.93
 C      -2.951257    -0.313224    -1.501993      21.97
 C      -4.161938    -0.781901    -2.399200      62.31
 H      -4.007853    -0.273191    -3.328757      26.31
 O      -4.134877    -2.236196    -2.617398     266.48
 H      -3.084014    -2.557642    -2.636303      23.74
 C      -5.569535    -0.423536    -1.867904      95.78
 H      -5.848682    -0.933005    -0.900217      26.59
 O      -5.646230     1.039011    -1.789942     238.50
 H      -5.780257     1.267515    -0.808698      25.71
 C      -6.725055    -0.909442    -2.739507     110.76
 O      -6.869541    -2.360031    -2.581748     305.53
 H      -6.014505    -2.750227    -2.738583      33.34
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 H      -6.614535    -0.576720    -3.732862      31.05
 H      -7.633724    -0.507127    -2.395402      29.84
55
name = lig-ACN-frame_67
 C       3.427684     2.914309    -0.373092      77.56
 H       2.928988     3.834646    -0.540948      26.07
 C       4.035944     0.813057     0.689935      74.18
 H       3.942451     0.082141     1.453336      20.21
 C       5.079577     0.633989    -0.282018       6.38
 O       5.936412    -0.431736    -0.254435     214.72
 C       5.888324    -1.330278     0.844088     126.13
 H       6.339820    -0.826024     1.671268      27.14
 H       6.616151    -2.105923     0.648580      25.02
 H       4.944805    -1.936126     0.936654      25.65
 C       5.361240     1.623922    -1.311425      18.22
 O       6.371455     1.502592    -2.272931     187.16
 H       7.053643     0.925038    -1.985197      23.95
 C       4.578577     2.780699    -1.275751      47.02
 H       4.660393     3.566209    -2.047601      20.15
 C       3.255542     1.927383     0.706828      19.33
 C       2.203796     2.150993     1.855534      89.68
 H       2.393219     3.217063     2.213907      20.58
 O       2.341183     1.191006     2.892389     309.49
 H       2.004063     0.390703     2.587130      27.58
 C       0.712747     2.202474     1.300871      69.71
 H       0.648015     2.735075     0.276003      16.18
 C      -0.334932     2.810354     2.307075     109.02
 O       0.099871     4.051994     2.916740     256.22
 H       0.572699     4.620283     2.087248      25.60
 H      -0.385176     2.108249     3.140789      24.96
 H      -1.353724     2.787485     2.008435      25.52
 C      -2.596874    -1.090661    -0.352682      59.31
 H      -3.304891    -1.858303     0.032089      20.29
 C      -2.085815     0.722673    -1.896719      41.56
 H      -2.411877     1.192024    -2.800003      20.54
 C      -0.979678     1.113139    -1.113579      13.89
 O      -0.006101     2.036446    -1.511556     208.67
 C      -0.439537     3.158423    -2.415912     102.41
 H       0.330861     3.835975    -2.042654      24.13
 H      -0.323163     2.878233    -3.464604      24.90
 H      -1.519283     3.403483    -2.092321      24.00
 C      -0.730739     0.481081     0.165946      15.51
 O       0.316235     0.820775     1.045217     220.90
 C      -1.554672    -0.615491     0.460739      49.28
 H      -1.354688    -1.233200     1.452262      18.49
 C      -2.962134    -0.310480    -1.485986      63.27
 C      -4.082112    -0.755981    -2.390298      64.33
 H      -4.026796    -0.290039    -3.359863      28.60
 O      -4.047438    -2.235859    -2.616852     275.46
 H      -3.096882    -2.510837    -2.675447      29.62
 C      -5.542206    -0.389936    -1.884242      94.45
 H      -5.561880    -0.829759    -0.833785      26.06
 O      -5.636847     1.059501    -1.770147     246.86
 H      -5.781459     1.239660    -0.868996      28.60
 C      -6.710831    -0.917937    -2.753657     110.38
 O      -6.907138    -2.335196    -2.598745     284.74
 H      -5.969602    -2.765557    -2.647337      30.19
 H      -6.541404    -0.633482    -3.775171      30.89
 H      -7.604901    -0.470795    -2.393972      29.49
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name = lig-ACN-frame_68
 C       3.521915     2.912323    -0.351460      54.59
 H       2.855746     3.765764    -0.359808      21.52
 C       4.129179     0.801988     0.723122      56.25
 H       4.062749     0.133750     1.524659      19.73
 C       5.102002     0.676900    -0.263836      16.97
 O       5.932440    -0.440060    -0.314543     231.27
 C       5.990412    -1.342827     0.876186     111.65
 H       6.189363    -0.825955     1.792237      28.27
 H       6.632364    -2.105968     0.626441      25.51
 H       4.935447    -1.577363     1.110260      26.51
 C       5.358719     1.620120    -1.295524      11.22
 O       6.376318     1.507469    -2.262658     130.10
 H       7.013463     0.790715    -1.950431      22.84
 C       4.522442     2.753497    -1.305868      65.72
 H       4.906485     3.589265    -1.963779      25.45
 C       3.239838     1.977868     0.644693       7.82
 C       2.182290     2.145763     1.767369     106.03
 H       2.436400     3.136549     2.370826      22.25
 O       2.303270     1.212866     2.879932     252.01
 H       2.285339     0.277033     2.461365      23.13
 C       0.716434     2.207888     1.224582      77.65
 H       0.807252     2.885894     0.271148      19.21
 C      -0.333780     2.803355     2.303835     105.23
 O       0.065053     4.082252     2.830607     271.66
 H       0.406933     4.766174     2.065928      28.13
 H      -0.320321     2.083172     3.175690      24.39
 H      -1.238461     2.910936     1.824749      25.35
 C      -2.607361    -1.011558    -0.284171      69.61
 H      -3.135452    -1.969292     0.062432      21.70
 C      -2.085567     0.707070    -1.868195      78.73
 H      -2.005599     1.196685    -2.853268      17.60
 C      -0.963932     1.102904    -1.074657      23.49
 O      -0.008325     2.026265    -1.542784     245.39
 C      -0.477583     3.090245    -2.369829     118.24
 H       0.061739     3.979911    -2.079098      25.95
 H      -0.470809     2.755587    -3.405860      25.54
 H      -1.511907     3.482868    -2.177190      27.09
 C      -0.732232     0.481665     0.159398      24.80
 O       0.306613     0.799411     1.011839     178.75
 C      -1.521649    -0.636590     0.547411      43.35
 H      -1.138588    -1.234018     1.448701      16.45
 C      -2.926455    -0.355680    -1.497142      47.72
 C      -4.058934    -0.767364    -2.459315      39.28
 H      -3.866258    -0.230212    -3.389279      27.65
 O      -3.992715    -2.189974    -2.605521     322.04
 H      -3.125707    -2.442630    -2.681316      29.14
 C      -5.459443    -0.382496    -1.841264      79.45
 H      -5.586824    -0.825587    -0.793922      25.99
 O      -5.645644     1.082174    -1.759513     239.09
 H      -5.278418     1.300333    -0.842794      26.59
 C      -6.671703    -0.924187    -2.740424     100.75
 O      -6.925136    -2.348565    -2.618930     279.75
 H      -6.010088    -2.762435    -2.657596      31.54
 H      -6.432603    -0.640316    -3.775933      29.79
 H      -7.594933    -0.409931    -2.469080      28.65
55
name = lig-ACN-frame_69
 C       3.538641     2.943782    -0.326578      48.06
 H       2.924852     3.879035    -0.420202      18.84
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 C       4.169187     0.904906     0.711382      77.28
 H       4.102730     0.192577     1.519078      20.42
 C       5.172694     0.640847    -0.253242      12.54
 O       6.007744    -0.495223    -0.328850     213.05
 C       6.000753    -1.288387     0.891336     129.09
 H       6.512009    -0.770931     1.662746      28.29
 H       6.659683    -2.061889     0.665386      26.09
 H       5.110200    -1.855692     1.088115      26.99
 C       5.361899     1.630836    -1.281843      12.54
 O       6.353000     1.494915    -2.210004     102.92
 H       7.090022     0.781470    -1.978411      21.06
 C       4.536983     2.783556    -1.321837      59.05
 H       4.638092     3.635408    -2.082799      24.58
 C       3.277548     1.927182     0.656210      33.01
 C       2.169144     2.158482     1.698402      97.29
 H       2.292000     3.276989     2.158614      23.70
 O       2.283005     1.219053     2.853858     230.45
 H       2.233079     0.182785     2.521297      21.47
 C       0.716355     2.217525     1.256590      92.89
 H       0.526222     2.768991     0.259379      18.00
 C      -0.249146     2.789705     2.213642     109.14
 O       0.025703     4.128304     2.779465     302.65
 H       0.421853     4.608080     2.056522      32.40
 H      -0.515904     2.097670     3.121964      24.45
 H      -1.152500     2.774747     1.741534      27.06
 C      -2.628108    -0.984546    -0.191753      48.15
 H      -3.202878    -1.967275    -0.106819      21.07
 C      -2.008567     0.720200    -1.871290      55.28
 H      -2.288597     1.037433    -2.920454      18.41
 C      -0.954573     1.101253    -1.080403      18.18
 O      -0.028734     1.986755    -1.533783     229.78
 C      -0.571804     3.084905    -2.352164     105.94
 H       0.157183     3.924028    -2.246387      23.77
 H      -0.412646     2.936022    -3.446958      24.28
 H      -1.598771     3.152078    -2.104418      26.31
 C      -0.723007     0.473070     0.191897      28.59
 O       0.350727     0.804707     0.973528     210.08
 C      -1.496795    -0.640487     0.571110      42.83
 H      -1.349333    -1.117644     1.526609      20.24
 C      -2.850873    -0.337002    -1.471514      33.20
 C      -4.011196    -0.739335    -2.423068      74.38
 H      -4.005817    -0.251413    -3.413279      23.91
 O      -4.012150    -2.181729    -2.626601     305.58
 H      -3.073786    -2.496553    -2.645997      25.83
 C      -5.453945    -0.396718    -1.859848      85.50
 H      -5.511009    -0.936632    -0.855956      26.73
 O      -5.623450     1.051669    -1.732889     257.56
 H      -4.991855     1.386476    -0.977794      26.99
 C      -6.578020    -0.907015    -2.716393     103.58
 O      -6.904773    -2.358583    -2.623419     266.23
 H      -6.113767    -2.849157    -2.731935      34.04
 H      -6.409248    -0.626773    -3.796898      28.96
 H      -7.548560    -0.438681    -2.385102      27.87
55
name = lig-ACN-frame_70
 C       3.500526     2.970784    -0.352715      62.50
 H       2.842926     3.885076    -0.447802      23.78
 C       4.234484     0.849774     0.720350      44.38
 H       4.051522     0.119670     1.552311      17.41
 C       5.221988     0.649799    -0.276000      15.23
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 O       6.037120    -0.485922    -0.302827     227.53
 C       6.101402    -1.314393     0.885362     109.94
 H       6.333353    -0.683751     1.713147      29.01
 H       6.811679    -2.115636     0.728869      24.77
 H       5.111545    -1.542515     1.144587      29.00
 C       5.379583     1.647590    -1.250182      17.76
 O       6.375157     1.484778    -2.224030     149.57
 H       7.006440     0.838626    -1.848688      22.48
 C       4.565744     2.794773    -1.270106      49.83
 H       4.692546     3.431076    -2.191098      21.10
 C       3.311903     2.011246     0.644389      -1.94
 C       2.208514     2.147542     1.744896     108.88
 H       2.513856     3.222373     2.232705      22.75
 O       2.281743     1.261291     2.813696     280.74
 H       1.935998     0.404085     2.406597      22.66
 C       0.758605     2.176345     1.177494      92.70
 H       0.853266     2.813355     0.264811      19.45
 C      -0.321787     2.814813     2.216253     101.66
 O      -0.010962     4.124057     2.721093     328.03
 H       0.532109     4.589751     2.158440      33.91
 H      -0.225143     2.093053     3.161051      23.30
 H      -1.230059     2.838556     1.768060      26.51
 C      -2.623671    -1.006006    -0.235287      66.72
 H      -3.321037    -1.698402     0.270477      18.70
 C      -2.020398     0.663544    -1.905671      36.38
 H      -2.113949     1.297229    -2.836613      15.61
 C      -0.927365     1.057460    -1.081276      13.24
 O      -0.002259     2.014720    -1.542272     231.52
 C      -0.615653     3.083896    -2.371334     103.79
 H      -0.146052     4.048042    -1.938071      23.10
 H      -0.549458     2.730535    -3.434506      22.79
 H      -1.600079     3.346228    -2.126602      27.00
 C      -0.707600     0.467270     0.187822      18.48
 O       0.427430     0.796955     0.971965     204.18
 C      -1.557720    -0.610167     0.607767      37.06
 H      -1.339118    -1.041613     1.507008      17.54
 C      -2.881535    -0.322189    -1.423222      63.25
 C      -3.985554    -0.737515    -2.336818      43.80
 H      -3.731743    -0.155535    -3.250622      29.05
 O      -4.054799    -2.186908    -2.656936     230.35
 H      -3.026839    -2.577287    -2.683326      24.84
 C      -5.380743    -0.427355    -1.822078      94.18
 H      -5.539966    -0.831641    -0.777423      26.09
 O      -5.587872     1.000230    -1.740112     276.90
 H      -5.195555     1.210313    -0.899864      28.69
 C      -6.575229    -0.950592    -2.740853      96.99
 O      -6.849761    -2.333070    -2.611594     261.17
 H      -5.938647    -2.740770    -2.781427      31.67
 H      -6.397118    -0.576663    -3.820456      29.35
 H      -7.466580    -0.360098    -2.317122      28.01
55
name = lig-ACN-frame_71
 C       3.507870     2.950596    -0.386385      51.23
 H       2.748657     3.750469    -0.501996      22.79
 C       4.195748     0.878275     0.711707      76.79
 H       4.121552     0.137470     1.566015      20.94
 C       5.206581     0.660106    -0.206592       7.86
 O       6.096476    -0.432276    -0.310107     204.41
 C       6.127513    -1.278241     0.937955     121.69
 H       6.531880    -0.781804     1.800168      28.53
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 H       6.862721    -2.108399     0.678155      24.65
 H       5.270932    -1.837447     1.083050      28.38
 C       5.448498     1.635489    -1.240422       2.44
 O       6.401930     1.486241    -2.252444      79.73
 H       7.099338     0.884753    -2.049490      23.86
 C       4.572744     2.789387    -1.283545      54.71
 H       4.834735     3.587007    -1.984894      23.23
 C       3.390277     1.996216     0.679520      30.78
 C       2.275975     2.235552     1.756259      88.51
 H       2.320360     3.284887     2.341994      21.52
 O       2.302117     1.243933     2.837654     280.40
 H       1.991698     0.424650     2.570593      26.53
 C       0.801876     2.266488     1.172973      68.61
 H       0.709621     2.689535     0.200357      19.55
 C      -0.304675     2.782260     2.173731     101.23
 O      -0.036445     4.123584     2.701543     277.54
 H       0.406538     4.654847     1.925566      28.51
 H      -0.385030     2.046092     3.104876      23.64
 H      -1.250090     2.701130     1.787880      26.46
 C      -2.629219    -0.988292    -0.169755      58.62
 H      -3.354718    -1.711238     0.133562      20.10
 C      -1.991137     0.639552    -1.846199      45.63
 H      -2.224150     0.995669    -2.870036      18.90
 C      -0.870391     1.039310    -1.116833      11.99
 O      -0.022614     2.059616    -1.555836     233.73
 C      -0.644616     3.101390    -2.343245     108.15
 H       0.050172     4.039943    -2.319935      23.25
 H      -0.505162     2.958593    -3.487170      24.03
 H      -1.666061     3.104052    -2.138635      26.62
 C      -0.641430     0.441952     0.173626      19.82
 O       0.451301     0.747790     0.937192     191.54
 C      -1.552992    -0.529754     0.641991      42.12
 H      -1.413204    -1.016172     1.527910      20.70
 C      -2.899747    -0.361318    -1.415222      67.08
 C      -4.015738    -0.797722    -2.359695      48.81
 H      -4.028034    -0.225197    -3.332856      27.44
 O      -4.061542    -2.173867    -2.679401     269.47
 H      -3.047513    -2.563210    -2.702622      25.57
 C      -5.421629    -0.460680    -1.804520      97.62
 H      -5.537537    -1.014760    -0.839457      26.49
 O      -5.533516     0.997286    -1.727096     236.71
 H      -5.710151     1.236825    -0.812117      27.92
 C      -6.553210    -0.912767    -2.699095      98.06
 O      -6.767841    -2.347290    -2.604741     229.59
 H      -5.854585    -2.823061    -2.691658      28.72
 H      -6.347681    -0.645027    -3.815107      29.63
 H      -7.593854    -0.472658    -2.429203      27.85
55
name = lig-ACN-frame_72
 C       3.556568     2.879976    -0.380951      68.30
 H       2.975842     3.777884    -0.518362      26.30
 C       4.195681     0.878348     0.762727      41.63
 H       4.041494     0.175825     1.604424      21.25
 C       5.262083     0.688435    -0.240594      14.59
 O       6.126421    -0.386365    -0.209126     216.92
 C       6.183492    -1.280709     0.904611     110.69
 H       6.434873    -0.657819     1.771822      27.71
 H       7.063891    -1.976750     0.645679      23.50
 H       5.225626    -1.665047     1.091235      26.92
 C       5.465153     1.661134    -1.255068      17.90
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 O       6.412347     1.509206    -2.273372      86.97
 H       7.149589     0.873594    -1.943168      21.35
 C       4.628016     2.762354    -1.327400      43.40
 H       4.742359     3.555501    -2.024827      22.38
 C       3.338712     2.036723     0.718265      10.15
 C       2.250564     2.248033     1.770610     102.08
 H       2.571714     3.285464     2.190087      20.63
 O       2.348909     1.264940     2.894896     233.80
 H       2.221645     0.408102     2.356137      20.53
 C       0.805428     2.243165     1.205643      97.14
 H       0.792012     2.861105     0.363337      21.09
 C      -0.250634     2.745605     2.135732     102.07
 O      -0.059775     4.095722     2.671839     255.72
 H       0.258462     4.827383     1.889841      27.00
 H      -0.300275     2.085717     3.076038      22.96
 H      -1.121467     2.729860     1.550525      24.09
 C      -2.676091    -0.930940    -0.096316      60.65
 H      -3.077982    -1.838989     0.243199      25.51
 C      -1.997183     0.598039    -1.856403      69.31
 H      -2.072068     0.998548    -2.851751      19.78
 C      -0.851699     1.031790    -1.136391       9.51
 O      -0.028967     2.078856    -1.567094     233.85
 C      -0.653309     3.124293    -2.397543      97.51
 H      -0.166388     4.073849    -1.994762      24.26
 H      -0.606476     2.754634    -3.493889      23.33
 H      -1.647340     3.371830    -2.061882      26.81
 C      -0.591895     0.444602     0.126966      19.89
 O       0.517283     0.776945     0.934409     194.35
 C      -1.540642    -0.516130     0.646574      48.05
 H      -1.320893    -0.814183     1.660232      17.91
 C      -2.868393    -0.411149    -1.419932      32.97
 C      -4.089116    -0.779760    -2.394692      39.47
 H      -3.888902    -0.169309    -3.330284      24.69
 O      -4.028020    -2.231046    -2.707294     311.84
 H      -3.095772    -2.493347    -2.693064      23.81
 C      -5.480671    -0.441469    -1.767072      93.57
 H      -5.588440    -0.815592    -0.739321      29.37
 O      -5.490609     1.017409    -1.679154     206.23
 H      -5.864061     1.170937    -0.714257      25.67
 C      -6.577566    -0.961605    -2.705569      99.29
 O      -6.705750    -2.400278    -2.589604     253.07
 H      -5.785991    -2.698977    -2.629530      31.42
 H      -6.299676    -0.538839    -3.753857      30.28
 H      -7.565251    -0.451123    -2.363678      28.62
55
name = lig-ACN-frame_73
 C       3.589174     2.931149    -0.368798      46.89
 H       2.994761     3.802205    -0.404852      24.04
 C       4.272237     0.900904     0.755776      73.34
 H       4.244270     0.138774     1.497519      18.89
 C       5.240499     0.738894    -0.172203      16.02
 O       6.183986    -0.318344    -0.190100     232.56
 C       6.212753    -1.230692     0.933833     122.72
 H       6.417703    -0.793251     1.939727      28.19
 H       6.978186    -2.061406     0.765928      24.51
 H       5.329143    -1.851099     1.002985      27.76
 C       5.489108     1.621977    -1.285236       5.44
 O       6.439795     1.522666    -2.274485     121.72
 H       7.237966     0.887112    -1.994793      21.39
 C       4.591946     2.761485    -1.321975      50.24
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 H       4.716491     3.344817    -2.194405      23.16
 C       3.352225     1.968731     0.668727      13.80
 C       2.270783     2.203901     1.832983     105.46
 H       2.257033     3.210859     2.349308      23.49
 O       2.406926     1.325832     2.896168     255.81
 H       2.318149     0.278151     2.686625      21.95
 C       0.886569     2.196757     1.207989      85.95
 H       0.937613     2.715128     0.291036      21.79
 C      -0.278018     2.764241     2.144603     108.02
 O      -0.079184     4.068984     2.652883     291.88
 H       0.416776     4.595049     1.888417      28.00
 H      -0.402020     2.071467     3.016571      25.36
 H      -1.240479     2.670312     1.679659      26.44
 C      -2.640491    -0.926329    -0.082524      49.21
 H      -3.374834    -1.545216     0.395031      21.12
 C      -1.967882     0.561678    -1.926439      31.16
 H      -2.198017     1.052310    -2.832884      16.61
 C      -0.875778     1.033676    -1.145831      12.60
 O      -0.047762     2.077107    -1.586853     227.99
 C      -0.662649     3.147204    -2.391098     106.00
 H       0.026884     3.995242    -2.400313      24.26
 H      -0.602391     2.962354    -3.546793      24.06
 H      -1.773171     3.229250    -2.170945      25.18
 C      -0.569328     0.474903     0.137068      13.49
 O       0.563962     0.838745     0.899335     234.44
 C      -1.473240    -0.465239     0.631290      48.65
 H      -1.323281    -0.979228     1.644022      18.61
 C      -2.908150    -0.418146    -1.409522      67.61
 C      -4.025538    -0.799921    -2.300494      55.53
 H      -4.012489    -0.201616    -3.267541      28.14
 O      -4.002139    -2.241941    -2.736042     290.48
 H      -3.136140    -2.518692    -2.708511      29.33
 C      -5.447705    -0.403223    -1.759281      94.75
 H      -5.584239    -0.931852    -0.818443      27.52
 O      -5.504897     1.051541    -1.631169     259.00
 H      -5.408805     1.285968    -0.656224      26.59
 C      -6.633861    -1.000329    -2.668562     102.00
 O      -6.659379    -2.440853    -2.576961     248.57
 H      -5.775707    -2.778457    -2.692808      30.94
 H      -6.547678    -0.733498    -3.780615      29.50
 H      -7.698886    -0.684196    -2.366608      27.84
55
name = lig-ACN-frame_74
 C       3.569267     2.977155    -0.323655      57.98
 H       2.896667     3.794337    -0.461207      19.58
 C       4.289323     0.904716     0.780315      62.68
 H       4.170319     0.272113     1.615207      21.23
 C       5.381876     0.726513    -0.210576      15.07
 O       6.278972    -0.268686    -0.162851     195.94
 C       6.209393    -1.245204     0.980078     102.30
 H       6.380283    -0.659451     1.940843      26.64
 H       7.118733    -1.771173     0.713979      24.14
 H       5.208664    -1.753150     0.956726      25.97
 C       5.428325     1.646601    -1.288904      20.36
 O       6.449598     1.522882    -2.266039     162.09
 H       7.184132     0.917898    -2.018688      24.35
 C       4.555637     2.715533    -1.363825      62.30
 H       4.659777     3.518046    -2.071903      27.52
 C       3.399005     1.990924     0.698338      13.25
 C       2.336362     2.190099     1.782209      98.36
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 H       2.634257     3.184181     2.108577      26.22
 O       2.489617     1.311232     2.994951     255.27
 H       2.194618     0.466384     2.572431      25.91
 C       0.841547     2.219705     1.194064      86.15
 H       0.867604     2.907075     0.340417      21.96
 C      -0.297129     2.698601     2.141456     104.00
 O      -0.065391     4.091055     2.635006     307.24
 H       0.442402     4.584323     2.076385      34.05
 H      -0.329400     2.083909     3.010222      26.64
 H      -1.234941     2.671842     1.547136      25.52
 C      -2.576138    -0.870079    -0.100090      67.90
 H      -3.373080    -1.412970     0.434433      21.86
 C      -1.962640     0.534216    -1.926981      33.58
 H      -2.179247     0.855689    -2.917448      17.27
 C      -0.889699     1.067635    -1.183238      15.45
 O      -0.071541     2.087647    -1.623349     226.57
 C      -0.644013     3.126368    -2.454678     105.13
 H      -0.132443     4.004168    -2.185409      24.27
 H      -0.687682     2.704985    -3.526167      22.52
 H      -1.678566     3.427896    -1.990783      24.04
 C      -0.576102     0.529845     0.123674      30.88
 O       0.572110     0.795564     0.830841     197.27
 C      -1.451851    -0.494302     0.625294      58.46
 H      -1.164863    -0.938700     1.691363      17.88
 C      -2.833600    -0.357554    -1.363741      57.60
 C      -4.030714    -0.829565    -2.294916      39.19
 H      -3.808508    -0.191529    -3.210554      26.64
 O      -3.983984    -2.194418    -2.732254     277.04
 H      -3.005268    -2.531193    -2.667310      27.42
 C      -5.473138    -0.455234    -1.759225      93.24
 H      -5.614878    -0.800621    -0.747966      27.34
 O      -5.538142     1.061305    -1.590344     266.18
 H      -5.059496     1.155382    -0.799457      30.04
 C      -6.634809    -1.024503    -2.612312     109.30
 O      -6.643925    -2.499119    -2.544885     211.36
 H      -5.674318    -2.744524    -2.789038      28.47
 H      -6.568533    -0.567403    -3.630644      29.54
 H      -7.558994    -0.671806    -2.087306      28.04
55
name = lig-ACN-frame_75
 C       3.557195     2.915413    -0.344515      37.63
 H       2.917583     3.806849    -0.392830      22.99
 C       4.368803     0.905879     0.752652      59.81
 H       4.294263     0.201339     1.557664      19.84
 C       5.345727     0.764449    -0.171959      13.21
 O       6.406885    -0.275157    -0.113412     236.22
 C       6.257798    -1.185757     0.956957     118.60
 H       6.208946    -0.651468     1.983677      27.32
 H       6.932167    -1.989457     1.042699      25.72
 H       5.243701    -1.774285     0.910311      25.65
 C       5.445052     1.654588    -1.303144       6.21
 O       6.406623     1.545333    -2.268934     141.13
 H       7.058448     0.954052    -1.927682      26.02
 C       4.479345     2.756109    -1.347481      60.21
 H       4.646991     3.471983    -2.173843      24.58
 C       3.467984     2.019351     0.707381      30.02
 C       2.371707     2.242419     1.785030      92.53
 H       2.439436     3.176496     2.267462      24.02
 O       2.533677     1.305580     2.992135     251.93
 H       2.230666     0.455278     2.850111      27.30
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 C       0.866222     2.214662     1.221020      76.66
 H       0.826704     2.847358     0.277489      19.42
 C      -0.246368     2.719480     2.159475     108.16
 O      -0.060096     4.067472     2.632046     306.48
 H       0.363118     4.567301     1.928727      31.19
 H      -0.403274     2.100921     2.968181      26.22
 H      -1.227282     2.659553     1.575650      23.71
 C      -2.596508    -0.854952    -0.034251      56.90
 H      -3.089255    -1.813488     0.332484      25.17
 C      -1.928320     0.597772    -1.951330      63.28
 H      -1.897709     0.898254    -3.007106      19.21
 C      -0.871936     1.097267    -1.180580       6.72
 O      -0.047418     2.095684    -1.650025     230.68
 C      -0.655275     3.120723    -2.476626     105.30
 H       0.002932     3.897716    -2.491910      26.25
 H      -0.698828     2.919496    -3.599083      24.52
 H      -1.828556     3.317078    -2.217252      24.38
 C      -0.615401     0.510425     0.060698      25.71
 O       0.591200     0.803055     0.765709     218.48
 C      -1.385115    -0.479020     0.625701      34.35
 H      -1.151820    -0.898475     1.705977      18.70
 C      -2.867258    -0.383435    -1.389064      40.67
 C      -4.016488    -0.741780    -2.304799      69.76
 H      -4.050252    -0.110408    -3.240854      27.08
 O      -3.955456    -2.172455    -2.702381     238.77
 H      -2.885744    -2.491866    -2.659883      20.65
 C      -5.430552    -0.466005    -1.686255      96.26
 H      -5.500316    -0.983339    -0.737977      28.51
 O      -5.577391     0.972780    -1.620814     261.27
 H      -5.208191     1.304854    -0.721749      27.39
 C      -6.621747    -1.036455    -2.507218     111.75
 O      -6.637441    -2.493926    -2.530605     219.76
 H      -5.683590    -2.836147    -2.699588      28.29
 H      -6.663670    -0.711672    -3.541726      29.94
 H      -7.579439    -0.738790    -2.077283      28.80
55
name = lig-ACN-frame_76
 C       3.522706     2.901975    -0.375695      76.24
 H       2.822639     3.790350    -0.366353      25.26
 C       4.380233     0.925567     0.806640      52.73
 H       4.272727     0.175946     1.622050      21.39
 C       5.433083     0.739773    -0.207157      12.18
 O       6.465613    -0.198750    -0.106165     190.82
 C       6.239944    -1.186478     1.016497     109.30
 H       6.290599    -0.673361     2.055916      26.87
 H       7.110814    -1.729289     0.844291      25.62
 H       5.218296    -1.729610     0.777296      24.18
 C       5.423368     1.687767    -1.272763      26.78
 O       6.355730     1.574772    -2.285492     162.73
 H       7.190245     1.018570    -2.123341      22.22
 C       4.534476     2.736150    -1.382724      38.72
 H       4.505110     3.398160    -2.285468      20.66
 C       3.468767     2.001712     0.772312      14.50
 C       2.339107     2.202362     1.879260     110.53
 H       2.424848     3.171651     2.211446      25.37
 O       2.554659     1.351835     2.939672     255.31
 H       2.328099     0.447674     2.484045      23.84
 C       0.958106     2.160565     1.202765      81.07
 H       1.049159     2.914998     0.314363      18.87
 C      -0.228017     2.715146     2.176354     100.35
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 O      -0.031231     4.054915     2.638141     261.49
 H       0.297399     4.744729     1.842776      26.56
 H      -0.260350     2.153129     3.017921      26.86
 H      -1.241759     2.609440     1.603445      23.89
 C      -2.588685    -0.908515    -0.110970      63.56
 H      -3.241074    -1.765369     0.301752      21.35
 C      -1.962742     0.599883    -1.933700      16.31
 H      -2.244078     0.937441    -2.969910      17.42
 C      -0.863109     1.106685    -1.205813      13.57
 O      -0.002666     2.116846    -1.680862     213.79
 C      -0.648800     3.131001    -2.567570     100.28
 H      -0.159961     4.035545    -2.386827      25.33
 H      -0.654667     2.662836    -3.565112      24.23
 H      -1.754804     3.373159    -2.058265      23.76
 C      -0.513666     0.539562     0.088917      19.70
 O       0.630473     0.853379     0.737773     216.91
 C      -1.445701    -0.469769     0.600007      56.89
 H      -1.078855    -0.989827     1.544492      18.52
 C      -2.824426    -0.313243    -1.396934      41.57
 C      -4.020148    -0.729816    -2.309175      62.18
 H      -3.937170    -0.113928    -3.236072      27.75
 O      -3.920056    -2.138364    -2.666709     255.91
 H      -2.906570    -2.417135    -2.711544      26.57
 C      -5.383042    -0.513398    -1.614331      97.52
 H      -5.321390    -0.841043    -0.578504      28.38
 O      -5.632575     0.909635    -1.639003     236.59
 H      -5.716929     1.201902    -0.648452      26.91
 C      -6.608679    -1.072907    -2.443364     115.67
 O      -6.641687    -2.496003    -2.496469     245.63
 H      -5.723894    -2.741907    -2.590190      31.68
 H      -6.505955    -0.568471    -3.378090      31.41
 H      -7.498487    -0.750531    -1.957498      29.45
55
name = lig-ACN-frame_77
 C       3.531725     2.874997    -0.343982      42.97
 H       2.771432     3.663953    -0.620988      19.40
 C       4.419263     0.950508     0.826620      64.85
 H       4.408741     0.276856     1.725483      20.90
 C       5.402158     0.806909    -0.132381      24.37
 O       6.444713    -0.128953    -0.052506     233.21
 C       6.311218    -1.158192     0.965623     114.50
 H       6.277345    -0.665346     2.005589      26.52
 H       7.088298    -1.907055     0.954223      25.57
 H       5.308199    -1.824559     0.935403      25.37
 C       5.478057     1.671571    -1.263258      11.30
 O       6.349357     1.611850    -2.362807      96.03
 H       7.163156     1.042559    -2.004878      22.84
 C       4.484646     2.702990    -1.344641      61.99
 H       4.611902     3.401595    -2.210176      28.29
 C       3.455684     2.013477     0.731225      27.21
 C       2.400458     2.239164     1.803808     103.36
 H       2.534605     3.154488     2.249094      26.64
 O       2.536974     1.295552     2.945387     213.46
 H       2.499645     0.254402     2.684713      22.53
 C       0.929739     2.245654     1.232776      79.56
 H       0.974901     2.963194     0.291599      20.48
 C      -0.148194     2.672749     2.151290     101.06
 O       0.004127     4.072872     2.655327     247.93
 H       0.400482     4.661576     1.819670      26.69
 H      -0.181676     2.061639     2.985113      26.59
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 H      -1.204111     2.568217     1.612046      23.81
 C      -2.516612    -0.912318    -0.216022      49.05
 H      -3.299577    -1.537184     0.305762      20.84
 C      -1.962183     0.687712    -1.908690      47.28
 H      -2.230247     1.269272    -2.844143      18.91
 C      -0.800925     1.123824    -1.220735       4.10
 O       0.015310     2.147061    -1.710235     224.41
 C      -0.634604     3.101237    -2.580397     103.36
 H      -0.031606     4.025903    -2.542532      24.38
 H      -0.657620     2.888157    -3.649525      25.49
 H      -1.846801     3.202216    -2.345540      24.05
 C      -0.562709     0.535820     0.045039      19.78
 O       0.714313     0.829882     0.753846     176.94
 C      -1.418550    -0.457727     0.544953      46.24
 H      -1.269677    -0.930333     1.487800      20.70
 C      -2.866034    -0.319887    -1.399849      57.05
 C      -3.977129    -0.751203    -2.259311      72.95
 H      -4.032997    -0.129471    -3.165482      30.45
 O      -3.882374    -2.135226    -2.642062     289.92
 H      -3.008862    -2.380564    -2.711429      31.93
 C      -5.380950    -0.541112    -1.597322      97.92
 H      -5.392940    -0.954818    -0.577140      29.80
 O      -5.694893     0.926686    -1.600306     217.17
 H      -5.965099     1.128257    -0.729713      30.38
 C      -6.550649    -1.080323    -2.342515     121.41
 O      -6.634198    -2.534309    -2.455576     226.76
 H      -5.758114    -2.875995    -2.669065      32.11
 H      -6.586715    -0.688447    -3.315294      31.48
 H      -7.438172    -0.755229    -1.895688      30.38
55
name = lig-ACN-frame_78
 C       3.505816     2.877210    -0.393827      31.76
 H       2.745780     3.682223    -0.388449      20.41
 C       4.422711     1.026105     0.874603      63.57
 H       4.433314     0.380226     1.777216      21.05
 C       5.441592     0.870896    -0.102629      30.56
 O       6.429661    -0.108925    -0.010354     221.33
 C       6.359361    -1.142776     0.972869     110.40
 H       6.454559    -0.759883     2.043685      26.46
 H       7.282656    -1.749375     0.717954      24.17
 H       5.325020    -1.683045     0.757445      25.05
 C       5.477762     1.691797    -1.286072      26.99
 O       6.368759     1.611019    -2.359601     140.92
 H       7.180513     1.068675    -2.227300      24.47
 C       4.496202     2.689830    -1.339380      64.99
 H       4.530593     3.411774    -2.166343      26.90
 C       3.448931     1.985126     0.717711      40.37
 C       2.422361     2.212105     1.801299     102.58
 H       2.627390     3.147202     2.240763      26.14
 O       2.513248     1.249921     2.948392     236.46
 H       2.253107     0.398205     2.514007      25.19
 C       0.982761     2.267705     1.173871      73.85
 H       0.796442     2.915636     0.223997      18.13
 C      -0.124646     2.708563     2.216213      98.68
 O       0.040100     4.043258     2.650384     315.94
 H       0.529442     4.585031     2.052085      31.85
 H      -0.133738     2.032577     3.069571      25.25
 H      -1.173885     2.600192     1.631995      23.09
 C      -2.492989    -0.893121    -0.192236      59.82
 H      -3.003904    -1.795795     0.183001      23.90
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 C      -1.985051     0.808930    -1.898435      59.03
 H      -2.202740     1.240031    -2.900494      21.73
 C      -0.795132     1.139285    -1.232295      11.61
 O       0.013271     2.151455    -1.724316     213.22
 C      -0.616694     3.111088    -2.641219      93.31
 H      -0.076364     4.101812    -2.385694      24.27
 H      -0.458971     2.718992    -3.617732      25.21
 H      -1.758505     3.383352    -2.259699      24.20
 C      -0.435566     0.553604     0.037215      22.73
 O       0.681376     0.809385     0.746728     193.41
 C      -1.335649    -0.468493     0.517535      35.24
 H      -1.151354    -0.750633     1.474241      21.36
 C      -2.776678    -0.238753    -1.474733      34.52
 C      -4.029464    -0.721476    -2.264158      67.79
 H      -4.054947    -0.156671    -3.187167      25.59
 O      -3.859773    -2.181322    -2.625691     265.78
 H      -2.910098    -2.366655    -2.638214      27.32
 C      -5.381835    -0.488355    -1.549030      89.09
 H      -5.326487    -0.893243    -0.511311      28.26
 O      -5.728998     0.929846    -1.537252     236.06
 H      -5.682063     1.222078    -0.586365      27.89
 C      -6.584802    -1.159800    -2.357985     112.94
 O      -6.617135    -2.589427    -2.388151     204.05
 H      -5.689297    -2.872580    -2.745735      29.09
 H      -6.591333    -0.693165    -3.292872      31.01
 H      -7.427630    -0.900834    -1.797887      29.42
55
name = lig-ACN-frame_79
 C       3.458609     2.860879    -0.401612      74.50
 H       2.882174     3.754303    -0.555650      24.68
 C       4.497701     1.055895     0.888353      69.12
 H       4.435890     0.407999     1.753086      22.80
 C       5.492432     0.892513    -0.099999      22.83
 O       6.478549    -0.059160    -0.020003     216.15
 C       6.384400    -1.144880     0.980854     109.09
 H       6.540000    -0.799144     2.029278      25.84
 H       7.261445    -1.854898     0.676983      24.32
 H       5.454306    -1.858102     1.010943      25.69
 C       5.460248     1.715063    -1.262801      25.49
 O       6.390755     1.592690    -2.310586     175.68
 H       7.106207     1.069995    -1.995219      26.92
 C       4.510832     2.765628    -1.411556      38.65
 H       4.545808     3.389252    -2.303427      21.22
 C       3.444611     2.005065     0.729067      27.20
 C       2.369879     2.181401     1.841841     109.25
 H       2.503397     3.168374     2.297540      25.36
 O       2.460072     1.242627     2.866587     292.69
 H       2.112957     0.424180     2.656509      29.64
 C       0.965755     2.195661     1.188000      85.90
 H       1.200325     2.886616     0.330587      21.28
 C      -0.101388     2.693947     2.197460      95.67
 O       0.090853     4.060886     2.697864     309.06
 H       0.522178     4.544116     2.043829      32.56
 H      -0.029348     2.057857     3.130066      25.25
 H      -1.233846     2.579504     1.788846      24.49
 C      -2.397025    -0.838384    -0.229960      60.64
 H      -2.937163    -1.724261     0.013833      24.47
 C      -1.999641     0.854876    -1.921285      66.89
 H      -2.211234     1.285598    -2.886908      22.22
 C      -0.796850     1.213009    -1.230719      12.94
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 O       0.035681     2.184972    -1.725627     206.41
 C      -0.557856     3.159794    -2.635589     103.77
 H       0.052960     4.206585    -2.537122      23.32
 H      -0.539583     2.919317    -3.712095      26.16
 H      -1.724431     3.186122    -2.502219      25.56
 C      -0.422017     0.524733    -0.033411      20.31
 O       0.699634     0.864318     0.779377     212.15
 C      -1.247229    -0.458449     0.508055      46.81
 H      -0.939822    -1.016555     1.299694      21.55
 C      -2.786805    -0.246594    -1.431101      33.59
 C      -3.983135    -0.703203    -2.304287      64.95
 H      -4.043480    -0.195616    -3.235102      28.11
 O      -3.873583    -2.168661    -2.583162     239.25
 H      -2.798089    -2.430981    -2.633682      24.45
 C      -5.430805    -0.496666    -1.547224      83.87
 H      -5.338363    -0.887649    -0.491925      27.84
 O      -5.744432     0.937038    -1.451996     211.73
 H      -5.213215     1.303523    -0.621299      26.85
 C      -6.621251    -1.184312    -2.318357     115.60
 O      -6.556328    -2.652236    -2.342995     208.26
 H      -5.642504    -2.921696    -2.614497      29.22
 H      -6.649578    -0.843522    -3.313236      29.61
 H      -7.589155    -0.911937    -1.947284      29.02
55
name = lig-ACN-frame_80
 C       3.502666     2.891304    -0.443731      20.79
 H       2.662734     3.502561    -0.532435      20.51
 C       4.506693     1.089946     0.892472      60.93
 H       4.552085     0.436987     1.724362      23.09
 C       5.467733     0.938301    -0.094838      20.47
 O       6.560863    -0.078964    -0.028532     215.32
 C       6.437533    -1.135736     0.979438     108.56
 H       6.617326    -0.670183     1.959866      27.58
 H       7.260938    -1.953255     0.824376      24.63
 H       5.369716    -1.478588     0.886642      26.55
 C       5.486829     1.765228    -1.256789      20.38
 O       6.405635     1.564403    -2.222550     120.53
 H       7.221929     1.018606    -1.942717      22.07
 C       4.468744     2.771513    -1.390625      68.70
 H       4.554261     3.450816    -2.232863      29.99
 C       3.480997     2.065709     0.721672      38.30
 C       2.346682     2.191603     1.791092     106.90
 H       2.444918     3.169472     2.346972      24.05
 O       2.422065     1.201393     2.884480     236.35
 H       2.252003     0.311266     2.404175      24.51
 C       0.943767     2.244095     1.215692      95.89
 H       0.752656     2.897467     0.372263      21.74
 C      -0.097921     2.699103     2.213006      89.16
 O       0.149841     4.057339     2.734234     257.85
 H       0.391814     4.742306     1.953113      27.94
 H      -0.118848     1.927282     3.109211      23.74
 H      -1.161887     2.629109     1.669149      23.36
 C      -2.350230    -0.891877    -0.268309      65.05
 H      -2.940765    -1.594438     0.256864      22.71
 C      -1.982896     0.830846    -1.920236      47.51
 H      -2.279209     1.343368    -2.792438      20.37
 C      -0.819614     1.269535    -1.250271      13.85
 O       0.072466     2.260138    -1.734362     217.10
 C      -0.519009     3.214568    -2.657239     103.36
 H       0.094155     4.252531    -2.353411      22.02
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 H      -0.281031     2.847562    -3.679754      24.37
 H      -1.583951     3.497019    -2.356497      25.14
 C      -0.407126     0.605048    -0.026969      14.55
 O       0.711805     0.851232     0.749687     187.43
 C      -1.181506    -0.517261     0.420184      36.31
 H      -0.851911    -1.062370     1.295826      20.10
 C      -2.820316    -0.174599    -1.436467      45.74
 C      -3.986342    -0.733549    -2.248787      81.34
 H      -3.939990    -0.171946    -3.152421      29.91
 O      -3.877479    -2.126119    -2.527831     232.65
 H      -2.884344    -2.465450    -2.752610      27.67
 C      -5.426005    -0.513830    -1.584669      89.75
 H      -5.387795    -1.097026    -0.611858      28.80
 O      -5.743842     0.913024    -1.405626     244.44
 H      -5.231145     1.256009    -0.647829      28.38
 C      -6.609045    -1.207988    -2.334525     117.13
 O      -6.514244    -2.672707    -2.300727     213.99
 H      -5.586991    -2.826161    -2.422766      31.16
 H      -6.577093    -0.850196    -3.337811      30.11
 H      -7.552729    -0.945103    -1.817238      28.02
55
name = lig-ACN-frame_81
 C       3.450227     2.913646    -0.395819      70.12
 H       2.711143     3.618528    -0.651567      21.49
 C       4.499973     1.119954     0.911312      70.71
 H       4.408821     0.593557     1.837985      24.88
 C       5.550881     0.883053    -0.072366      29.98
 O       6.576649    -0.031587    -0.064215     234.60
 C       6.426384    -1.038909     0.987589     115.81
 H       6.630866    -0.720133     2.009642      27.59
 H       7.146499    -1.829570     0.648351      26.49
 H       5.452540    -1.544973     1.023151      28.01
 C       5.508832     1.774699    -1.184758      24.47
 O       6.454657     1.567406    -2.211383      73.58
 H       7.225498     0.955024    -1.850773      21.80
 C       4.525686     2.757080    -1.397495      66.78
 H       4.513123     3.418428    -2.277217      28.48
 C       3.492854     2.087343     0.752013      35.59
 C       2.395012     2.239657     1.778956      99.93
 H       2.641020     3.240815     2.327047      24.24
 O       2.402013     1.197007     2.860868     199.65
 H       2.373974     0.172736     2.492769      22.16
 C       0.922397     2.286396     1.164831      81.25
 H       0.964142     2.947913     0.350189      22.33
 C      -0.150744     2.741129     2.263768      90.88
 O       0.188145     4.007824     2.772866     236.59
 H       0.436463     4.660183     1.897235      26.40
 H      -0.287736     2.066883     3.266444      22.54
 H      -1.216349     2.797824     1.731111      22.93
 C      -2.366934    -0.933165    -0.261336      57.61
 H      -2.944064    -1.784814     0.060497      22.88
 C      -1.972368     0.871175    -1.926422      49.39
 H      -2.259560     1.311790    -2.851237      22.63
 C      -0.770929     1.299357    -1.235326       7.88
 O       0.056237     2.300414    -1.709957     209.45
 C      -0.445255     3.323725    -2.630446     105.69
 H       0.243580     4.376502    -2.522757      22.05
 H      -0.422106     3.030088    -3.742425      25.05
 H      -1.516111     3.433022    -2.549294      27.02
 C      -0.437384     0.623557    -0.024202      22.69
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 O       0.710916     0.867783     0.693906     183.61
 C      -1.130863    -0.543801     0.292720      47.65
 H      -0.816731    -0.959608     1.318222      21.86
 C      -2.790481    -0.203461    -1.377832      23.39
 C      -4.027582    -0.660153    -2.209723      85.41
 H      -4.087437    -0.182380    -3.173098      27.65
 O      -3.865043    -2.144262    -2.479145     263.49
 H      -2.991178    -2.228798    -2.705306      32.13
 C      -5.390792    -0.552276    -1.569624      96.57
 H      -5.368021    -0.953711    -0.515165      27.85
 O      -5.736224     0.840319    -1.418718     231.78
 H      -5.627727     1.068266    -0.509810      29.45
 C      -6.549474    -1.218964    -2.388923     114.83
 O      -6.495088    -2.638984    -2.274445     215.02
 H      -5.558724    -2.953552    -2.461491      27.74
 H      -6.716194    -0.859102    -3.404424      29.48
 H      -7.500810    -0.890311    -1.854284      27.58
55
name = lig-ACN-frame_82
 C       3.519313     2.910880    -0.439349      36.69
 H       2.843053     3.757082    -0.481777      24.77
 C       4.544000     1.113099     0.941308      64.46
 H       4.577606     0.434759     1.801484      23.06
 C       5.508997     0.974493    -0.022161      30.54
 O       6.529318     0.003115    -0.033671     236.21
 C       6.443655    -1.010776     0.981448     122.94
 H       6.739659    -0.490587     1.891285      27.42
 H       7.168799    -1.771690     0.821158      27.25
 H       5.438929    -1.367836     1.013046      28.24
 C       5.562866     1.747175    -1.179019      25.12
 O       6.492128     1.601487    -2.205488     181.20
 H       7.247674     1.037567    -1.963508      25.95
 C       4.530257     2.737509    -1.315747      65.39
 H       4.642832     3.266300    -2.281905      22.24
 C       3.486981     2.090012     0.719327      34.82
 C       2.366883     2.209940     1.843193     106.14
 H       2.411383     3.243365     2.436900      22.26
 O       2.426688     1.253541     2.827581     258.74
 H       2.058621     0.408412     2.361993      24.37
 C       0.950377     2.274319     1.208102     101.95
 H       0.892333     2.966020     0.436723      22.36
 C      -0.192738     2.755875     2.208475      88.69
 O       0.228809     4.022463     2.830544     264.63
 H       0.631593     4.642640     2.135656      29.93
 H      -0.137761     1.839613     3.044215      23.47
 H      -1.274782     2.794314     1.767550      24.15
 C      -2.344520    -0.942007    -0.299634      58.48
 H      -2.758611    -1.926361    -0.000671      23.35
 C      -1.987192     0.881570    -1.872300      55.92
 H      -2.219985     1.314162    -2.847959      23.06
 C      -0.815055     1.323933    -1.282644      18.95
 O       0.052012     2.362597    -1.681869     210.89
 C      -0.430272     3.382225    -2.634467     105.34
 H       0.354716     4.343964    -2.315703      22.30
 H      -0.207012     2.975894    -3.676558      25.57
 H      -1.385087     3.712526    -2.400412      28.71
 C      -0.427016     0.604768    -0.108554      20.70
 O       0.721628     0.963340     0.661022     188.25
 C      -1.147798    -0.564725     0.340934      47.56
 H      -0.644056    -1.288944     1.158422      19.61
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 C      -2.778244    -0.188113    -1.434658      37.42
 C      -3.971137    -0.683053    -2.194563      75.85
 H      -3.991917    -0.060225    -3.121735      28.48
 O      -3.833841    -2.123142    -2.436414     257.24
 H      -2.945338    -2.402439    -2.704510      29.87
 C      -5.409543    -0.566153    -1.517057      87.31
 H      -5.394654    -1.196878    -0.584500      29.17
 O      -5.750273     0.832702    -1.442591     195.86
 H      -5.910045     1.151956    -0.474529      26.66
 C      -6.499644    -1.208521    -2.373339     107.36
 O      -6.515495    -2.645007    -2.293481     181.73
 H      -5.592157    -2.906902    -2.652307      28.63
 H      -6.268509    -0.881281    -3.411677      29.67
 H      -7.540416    -0.874042    -2.009222      28.14
55
name = lig-ACN-frame_83
 C       3.581992     2.899832    -0.355076      64.54
 H       2.819115     3.698080    -0.608783      17.34
 C       4.493477     1.154361     0.969843      65.28
 H       4.399744     0.484712     1.868937      21.98
 C       5.549285     1.005163    -0.014096      28.05
 O       6.502231     0.008148    -0.010929     228.41
 C       6.467530    -0.967380     1.054900     124.29
 H       6.660821    -0.615139     2.062796      27.75
 H       7.148955    -1.673416     0.733217      27.82
 H       5.521648    -1.417012     1.141045      28.61
 C       5.566511     1.790155    -1.217682      26.97
 O       6.514712     1.650006    -2.196230     161.12
 H       7.248665     1.125355    -1.905179      25.79
 C       4.630056     2.738883    -1.386146      67.80
 H       4.631212     3.511036    -2.168068      31.52
 C       3.462282     2.066523     0.792759      39.87
 C       2.329812     2.283491     1.789283      99.32
 H       2.620345     3.333118     2.292941      25.20
 O       2.452870     1.228601     2.857744     257.32
 H       2.068086     0.431423     2.601895      27.78
 C       0.910878     2.356369     1.178905      93.42
 H       1.011910     3.067527     0.410022      21.78
 C      -0.111771     2.744997     2.182948      98.06
 O       0.231728     4.007146     2.891159     294.09
 H       0.578149     4.542685     2.269508      35.93
 H      -0.386488     2.026963     3.139281      23.60
 H      -1.081686     2.896620     1.577663      24.43
 C      -2.243912    -0.950910    -0.342360      57.01
 H      -2.909412    -1.807524    -0.032430      22.20
 C      -2.046208     0.932205    -1.943564      47.56
 H      -2.486534     1.497963    -2.812281      20.83
 C      -0.824262     1.337482    -1.244985       7.34
 O       0.007793     2.391881    -1.641071     209.60
 C      -0.378316     3.407942    -2.574848     112.80
 H       0.431998     4.366225    -2.484997      21.35
 H      -0.408812     3.087671    -3.679478      25.05
 H      -1.383654     3.700765    -2.476903      27.11
 C      -0.370346     0.593697    -0.081045      19.50
 O       0.712490     0.978481     0.607128     204.87
 C      -1.116878    -0.524254     0.347623      47.14
 H      -0.624315    -1.206116     1.216586      19.02
 C      -2.752780    -0.197564    -1.410217      34.71
 C      -3.943446    -0.737237    -2.186137      76.46
 H      -4.027406    -0.266598    -3.220528      27.90
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 O      -3.811109    -2.136480    -2.425264     214.07
 H      -2.744757    -2.287053    -2.696779      26.58
 C      -5.375166    -0.568288    -1.473467      84.87
 H      -5.345966    -0.847885    -0.396853      28.64
 O      -5.787322     0.864439    -1.442666     188.87
 H      -5.537475     1.195329    -0.492896      26.88
 C      -6.450526    -1.219738    -2.413118     105.14
 O      -6.549493    -2.669449    -2.343812     222.56
 H      -5.696576    -3.016517    -2.597342      30.95
 H      -6.249980    -0.869245    -3.484632      28.23
 H      -7.496203    -0.756616    -2.217416      27.37
55
name = lig-ACN-frame_84
 C       3.618977     2.925782    -0.366143      27.07
 H       2.779572     3.691744    -0.530646      19.08
 C       4.506208     1.142501     0.956474      59.66
 H       4.518102     0.461604     1.854574      22.72
 C       5.514350     1.001670    -0.004731      26.37
 O       6.513241     0.005769     0.043518     224.62
 C       6.474547    -0.980930     1.137760     123.60
 H       6.779143    -0.461201     2.029482      27.80
 H       7.240050    -1.676464     0.951391      27.83
 H       5.570892    -1.490226     1.177703      28.96
 C       5.589454     1.817607    -1.181795      20.87
 O       6.576743     1.682260    -2.205034     141.46
 H       7.367735     1.079524    -1.908336      23.98
 C       4.568596     2.862195    -1.339999      71.55
 H       4.667532     3.528305    -2.183019      29.34
 C       3.498282     2.113475     0.742808      43.42
 C       2.377350     2.259402     1.792087     101.65
 H       2.447167     3.244591     2.432023      22.80
 O       2.448049     1.278094     2.898186     234.12
 H       2.271191     0.427307     2.425860      26.82
 C       0.992440     2.375832     1.122299      91.85
 H       0.846676     3.065885     0.298462      21.22
 C      -0.154198     2.829851     2.203305      96.08
 O       0.225236     3.959965     2.933777     271.24
 H       0.449131     4.692405     2.274172      30.52
 H      -0.300145     1.850442     2.896743      23.95
 H      -1.138597     3.016927     1.668543      24.41
 C      -2.198529    -0.937006    -0.356917      54.79
 H      -2.677375    -1.848165     0.100166      21.23
 C      -2.042989     0.985169    -1.903030      61.13
 H      -2.453815     1.629988    -2.740934      21.97
 C      -0.885171     1.357133    -1.270058      16.59
 O      -0.020343     2.395207    -1.571489     217.06
 C      -0.403687     3.394820    -2.572966     109.26
 H       0.420638     4.293370    -2.377299      22.25
 H      -0.282149     2.930371    -3.584692      25.94
 H      -1.405943     3.731111    -2.375519      27.50
 C      -0.424359     0.664402    -0.106406      18.97
 O       0.779989     1.006552     0.608381     172.29
 C      -1.034235    -0.512227     0.340861      38.28
 H      -0.806169    -0.864519     1.430259      20.84
 C      -2.714209    -0.184237    -1.455258      33.56
 C      -3.975988    -0.734811    -2.142021      65.35
 H      -4.043942    -0.145093    -3.122707      25.72
 O      -3.761646    -2.225217    -2.421908     206.16
 H      -2.748186    -2.377437    -2.690663      26.21
 C      -5.347552    -0.510372    -1.508308      95.21
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 H      -5.401115    -1.079193    -0.561018      28.36
 O      -5.787860     0.880393    -1.420632     228.47
 H      -5.217895     1.359965    -0.852729      30.45
 C      -6.408555    -1.243698    -2.445606      97.12
 O      -6.595679    -2.670403    -2.388359     221.10
 H      -5.708965    -3.078955    -2.479221      30.02
 H      -6.168552    -0.920227    -3.542210      27.39
 H      -7.426411    -0.885161    -2.064001      25.74
55
name = lig-ACN-frame_85
 C       3.518648     3.042327    -0.392731      87.34
 H       2.806898     3.934569    -0.446862      24.80
 C       4.547065     1.121276     0.913578      64.80
 H       4.502101     0.505418     1.840733      23.17
 C       5.534068     0.956597    -0.059412      36.11
 O       6.536378    -0.015431     0.093983     225.13
 C       6.511305    -0.955583     1.208916     119.81
 H       6.587127    -0.465584     2.155727      28.29
 H       7.322952    -1.656079     1.007131      26.43
 H       5.565126    -1.397292     1.279559      28.98
 C       5.619638     1.878426    -1.174290      27.08
 O       6.585832     1.721737    -2.147127     138.78
 H       7.300970     1.070000    -1.791299      24.14
 C       4.660293     2.873111    -1.296790      39.64
 H       4.684467     3.503337    -2.155852      18.92
 C       3.557004     2.136585     0.765822      34.35
 C       2.425895     2.299189     1.838511     103.05
 H       2.633864     3.327897     2.277837      24.76
 O       2.426262     1.328934     2.867661     247.08
 H       2.307270     0.323079     2.507348      21.74
 C       0.976964     2.362708     1.145141     104.21
 H       1.257905     3.099400     0.351125      18.66
 C      -0.163746     2.794541     2.108543      96.54
 O       0.227051     3.960724     3.003442     218.51
 H       0.473194     4.807631     2.305155      28.42
 H      -0.240022     1.991924     2.951653      23.80
 H      -1.165902     2.939018     1.666826      24.92
 C      -2.160298    -0.912154    -0.337223      44.21
 H      -2.695531    -1.838850    -0.108858      21.23
 C      -2.089740     0.996479    -1.857139      68.14
 H      -2.414419     1.481187    -2.820935      23.57
 C      -0.847668     1.404579    -1.214398      12.61
 O      -0.041881     2.447570    -1.544090     215.36
 C      -0.416407     3.330349    -2.561800     119.99
 H       0.293408     4.247931    -2.438758      24.00
 H      -0.324585     2.941606    -3.589516      27.28
 H      -1.501584     3.713825    -2.512207      27.65
 C      -0.368414     0.717485    -0.050067      24.73
 O       0.780777     1.040021     0.578809     201.12
 C      -1.047569    -0.439749     0.342762      44.47
 H      -0.641078    -0.995827     1.202090      21.13
 C      -2.698885    -0.223311    -1.442962      39.72
 C      -3.890717    -0.750599    -2.183042      66.76
 H      -3.921924    -0.321522    -3.219835      25.39
 O      -3.752999    -2.235099    -2.395551     289.65
 H      -2.900696    -2.366985    -2.654564      31.24
 C      -5.374404    -0.591954    -1.552253      88.42
 H      -5.417193    -0.967949    -0.522879      27.74
 O      -5.760780     0.846275    -1.439081     199.79
 H      -5.083896     1.271475    -0.845901      29.34
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 C      -6.434925    -1.211035    -2.464340     106.01
 O      -6.594804    -2.664716    -2.389678     212.67
 H      -5.666174    -3.084408    -2.546333      27.71
 H      -6.248857    -0.871438    -3.589968      26.58
 H      -7.426040    -0.725755    -2.236617      26.39
55
name = lig-ACN-frame_86
 C       3.634405     3.035437    -0.342999      43.54
 H       2.947811     3.859912    -0.583958      20.37
 C       4.507239     1.178279     0.866626      54.11
 H       4.446691     0.489228     1.711312      22.57
 C       5.583910     0.925746    -0.057220      32.86
 O       6.594828    -0.028149     0.085833     230.85
 C       6.490571    -0.895166     1.277232     119.60
 H       6.709502    -0.383273     2.177675      28.67
 H       7.363219    -1.622533     1.117146      26.29
 H       5.639372    -1.534633     1.238763      28.03
 C       5.618762     1.849655    -1.109906      28.26
 O       6.616303     1.763156    -2.088383     158.77
 H       7.308022     1.176321    -1.844002      25.31
 C       4.655292     2.913176    -1.265017      56.89
 H       4.862956     3.622285    -2.039355      30.48
 C       3.520774     2.199657     0.746507      45.69
 C       2.428757     2.350151     1.814780     110.51
 H       2.555894     3.246839     2.412947      24.75
 O       2.441513     1.335758     2.883995     237.62
 H       2.080196     0.506043     2.400991      24.35
 C       1.059620     2.435415     1.184751      87.81
 H       0.827270     3.159131     0.319530      19.94
 C      -0.098211     2.781987     2.147457     102.73
 O       0.195794     3.936752     2.982155     273.94
 H       0.597477     4.668122     2.357440      30.89
 H      -0.410162     1.916746     2.783233      26.46
 H      -0.915146     3.018647     1.477157      25.39
 C      -2.185759    -0.930665    -0.321451      65.98
 H      -2.535980    -1.869877     0.029001      22.48
 C      -2.022663     0.990022    -1.812479      59.45
 H      -2.377855     1.462857    -2.730803      22.24
 C      -0.890436     1.435989    -1.143939      15.08
 O      -0.042645     2.508777    -1.521769     215.76
 C      -0.455158     3.346854    -2.650387     110.29
 H       0.152594     4.252711    -2.616835      24.53
 H      -0.252383     2.835547    -3.581891      26.79
 H      -1.629670     3.432074    -2.536040      24.80
 C      -0.396215     0.730464    -0.029821      20.71
 O       0.830896     1.075931     0.585215     205.15
 C      -1.047491    -0.436471     0.400046      50.40
 H      -0.530853    -1.074765     1.010172      19.41
 C      -2.700407    -0.190814    -1.402303      36.91
 C      -3.879571    -0.838246    -2.257968      70.53
 H      -3.871936    -0.318031    -3.219549      28.78
 O      -3.757076    -2.224436    -2.350293     285.75
 H      -2.886881    -2.485165    -2.705042      30.88
 C      -5.329030    -0.613019    -1.599457      82.62
 H      -5.317961    -1.166951    -0.652265      29.20
 O      -5.699982     0.767064    -1.491505     202.34
 H      -5.296190     1.160438    -0.594474      26.00
 C      -6.495509    -1.203427    -2.518188     102.44
 O      -6.581503    -2.623426    -2.375199     221.06
 H      -5.706540    -2.948867    -2.641392      30.12
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 H      -6.198062    -0.893480    -3.639189      27.50
 H      -7.480686    -0.835712    -2.207603      28.11
55
name = lig-ACN-frame_87
 C       3.712819     3.111869    -0.331247      11.75
 H       2.967232     3.851465    -0.428826      18.48
 C       4.484696     1.135111     0.901008      60.15
 H       4.274478     0.496720     1.743985      21.82
 C       5.533632     0.987638     0.021420      36.01
 O       6.606302    -0.022445     0.089065     221.71
 C       6.539616    -0.867112     1.278023     115.06
 H       6.495921    -0.203817     2.113913      28.75
 H       7.462132    -1.585258     1.306021      24.92
 H       5.533110    -1.310210     1.360907      27.02
 C       5.669243     1.832609    -1.128214      28.02
 O       6.668356     1.818536    -2.057733     190.72
 H       7.382926     1.203462    -1.770796      26.78
 C       4.761134     2.887465    -1.251098      70.70
 H       4.888279     3.653398    -2.025697      28.72
 C       3.539552     2.189150     0.757241      37.12
 C       2.448603     2.399349     1.837099     107.55
 H       2.637112     3.329063     2.282213      27.91
 O       2.458007     1.332901     2.850859     273.19
 H       2.041574     0.592478     2.520178      27.44
 C       1.042803     2.453255     1.173948      99.18
 H       1.243245     3.232396     0.340514      19.53
 C      -0.097149     2.784835     2.165135     120.34
 O       0.177622     3.917864     2.960962     327.08
 H       0.552315     4.514140     2.407481      37.00
 H      -0.322884     1.979576     2.830126      26.96
 H      -0.980254     2.998478     1.593265      26.30
 C      -2.187678    -0.934318    -0.250483      60.48
 H      -2.691026    -1.827943    -0.009443      21.69
 C      -2.010794     0.968694    -1.811876      47.26
 H      -2.327236     1.535256    -2.654075      20.92
 C      -0.867824     1.517289    -1.095630       6.71
 O      -0.080005     2.568807    -1.517747     204.43
 C      -0.512071     3.299451    -2.740098     111.07
 H      -0.032113     4.217282    -2.652917      25.17
 H      -0.310357     2.716344    -3.609096      26.77
 H      -1.692297     3.692113    -2.829180      24.83
 C      -0.388839     0.756403     0.047015      27.01
 O       0.870434     1.095712     0.606935     188.53
 C      -1.018931    -0.495813     0.416271      29.06
 H      -0.718869    -0.903106     1.278008      22.55
 C      -2.743163    -0.208027    -1.386930      30.82
 C      -3.876115    -0.774300    -2.237693      80.15
 H      -3.817878    -0.420699    -3.232144      29.91
 O      -3.747020    -2.312347    -2.326044     203.89
 H      -2.707685    -2.452987    -2.714048      25.08
 C      -5.307699    -0.651442    -1.711682      97.06
 H      -5.367159    -1.194486    -0.767010      29.54
 O      -5.611845     0.739380    -1.494499     203.44
 H      -5.575064     1.022807    -0.569535      28.26
 C      -6.459967    -1.204928    -2.538650     112.23
 O      -6.584092    -2.623473    -2.384658     224.11
 H      -5.744830    -3.027802    -2.611554      30.57
 H      -6.480801    -0.872491    -3.694798      28.14
 H      -7.350752    -0.745352    -2.133826      29.42
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name = lig-ACN-frame_88
 C       3.755287     3.129835    -0.290833      72.00
 H       3.296101     4.040968    -0.439599      31.56
 C       4.456422     1.078053     0.971482      57.87
 H       4.376490     0.372196     1.793130      22.23
 C       5.600409     0.965002     0.023285      26.43
 O       6.549013     0.020479     0.099840     217.65
 C       6.532197    -0.765391     1.304637     115.78
 H       6.706880    -0.223517     2.223010      27.69
 H       7.447523    -1.489985     1.169944      24.56
 H       5.699874    -1.550715     1.281845      24.95
 C       5.696731     1.869447    -1.090544      23.20
 O       6.771390     1.821051    -2.044181     177.43
 H       7.523018     1.142176    -1.757733      27.01
 C       4.809455     2.931934    -1.233673      69.91
 H       5.008110     3.550496    -2.147219      17.04
 C       3.588453     2.197288     0.773941      29.95
 C       2.470495     2.373945     1.840033     102.10
 H       2.637051     3.214559     2.388144      23.90
 O       2.490181     1.366803     2.836726     254.58
 H       2.163225     0.551237     2.361297      24.43
 C       1.050606     2.437026     1.168499      95.76
 H       0.963459     3.131283     0.276854      20.10
 C      -0.153050     2.756107     2.123084     108.01
 O       0.191389     3.960396     2.981763     272.33
 H       0.404967     4.698784     2.368966      31.32
 H      -0.101731     1.993706     2.797277      26.99
 H      -1.123678     2.730407     1.709160      26.48
 C      -2.218681    -0.894587    -0.234528      58.58
 H      -2.709409    -1.746788     0.203166      20.82
 C      -2.018051     0.976798    -1.762692      53.83
 H      -2.374125     1.370920    -2.669260      21.66
 C      -0.892854     1.453598    -1.080977       7.18
 O      -0.194513     2.644258    -1.546889     202.36
 C      -0.544857     3.266098    -2.790157     105.18
 H       0.150083     4.083535    -2.928016      24.26
 H      -0.304676     2.682228    -3.674988      27.41
 H      -1.793553     3.366097    -2.747671      23.89
 C      -0.350451     0.755341     0.068252      36.50
 O       0.848094     1.095787     0.635503     203.30
 C      -1.021176    -0.428644     0.449291      42.29
 H      -0.720138    -0.954812     1.298894      22.00
 C      -2.664632    -0.204352    -1.340520      39.11
 C      -3.822039    -0.854376    -2.227299      61.14
 H      -3.744501    -0.359821    -3.156091      28.73
 O      -3.700448    -2.332112    -2.320159     231.87
 H      -2.675342    -2.557524    -2.618459      25.12
 C      -5.284273    -0.646551    -1.722411      91.89
 H      -5.350002    -1.190534    -0.773672      28.62
 O      -5.553094     0.786680    -1.488676     211.44
 H      -5.341951     0.908035    -0.562297      28.34
 C      -6.450196    -1.219016    -2.567845     107.52
 O      -6.614320    -2.666394    -2.418032     210.90
 H      -5.680493    -3.068181    -2.584129      28.83
 H      -6.365357    -0.867985    -3.702631      27.78
 H      -7.341437    -0.823949    -2.126781      28.45
55
name = lig-ACN-frame_89
 C       3.844578     3.122137    -0.251070      35.58
 H       3.140043     3.900186    -0.239961      18.34
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 C       4.532635     1.121905     0.882193      66.73
 H       4.387817     0.408070     1.699030      22.42
 C       5.530856     1.015238     0.015463      27.90
 O       6.544782     0.023646     0.126899     234.58
 C       6.602099    -0.786423     1.308485     110.76
 H       6.648856    -0.098077     2.191791      27.64
 H       7.565480    -1.387487     1.168465      24.64
 H       5.588465    -1.357923     1.481346      25.38
 C       5.790330     1.892626    -1.052225      18.75
 O       6.829511     1.784240    -1.991014     174.98
 H       7.521586     1.154776    -1.673129      24.37
 C       4.837880     2.953863    -1.210712      75.01
 H       4.930503     3.801561    -1.946250      30.77
 C       3.625695     2.208114     0.812834      27.40
 C       2.454428     2.406856     1.799669      95.93
 H       2.532105     3.315428     2.260801      27.12
 O       2.510391     1.345929     2.850473     210.66
 H       2.355691     0.373197     2.412355      22.59
 C       1.006294     2.462866     1.138921      82.48
 H       1.035242     3.195930     0.327770      20.65
 C      -0.075532     2.749293     2.232195     114.00
 O       0.153812     3.966564     2.942094     255.58
 H       0.357919     4.723874     2.149814      27.59
 H      -0.207512     2.013042     2.873556      28.79
 H      -0.937823     2.949909     1.664178      25.21
 C      -2.173015    -0.847870    -0.127434      61.57
 H      -2.665776    -1.780436     0.228800      22.84
 C      -2.050548     0.947476    -1.748801      53.39
 H      -2.298870     1.468729    -2.656426      21.54
 C      -0.873346     1.474189    -1.136641      22.39
 O      -0.298616     2.635956    -1.503673     215.40
 C      -0.600683     3.190253    -2.846492     100.29
 H      -0.071290     4.198588    -2.874627      23.07
 H      -0.465323     2.368533    -3.568135      26.32
 H      -1.763414     3.697706    -3.018535      24.27
 C      -0.365677     0.755935    -0.023001      22.06
 O       0.830902     1.050964     0.668659     198.35
 C      -1.074089    -0.354435     0.515800      55.46
 H      -0.481648    -0.946772     1.257991      18.11
 C      -2.687789    -0.263879    -1.349231      36.81
 C      -3.748594    -0.909035    -2.208322      73.31
 H      -3.708756    -0.492485    -3.184064      28.26
 O      -3.635625    -2.318702    -2.316349     302.68
 H      -2.742020    -2.496752    -2.594764      29.94
 C      -5.246410    -0.622333    -1.631893      83.34
 H      -5.325551    -1.133139    -0.656878      28.58
 O      -5.502504     0.801410    -1.490468     205.61
 H      -5.030850     1.306660    -0.708632      25.54
 C      -6.441124    -1.254926    -2.570559     100.91
 O      -6.620768    -2.687191    -2.473678     225.98
 H      -5.740697    -3.128952    -2.602497      29.54
 H      -6.180283    -0.989663    -3.683501      27.46
 H      -7.402394    -0.810682    -2.371633      28.35
55
name = lig-ACN-frame_90
 C       3.840464     3.152835    -0.200223      56.06
 H       3.186432     3.969482    -0.511351      20.23
 C       4.506985     1.170913     0.911452      49.31
 H       4.390954     0.379135     1.669241      20.33
 C       5.640340     0.997689    -0.042475      18.09
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 O       6.576518     0.003042     0.100243     219.49
 C       6.648241    -0.770044     1.349158     102.87
 H       6.871265    -0.106005     2.253340      27.61
 H       7.431465    -1.548117     1.285323      26.05
 H       5.685476    -1.466048     1.447173      24.87
 C       5.815939     1.976865    -1.089143      16.61
 O       6.867071     1.746081    -1.928443     167.82
 H       7.474915     1.134055    -1.560621      24.43
 C       4.901102     2.994982    -1.164494      76.14
 H       5.037390     3.716406    -2.002355      29.42
 C       3.616890     2.230082     0.829099      40.82
 C       2.450112     2.369128     1.794468     108.05
 H       2.604198     3.251647     2.339050      25.51
 O       2.521466     1.361705     2.851270     248.25
 H       2.245732     0.519609     2.366776      24.53
 C       1.062566     2.375696     1.198859      83.22
 H       0.964687     3.051216     0.394850      22.32
 C      -0.068711     2.762757     2.229519     114.34
 O       0.142061     4.008085     2.918505     269.36
 H       0.559212     4.744494     2.208548      26.89
 H      -0.107654     2.067071     2.947625      27.86
 H      -1.013304     2.676166     1.755320      27.36
 C      -2.228715    -0.869710    -0.098070      64.56
 H      -2.644868    -1.850929     0.291737      21.22
 C      -2.065182     0.898565    -1.799839      52.25
 H      -2.637122     1.343930    -2.638721      19.52
 C      -0.949598     1.435040    -1.153681      16.85
 O      -0.373976     2.693333    -1.507081     217.57
 C      -0.674126     3.158632    -2.840431      90.15
 H       0.237822     3.879363    -3.085005      22.02
 H      -0.446118     2.405208    -3.681410      25.54
 H      -1.902417     3.443313    -2.924039      22.58
 C      -0.354366     0.770837    -0.015632      30.18
 O       0.795688     1.068896     0.645224     225.80
 C      -1.044874    -0.300317     0.529118      68.32
 H      -0.686867    -0.705184     1.589860      18.90
 C      -2.652264    -0.279835    -1.290397      46.95
 C      -3.815231    -0.865415    -2.149615      56.15
 H      -3.787451    -0.338299    -3.101318      29.25
 O      -3.584635    -2.362173    -2.300172     277.14
 H      -2.728878    -2.447240    -2.569633      29.64
 C      -5.230787    -0.649776    -1.562949      91.15
 H      -5.288803    -1.040825    -0.528429      28.38
 O      -5.476070     0.804703    -1.544420     220.64
 H      -4.864502     1.050201    -0.773875      27.76
 C      -6.317144    -1.245740    -2.556865     105.27
 O      -6.613005    -2.689097    -2.505132     238.73
 H      -5.778535    -3.098156    -2.670232      32.07
 H      -5.987464    -0.897173    -3.577108      28.55
 H      -7.273263    -0.743467    -2.324229      28.04
55
name = lig-ACN-frame_91
 C       3.827924     3.231798    -0.280818      23.47
 H       3.121539     4.122063    -0.313259      23.59
 C       4.587768     1.145028     0.901022      56.42
 H       4.417238     0.434285     1.706311      21.30
 C       5.635522     1.022019     0.057436      33.11
 O       6.645902    -0.037675     0.070451     222.88
 C       6.673455    -0.772783     1.344635     108.96
 H       6.950839    -0.071327     2.256520      26.03
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 H       7.461427    -1.436232     1.119120      25.23
 H       5.613804    -1.242141     1.599320      24.45
 C       5.825919     1.895300    -1.003114      17.19
 O       6.907759     1.763199    -1.941046     178.23
 H       7.579703     1.069910    -1.575104      26.16
 C       4.918932     3.057323    -1.138487      59.44
 H       5.020428     3.746304    -1.966793      19.33
 C       3.633791     2.243789     0.772342      19.05
 C       2.493780     2.337789     1.873290      93.72
 H       2.522925     3.315253     2.345352      25.59
 O       2.524186     1.340710     2.859751     280.08
 H       2.168627     0.555742     2.564772      28.07
 C       1.033499     2.404011     1.211633      97.06
 H       1.137605     3.153041     0.487777      22.68
 C      -0.073610     2.710660     2.239505     111.52
 O       0.149625     4.049252     2.876415     280.16
 H       0.502131     4.673092     2.192366      30.87
 H       0.030529     2.043219     3.010475      27.29
 H      -1.035198     2.697228     1.788628      26.86
 C      -2.195271    -0.887691    -0.070384      59.96
 H      -2.805934    -1.675169     0.451259      23.09
 C      -2.083583     0.838742    -1.805753      58.56
 H      -2.467200     1.381269    -2.723202      19.25
 C      -0.967391     1.475104    -1.148217      16.69
 O      -0.444307     2.690869    -1.513788     221.22
 C      -0.694338     3.118824    -2.862950      96.36
 H      -0.141997     4.167119    -3.124367      22.06
 H      -0.699834     2.159207    -3.513175      23.57
 H      -1.854722     3.644486    -2.967874      23.56
 C      -0.444764     0.796691    -0.003050      29.15
 O       0.824423     1.084029     0.608633     189.62
 C      -1.123980    -0.337292     0.544852      42.41
 H      -0.806083    -0.670587     1.661025      17.80
 C      -2.704273    -0.307684    -1.269402      42.13
 C      -3.813304    -0.923075    -2.040649      55.56
 H      -3.856702    -0.447336    -3.041169      30.22
 O      -3.614791    -2.337659    -2.271692     249.41
 H      -2.660039    -2.414247    -2.487349      27.99
 C      -5.226672    -0.697018    -1.539241     102.65
 H      -5.439711    -1.144631    -0.539131      29.18
 O      -5.437370     0.765595    -1.594227     218.43
 H      -5.245686     1.207436    -0.789050      29.39
 C      -6.227105    -1.227748    -2.512569     109.18
 O      -6.556764    -2.629884    -2.525801     224.83
 H      -5.739509    -3.204328    -2.694052      29.50
 H      -5.940600    -0.896871    -3.520116      29.64
 H      -7.211573    -0.744556    -2.255646      28.35
55
name = lig-ACN-frame_92
 C       3.840590     3.182932    -0.257398      70.61
 H       3.204604     4.144709    -0.376140      22.13
 C       4.555266     1.181616     0.949059      63.04
 H       4.353144     0.555168     1.795586      22.77
 C       5.731690     0.982609     0.077684      28.29
 O       6.634906    -0.028450     0.098011     214.54
 C       6.724760    -0.777076     1.305996     108.35
 H       7.077212     0.001344     2.139585      25.35
 H       7.320368    -1.637267     1.306358      26.37
 H       5.681594    -1.214982     1.559957      25.20
 C       5.846243     1.945659    -1.021538      16.96
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 O       6.856208     1.808296    -1.916908      91.17
 H       7.636392     1.189126    -1.620690      22.52
 C       4.957214     3.006041    -1.163275      67.15
 H       5.305496     3.762666    -1.829269      25.23
 C       3.663406     2.236310     0.754222      34.13
 C       2.476411     2.368313     1.822912      70.43
 H       2.764034     3.241699     2.458386      24.00
 O       2.543980     1.279443     2.932350     189.16
 H       2.253609     0.468972     2.402233      24.38
 C       1.062365     2.460210     1.192249      86.35
 H       0.944460     3.200996     0.442613      22.93
 C      -0.038262     2.740686     2.289548     112.55
 O       0.148843     4.028524     2.821759     313.68
 H       0.272033     4.580340     2.138060      34.74
 H      -0.124235     1.990470     3.054384      26.73
 H      -1.009735     2.671946     1.817141      26.46
 C      -2.277391    -0.897632    -0.055349      57.55
 H      -2.828249    -1.724344     0.410224      22.90
 C      -2.063501     0.838656    -1.761680      54.18
 H      -2.418710     1.111427    -2.793232      20.62
 C      -1.025205     1.453051    -1.105931      13.11
 O      -0.469057     2.685691    -1.511757     198.70
 C      -0.801354     3.126818    -2.893293      88.02
 H       0.146596     3.822960    -3.074858      22.64
 H      -0.500688     2.353352    -3.730658      24.33
 H      -2.004640     3.429996    -3.016905      23.13
 C      -0.464632     0.809796     0.064118      29.52
 O       0.799993     1.114001     0.543176     204.03
 C      -1.131519    -0.294592     0.602885      55.97
 H      -0.557147    -0.887718     1.452325      17.62
 C      -2.701975    -0.315459    -1.243565      40.58
 C      -3.806128    -0.975120    -2.030714      55.96
 H      -3.788735    -0.426826    -3.012188      27.59
 O      -3.677874    -2.369535    -2.209529     227.17
 H      -2.665963    -2.568977    -2.561306      24.93
 C      -5.219950    -0.689053    -1.477050      95.79
 H      -5.389150    -1.020826    -0.415185      29.43
 O      -5.421775     0.734547    -1.619581     208.98
 H      -5.505586     1.024260    -0.677613      28.31
 C      -6.275757    -1.217148    -2.550314     104.41
 O      -6.488141    -2.614589    -2.524784     229.47
 H      -5.557071    -2.994538    -2.667237      29.54
 H      -5.939144    -0.831999    -3.493398      30.17
 H      -7.278714    -0.696823    -2.353725      28.44
55
name = lig-ACN-frame_93
 C       3.908819     3.118543    -0.268855      38.59
 H       3.195395     3.987821    -0.508398      17.72
 C       4.620874     1.180363     0.965415      51.13
 H       4.560877     0.446397     1.746886      20.12
 C       5.659564     1.047943     0.068339      33.32
 O       6.650088    -0.027107     0.094815     216.24
 C       6.719936    -0.796278     1.359649     106.85
 H       7.204890    -0.224819     2.298076      26.04
 H       7.409651    -1.532834     0.992464      25.07
 H       5.724495    -1.174192     1.663531      27.06
 C       5.857905     1.924594    -0.963739      26.33
 O       6.853515     1.858533    -1.946054     174.80
 H       7.552498     1.310678    -1.596258      25.28
 C       4.962879     2.983187    -1.148227      45.48
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 H       4.994091     3.670024    -1.968105      24.98
 C       3.634160     2.207713     0.809683      22.60
 C       2.523062     2.328418     1.815739      78.81
 H       2.511977     3.359784     2.356343      25.88
 O       2.533983     1.289195     2.876239     197.17
 H       2.377796     0.277594     2.505852      21.56
 C       1.047407     2.431964     1.219897      91.32
 H       1.082697     3.235561     0.483973      23.84
 C      -0.043668     2.721103     2.239130     107.89
 O       0.143662     4.050062     2.832486     265.33
 H       0.336775     4.775202     2.156274      29.67
 H       0.148519     2.074044     3.130717      25.00
 H      -1.010735     2.619309     1.742048      25.96
 C      -2.288164    -0.848287     0.053706      52.16
 H      -2.585235    -1.837095     0.306315      21.05
 C      -2.099005     0.797943    -1.756819      55.61
 H      -2.384647     1.229849    -2.719825      20.82
 C      -1.052120     1.473100    -1.038636      11.60
 O      -0.498787     2.645737    -1.545583     206.34
 C      -0.786166     3.097179    -2.881391     103.67
 H      -0.351847     4.167132    -3.063590      22.82
 H      -0.643649     2.199977    -3.593609      24.21
 H      -1.973969     3.470796    -3.008652      24.35
 C      -0.492767     0.842534     0.104234      32.95
 O       0.804549     1.190722     0.510981     204.25
 C      -1.130057    -0.332303     0.623802      54.63
 H      -0.609739    -0.880693     1.445594      21.63
 C      -2.700706    -0.338371    -1.209956      42.80
 C      -3.832433    -0.936629    -2.058586      62.48
 H      -3.855540    -0.535921    -3.115621      28.66
 O      -3.734646    -2.488668    -2.143322     201.86
 H      -2.678728    -2.647359    -2.518387      23.00
 C      -5.278523    -0.663248    -1.556685      99.39
 H      -5.359487    -1.098331    -0.521938      28.80
 O      -5.433204     0.774275    -1.581551     217.71
 H      -5.192003     1.249096    -0.658252      25.52
 C      -6.320563    -1.182020    -2.529386     114.20
 O      -6.417946    -2.657615    -2.540284     231.80
 H      -5.530095    -2.993541    -2.566918      31.90
 H      -5.993510    -0.836690    -3.475736      30.06
 H      -7.384384    -0.799249    -2.330571      28.11
55
name = lig-ACN-frame_94
 C       3.826717     3.085278    -0.229183      50.35
 H       3.022126     3.839698    -0.379942      22.55
 C       4.651029     1.150456     1.005557      66.76
 H       4.489395     0.450247     1.842171      21.72
 C       5.706123     1.006396     0.074365      26.52
 O       6.617641     0.026886     0.162974     209.65
 C       6.729148    -0.829301     1.344901     107.08
 H       7.162121    -0.132748     2.205228      25.68
 H       7.400540    -1.727846     1.200537      25.55
 H       5.799971    -1.259241     1.620301      28.04
 C       5.893410     1.964755    -1.030335      16.42
 O       6.891458     1.870016    -1.959721     133.53
 H       7.630538     1.287099    -1.738956      23.04
 C       4.918353     2.991301    -1.142743      75.53
 H       5.056298     3.575015    -2.063018      22.91
 C       3.692701     2.177972     0.834922      21.25
 C       2.447537     2.287780     1.850377      87.92
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 H       2.726662     3.266032     2.464426      23.39
 O       2.533224     1.325307     2.818373     249.33
 H       2.283986     0.455940     2.283048      24.13
 C       1.090911     2.438094     1.178222      95.27
 H       1.146782     3.302513     0.482192      22.88
 C      -0.005039     2.752807     2.247464     102.22
 O       0.119359     4.076361     2.859776     227.47
 H       0.492568     4.722655     2.021991      24.92
 H      -0.030871     1.903462     3.050312      24.64
 H      -1.056157     2.656900     1.871494      24.97
 C      -2.263277    -0.870387     0.044328      71.22
 H      -2.740502    -1.682548     0.545484      21.95
 C      -2.124862     0.813127    -1.710675      68.59
 H      -2.545930     1.179992    -2.609589      23.15
 C      -1.105483     1.475485    -1.069129      14.56
 O      -0.478085     2.623854    -1.527358     207.21
 C      -0.857127     3.072023    -2.852690     106.90
 H      -0.186616     3.943223    -3.010454      24.25
 H      -0.418314     2.410751    -3.693659      25.24
 H      -2.068949     3.109690    -2.933836      24.23
 C      -0.504204     0.865723     0.111128      45.37
 O       0.797453     1.207851     0.491348     206.47
 C      -1.073047    -0.305502     0.660116      30.19
 H      -0.719835    -0.684228     1.564729      22.33
 C      -2.778411    -0.367636    -1.200048      52.63
 C      -3.869066    -1.051576    -2.040916      55.39
 H      -3.705293    -0.608121    -3.094295      27.73
 O      -3.765672    -2.504417    -2.077606     237.58
 H      -2.777453    -2.695616    -2.322798      27.21
 C      -5.302907    -0.611514    -1.602016      94.39
 H      -5.561764    -1.053917    -0.601820      28.51
 O      -5.466704     0.861336    -1.539683     242.60
 H      -4.905345     1.056938    -0.726316      27.50
 C      -6.362164    -1.243212    -2.556643     118.80
 O      -6.375863    -2.672820    -2.552205     236.70
 H      -5.433792    -2.965649    -2.535243      29.84
 H      -6.314367    -0.818591    -3.514976      29.86
 H      -7.359470    -0.908159    -2.138821      28.09
55
name = lig-ACN-frame_95
 C       3.768714     3.057174    -0.238573      49.70
 H       3.078116     3.857494    -0.415913      20.60
 C       4.647986     1.152925     1.012804      56.85
 H       4.587682     0.401237     1.856120      21.04
 C       5.736715     1.044053     0.092479      25.33
 O       6.694972    -0.007500     0.192882     205.55
 C       6.690506    -0.817738     1.358896     110.43
 H       7.038993    -0.242622     2.325441      24.77
 H       7.495589    -1.590297     1.049358      23.82
 H       5.760689    -1.252034     1.536763      27.69
 C       5.847156     1.955837    -0.994825      18.60
 O       6.931737     1.875301    -1.978538      65.33
 H       7.639388     1.248099    -1.521671      23.98
 C       4.866540     2.965639    -1.151334      65.90
 H       4.964186     3.850976    -1.825799      26.37
 C       3.675218     2.166496     0.855922      33.69
 C       2.540479     2.367612     1.791417      61.31
 H       2.565115     3.398170     2.430750      23.80
 O       2.491019     1.247628     2.833969     216.81
 H       2.223598     0.403771     2.486016      25.62
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 C       1.075263     2.521825     1.173360      74.90
 H       0.976932     3.282116     0.334148      21.98
 C      -0.019653     2.805818     2.254167      96.55
 O       0.128956     4.074073     2.869146     228.94
 H       0.395508     4.857287     2.148519      26.31
 H       0.083109     2.066930     3.190711      23.20
 H      -0.952317     2.756364     1.609375      24.56
 C      -2.216183    -0.895527     0.034824      66.81
 H      -2.818007    -1.626929     0.572646      24.79
 C      -2.259373     0.800352    -1.695597      52.06
 H      -2.567309     1.147399    -2.633142      22.36
 C      -1.090499     1.427315    -1.055780      10.16
 O      -0.462399     2.600040    -1.509551     204.76
 C      -0.853351     3.044673    -2.837386     112.94
 H      -0.561019     4.059834    -2.910790      25.87
 H      -0.492888     2.276558    -3.558257      25.92
 H      -2.033684     3.229674    -3.033038      25.10
 C      -0.490778     0.854653     0.058544      24.28
 O       0.793656     1.192632     0.480207     192.91
 C      -1.137290    -0.242843     0.656902      53.81
 H      -0.695307    -0.612075     1.479270      20.12
 C      -2.760208    -0.377276    -1.139800      48.12
 C      -3.873778    -1.056175    -1.988321      58.13
 H      -3.752001    -0.733327    -3.086817      26.73
 O      -3.770507    -2.505875    -1.988772     272.17
 H      -2.922639    -2.671348    -2.211600      32.59
 C      -5.348618    -0.614455    -1.622717      94.54
 H      -5.461648    -0.968628    -0.574348      28.75
 O      -5.477334     0.849690    -1.587948     217.44
 H      -5.314641     1.159760    -0.699932      28.69
 C      -6.446813    -1.232228    -2.557087     114.18
 O      -6.345497    -2.697619    -2.558108     210.70
 H      -5.359312    -2.966098    -2.663444      28.05
 H      -6.284698    -0.828103    -3.525144      29.90
 H      -7.456037    -1.033815    -2.173810      29.07
55
name = lig-ACN-frame_96
 C       3.781971     3.038911    -0.290336      55.30
 H       3.106977     3.829507    -0.366478      26.23
 C       4.668807     1.177021     0.983094      57.81
 H       4.532749     0.462848     1.865357      22.39
 C       5.747380     1.055285     0.115034      27.32
 O       6.755666     0.044973     0.165257     193.91
 C       6.656583    -0.840142     1.398076     109.22
 H       6.869879    -0.254785     2.359585      25.24
 H       7.471736    -1.655696     1.304238      24.93
 H       5.726373    -1.338030     1.431750      27.40
 C       5.855145     1.936485    -1.009714      17.76
 O       6.874500     1.887147    -1.873007      78.73
 H       7.738785     1.393487    -1.600322      23.62
 C       4.853508     2.949405    -1.135153      69.33
 H       5.043641     3.685214    -1.959770      22.81
 C       3.647455     2.168260     0.809332      18.84
 C       2.485589     2.321175     1.841745      72.03
 H       2.829213     3.294168     2.483529      24.45
 O       2.438305     1.285828     2.850785     256.39
 H       2.279997     0.512853     2.339275      29.06
 C       1.058173     2.510970     1.160098      90.85
 H       1.158905     3.415465     0.437949      23.79
 C      -0.019678     2.851070     2.178061      98.41
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 O       0.166111     4.143526     2.890754     266.89
 H       0.140009     4.801822     2.237282      32.14
 H      -0.022851     1.955347     3.017916      24.43
 H      -1.123475     2.769875     1.861205      25.89
 C      -2.263524    -0.902228     0.071597      59.94
 H      -2.439215    -1.959403     0.424723      21.17
 C      -2.244492     0.854398    -1.658897      67.15
 H      -2.708738     1.217913    -2.551877      24.83
 C      -1.120114     1.415994    -1.127365      19.68
 O      -0.496512     2.573747    -1.525670     220.28
 C      -0.856696     3.054550    -2.833506     121.41
 H      -0.353327     3.909756    -3.054540      28.19
 H      -0.463674     2.430514    -3.645918      27.61
 H      -2.020496     2.999811    -2.829968      25.53
 C      -0.471619     0.812201     0.033090      22.12
 O       0.806049     1.212663     0.514673     189.04
 C      -1.155898    -0.245227     0.684951      57.15
 H      -0.752919    -0.674952     1.537360      21.91
 C      -2.789751    -0.378005    -1.157459      45.81
 C      -3.892992    -0.988668    -1.959866      63.30
 H      -3.733241    -0.631344    -3.026126      28.67
 O      -3.759418    -2.517561    -1.875371     236.84
 H      -2.868731    -2.704179    -2.232077      29.62
 C      -5.380553    -0.650377    -1.555388      96.67
 H      -5.618259    -1.032342    -0.549087      30.29
 O      -5.513591     0.795509    -1.708207     201.86
 H      -5.531580     1.146201    -0.782211      28.79
 C      -6.430621    -1.254482    -2.515153     116.59
 O      -6.344286    -2.705133    -2.570097     225.21
 H      -5.395800    -2.878828    -2.694030      30.81
 H      -6.254687    -0.808281    -3.510167      29.68
 H      -7.417371    -0.952806    -2.275941      30.72
55
name = lig-ACN-frame_97
 C       3.757731     3.064701    -0.299771      56.75
 H       3.052989     3.809381    -0.561767      22.91
 C       4.636264     1.184174     0.992784      64.24
 H       4.531349     0.484526     1.867566      23.16
 C       5.763628     1.011172     0.117945      28.29
 O       6.771975     0.091047     0.238135     200.13
 C       6.634845    -0.822430     1.365794     115.54
 H       6.633808    -0.178396     2.261247      26.23
 H       7.492631    -1.519009     1.343263      25.85
 H       5.673927    -1.368419     1.297319      26.35
 C       5.826273     1.935248    -0.934833      24.83
 O       6.877399     1.918821    -1.845249     165.41
 H       7.563560     1.385694    -1.477052      24.55
 C       4.919427     2.930993    -1.194481      51.60
 H       5.031751     3.502091    -2.132065      21.38
 C       3.618769     2.126289     0.782846       9.95
 C       2.431724     2.303127     1.854347      80.34
 H       2.537733     3.356498     2.434126      23.83
 O       2.392726     1.339162     2.866470     249.27
 H       2.228841     0.369852     2.544619      23.89
 C       1.082357     2.521031     1.166149      80.62
 H       1.163582     3.249105     0.249624      22.61
 C      -0.063665     2.906134     2.200686      94.04
 O       0.200794     4.168950     2.873612     268.75
 H       0.221507     4.878031     2.245894      31.25
 H      -0.003541     2.082390     3.092621      24.17
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 H      -1.023455     2.978292     1.549936      25.05
 C      -2.263036    -0.893115     0.042756      73.27
 H      -2.732361    -1.882751     0.373123      22.65
 C      -2.262011     0.843423    -1.652892      52.11
 H      -2.770099     1.386700    -2.478783      23.12
 C      -1.054622     1.399368    -1.075164      19.97
 O      -0.493557     2.586358    -1.569554     218.45
 C      -0.859424     3.049608    -2.884278     121.75
 H      -0.376148     3.921250    -2.847087      28.69
 H      -0.590656     2.267180    -3.554035      28.83
 H      -1.918844     3.400817    -3.116177      27.39
 C      -0.478661     0.813737     0.072084      41.12
 O       0.773328     1.222434     0.526187     195.84
 C      -1.127744    -0.299344     0.672834      50.63
 H      -0.664221    -0.659295     1.613599      19.55
 C      -2.813301    -0.317909    -1.107988      40.66
 C      -3.931267    -1.061838    -1.914621      61.94
 H      -3.911157    -0.776376    -2.992769      29.18
 O      -3.742255    -2.459639    -1.810551     220.56
 H      -2.725086    -2.691444    -2.204949      25.32
 C      -5.371746    -0.679485    -1.516284     100.27
 H      -5.496223    -0.844422    -0.443774      29.51
 O      -5.592208     0.743339    -1.782885     188.50
 H      -5.111346     1.246838    -0.977959      26.86
 C      -6.347842    -1.305903    -2.508760     116.77
 O      -6.371029    -2.711234    -2.585186     244.70
 H      -5.493453    -3.063266    -2.506591      31.93
 H      -6.093683    -0.790119    -3.484590      27.88
 H      -7.319273    -1.094079    -2.148915      28.84
55
name = lig-ACN-frame_98
 C       3.771075     3.035909    -0.340959      54.33
 H       2.984417     3.756815    -0.561052      21.53
 C       4.582976     1.133837     1.022739      60.44
 H       4.453453     0.456899     1.864240      22.88
 C       5.675219     1.047359     0.161675      19.10
 O       6.782655     0.125400     0.313310     214.24
 C       6.603950    -0.793629     1.362794     126.29
 H       6.571445    -0.412297     2.357166      28.08
 H       7.485733    -1.394485     1.278994      27.18
 H       5.717457    -1.492546     1.195833      26.80
 C       5.875151     1.948024    -0.934633      13.06
 O       6.923175     1.928741    -1.832654     132.89
 H       7.671796     1.337040    -1.638584      21.58
 C       4.828718     2.919596    -1.176016      71.30
 H       4.966558     3.618997    -1.980175      27.40
 C       3.586815     2.178848     0.773685      13.43
 C       2.444841     2.369084     1.746372      70.35
 H       2.679506     3.350582     2.349428      23.60
 O       2.360733     1.342931     2.945448     177.59
 H       2.079954     0.469590     2.358016      23.17
 C       1.013697     2.498742     1.166104      84.53
 H       1.024356     3.411356     0.412785      22.47
 C      -0.042230     2.980369     2.161439     101.77
 O       0.227959     4.196464     2.848525     237.44
 H       0.554308     4.958694     2.112139      25.79
 H      -0.375456     2.211309     2.995463      24.85
 H      -1.070382     3.056357     1.591704      24.73
 C      -2.243353    -0.882190     0.036594      73.28
 H      -2.835352    -1.549438     0.702282      25.59
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 C      -2.227729     0.882970    -1.620651      60.75
 H      -2.617570     1.346323    -2.581826      23.52
 C      -1.091083     1.412290    -1.065132      14.14
 O      -0.495679     2.588395    -1.568319     206.61
 C      -0.821761     3.073657    -2.953089     122.70
 H      -0.239139     3.854339    -3.293128      27.80
 H      -0.605322     2.380383    -3.714410      28.90
 H      -1.893025     3.255174    -2.956270      27.26
 C      -0.502419     0.824988     0.114958      41.12
 O       0.748637     1.189207     0.556341     196.78
 C      -1.092264    -0.346478     0.629116      40.27
 H      -0.675909    -0.910081     1.572061      20.16
 C      -2.846222    -0.285358    -1.111123      53.70
 C      -3.893259    -1.022183    -1.874632      63.25
 H      -3.745599    -0.723719    -2.916741      28.40
 O      -3.714372    -2.481736    -1.773475     177.10
 H      -2.662045    -2.638602    -2.054127      25.94
 C      -5.348144    -0.683890    -1.491994     101.75
 H      -5.586320    -0.961641    -0.470150      29.44
 O      -5.621660     0.723237    -1.799774     200.37
 H      -5.007631     1.256941    -1.210292      29.77
 C      -6.334487    -1.340577    -2.463890     107.87
 O      -6.381725    -2.807209    -2.593165     214.84
 H      -5.429779    -3.145464    -2.397141      30.39
 H      -6.061275    -0.927591    -3.505743      27.52
 H      -7.338448    -0.957073    -2.333516      28.58
55
name = lig-ACN-frame_99
 C       3.682289     2.988484    -0.317361      54.65
 H       2.980628     3.851802    -0.490693      23.57
 C       4.498852     1.152845     1.001079      92.40
 H       4.310024     0.484736     1.799189      25.32
 C       5.689916     1.089705     0.171881      15.58
 O       6.714422     0.234513     0.368667     165.76
 C       6.621920    -0.889650     1.414776     110.58
 H       6.473460    -0.392467     2.305444      27.56
 H       7.474459    -1.470118     1.422458      28.56
 H       5.671238    -1.517896     1.157041      25.40
 C       5.859777     1.975667    -0.959668      18.30
 O       6.939073     1.947741    -1.819492      33.51
 H       7.731788     1.428339    -1.374691      20.96
 C       4.863735     2.902582    -1.195207      53.27
 H       5.045020     3.626474    -1.959932      23.68
 C       3.581432     2.133995     0.797406      32.16
 C       2.412689     2.379733     1.829894      86.03
 H       2.644537     3.371353     2.333495      26.02
 O       2.352223     1.423717     2.879459     237.89
 H       2.083349     0.497760     2.575818      26.92
 C       0.993276     2.524411     1.149215      83.82
 H       1.026528     3.155825     0.174008      23.34
 C      -0.140633     3.004825     2.129305      97.84
 O       0.291254     4.260291     2.818831     214.62
 H       0.566083     4.978785     2.020551      25.94
 H      -0.195648     2.217156     2.935805      26.14
 H      -1.096067     3.244285     1.509530      25.32
 C      -2.290712    -0.837697     0.105981      42.28
 H      -2.705419    -1.804685     0.377330      20.23
 C      -2.238763     0.889736    -1.650866      55.90
 H      -2.581119     1.136859    -2.703929      24.06
 C      -1.105842     1.511021    -1.048496      11.41
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 O      -0.447384     2.619794    -1.601806     199.39
 C      -0.805727     3.006403    -2.964688     125.22
 H      -0.172761     3.883275    -2.962839      26.23
 H      -0.670900     2.157730    -3.565780      28.54
 H      -1.800028     3.341184    -3.069396      28.67
 C      -0.508521     0.830591     0.082661      28.31
 O       0.749625     1.181807     0.618747     179.29
 C      -1.078292    -0.362234     0.591052      54.57
 H      -0.469454    -0.854928     1.506723      23.25
 C      -2.784077    -0.271754    -1.079944      39.68
 C      -3.858765    -0.985662    -1.893798      76.65
 H      -3.783277    -0.707378    -2.925812      29.41
 O      -3.680145    -2.497665    -1.748407     246.18
 H      -2.792452    -2.730566    -1.997444      30.64
 C      -5.363165    -0.701743    -1.528219      94.43
 H      -5.457254    -0.886440    -0.459902      29.77
 O      -5.604208     0.721150    -1.781537     212.19
 H      -5.277666     1.167621    -1.009870      31.64
 C      -6.344698    -1.442348    -2.531531     103.94
 O      -6.374770    -2.881794    -2.539948     213.40
 H      -5.393599    -3.144760    -2.515976      29.84
 H      -5.981335    -1.008519    -3.549613      27.87
 H      -7.394850    -1.171775    -2.260116      27.81
55
name = lig-ACN-frame_100
 C       3.695476     2.986679    -0.341334      51.42
 H       2.940926     3.819170    -0.556352      24.12
 C       4.516158     1.137595     0.969461      49.89
 H       4.515042     0.400503     1.728850      23.87
 C       5.652602     1.122192     0.188899      18.90
 O       6.736357     0.204338     0.467173     209.23
 C       6.578499    -0.846357     1.410159     124.92
 H       6.500640    -0.583103     2.401010      28.19
 H       7.489594    -1.326248     1.246023      27.44
 H       5.703360    -1.620744     1.192770      25.33
 C       5.806407     1.973473    -0.920861      17.51
 O       6.916812     1.976401    -1.785256     157.06
 H       7.781205     1.499803    -1.455203      21.91
 C       4.803428     2.948302    -1.167696      57.64
 H       4.863262     3.583084    -2.041127      23.74
 C       3.450870     2.160331     0.787826       0.07
 C       2.349104     2.436543     1.835538      97.35
 H       2.475646     3.392021     2.357793      26.06
 O       2.351046     1.460355     2.868532     272.49
 H       2.157662     0.687431     2.422404      31.23
 C       0.986691     2.552125     1.106909      90.30
 H       1.137328     3.333293     0.297190      24.49
 C      -0.129543     3.089183     2.094759     108.03
 O       0.331886     4.286933     2.754513     289.89
 H       0.253854     5.015891     2.144967      30.92
 H      -0.343333     2.390401     2.907745      26.85
 H      -1.169012     3.184480     1.603716      26.25
 C      -2.291692    -0.854321     0.116567      48.66
 H      -2.614224    -1.814611     0.446857      20.55
 C      -2.197915     0.893100    -1.674448      60.31
 H      -2.597775     1.309111    -2.617562      23.16
 C      -1.102277     1.541713    -1.042696      20.16
 O      -0.419445     2.631206    -1.582872     231.91
 C      -0.774845     2.950823    -2.926095     131.87
 H      -0.176427     3.827847    -3.438153      25.76
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 H      -0.476935     2.217210    -3.638726      28.08
 H      -1.748498     3.188296    -3.061133      29.38
 C      -0.483471     0.868549     0.044731      28.17
 O       0.715653     1.161983     0.670986     188.11
 C      -1.068250    -0.296809     0.598530      53.05
 H      -0.441437    -0.858211     1.429828      20.82
 C      -2.795647    -0.259671    -1.092458      38.22
 C      -3.841483    -1.058005    -1.925628      93.43
 H      -3.672313    -0.827089    -2.944218      30.57
 O      -3.670052    -2.454585    -1.766941     294.93
 H      -2.852907    -2.622647    -2.118922      33.08
 C      -5.326828    -0.733925    -1.610032      93.79
 H      -5.580319    -1.075068    -0.601517      29.24
 O      -5.589549     0.719226    -1.733344     205.23
 H      -5.570397     1.118516    -0.784712      26.88
 C      -6.323177    -1.510665    -2.568126     104.02
 O      -6.324612    -2.952324    -2.457149     233.15
 H      -5.474750    -3.292676    -2.649343      33.33
 H      -6.176908    -1.177379    -3.673236      28.99
 H      -7.391147    -1.164999    -2.367049      28.22
55
name = lig-ACN-frame_101
 C       3.624628     3.050252    -0.326926      61.23
 H       2.803643     3.767080    -0.640234      23.28
 C       4.436164     1.187146     1.008268      80.29
 H       4.232190     0.592322     1.895692      25.95
 C       5.657187     1.075058     0.218267      13.16
 O       6.732551     0.248841     0.496662     190.59
 C       6.576801    -0.863530     1.425976     117.25
 H       6.509446    -0.488890     2.389380      27.69
 H       7.403062    -1.567920     1.382199      27.75
 H       5.599579    -1.434296     1.121842      25.37
 C       5.822746     2.004076    -0.905914      18.10
 O       6.854349     2.021405    -1.757214     137.86
 H       7.513593     1.400786    -1.477984      23.64
 C       4.768663     2.925017    -1.148324      53.76
 H       5.004763     3.635975    -2.008637      22.72
 C       3.483880     2.151519     0.757591      29.35
 C       2.338056     2.500657     1.752196      82.39
 H       2.605409     3.403040     2.187002      26.20
 O       2.333065     1.450598     2.896991     203.06
 H       2.137061     0.557781     2.490401      27.78
 C       0.934257     2.581478     1.128747      98.38
 H       0.923389     3.174429     0.207864      24.52
 C      -0.101686     3.124880     2.071423     113.29
 O       0.328743     4.342501     2.703642     306.52
 H       0.284131     5.044277     2.121823      32.09
 H      -0.263879     2.386362     2.810710      27.78
 H      -1.014070     3.368323     1.458653      26.22
 C      -2.204015    -0.833237     0.018645      70.91
 H      -2.754510    -1.508495     0.627283      27.85
 C      -2.187938     0.895117    -1.637791      68.50
 H      -2.660320     1.324241    -2.494681      24.81
 C      -1.049755     1.484074    -1.068843      14.75
 O      -0.397941     2.660205    -1.551312     196.47
 C      -0.737493     2.916345    -2.991252     112.16
 H      -0.230412     4.003848    -3.069944      24.40
 H      -0.554794     1.996735    -3.549704      26.92
 H      -1.749678     3.024936    -3.027930      28.22
 C      -0.490210     0.867880     0.092137      25.71
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 O       0.704219     1.233091     0.682423     195.97
 C      -1.119261    -0.254041     0.611955      43.95
 H      -0.651612    -0.706583     1.516092      20.92
 C      -2.824695    -0.284048    -1.121202      50.11
 C      -3.823190    -1.013334    -1.985162      77.45
 H      -3.632827    -0.713850    -2.976968      29.81
 O      -3.652616    -2.474159    -1.824610     210.94
 H      -2.659107    -2.782622    -2.055805      27.39
 C      -5.331164    -0.775870    -1.692022      98.30
 H      -5.478497    -1.190333    -0.678881      29.19
 O      -5.588740     0.670983    -1.683642     210.90
 H      -5.367634     1.049135    -0.691776      24.43
 C      -6.287144    -1.537123    -2.614590     105.49
 O      -6.292707    -3.013173    -2.363859     190.39
 H      -5.329270    -3.242269    -2.551909      30.80
 H      -5.967892    -1.331797    -3.705451      29.15
 H      -7.324186    -1.190454    -2.347926      28.45
55
name = lig-ACN-frame_102
 C       3.593711     3.069023    -0.372869      63.56
 H       2.866954     3.871334    -0.561369      24.83
 C       4.452511     1.216321     1.051633      59.17
 H       4.330392     0.572134     1.961306      24.81
 C       5.586885     1.093958     0.263654      10.22
 O       6.750339     0.287747     0.480336     163.79
 C       6.520218    -0.865278     1.461637     107.08
 H       6.560676    -0.455896     2.455292      26.36
 H       7.380118    -1.571093     1.254250      26.30
 H       5.484910    -1.338710     1.366275      24.93
 C       5.716168     1.991379    -0.800268      14.63
 O       6.841460     2.038557    -1.752779     115.18
 H       7.571778     1.431015    -1.531199      23.38
 C       4.768110     2.938381    -1.133286      49.86
 H       4.959688     3.673432    -2.004109      22.95
 C       3.463890     2.224350     0.726357       2.36
 C       2.392079     2.415879     1.776244      86.48
 H       2.549832     3.287404     2.276291      28.18
 O       2.304469     1.518660     2.862221     210.66
 H       1.935272     0.584730     2.442069      25.55
 C       0.976276     2.637191     1.071531      94.50
 H       1.039206     3.334267     0.274789      26.42
 C      -0.151400     3.162429     2.067021     106.06
 O       0.307200     4.418223     2.707964     253.50
 H       0.602318     5.035338     1.886684      27.26
 H      -0.355002     2.539184     2.874001      28.41
 H      -1.092785     3.292084     1.494431      26.79
 C      -2.262479    -0.853509    -0.003075      43.03
 H      -2.719535    -1.797624     0.345617      19.07
 C      -2.212290     0.921976    -1.642239      50.69
 H      -2.584677     1.319194    -2.542082      21.82
 C      -0.991412     1.444037    -1.078634      15.53
 O      -0.418375     2.631372    -1.571492     233.78
 C      -0.748735     2.914150    -2.934938     125.90
 H      -0.113600     3.867933    -3.383032      25.09
 H      -0.208531     2.233095    -3.647828      27.48
 H      -1.679668     3.116802    -3.196984      29.69
 C      -0.484062     0.895940     0.118798      30.52
 O       0.692378     1.272167     0.691786     200.74
 C      -1.134420    -0.241937     0.695638      48.84
 H      -0.893646    -0.544591     1.660630      24.30
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 C      -2.743207    -0.269460    -1.184982      35.44
 C      -3.804971    -1.010744    -2.063379      75.48
 H      -3.660373    -0.763841    -3.094911      25.69
 O      -3.635033    -2.499922    -1.922644     225.37
 H      -2.515788    -2.650131    -2.036312      24.06
 C      -5.296242    -0.801961    -1.663143      92.77
 H      -5.464852    -1.204030    -0.640216      28.95
 O      -5.606736     0.596770    -1.653650     260.72
 H      -5.103838     0.984145    -0.879738      28.63
 C      -6.249667    -1.609369    -2.652992     108.42
 O      -6.253159    -2.987506    -2.281462     218.00
 H      -5.287255    -3.329071    -2.162412      29.36
 H      -5.922780    -1.433668    -3.734889      29.63
 H      -7.306060    -1.274232    -2.640497      28.53
55
name = lig-ACN-frame_103
 C       3.602623     3.070811    -0.382298      60.00
 H       2.929958     3.863788    -0.612455      24.47
 C       4.455826     1.267815     1.085361      73.99
 H       4.296495     0.615065     2.000085      23.55
 C       5.628333     1.141256     0.280999      17.80
 O       6.676278     0.249473     0.510053     208.45
 C       6.485059    -0.760977     1.465408     124.71
 H       6.751235    -0.522203     2.519066      26.74
 H       7.244220    -1.597309     1.128397      25.71
 H       5.515167    -1.247445     1.339418      25.64
 C       5.759360     2.000584    -0.883747      16.00
 O       6.780889     2.020228    -1.687365     126.92
 H       7.636175     1.541205    -1.315071      20.70
 C       4.748317     3.002550    -1.136491      47.57
 H       4.996602     3.624971    -2.070742      23.19
 C       3.463256     2.202064     0.794895      25.60
 C       2.337368     2.525682     1.807312     105.14
 H       2.632594     3.392326     2.267944      27.89
 O       2.271189     1.504471     2.835143     244.75
 H       1.859703     0.671861     2.456865      26.19
 C       1.002924     2.683513     1.131938      92.17
 H       1.128065     3.272381     0.293475      25.89
 C      -0.137927     3.241928     2.073273     110.26
 O       0.257921     4.463677     2.693371     245.97
 H       0.502446     5.252721     1.920341      25.60
 H      -0.284219     2.504637     2.818540      27.76
 H      -1.081581     3.371540     1.561334      26.84
 C      -2.269988    -0.851253     0.025003      59.69
 H      -2.552051    -1.897725     0.358460      20.35
 C      -2.153559     0.951035    -1.710374      49.25
 H      -2.493471     1.406228    -2.620753      20.71
 C      -1.048017     1.461026    -1.087222      19.79
 O      -0.441284     2.590630    -1.593476     225.19
 C      -0.671392     2.972400    -2.987976     110.23
 H      -0.146160     4.049615    -2.920657      23.62
 H      -0.461985     2.061809    -3.655185      26.74
 H      -1.675281     3.054750    -3.102783      28.41
 C      -0.538424     0.852759     0.134813      23.79
 O       0.697141     1.288049     0.684518     180.75
 C      -1.239158    -0.228220     0.729951      40.35
 H      -0.833791    -0.633341     1.555087      21.22
 C      -2.714892    -0.331232    -1.250027      50.02
 C      -3.759953    -1.090720    -2.074176      79.00
 H      -3.671316    -0.739927    -3.124071      25.45
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 O      -3.587244    -2.485949    -2.023168     271.70
 H      -2.616229    -2.835711    -2.315581      25.57
 C      -5.262891    -0.839626    -1.656611      91.73
 H      -5.390825    -1.331771    -0.662366      29.59
 O      -5.647125     0.554917    -1.661592     273.59
 H      -5.227534     1.059534    -0.978530      30.44
 C      -6.164386    -1.625859    -2.646623     108.96
 O      -6.244530    -2.999111    -2.195333     242.57
 H      -5.306354    -3.191121    -2.087893      31.83
 H      -5.684331    -1.578073    -3.662709      30.81
 H      -7.160673    -1.199502    -2.626417      29.46
55
name = lig-ACN-frame_104
 C       3.609641     3.053355    -0.299125      65.80
 H       2.793017     3.650963    -0.568885      25.36
 C       4.485773     1.319459     1.103027      50.37
 H       4.372442     0.687062     2.016731      24.62
 C       5.603187     1.222430     0.285353      24.03
 O       6.610340     0.278879     0.485417     191.85
 C       6.463857    -0.785058     1.484209     117.53
 H       6.704397    -0.267016     2.479271      25.16
 H       7.193825    -1.668921     1.206350      25.38
 H       5.452803    -1.064576     1.613036      26.03
 C       5.702291     2.048408    -0.838763      14.92
 O       6.868326     1.981677    -1.720653     130.76
 H       7.610117     1.484800    -1.273743      21.45
 C       4.772127     2.977902    -1.159318      60.22
 H       4.894325     3.714234    -1.974369      22.77
 C       3.459940     2.273572     0.804321       1.14
 C       2.348180     2.590049     1.841583      75.29
 H       2.476708     3.474953     2.400709      25.95
 O       2.237337     1.483105     2.854357     236.05
 H       1.959429     0.784357     2.337607      30.98
 C       0.920895     2.711229     1.136184      93.31
 H       0.902548     3.307635     0.286231      26.09
 C      -0.114728     3.267527     2.064523     110.89
 O       0.211478     4.539997     2.713407     269.70
 H       0.094515     5.229710     1.978703      28.51
 H      -0.266383     2.630258     2.930243      26.79
 H      -0.975842     3.379774     1.440042      26.91
 C      -2.270490    -0.848678    -0.040902      63.68
 H      -2.873496    -1.686204     0.440989      23.67
 C      -2.167049     0.786535    -1.770636      49.12
 H      -2.614987     1.155772    -2.718091      21.29
 C      -1.106941     1.478371    -1.052834       9.35
 O      -0.385223     2.576828    -1.577886     201.27
 C      -0.683417     3.028376    -2.966402     119.39
 H      -0.022645     3.941006    -3.241369      25.71
 H      -0.195212     2.380611    -3.789443      25.54
 H      -1.629478     3.381581    -3.173763      28.31
 C      -0.574758     0.926261     0.146308      21.25
 O       0.660159     1.282518     0.677203     187.20
 C      -1.249500    -0.195944     0.716690      45.77
 H      -0.852533    -0.678717     1.541495      20.68
 C      -2.695920    -0.353485    -1.244692      43.12
 C      -3.706273    -1.056787    -2.079250      73.83
 H      -3.574818    -0.706219    -3.160381      25.77
 O      -3.551729    -2.560395    -2.108619     284.85
 H      -2.660542    -2.717651    -2.345709      30.91
 C      -5.190466    -0.859754    -1.659268      96.45
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 H      -5.352256    -1.202792    -0.607686      28.16
 O      -5.684991     0.522560    -1.704589     233.00
 H      -5.448517     0.914973    -0.766859      26.19
 C      -6.084582    -1.633218    -2.611702     110.20
 O      -6.258561    -3.025301    -2.124603     228.72
 H      -5.417019    -3.470662    -2.235643      32.40
 H      -5.688350    -1.627085    -3.637509      32.26
 H      -7.063743    -1.199478    -2.637655      30.32
55
name = lig-ACN-frame_105
 C       3.591326     3.109246    -0.326797      59.28
 H       2.887096     3.863451    -0.615823      23.87
 C       4.468805     1.391739     1.182092      82.65
 H       4.424882     0.774261     2.068807      24.25
 C       5.573280     1.230992     0.293333       8.05
 O       6.591917     0.279619     0.422232     171.66
 C       6.401059    -0.723396     1.547920     115.63
 H       6.891590    -0.386766     2.569393      25.42
 H       7.127253    -1.556591     1.167394      25.73
 H       5.473451    -1.183275     1.578455      26.82
 C       5.840164     2.071341    -0.869690       8.96
 O       6.893454     1.951414    -1.721958     149.88
 H       7.567253     1.357063    -1.452079      23.98
 C       4.706783     3.000692    -1.136733      46.10
 H       4.809490     3.597700    -1.998748      24.66
 C       3.482893     2.347486     0.922325      24.88
 C       2.297003     2.516619     1.857382     104.34
 H       2.521090     3.439705     2.407570      25.77
 O       2.215597     1.517828     2.840129     253.22
 H       2.020154     0.599941     2.429534      25.77
 C       0.947777     2.697125     1.099456      90.46
 H       1.061429     3.357845     0.260004      24.28
 C      -0.215730     3.281245     2.122462     100.76
 O       0.150157     4.604516     2.719500     290.54
 H       0.271907     5.200525     2.075298      33.62
 H      -0.406022     2.523650     2.953619      26.19
 H      -1.180787     3.351958     1.678508      26.99
 C      -2.286048    -0.856564     0.043762      64.47
 H      -2.800522    -1.710164     0.557109      19.94
 C      -2.080614     0.771281    -1.808742      60.06
 H      -2.313995     1.076986    -2.879409      19.56
 C      -1.127426     1.498860    -1.122940      16.87
 O      -0.366485     2.581614    -1.607155     217.09
 C      -0.636703     3.106461    -2.938309     116.19
 H       0.026472     3.993754    -2.878075      24.77
 H      -0.490759     2.203234    -3.623606      26.01
 H      -1.680144     3.237324    -3.064323      28.84
 C      -0.651201     0.978273     0.143653      36.77
 O       0.600643     1.341502     0.704303     180.13
 C      -1.212318    -0.197933     0.659857      43.68
 H      -0.938896    -0.449601     1.696408      22.15
 C      -2.699504    -0.410045    -1.252350      36.07
 C      -3.712304    -1.112340    -2.116371      70.73
 H      -3.556824    -0.724798    -3.187537      25.79
 O      -3.555651    -2.573006    -2.175195     298.87
 H      -2.701781    -2.818642    -2.097590      31.93
 C      -5.159111    -0.842458    -1.653581      87.28
 H      -5.205844    -1.320969    -0.638302      28.24
 O      -5.670708     0.501996    -1.733045     249.83
 H      -5.606251     1.100071    -0.860673      25.55
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 C      -6.075927    -1.738012    -2.568651     109.33
 O      -6.298800    -3.046200    -2.093590     231.20
 H      -5.491219    -3.588886    -2.423061      30.28
 H      -5.685410    -1.715299    -3.574116      32.96
 H      -7.038042    -1.260259    -2.566832      30.42
55
name = lig-ACN-frame_106
 C       3.612868     3.162353    -0.269093      56.13
 H       2.868627     3.938446    -0.540254      23.32
 C       4.527806     1.473179     1.201808      65.91
 H       4.363369     0.866476     2.054767      25.33
 C       5.619427     1.253578     0.281838      11.96
 O       6.548618     0.216835     0.455051     187.72
 C       6.429733    -0.675144     1.503825     124.25
 H       6.596283    -0.118421     2.572327      24.33
 H       7.110036    -1.553101     1.304833      25.80
 H       5.412723    -0.920360     1.620075      25.95
 C       5.771272     2.102812    -0.831641      21.21
 O       6.847967     1.956425    -1.743562     109.47
 H       7.583483     1.370102    -1.362993      21.04
 C       4.795491     2.990333    -1.135737      62.28
 H       4.854911     3.490705    -2.027921      24.66
 C       3.491529     2.430363     0.905936      -3.23
 C       2.244935     2.525977     1.851636      89.93
 H       2.292463     3.472254     2.465723      25.14
 O       2.201209     1.490942     2.884130     219.98
 H       1.961279     0.571942     2.352624      24.03
 C       0.852046     2.729406     1.182694      90.07
 H       1.017520     3.380377     0.283334      23.88
 C      -0.248399     3.317791     2.141870     107.96
 O       0.077697     4.585468     2.723432     267.10
 H       0.474520     5.082291     1.940934      29.59
 H      -0.171921     2.622250     3.069065      25.23
 H      -1.150946     3.350707     1.573443      26.86
 C      -2.304991    -0.838257     0.074287      53.96
 H      -2.632325    -1.760221     0.534714      19.65
 C      -2.023644     0.737061    -1.852859      66.51
 H      -2.216078     0.920874    -2.956808      18.93
 C      -1.034024     1.491824    -1.152884      18.71
 O      -0.369443     2.580651    -1.594800     237.41
 C      -0.641138     3.116475    -2.890597     131.07
 H      -0.071036     3.990804    -3.109907      27.16
 H      -0.310457     2.535681    -3.788691      27.64
 H      -1.651373     3.567096    -2.968661      27.90
 C      -0.661610     1.009484     0.107754      29.58
 O       0.507992     1.409355     0.718570     197.27
 C      -1.238145    -0.155212     0.687312      45.27
 H      -0.721002    -0.520968     1.675337      21.25
 C      -2.634913    -0.419847    -1.266285      38.76
 C      -3.687328    -1.145343    -2.148306      72.89
 H      -3.630195    -0.731146    -3.188328      27.02
 O      -3.609258    -2.581386    -2.198377     271.76
 H      -2.611044    -2.777507    -2.239047      26.38
 C      -5.186085    -0.921214    -1.654012      82.02
 H      -5.293748    -1.152094    -0.560530      28.20
 O      -5.632691     0.498154    -1.774481     272.01
 H      -5.226915     0.880058    -0.995709      29.77
 C      -6.141300    -1.745580    -2.544152     108.90
 O      -6.345857    -3.142697    -2.072863     237.54
 H      -5.519159    -3.619626    -2.269053      32.03
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 H      -5.730645    -1.798260    -3.523259      32.33
 H      -7.123529    -1.282357    -2.562858      29.82
55
name = lig-ACN-frame_107
 C       3.707382     3.247038    -0.265686      56.14
 H       2.846960     3.893224    -0.644492      22.36
 C       4.546238     1.542967     1.185115      77.48
 H       4.449086     0.900591     2.033282      24.94
 C       5.637282     1.269910     0.364328      21.78
 O       6.550656     0.227124     0.395488     195.24
 C       6.369532    -0.660743     1.577848     116.18
 H       6.761643    -0.035522     2.534505      24.16
 H       7.119292    -1.430139     1.469335      26.90
 H       5.432671    -1.212451     1.620243      25.96
 C       5.765994     2.042423    -0.820230       9.60
 O       6.749405     1.972520    -1.752005     127.69
 H       7.638182     1.553866    -1.383541      22.01
 C       4.756767     3.064712    -1.119874      49.31
 H       4.908495     3.662154    -1.973248      24.64
 C       3.495127     2.438649     0.892435      16.15
 C       2.227065     2.606857     1.915192      78.98
 H       2.505388     3.531020     2.573462      23.81
 O       2.188767     1.453364     2.888130     236.81
 H       1.866764     0.649097     2.420448      26.28
 C       0.792132     2.779616     1.220134      89.53
 H       0.727709     3.570763     0.386064      22.52
 C      -0.237752     3.272208     2.179045     103.28
 O       0.045294     4.581139     2.701496     219.59
 H       0.261330     5.382338     1.937122      26.28
 H      -0.582165     2.557535     3.050469      25.42
 H      -1.194173     3.289091     1.661927      26.42
 C      -2.266190    -0.809551    -0.010202      50.79
 H      -2.819897    -1.609073     0.404723      23.86
 C      -1.971728     0.658849    -1.895855      57.72
 H      -2.309785     0.980215    -2.902303      20.96
 C      -1.020799     1.406197    -1.188817       9.44
 O      -0.319052     2.620796    -1.597491     203.55
 C      -0.646566     3.211537    -2.927825     109.22
 H       0.005240     4.016623    -2.841031      25.85
 H      -0.418036     2.399088    -3.622235      26.93
 H      -1.792726     3.266593    -3.088993      26.51
 C      -0.651114     0.978494     0.124893      29.57
 O       0.471115     1.456007     0.763867     202.19
 C      -1.279741    -0.094987     0.721371      56.25
 H      -0.791062    -0.633086     1.683318      17.62
 C      -2.616032    -0.432865    -1.291956      46.87
 C      -3.728479    -1.119938    -2.108238      73.08
 H      -3.622241    -0.748048    -3.111371      28.02
 O      -3.604794    -2.623747    -2.187807     212.27
 H      -2.621543    -2.961124    -2.607133      24.39
 C      -5.208385    -0.932732    -1.670008      93.86
 H      -5.299020    -1.367160    -0.633808      28.17
 O      -5.556075     0.453700    -1.815640     286.13
 H      -5.173355     1.049263    -1.175258      29.44
 C      -6.225342    -1.813461    -2.527678     107.85
 O      -6.402530    -3.201331    -2.068731     246.88
 H      -5.501775    -3.513485    -2.052055      32.70
 H      -5.950811    -1.736901    -3.556535      31.94
 H      -7.225220    -1.348662    -2.444000      29.04
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name = lig-ACN-frame_108
 C       3.635928     3.303146    -0.241798      56.44
 H       2.912441     4.150649    -0.532664      22.74
 C       4.498739     1.515124     1.256359      41.11
 H       4.321862     0.965002     2.191082      22.36
 C       5.631294     1.318902     0.323734      11.86
 O       6.534738     0.207746     0.420129     174.53
 C       6.411948    -0.657062     1.618761     110.85
 H       6.428481    -0.123172     2.700921      23.96
 H       7.182328    -1.334935     1.447546      26.63
 H       5.357344    -1.070895     1.627422      24.72
 C       5.714055     2.125539    -0.859956      26.27
 O       6.715374     1.960685    -1.796308     153.72
 H       7.500159     1.495091    -1.467272      21.91
 C       4.795961     3.096832    -1.077006      57.17
 H       4.927854     3.688084    -2.001805      23.99
 C       3.468176     2.482935     0.927718      13.59
 C       2.288539     2.588642     1.928866      96.21
 H       2.428285     3.549706     2.644962      23.47
 O       2.178969     1.500845     2.838917     284.21
 H       1.875331     0.787674     2.344051      28.20
 C       0.847592     2.811981     1.267548      73.63
 H       1.045036     3.447064     0.292724      21.52
 C      -0.364525     3.277837     2.231296      97.58
 O       0.020067     4.606099     2.728715     229.39
 H      -0.018595     5.082634     1.787088      27.68
 H      -0.280989     2.581030     3.170695      24.41
 H      -1.247177     3.319966     1.575286      25.00
 C      -2.271335    -0.832333    -0.022802      54.75
 H      -2.779988    -1.595554     0.519989      22.70
 C      -1.926770     0.670913    -1.973958      52.12
 H      -2.232283     1.021949    -2.945829      20.43
 C      -0.957889     1.425558    -1.212414      11.25
 O      -0.344617     2.589322    -1.598900     223.43
 C      -0.619573     3.181747    -2.925084     123.08
 H      -0.287564     4.177366    -3.080864      26.34
 H      -0.264943     2.650359    -3.762930      28.01
 H      -1.780274     3.475475    -2.981169      25.60
 C      -0.623435     0.988040     0.130422      22.76
 O       0.516571     1.455469     0.821085     172.53
 C      -1.310928    -0.146207     0.699314      40.45
 H      -1.182377    -0.301378     1.880132      18.63
 C      -2.664065    -0.443121    -1.371632      47.81
 C      -3.752008    -1.214547    -2.133500      73.27
 H      -3.759079    -0.829440    -3.115853      28.13
 O      -3.602545    -2.640099    -2.157510     236.73
 H      -2.545977    -2.788734    -2.425238      24.64
 C      -5.213400    -0.981667    -1.666393      89.42
 H      -5.361338    -1.185997    -0.568128      27.64
 O      -5.523961     0.423725    -1.881846     260.52
 H      -5.257888     0.859514    -0.957535      25.31
 C      -6.312689    -1.835561    -2.505811     105.94
 O      -6.423392    -3.203116    -2.080914     228.70
 H      -5.480825    -3.604700    -2.041236      30.26
 H      -6.134998    -1.840940    -3.559538      31.21
 H      -7.290229    -1.363545    -2.230461      28.67
55
name = lig-ACN-frame_109
 C       3.605389     3.302130    -0.173531      59.25
 H       2.896620     4.156854    -0.338498      24.16
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 C       4.468150     1.532724     1.199942      80.53
 H       4.419904     0.834359     2.067233      23.94
 C       5.529328     1.281503     0.355410      14.48
 O       6.497774     0.269241     0.506052     210.20
 C       6.406230    -0.631553     1.594981     122.83
 H       6.598486     0.030832     2.548335      25.41
 H       7.167427    -1.348316     1.582111      27.92
 H       5.439084    -1.285287     1.589939      25.20
 C       5.719212     2.138683    -0.826687       3.43
 O       6.709605     1.935132    -1.855588     144.27
 H       7.355060     1.332832    -1.495524      23.77
 C       4.697828     3.174808    -1.050259      43.93
 H       4.721361     3.780566    -2.029437      23.07
 C       3.492741     2.513933     0.958745      39.25
 C       2.262824     2.639648     1.929751      94.58
 H       2.472633     3.634017     2.602924      23.70
 O       2.199768     1.526297     2.829180     237.66
 H       1.891190     0.673023     2.302039      23.66
 C       0.867291     2.781406     1.293677      86.30
 H       0.824508     3.584545     0.415768      21.80
 C      -0.252840     3.312471     2.220749     105.60
 O      -0.051371     4.617728     2.729622     295.37
 H       0.208713     5.227724     2.139604      34.70
 H      -0.453338     2.612652     3.129593      25.60
 H      -1.287274     3.196281     1.764198      25.90
 C      -2.345804    -0.837977    -0.076140      58.90
 H      -2.875769    -1.684270     0.369078      22.68
 C      -1.937082     0.677948    -1.963234      61.26
 H      -2.048278     0.897554    -2.992040      19.86
 C      -0.953656     1.385709    -1.207643      18.07
 O      -0.328395     2.590749    -1.650028     203.71
 C      -0.647761     3.179131    -2.920272     114.84
 H      -0.113170     4.102228    -2.714397      24.88
 H      -0.195028     2.593807    -3.680851      29.79
 H      -1.833381     3.027639    -3.103120      26.90
 C      -0.574012     0.975548     0.118614      31.34
 O       0.548582     1.388234     0.848228     183.90
 C      -1.314275    -0.090980     0.652185      46.25
 H      -1.144004    -0.398617     1.748923      20.29
 C      -2.622215    -0.439842    -1.395696      45.47
 C      -3.787382    -1.252659    -2.221155      52.35
 H      -3.759756    -0.977766    -3.236389      29.21
 O      -3.549255    -2.695533    -2.109218     288.25
 H      -2.641156    -2.920805    -2.028857      31.13
 C      -5.270203    -1.022498    -1.685624      90.11
 H      -5.318984    -1.308984    -0.609156      28.84
 O      -5.510604     0.412373    -1.925225     220.79
 H      -5.573761     0.976888    -1.076387      26.61
 C      -6.340012    -1.798887    -2.425931     110.88
 O      -6.435342    -3.229768    -2.072165     219.61
 H      -5.532938    -3.576812    -2.345627      29.79
 H      -6.140995    -1.567203    -3.471453      30.68
 H      -7.364679    -1.359851    -2.269435      28.82
55
name = lig-ACN-frame_110
 C       3.619520     3.359729    -0.128430      44.27
 H       2.776835     3.963833    -0.441735      22.45
 C       4.429504     1.491769     1.188025      59.17
 H       4.185737     0.819316     2.051162      22.06
 C       5.506368     1.306089     0.265466      20.48
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 O       6.477233     0.367280     0.517360     197.23
 C       6.400747    -0.608233     1.632993     110.34
 H       6.488461    -0.190740     2.699459      26.33
 H       7.264085    -1.151777     1.303239      26.24
 H       5.371431    -1.190794     1.652562      25.26
 C       5.660417     2.154321    -0.855892      19.79
 O       6.619472     1.920568    -1.806345     153.33
 H       7.461771     1.375042    -1.534713      20.83
 C       4.680295     3.131595    -1.036002      61.76
 H       4.790759     3.876267    -1.932523      25.87
 C       3.443364     2.514689     1.017629      21.02
 C       2.256587     2.664836     1.933252      95.19
 H       2.372192     3.625762     2.677156      23.13
 O       2.243787     1.538573     2.890558     237.84
 H       1.927732     0.700314     2.282189      21.95
 C       0.839916     2.747798     1.240431      78.89
 H       0.865576     3.306367     0.210936      21.13
 C      -0.194651     3.266423     2.234131     101.35
 O      -0.062897     4.636673     2.781573     269.08
 H       0.392722     5.102435     2.039702      31.22
 H      -0.216234     2.613228     3.136754      25.40
 H      -1.066100     3.292393     1.495810      24.69
 C      -2.344919    -0.753733    -0.109906      66.81
 H      -2.866003    -1.595330     0.417802      24.05
 C      -1.930319     0.658851    -1.942630      47.04
 H      -2.114015     0.944731    -2.956442      21.45
 C      -0.943129     1.403580    -1.216528      17.11
 O      -0.303313     2.520016    -1.633633     231.27
 C      -0.641803     3.130656    -2.931366     119.00
 H      -0.531242     4.281944    -3.026262      24.65
 H      -0.143313     2.665211    -3.762948      27.44
 H      -1.812520     3.236544    -3.205124      25.97
 C      -0.582557     0.926807     0.084289      24.62
 O       0.563268     1.343928     0.843985     189.37
 C      -1.371001    -0.124189     0.624345      43.36
 H      -0.916711    -0.596630     1.468365      17.99
 C      -2.686028    -0.467696    -1.468873      45.10
 C      -3.733928    -1.263220    -2.227031      65.43
 H      -3.694469    -0.975935    -3.251833      27.71
 O      -3.511820    -2.773616    -2.039445     274.94
 H      -2.617811    -2.826438    -2.195948      30.61
 C      -5.210843    -0.970838    -1.672313      88.78
 H      -5.190355    -1.209049    -0.591893      28.35
 O      -5.544013     0.402769    -1.963977     267.83
 H      -5.463871     0.866631    -1.159838      29.92
 C      -6.381985    -1.789174    -2.402101     103.64
 O      -6.423906    -3.211961    -2.102723     224.69
 H      -5.655242    -3.627739    -2.437115      32.81
 H      -6.285973    -1.740775    -3.500590      30.01
 H      -7.362935    -1.384324    -2.027853      28.92
55
name = lig-ACN-frame_111
 C       3.602747     3.366034    -0.119928      68.49
 H       2.970904     4.161086    -0.374450      25.75
 C       4.344576     1.474376     1.182045      66.22
 H       4.372099     0.754802     2.003016      22.76
 C       5.428029     1.335280     0.324110      22.44
 O       6.500362     0.430930     0.520579     229.45
 C       6.405522    -0.552521     1.597197     119.02
 H       6.539250    -0.056983     2.567857      27.15
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 H       7.161539    -1.386231     1.540038      26.16
 H       5.392769    -1.143972     1.461747      24.41
 C       5.552106     2.115937    -0.849192      23.89
 O       6.571108     1.925128    -1.799328     141.72
 H       7.347405     1.577340    -1.214066      22.38
 C       4.672591     3.155549    -1.039718      56.17
 H       4.808281     3.801059    -1.992721      21.70
 C       3.447577     2.521644     0.976282      32.65
 C       2.249449     2.593344     1.972816     102.96
 H       2.298008     3.661594     2.534900      21.55
 O       2.265377     1.572222     2.956701     279.72
 H       1.960402     0.753616     2.575077      26.63
 C       0.909211     2.690719     1.178938      75.38
 H       1.015886     3.414986     0.320991      21.57
 C      -0.257368     3.240530     2.208617      96.33
 O       0.012440     4.577923     2.792887     216.48
 H       0.292763     5.315157     1.980840      26.41
 H      -0.260418     2.516549     3.000977      25.68
 H      -1.376138     3.173167     1.953774      24.77
 C      -2.416741    -0.777495    -0.118062      59.85
 H      -2.947858    -1.636821     0.396026      19.97
 C      -1.949545     0.660673    -2.023049      47.10
 H      -2.211879     1.087328    -2.996489      18.70
 C      -0.989278     1.351775    -1.210559      10.75
 O      -0.264035     2.526457    -1.678717     202.95
 C      -0.669272     3.106984    -2.980503      89.98
 H      -0.280186     4.196955    -2.737088      22.73
 H      -0.081919     2.653969    -3.828357      25.97
 H      -1.812974     2.774994    -3.019886      24.25
 C      -0.585871     0.912633     0.096419      28.87
 O       0.527866     1.292058     0.813130     196.76
 C      -1.297816    -0.191266     0.608455      36.76
 H      -1.187151    -0.510511     1.560450      22.76
 C      -2.667304    -0.408213    -1.434740      46.54
 C      -3.710102    -1.328842    -2.192905      85.26
 H      -3.695368    -1.157505    -3.265016      27.53
 O      -3.476427    -2.742881    -1.988664     237.75
 H      -2.597295    -3.096507    -2.451553      25.43
 C      -5.148699    -0.976669    -1.733714      92.25
 H      -5.225213    -1.088892    -0.653372      28.30
 O      -5.589756     0.416792    -1.985922     255.12
 H      -5.129605     1.004225    -1.334469      28.86
 C      -6.337939    -1.804626    -2.373099     111.81
 O      -6.427578    -3.206243    -2.118491     219.68
 H      -5.497620    -3.545675    -2.353210      30.07
 H      -6.416836    -1.429667    -3.439964      29.16
 H      -7.247661    -1.337630    -1.963691      28.18
55
name = lig-ACN-frame_112
 C       3.579846     3.392311    -0.153963      64.32
 H       2.982184     4.240087    -0.150578      26.33
 C       4.327543     1.441487     1.204394      63.14
 H       4.062644     0.941318     2.109288      22.98
 C       5.452364     1.290460     0.361686      20.88
 O       6.538215     0.465413     0.512115     242.24
 C       6.367736    -0.487894     1.543609     119.07
 H       6.469324    -0.022325     2.502452      26.98
 H       7.316156    -1.135251     1.297940      24.94
 H       5.338937    -1.012282     1.588341      24.81
 C       5.503642     2.079266    -0.849479      18.31
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 O       6.552555     1.919479    -1.757001     210.08
 H       7.350363     1.470951    -1.502944      25.49
 C       4.609159     3.210340    -1.060046      50.17
 H       4.705350     3.847556    -1.973325      22.35
 C       3.387103     2.485337     0.968215      27.78
 C       2.225003     2.581229     1.931094      94.43
 H       2.357960     3.569991     2.556673      21.99
 O       2.268637     1.595022     3.050714     264.04
 H       1.982119     0.784274     2.678425      27.99
 C       0.803746     2.657328     1.237642      83.59
 H       0.918244     3.226710     0.327456      22.42
 C      -0.246214     3.203321     2.202710     107.35
 O       0.098114     4.477612     2.760658     256.84
 H       0.059046     5.184343     1.967245      28.14
 H      -0.256307     2.621411     3.064268      26.43
 H      -1.188016     3.225700     1.526095      24.48
 C      -2.377305    -0.813655    -0.076646      55.94
 H      -3.024118    -1.634269     0.314692      21.14
 C      -1.975412     0.696155    -2.019370      72.30
 H      -2.147085     0.834224    -3.123361      20.30
 C      -0.950583     1.379026    -1.277221      11.83
 O      -0.251363     2.459800    -1.713954     229.16
 C      -0.670810     3.057842    -2.940031     113.10
 H      -0.474698     4.253709    -3.024873      24.34
 H      -0.150209     2.531410    -3.871705      25.71
 H      -1.785420     3.195946    -3.249275      26.15
 C      -0.636149     0.859703     0.053686      27.06
 O       0.533878     1.288906     0.779681     187.37
 C      -1.341899    -0.253545     0.635452      22.35
 H      -1.107047    -0.440728     1.589803      20.82
 C      -2.670262    -0.415095    -1.429167      36.40
 C      -3.682065    -1.279760    -2.217944      66.34
 H      -3.584779    -0.996863    -3.297950      27.42
 O      -3.478259    -2.725236    -1.926637     198.32
 H      -2.428731    -2.872872    -2.347551      23.29
 C      -5.184538    -0.993583    -1.718411      93.39
 H      -5.158305    -1.276823    -0.672261      29.71
 O      -5.576330     0.394009    -2.050077     215.09
 H      -5.099479     1.027994    -1.332075      26.21
 C      -6.306663    -1.726095    -2.367298     112.05
 O      -6.386173    -3.207822    -2.147401     187.25
 H      -5.443271    -3.594640    -2.114874      30.51
 H      -6.244049    -1.668712    -3.498840      28.57
 H      -7.231765    -1.322442    -1.998232      29.25
55
name = lig-ACN-frame_113
 C       3.520689     3.378240    -0.090919      59.63
 H       2.773956     4.100239    -0.421172      20.88
 C       4.328473     1.447003     1.210468      63.98
 H       4.300914     0.758815     2.006382      20.66
 C       5.414727     1.342175     0.298756      12.27
 O       6.539246     0.500594     0.489520     236.16
 C       6.406615    -0.475087     1.566830     117.55
 H       6.499223    -0.072809     2.526229      28.38
 H       7.189926    -1.362847     1.437001      25.08
 H       5.448919    -1.028856     1.380517      26.07
 C       5.511006     2.136715    -0.847473      14.53
 O       6.526890     1.925269    -1.761404     199.92
 H       7.100056     1.303684    -1.293608      22.51
 C       4.598955     3.142212    -1.051430      65.61
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 H       4.822733     3.853273    -1.820991      27.81
 C       3.349117     2.424523     0.919492      32.66
 C       2.178598     2.605721     1.950936      97.10
 H       2.251924     3.635443     2.403990      24.27
 O       2.242681     1.632284     3.080900     246.26
 H       1.937035     0.692920     2.675554      22.83
 C       0.794251     2.601140     1.255240      88.57
 H       0.775744     3.337219     0.510187      22.51
 C      -0.276739     3.129035     2.203358     109.39
 O       0.153749     4.428663     2.715147     316.09
 H       0.281180     4.977686     2.025774      35.70
 H      -0.630851     2.458221     2.908783      27.90
 H      -1.258288     3.351298     1.633541      24.88
 C      -2.378053    -0.870447    -0.098806      71.10
 H      -2.849912    -1.685860     0.441455      23.60
 C      -1.985324     0.651875    -1.968219      39.43
 H      -2.092138     0.924362    -3.056580      19.79
 C      -0.971653     1.302465    -1.270833      14.39
 O      -0.246934     2.429368    -1.745453     206.31
 C      -0.675225     3.086374    -3.004919      84.53
 H      -0.073437     4.103775    -2.869153      22.26
 H      -0.217052     2.454827    -3.956534      24.23
 H      -1.829992     2.965558    -2.947847      25.44
 C      -0.624110     0.851682     0.030358      27.83
 O       0.501615     1.249731     0.740132     218.25
 C      -1.361295    -0.173012     0.655697      52.38
 H      -0.997506    -0.676177     1.508781      16.90
 C      -2.666294    -0.437506    -1.409885      42.64
 C      -3.714601    -1.200931    -2.179183      60.01
 H      -3.729283    -1.036219    -3.312297      27.05
 O      -3.460955    -2.667408    -1.921381     219.02
 H      -2.454974    -2.871545    -1.874415      27.72
 C      -5.154768    -0.953890    -1.700587      92.85
 H      -5.261240    -0.984483    -0.629466      29.21
 O      -5.512877     0.360264    -2.081463     235.53
 H      -5.427215     0.964047    -1.270089      27.18
 C      -6.301685    -1.818178    -2.474153     110.00
 O      -6.335435    -3.181263    -2.137145     239.78
 H      -5.413611    -3.394729    -2.101201      31.61
 H      -6.088206    -1.510255    -3.578228      29.40
 H      -7.259941    -1.379019    -2.273237      29.59
55
name = lig-ACN-frame_114
 C       3.482503     3.253468    -0.143868      49.32
 H       2.657579     4.003720    -0.349368      22.12
 C       4.342254     1.458498     1.147093      63.90
 H       4.262905     0.813778     2.003059      23.37
 C       5.422883     1.348154     0.295465      30.63
 O       6.520122     0.507887     0.498698     232.88
 C       6.423953    -0.513645     1.551885     123.07
 H       6.542767    -0.016180     2.467409      28.77
 H       7.393410    -1.149404     1.371145      26.03
 H       5.476186    -1.054835     1.568291      26.91
 C       5.548449     2.177312    -0.853258      19.22
 O       6.512832     1.933095    -1.772827      91.09
 H       7.355739     1.396907    -1.445624      20.93
 C       4.532571     3.199712    -1.013964      60.08
 H       4.587709     3.813964    -1.853546      24.90
 C       3.291116     2.399863     0.987657      40.83
 C       2.151392     2.553959     1.964213     113.55
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 H       2.258359     3.512300     2.438040      22.55
 O       2.193656     1.686938     3.053627     273.42
 H       1.941079     0.720909     2.681984      23.16
 C       0.769495     2.564523     1.221497      87.83
 H       0.912178     3.133185     0.385172      22.32
 C      -0.412312     3.111178     2.185336     103.83
 O       0.173230     4.368458     2.725363     293.25
 H       0.536695     4.871130     1.991369      31.78
 H      -0.433746     2.570886     3.088411      25.55
 H      -1.363120     3.223097     1.578054      24.99
 C      -2.347466    -0.863564    -0.068988      59.66
 H      -2.821114    -1.739348     0.284997      24.73
 C      -1.977880     0.601497    -1.976623      65.80
 H      -2.382968     0.979958    -2.938445      21.60
 C      -0.956466     1.305747    -1.246142      17.39
 O      -0.232264     2.368796    -1.773939     216.05
 C      -0.664729     3.049093    -2.976232     111.56
 H      -0.166143     4.110954    -3.049478      23.71
 H      -0.469094     2.460870    -4.101778      23.44
 H      -1.696616     3.427143    -3.060629      26.89
 C      -0.624381     0.879319     0.073813      35.62
 O       0.546568     1.224692     0.728732     208.97
 C      -1.370303    -0.183203     0.607906      26.63
 H      -1.064731    -0.419306     1.676848      17.98
 C      -2.696691    -0.460476    -1.367696      52.89
 C      -3.740730    -1.260535    -2.110619      71.57
 H      -3.644685    -0.905929    -3.219536      29.37
 O      -3.475822    -2.624222    -1.933172     296.75
 H      -2.599575    -2.671700    -2.005026      35.16
 C      -5.235199    -0.953017    -1.716592      98.43
 H      -5.327689    -1.232882    -0.666044      30.39
 O      -5.484350     0.437631    -2.119715     253.24
 H      -5.404042     0.998881    -1.373870      29.74
 C      -6.210897    -1.798341    -2.544001     107.89
 O      -6.264016    -3.205410    -2.122269     195.40
 H      -5.384074    -3.627204    -2.201581      30.39
 H      -5.982569    -1.832873    -3.682318      28.97
 H      -7.217879    -1.447752    -2.364717      30.42
55
name = lig-ACN-frame_115
 C       3.342699     3.176457    -0.177412      73.85
 H       2.594945     4.052493    -0.301694      23.85
 C       4.314812     1.422916     1.192307      64.21
 H       4.230775     0.801540     2.105229      23.43
 C       5.459776     1.363933     0.317300      11.24
 O       6.491695     0.458003     0.501546     240.91
 C       6.473835    -0.485778     1.545149     125.76
 H       6.563838    -0.121816     2.545447      27.29
 H       7.361953    -1.141654     1.269467      25.36
 H       5.660450    -1.163990     1.472197      27.87
 C       5.540610     2.215774    -0.835833      20.91
 O       6.531770     1.981526    -1.842298     175.73
 H       7.398385     1.687922    -1.350774      23.58
 C       4.547294     3.201718    -1.035937      49.29
 H       4.502716     3.794113    -1.905799      23.14
 C       3.317833     2.382408     0.970268      25.54
 C       2.110380     2.575969     1.930100      89.72
 H       2.223336     3.505466     2.362316      21.83
 O       2.130863     1.634479     3.078247     302.23
 H       1.967882     0.777114     2.755441      27.82
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 C       0.695651     2.577592     1.197792     103.45
 H       0.653856     3.257512     0.441381      21.82
 C      -0.337500     3.120622     2.157726     106.76
 O       0.107217     4.319301     2.735883     279.36
 H       0.360217     5.071020     1.950736      27.26
 H      -0.576797     2.350478     2.886322      25.58
 H      -1.350851     3.281186     1.703136      24.78
 C      -2.355452    -0.884594    -0.029041      60.93
 H      -2.857946    -1.648764     0.505477      22.72
 C      -2.008225     0.626669    -1.941922      46.32
 H      -2.256712     0.927963    -2.949423      20.66
 C      -0.984177     1.311085    -1.288509      19.09
 O      -0.212379     2.333372    -1.809403     225.85
 C      -0.675004     3.068187    -2.979217     106.99
 H       0.107427     3.851953    -3.053867      23.83
 H      -0.447318     2.170836    -3.868892      23.43
 H      -1.740201     3.251387    -2.874036      28.25
 C      -0.632643     0.870591     0.055443      58.03
 O       0.604398     1.187382     0.745223     183.40
 C      -1.318616    -0.197804     0.678729      33.35
 H      -1.169360    -0.488432     1.833001      16.45
 C      -2.710200    -0.442619    -1.336186      47.21
 C      -3.776823    -1.213134    -2.096877      40.07
 H      -3.725292    -0.991410    -3.239882      28.07
 O      -3.484710    -2.689517    -1.952451     184.70
 H      -2.638582    -2.922247    -2.436865      26.23
 C      -5.244978    -0.936342    -1.783395      98.16
 H      -5.606386    -1.009726    -0.748209      29.33
 O      -5.504979     0.492021    -2.139839     226.87
 H      -5.036251     0.965197    -1.416788      27.63
 C      -6.155707    -1.860124    -2.612280     108.32
 O      -6.208137    -3.244641    -2.096404     169.56
 H      -5.281132    -3.587288    -2.401054      29.74
 H      -5.768691    -1.750582    -3.704705      29.22
 H      -7.169962    -1.432016    -2.607488      29.57
55
name = lig-ACN-frame_116
 C       3.373959     3.205398    -0.228717      48.84
 H       2.478372     3.855770    -0.560136      20.63
 C       4.340756     1.418589     1.238875      55.87
 H       4.352630     0.672100     2.086583      21.24
 C       5.428542     1.384148     0.358800      20.18
 O       6.493722     0.455305     0.449809     211.52
 C       6.524856    -0.553190     1.555472     125.15
 H       6.566846     0.007839     2.497873      28.30
 H       7.406116    -1.144167     1.477009      27.71
 H       5.631704    -1.101944     1.494279      27.83
 C       5.533531     2.213192    -0.818544      16.59
 O       6.509718     2.088506    -1.831957     132.01
 H       7.320294     1.655069    -1.512111      23.60
 C       4.469315     3.120894    -1.047904      62.08
 H       4.727027     3.814368    -1.848905      27.34
 C       3.259303     2.349045     0.922431      28.76
 C       2.104290     2.583823     1.921227     109.71
 H       2.196130     3.477876     2.396051      26.24
 O       2.062946     1.591771     3.068101     284.79
 H       1.863619     0.737057     2.685584      26.03
 C       0.774455     2.598776     1.163240      82.18
 H       0.842795     3.163242     0.301104      22.67
 C      -0.367363     3.057880     2.141786     102.08
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 O       0.024774     4.334987     2.805898     252.39
 H       0.066089     5.095347     1.980628      27.26
 H      -0.544606     2.405389     3.043385      23.98
 H      -1.218582     3.222193     1.482500      24.90
 C      -2.373029    -0.842707     0.040413      48.12
 H      -2.964122    -1.631469     0.496885      24.56
 C      -2.073224     0.665528    -1.926629      60.41
 H      -2.188805     0.798114    -2.971392      19.37
 C      -0.964153     1.282594    -1.217833       9.36
 O      -0.172769     2.313028    -1.793728     213.49
 C      -0.657853     2.986367    -2.982068     125.68
 H      -0.101713     3.884409    -3.147435      26.87
 H      -0.784267     2.476643    -4.047943      26.43
 H      -1.590785     3.424303    -2.836969      29.76
 C      -0.565583     0.787447     0.067078      24.17
 O       0.545412     1.205647     0.712939     208.87
 C      -1.338132    -0.197668     0.702559      56.19
 H      -0.818264    -0.617071     1.717331      16.57
 C      -2.716182    -0.445415    -1.278148      36.46
 C      -3.738482    -1.237772    -2.118180      45.35
 H      -3.640754    -0.869537    -3.212767      26.93
 O      -3.522968    -2.747431    -1.989382     166.94
 H      -2.558956    -2.862398    -2.577207      23.42
 C      -5.276183    -0.880748    -1.798444      95.81
 H      -5.349214    -1.102459    -0.698981      29.99
 O      -5.531387     0.454593    -2.168880     211.91
 H      -5.096988     1.160681    -1.495635      25.47
 C      -6.146352    -1.916907    -2.696522     106.27
 O      -6.152875    -3.229642    -2.124410     198.85
 H      -5.241918    -3.571860    -2.117641      30.41
 H      -5.714974    -2.017123    -3.754611      28.95
 H      -7.237026    -1.632391    -2.762826      29.24
55
name = lig-ACN-frame_117
 C       3.387686     3.173680    -0.203457      47.23
 H       2.565440     3.892062    -0.492672      20.69
 C       4.325660     1.497409     1.204981      63.33
 H       4.094815     0.906716     2.145971      19.85
 C       5.471916     1.328481     0.340107      33.11
 O       6.529605     0.423379     0.427003     224.17
 C       6.508383    -0.517865     1.541695     130.15
 H       6.563867    -0.004015     2.546260      28.32
 H       7.356114    -1.023330     1.338947      28.57
 H       5.716847    -1.210563     1.574904      29.39
 C       5.500533     2.173800    -0.798705      33.10
 O       6.467008     2.211860    -1.748572     146.46
 H       7.153446     1.584836    -1.536500      25.09
 C       4.490380     3.081032    -1.094222      54.27
 H       4.458949     3.753532    -1.993734      26.36
 C       3.260228     2.324343     0.932041      44.67
 C       2.135213     2.496840     1.951438     122.16
 H       2.291441     3.415095     2.399774      28.13
 O       2.010496     1.593121     2.990204     311.80
 H       1.787499     0.618706     2.589217      21.45
 C       0.787738     2.596984     1.182863      85.91
 H       0.889296     3.322284     0.382718      21.54
 C      -0.392030     3.092980     2.100215     101.24
 O      -0.103821     4.329061     2.845090     315.55
 H       0.200670     5.027820     2.222245      31.91
 H      -0.429995     2.227943     2.883036      24.51
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 H      -1.371206     3.064630     1.657981      26.77
 C      -2.447941    -0.801645     0.073392      56.18
 H      -2.877083    -1.718255     0.552967      22.00
 C      -2.040246     0.637979    -1.834631      52.55
 H      -2.344674     0.962814    -2.800077      21.21
 C      -0.973651     1.267932    -1.228947      19.19
 O      -0.149163     2.265190    -1.768819     230.47
 C      -0.686233     3.002022    -2.938748     125.18
 H       0.043256     3.697190    -3.117217      26.67
 H      -0.590808     2.156374    -3.693108      26.59
 H      -1.677851     3.252244    -2.830247      30.01
 C      -0.575771     0.777803     0.059982      34.43
 O       0.566399     1.235645     0.709772     200.11
 C      -1.311471    -0.244426     0.705372      72.06
 H      -0.974497    -0.634652     1.779347      19.53
 C      -2.751089    -0.444750    -1.267970      44.67
 C      -3.713495    -1.263955    -2.115584      80.35
 H      -3.478788    -1.028944    -3.200081      28.06
 O      -3.541176    -2.706659    -2.061171     239.19
 H      -2.489814    -2.922310    -2.143872      25.53
 C      -5.233785    -0.988976    -1.859298      88.84
 H      -5.622069    -1.169230    -0.805825      29.38
 O      -5.585865     0.424115    -2.212119     196.34
 H      -5.374346     0.987772    -1.372966      26.68
 C      -6.108044    -1.911135    -2.717974     119.24
 O      -6.133365    -3.248832    -2.136092     192.61
 H      -5.199901    -3.347757    -1.924789      30.05
 H      -5.659883    -1.870417    -3.754346      29.15
 H      -7.178632    -1.516588    -2.787192      28.62
55
name = lig-ACN-frame_118
 C       3.325704     3.169104    -0.191019      78.08
 H       2.626078     3.982597    -0.320066      23.77
 C       4.374050     1.441141     1.211071      63.67
 H       4.486426     0.828363     2.131932      23.07
 C       5.439789     1.313997     0.306775      24.24
 O       6.519462     0.405400     0.435234     225.17
 C       6.525214    -0.494600     1.529935     130.79
 H       6.573425     0.066238     2.533916      27.40
 H       7.296301    -1.134755     1.523076      28.57
 H       5.604305    -1.015693     1.416177      26.98
 C       5.454118     2.171095    -0.817003      29.36
 O       6.531689     2.269242    -1.708235     133.83
 H       7.354029     1.723757    -1.374720      24.93
 C       4.415215     3.080171    -1.057252      56.99
 H       4.550085     3.564581    -2.074345      23.74
 C       3.321940     2.371255     0.926615      33.96
 C       2.106260     2.539008     1.907599     110.60
 H       2.287770     3.415270     2.481826      24.12
 O       2.002110     1.513655     2.975038     267.00
 H       1.806099     0.549274     2.549455      19.92
 C       0.725685     2.675411     1.190441      84.72
 H       0.765822     3.324935     0.253938      20.20
 C      -0.389970     3.073260     2.135860     108.04
 O      -0.238438     4.303328     2.847193     346.62
 H       0.236083     4.853243     2.346177      34.86
 H      -0.604754     2.292531     2.987903      23.45
 H      -1.230426     3.202429     1.486048      25.59
 C      -2.454737    -0.843211     0.085204      57.57
 H      -3.077676    -1.619317     0.635344      21.32
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 C      -2.062261     0.615235    -1.840438      73.65
 H      -2.423838     0.995474    -2.798425      21.24
 C      -0.939945     1.235340    -1.175887       8.81
 O      -0.179488     2.257638    -1.719796     225.85
 C      -0.655035     2.900588    -2.906284     135.11
 H      -0.176548     3.783708    -2.994125      28.01
 H      -0.733691     2.376806    -3.877236      27.29
 H      -1.643384     3.253261    -2.731595      28.40
 C      -0.588230     0.809326     0.119968      44.44
 O       0.611188     1.241129     0.704969     192.22
 C      -1.316340    -0.259359     0.693152      40.29
 H      -1.108092    -0.518104     1.763439      21.13
 C      -2.780948    -0.451529    -1.211949      37.52
 C      -3.726717    -1.223757    -2.149538      69.93
 H      -3.606462    -0.783808    -3.162790      29.12
 O      -3.497480    -2.685004    -2.079462     277.37
 H      -2.625508    -2.797404    -1.958686      33.08
 C      -5.225670    -1.016482    -1.918658      98.01
 H      -5.369328    -1.241371    -0.797559      28.75
 O      -5.630128     0.344995    -2.218892     232.97
 H      -5.427453     0.867639    -1.474488      30.69
 C      -6.077690    -1.918342    -2.764250     116.50
 O      -6.142532    -3.249360    -2.153601     168.48
 H      -5.188763    -3.597872    -2.048585      28.54
 H      -5.780171    -1.979072    -3.825090      29.79
 H      -7.135940    -1.481115    -2.677210      28.44
55
name = lig-ACN-frame_119
 C       3.303717     3.209202    -0.183786      34.14
 H       2.464723     3.825880    -0.408304      21.72
 C       4.387330     1.393006     1.226002      62.78
 H       4.262238     0.813969     2.133507      23.44
 C       5.427401     1.298732     0.267146      17.79
 O       6.526008     0.458121     0.395669     189.62
 C       6.454798    -0.506617     1.577037     114.35
 H       6.567743     0.122614     2.529544      26.67
 H       7.301050    -1.087934     1.356167      27.37
 H       5.553834    -1.099123     1.716135      27.44
 C       5.494163     2.189388    -0.872184      17.33
 O       6.598097     2.288185    -1.671183     117.49
 H       7.460986     1.836108    -1.263394      23.05
 C       4.382111     3.071389    -1.094715      54.63
 H       4.461753     3.905175    -1.847750      26.65
 C       3.311153     2.359428     1.043165      14.97
 C       2.117120     2.572299     1.950371     103.20
 H       2.185595     3.514170     2.526633      24.59
 O       2.027055     1.487654     2.949161     303.43
 H       1.911729     0.636544     2.523031      25.08
 C       0.759420     2.641098     1.210521      77.24
 H       0.678360     3.406315     0.305958      19.91
 C      -0.508060     3.034967     2.140646      93.21
 O      -0.323077     4.308381     2.866704     296.20
 H       0.059184     4.999084     2.183986      29.47
 H      -0.721222     2.187203     2.906770      24.88
 H      -1.355337     3.048498     1.494356      26.40
 C      -2.422930    -0.882208     0.089223      58.35
 H      -3.046793    -1.606398     0.687086      24.27
 C      -2.062741     0.622666    -1.809487      57.77
 H      -2.168783     0.792818    -2.912472      21.64
 C      -0.991808     1.191537    -1.160398      10.01
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 O      -0.195001     2.236977    -1.692185     209.19
 C      -0.705263     2.910397    -2.880479     123.57
 H      -0.057208     3.707067    -3.048364      26.91
 H      -0.566990     2.227491    -3.763708      26.66
 H      -1.755643     3.079348    -2.799788      28.16
 C      -0.574227     0.782308     0.165369      21.78
 O       0.592997     1.264054     0.706214     206.32
 C      -1.358027    -0.231163     0.783026      47.67
 H      -0.992284    -0.575985     1.695339      18.33
 C      -2.790021    -0.434385    -1.244484      44.73
 C      -3.723455    -1.163075    -2.191743      63.55
 H      -3.457658    -0.906546    -3.207352      29.95
 O      -3.433997    -2.636022    -2.078455     220.75
 H      -2.505160    -2.691418    -2.334671      29.18
 C      -5.212943    -1.001099    -1.898217      92.81
 H      -5.492143    -1.344256    -0.827748      29.73
 O      -5.682482     0.298185    -2.201461     211.51
 H      -5.175073     0.987555    -1.669527      29.34
 C      -6.120748    -1.998401    -2.782130     107.42
 O      -6.174488    -3.271357    -2.176918     182.67
 H      -5.316797    -3.681847    -2.463665      30.68
 H      -5.739223    -2.022123    -3.795080      30.81
 H      -7.203118    -1.634941    -2.810094      29.09
55
name = lig-ACN-frame_120
 C       3.373351     3.117523    -0.112735      63.51
 H       2.582473     3.780883    -0.380109      22.60
 C       4.289220     1.459868     1.197530      62.17
 H       4.287068     0.729546     1.967425      22.78
 C       5.385080     1.336008     0.252656      15.25
 O       6.494088     0.446506     0.438484     198.45
 C       6.431637    -0.432685     1.568404     117.54
 H       6.663648     0.066986     2.563322      27.52
 H       7.240689    -1.250875     1.460564      25.88
 H       5.461106    -0.965506     1.488549      26.87
 C       5.460912     2.237225    -0.846977      18.13
 O       6.616104     2.312960    -1.646716     126.76
 H       7.289128     1.641276    -1.368314      25.32
 C       4.412478     3.115792    -1.094655      62.31
 H       4.460391     3.815100    -1.940461      26.01
 C       3.306523     2.403458     0.998956      40.89
 C       2.102465     2.527914     2.054727     107.91
 H       2.277326     3.503792     2.630010      23.35
 O       2.079591     1.540538     2.976463     338.04
 H       1.873329     0.723619     2.578978      26.86
 C       0.674483     2.593350     1.285307      77.65
 H       0.936596     3.369144     0.400902      20.42
 C      -0.553302     3.012808     2.118493     102.17
 O      -0.402771     4.273465     2.842030     257.16
 H      -0.153738     5.075830     2.066179      26.84
 H      -0.629067     2.285111     2.965388      24.69
 H      -1.483757     3.050640     1.573475      26.11
 C      -2.420956    -0.832300     0.081468      63.72
 H      -2.827322    -1.794450     0.421425      23.60
 C      -2.026165     0.604581    -1.826667      85.02
 H      -2.159622     0.837364    -2.932592      18.49
 C      -0.981777     1.244741    -1.104926      23.07
 O      -0.226462     2.226847    -1.670628     220.28
 C      -0.720583     2.868715    -2.891395     125.10
 H      -0.289319     3.861381    -2.919476      25.99
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 H      -0.587399     2.292565    -3.743812      27.50
 H      -1.811360     3.093050    -2.927482      28.39
 C      -0.627337     0.764274     0.152444      28.46
 O       0.570848     1.255018     0.720058     210.05
 C      -1.371768    -0.238629     0.844185      23.37
 H      -1.165132    -0.606023     1.740740      17.59
 C      -2.755629    -0.433121    -1.223708      45.35
 C      -3.699257    -1.221530    -2.179366      58.11
 H      -3.655544    -0.733627    -3.131634      31.37
 O      -3.365351    -2.579566    -2.097217     240.13
 H      -2.377349    -2.746245    -2.580624      23.79
 C      -5.300323    -1.078209    -1.909930      86.92
 H      -5.419871    -1.221569    -0.778807      29.01
 O      -5.741067     0.340739    -2.180046     177.98
 H      -4.994361     0.902042    -1.676630      28.69
 C      -6.128626    -1.979256    -2.772841     116.42
 O      -6.198443    -3.365154    -2.197943     200.45
 H      -5.416892    -3.816772    -2.480332      31.73
 H      -5.694293    -2.032696    -3.745244      30.69
 H      -7.156254    -1.540515    -2.875454      29.23
55
name = lig-ACN-frame_121
 C       3.346156     3.240675    -0.217573      54.25
 H       2.612490     4.037361    -0.336853      24.66
 C       4.307060     1.411030     1.172570      61.74
 H       4.236526     0.838666     2.070055      23.70
 C       5.365674     1.379981     0.308097      29.86
 O       6.428258     0.497521     0.456145     225.81
 C       6.388829    -0.415706     1.564560     114.50
 H       6.480701     0.164319     2.520299      26.57
 H       7.266764    -1.221346     1.365220      24.33
 H       5.379624    -0.919384     1.739184      25.26
 C       5.514341     2.242448    -0.800250      31.86
 O       6.566012     2.325868    -1.626318     196.50
 H       7.242634     1.702293    -1.421192      26.43
 C       4.457150     3.149577    -1.048045      54.03
 H       4.433360     3.643340    -1.994098      23.77
 C       3.213851     2.384326     1.039444       7.54
 C       2.046673     2.568994     2.010521      86.30
 H       2.151778     3.590589     2.588747      21.87
 O       2.153258     1.523976     3.138346     232.93
 H       1.770075     0.605219     2.784439      20.70
 C       0.684969     2.609555     1.330030      82.51
 H       0.566630     3.330977     0.362371      19.29
 C      -0.566425     2.978523     2.178149     103.61
 O      -0.473419     4.256288     2.776381     293.29
 H      -0.009287     4.969888     2.104136      28.16
 H      -0.790918     2.257909     2.960162      26.14
 H      -1.322212     2.924075     1.391669      25.56
 C      -2.446809    -0.859200     0.081474      60.02
 H      -2.941094    -1.709481     0.517102      23.24
 C      -1.994494     0.604304    -1.842087      46.43
 H      -2.327188     0.970166    -2.849503      21.16
 C      -1.018547     1.247604    -1.114150      14.95
 O      -0.226383     2.287574    -1.683384     204.87
 C      -0.760326     2.871215    -2.896908     117.83
 H      -0.209264     3.879967    -2.971809      24.90
 H      -0.544960     2.410707    -3.795864      27.75
 H      -1.828072     2.946350    -2.616286      26.70
 C      -0.643452     0.808778     0.236234      37.11
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```
 O       0.541807     1.206309     0.762935     181.43
 C      -1.395835    -0.246139     0.795121      23.72
 H      -1.116679    -0.476314     1.749640      16.75
 C      -2.743859    -0.424478    -1.242101      58.84
 C      -3.760891    -1.173620    -2.113457      67.11
 H      -3.582653    -0.864430    -3.122081      32.41
 O      -3.336375    -2.630129    -2.171097     174.71
 H      -2.174520    -2.514819    -2.191553      22.77
 C      -5.279080    -1.037062    -1.839761      89.85
 H      -5.625560    -1.416844    -0.815803      28.85
 O      -5.740627     0.323956    -2.143969     227.01
 H      -5.304532     0.975947    -1.572917      29.36
 C      -6.126065    -2.039380    -2.771448     104.99
 O      -6.228563    -3.391929    -2.214160     194.37
 H      -5.294263    -3.779306    -2.341781      30.35
 H      -5.761292    -2.028252    -3.774607      30.87
 H      -7.170741    -1.728513    -2.728519      29.23
55
name = lig-ACN-frame_122
 C       3.284615     3.312742    -0.143350      63.92
 H       2.505975     4.002840    -0.513498      21.38
 C       4.177285     1.466707     1.223456      63.63
 H       4.149098     0.840078     2.110852      23.00
 C       5.383588     1.404712     0.372734       9.61
 O       6.413201     0.507119     0.452295     179.56
 C       6.314863    -0.393061     1.624066     106.84
 H       6.625913     0.117474     2.545314      26.32
 H       7.286197    -1.131368     1.380119      23.83
 H       5.369290    -1.060740     1.581754      24.71
 C       5.468502     2.300547    -0.735639      15.92
 O       6.575182     2.304742    -1.665579     125.63
 H       7.392708     1.846569    -1.261137      24.49
 C       4.426002     3.181689    -1.019928      55.66
 H       4.651623     3.868129    -1.799438      24.91
 C       3.211066     2.423989     0.899634      30.23
 C       2.067860     2.524698     2.043949      87.11
 H       2.185800     3.589792     2.576628      23.99
 O       2.186538     1.595859     3.233449     233.62
 H       1.877375     0.627916     2.827631      22.03
 C       0.663647     2.522351     1.346161      83.48
 H       0.850450     3.334807     0.480135      19.67
 C      -0.582883     2.908268     2.183181      98.58
 O      -0.521478     4.289671     2.725726     325.15
 H       0.027565     4.776838     2.162576      32.62
 H      -0.735676     2.226384     2.986812      26.71
 H      -1.534843     2.861360     1.603216      25.19
 C      -2.471750    -0.885421     0.078831      50.83
 H      -3.148313    -1.499210     0.626059      22.91
 C      -2.044333     0.619350    -1.819083      59.02
 H      -2.213606     0.862302    -2.873860      19.39
 C      -0.963291     1.280444    -1.129849      10.52
 O      -0.213742     2.310666    -1.665842     221.44
 C      -0.801205     2.934666    -2.873196     117.64
 H      -0.345731     4.003806    -3.052724      24.68
 H      -0.637494     2.289944    -3.601498      28.97
 H      -1.913796     3.091384    -3.076113      26.83
 C      -0.685061     0.842848     0.167664      37.54
 O       0.528237     1.194522     0.867356     219.95
 C      -1.410014    -0.226817     0.767789      46.12
 H      -1.125997    -0.684563     1.727900      19.23
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 C      -2.787629    -0.449749    -1.238786      45.70
 C      -3.758358    -1.176871    -2.113880      45.79
 H      -3.758321    -0.677858    -3.094249      29.17
 O      -3.387327    -2.649241    -2.204294     165.02
 H      -2.286429    -2.737035    -2.191208      23.47
 C      -5.286926    -1.063670    -1.791488      91.75
 H      -5.454345    -1.214365    -0.677451      29.52
 O      -5.731949     0.282312    -2.092128     219.03
 H      -5.526443     0.785735    -1.331154      31.09
 C      -6.150780    -2.054826    -2.725191     116.40
 O      -6.191362    -3.383935    -2.213839     232.79
 H      -5.240162    -3.681654    -2.142075      32.01
 H      -5.760209    -2.048338    -3.736901      31.40
 H      -7.128032    -1.635051    -2.765661      30.81
55
name = lig-ACN-frame_123
 C       3.277888     3.325412    -0.160852      41.33
 H       2.414942     4.001404    -0.332093      21.33
 C       4.203732     1.541165     1.185913      68.48
 H       3.967725     0.863381     2.022935      21.12
 C       5.310525     1.465108     0.392734      14.18
 O       6.394890     0.482228     0.524066     207.96
 C       6.349813    -0.401345     1.625575     111.83
 H       6.244394     0.119403     2.587076      27.07
 H       7.197708    -1.290654     1.603662      23.67
 H       5.269501    -0.880359     1.631052      25.56
 C       5.464921     2.349247    -0.726605      17.91
 O       6.521255     2.282283    -1.637531      90.24
 H       7.351400     1.799043    -1.218167      23.07
 C       4.413746     3.298852    -0.978294      54.12
 H       4.475595     4.068064    -1.732557      24.50
 C       3.118655     2.427781     0.989450      13.15
 C       2.072691     2.512328     2.096787      99.97
 H       2.260458     3.623195     2.540740      23.47
 O       2.203266     1.691686     3.208965     275.50
 H       1.987606     0.758171     3.002179      26.30
 C       0.660860     2.485299     1.412563      78.96
 H       0.683290     3.137896     0.443907      20.71
 C      -0.581976     2.921873     2.221474     104.23
 O      -0.553704     4.274640     2.686949     339.14
 H      -0.115868     4.792767     2.074825      33.99
 H      -0.545673     2.346714     3.117963      26.75
 H      -1.431535     2.675579     1.514326      25.83
 C      -2.523613    -0.817685     0.091264      56.65
 H      -2.940501    -1.709777     0.537171      24.77
 C      -2.058700     0.627100    -1.795202      60.15
 H      -2.203271     0.779495    -2.839962      19.51
 C      -0.996229     1.282203    -1.149650      16.91
 O      -0.266873     2.385872    -1.675761     205.02
 C      -0.805386     2.954471    -2.920522     113.92
 H      -0.130426     3.953945    -2.980109      24.37
 H      -0.608360     2.504490    -3.760782      30.23
 H      -1.832759     3.173065    -2.470830      26.49
 C      -0.631326     0.775020     0.172486      40.23
 O       0.458269     1.122004     0.910426     208.98
 C      -1.431966    -0.235568     0.725022      69.95
 H      -1.055107    -0.494366     1.815064      16.97
 C      -2.793257    -0.435301    -1.222166      31.17
 C      -3.778077    -1.236986    -2.179616      59.06
 H      -3.636731    -0.832914    -3.218317      27.94
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 O      -3.494225    -2.627066    -2.216623     278.85
 H      -2.580974    -2.678579    -2.499746      28.93
 C      -5.297584    -1.129263    -1.756821      95.01
 H      -5.451416    -1.490721    -0.709052      29.56
 O      -5.733027     0.257724    -2.024901     209.60
 H      -5.422785     0.905941    -1.253110      26.70
 C      -6.144381    -1.982102    -2.641964     117.00
 O      -6.147629    -3.399591    -2.182566     234.53
 H      -5.224728    -3.594922    -2.154836      33.14
 H      -5.668851    -1.910355    -3.631089      31.31
 H      -7.154591    -1.718769    -2.673586      30.31
55
name = lig-ACN-frame_124
 C       3.220987     3.299286    -0.093021      71.23
 H       2.540313     4.114101    -0.347569      24.79
 C       4.200302     1.535052     1.226902      56.16
 H       4.295353     0.818456     2.054215      22.45
 C       5.354491     1.463100     0.340696      12.69
 O       6.358045     0.554055     0.556941     183.57
 C       6.230783    -0.414756     1.706577     106.11
 H       6.449354     0.120567     2.636712      25.95
 H       7.268415    -0.956285     1.518969      24.32
 H       5.379958    -1.230087     1.623561      24.14
 C       5.425178     2.408250    -0.727005      23.35
 O       6.460642     2.282227    -1.582981     194.17
 H       7.095267     1.635039    -1.278273      25.12
 C       4.421697     3.385363    -0.898514      58.96
 H       4.507524     3.946842    -1.852076      22.47
 C       3.155577     2.467514     1.025000      33.88
 C       1.988244     2.634567     2.038171      89.66
 H       1.934584     3.726984     2.535104      22.58
 O       2.226355     1.711858     3.218537     254.03
 H       1.900061     0.913061     2.909995      29.20
 C       0.631393     2.501333     1.411962      80.41
 H       0.639769     3.208653     0.546793      20.36
 C      -0.533525     2.887024     2.311179     102.60
 O      -0.586539     4.286811     2.648025     282.24
 H      -0.228514     4.905785     1.849456      28.27
 H      -0.764649     2.280204     3.170283      25.52
 H      -1.498733     2.697780     1.719537      24.58
 C      -2.551586    -0.824467     0.092566      48.42
 H      -3.029758    -1.735631     0.507740      22.86
 C      -2.058001     0.629354    -1.842387      64.69
 H      -2.317649     1.021764    -2.791167      20.84
 C      -1.008184     1.281692    -1.116553      25.11
 O      -0.308019     2.368963    -1.681576     222.76
 C      -0.796438     3.038735    -2.870933     119.83
 H      -0.171735     4.047655    -3.019549      23.92
 H      -0.811479     2.388463    -3.619611      28.60
 H      -1.909839     3.359749    -3.070605      26.88
 C      -0.631842     0.737960     0.128535      37.50
 O       0.463882     1.047363     0.970775     195.26
 C      -1.446181    -0.241138     0.746261      55.75
 H      -1.223117    -0.642840     1.875702      17.08
 C      -2.840248    -0.441666    -1.290017      59.97
 C      -3.806178    -1.192859    -2.155619      58.38
 H      -3.822148    -0.736460    -3.219560      29.06
 O      -3.553797    -2.672584    -2.228508     266.68
 H      -2.695227    -2.782792    -2.427106      31.15
 C      -5.253816    -1.080719    -1.727335      96.50
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 H      -5.368859    -1.382753    -0.671495      29.55
 O      -5.742651     0.241473    -1.902618     247.75
 H      -5.065794     0.854073    -1.408763      27.83
 C      -6.172053    -2.025633    -2.621079     111.06
 O      -6.113544    -3.379310    -2.163304     233.89
 H      -5.178471    -3.680201    -2.346055      29.79
 H      -6.011330    -1.917814    -3.725818      30.31
 H      -7.145188    -1.657054    -2.444265      29.77
55
name = lig-ACN-frame_125
 C       3.258974     3.380138    -0.049739      51.79
 H       2.353687     3.914592    -0.264294      22.13
 C       4.207863     1.537055     1.286139      68.33
 H       4.099267     1.012393     2.223215      23.35
 C       5.257153     1.492535     0.401250      22.95
 O       6.322672     0.591294     0.585099     197.35
 C       6.254022    -0.369431     1.703971     109.27
 H       6.041639     0.062035     2.710791      26.37
 H       7.152469    -1.016307     1.618559      25.57
 H       5.260399    -0.994036     1.558765      25.68
 C       5.379422     2.397339    -0.659156      27.49
 O       6.463330     2.313714    -1.608776     109.41
 H       7.067720     1.650004    -1.259826      25.25
 C       4.390086     3.354573    -0.865884      61.09
 H       4.453893     4.152365    -1.667681      24.03
 C       3.209325     2.512892     1.061651       7.22
 C       2.005425     2.666935     2.061028      97.47
 H       2.064753     3.750852     2.497194      25.28
 O       2.195023     1.758801     3.175655     229.87
 H       1.834723     0.815067     2.890242      22.81
 C       0.566180     2.447082     1.371783      90.20
 H       0.481159     3.002875     0.465877      23.00
 C      -0.626810     2.861825     2.344761      92.82
 O      -0.604746     4.317022     2.649851     240.66
 H      -0.049604     4.810760     1.764546      25.98
 H      -0.345639     2.404962     3.314070      24.60
 H      -1.584228     2.541706     1.805805      25.01
 C      -2.552302    -0.870418    -0.019587      62.28
 H      -3.307274    -1.451240     0.561885      22.81
 C      -2.091303     0.641272    -1.854319      36.31
 H      -2.379549     1.009014    -2.826721      20.60
 C      -1.035978     1.265333    -1.143737       6.75
 O      -0.354299     2.370551    -1.629026     195.79
 C      -0.814579     3.055896    -2.903516     104.11
 H      -0.009808     3.891894    -3.012435      24.24
 H      -0.525147     2.505559    -3.692109      27.81
 H      -1.880804     3.445726    -2.671875      25.74
 C      -0.657621     0.706911     0.203827      19.81
 O       0.497977     1.082360     0.989793     210.50
 C      -1.517502    -0.282244     0.729696      71.26
 H      -1.151523    -0.695586     1.798382      17.08
 C      -2.785181    -0.435786    -1.292324      42.52
 C      -3.827374    -1.184058    -2.172073      44.19
 H      -3.708711    -0.712480    -3.242745      25.26
 O      -3.556080    -2.687390    -2.232091     212.56
 H      -2.511460    -2.749545    -2.205912      25.80
 C      -5.285610    -1.094827    -1.716656      99.75
 H      -5.335298    -1.454705    -0.689615      28.74
 O      -5.751454     0.294877    -1.780561     257.98
 H      -5.107690     0.881414    -1.473290      31.57
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 C      -6.242758    -2.003984    -2.532077     108.37
 O      -6.103536    -3.394229    -2.167205     241.49
 H      -5.202470    -3.675736    -2.525912      30.22
 H      -6.032680    -1.868620    -3.636606      29.74
 H      -7.272840    -1.784671    -2.298971      28.43
55
name = lig-ACN-frame_126
 C       3.276676     3.435295     0.009802      57.56
 H       2.503884     4.126125    -0.272028      21.69
 C       4.131864     1.617649     1.406385      64.29
 H       4.035691     0.925667     2.222237      21.86
 C       5.260733     1.472257     0.492194       3.73
 O       6.345163     0.609077     0.613025     203.37
 C       6.194072    -0.318476     1.660795     120.14
 H       6.163480     0.296289     2.603070      26.26
 H       7.064802    -0.878772     1.747792      27.09
 H       5.307232    -1.044929     1.448191      25.46
 C       5.407688     2.374179    -0.685133      11.97
 O       6.420586     2.345974    -1.582116     112.11
 H       7.327680     1.920953    -1.277433      21.72
 C       4.361164     3.354446    -0.895444      65.87
 H       4.574335     4.124578    -1.710690      23.84
 C       3.129907     2.571155     1.125548      36.39
 C       2.009461     2.635048     2.039476     105.85
 H       2.017610     3.663037     2.526162      24.84
 O       2.117544     1.781042     3.158116     227.32
 H       1.843938     0.791811     2.806061      22.29
 C       0.530345     2.511274     1.369112      78.95
 H       0.468205     3.151752     0.572189      22.36
 C      -0.586548     2.894249     2.372915     100.17
 O      -0.634156     4.292637     2.624369     286.97
 H       0.032452     4.843062     1.990275      27.65
 H      -0.532847     2.326336     3.372860      23.90
 H      -1.640086     2.525594     2.098299      24.04
 C      -2.563023    -0.893630    -0.006152      55.37
 H      -3.174757    -1.760356     0.377954      21.71
 C      -2.085228     0.662110    -1.847302      72.91
 H      -2.207664     0.933686    -2.918462      18.59
 C      -1.038270     1.232991    -1.089705      14.78
 O      -0.372628     2.392940    -1.585646     216.31
 C      -0.736842     3.012749    -2.847937     123.08
 H      -0.184979     3.985986    -2.779989      25.12
 H      -0.865109     2.483850    -3.721305      28.93
 H      -1.842733     3.343836    -2.847093      26.42
 C      -0.692588     0.729753     0.201668      37.44
 O       0.442933     1.064857     0.928720     227.81
 C      -1.490308    -0.336337     0.715866      24.48
 H      -1.361506    -0.700340     1.779815      19.29
 C      -2.820875    -0.476418    -1.387942      45.10
 C      -3.813525    -1.238128    -2.222074      57.42
 H      -3.834789    -0.923208    -3.369827      24.31
 O      -3.493782    -2.621654    -2.223161     213.09
 H      -2.343326    -2.758860    -2.260974      20.65
 C      -5.327027    -1.082452    -1.645582      88.02
 H      -5.328275    -1.473327    -0.635389      29.88
 O      -5.777916     0.324849    -1.704245     253.89
 H      -5.216592     0.822784    -1.056854      29.64
 C      -6.316943    -1.963414    -2.457581     101.09
 O      -6.120418    -3.425231    -2.193757     253.97
 H      -5.230501    -3.592849    -2.483672      32.85
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 H      -6.187076    -1.715485    -3.562874      29.39
 H      -7.382548    -1.691080    -2.223158      27.74
55
name = lig-ACN-frame_127
 C       3.296314     3.476241     0.002922      52.80
 H       2.614675     4.303210    -0.209915      22.39
 C       4.187094     1.660672     1.385393      62.31
 H       4.054364     0.984538     2.225015      19.79
 C       5.271233     1.567128     0.488558      22.10
 O       6.345166     0.651905     0.599798     191.83
 C       6.187288    -0.321167     1.711043     118.42
 H       5.997593     0.129945     2.727500      27.08
 H       7.049970    -0.818467     1.661820      27.21
 H       5.316193    -1.041943     1.598905      26.54
 C       5.324835     2.369512    -0.608151      27.13
 O       6.419582     2.366650    -1.571944     173.89
 H       7.217590     1.992733    -1.056706      25.78
 C       4.401159     3.311448    -0.867791      56.12
 H       4.431568     3.897312    -1.812759      20.90
 C       3.144225     2.605538     1.094310      20.21
 C       1.824491     2.692351     2.069626     106.26
 H       1.789700     3.698641     2.525716      26.16
 O       2.017785     1.715237     3.188592     234.01
 H       1.798233     0.840016     2.843048      24.78
 C       0.547563     2.547855     1.387960     103.18
 H       0.487544     3.149774     0.583469      23.58
 C      -0.550482     2.877502     2.404455      99.05
 O      -0.666554     4.316052     2.627954     316.33
 H      -0.108540     4.736787     2.075280      35.49
 H      -0.340234     2.325027     3.398751      24.79
 H      -1.447659     2.614465     1.766163      25.05
 C      -2.555620    -0.931134    -0.076874      83.63
 H      -2.864219    -1.908826     0.322034      22.68
 C      -2.068477     0.599349    -1.861204      34.25
 H      -2.195426     1.010446    -2.903926      17.25
 C      -1.073636     1.273718    -1.096885      33.80
 O      -0.346526     2.365276    -1.522465     238.95
 C      -0.770997     3.001022    -2.762272     124.31
 H      -0.105696     3.805499    -3.009229      25.85
 H      -0.284370     2.353662    -3.414308      26.66
 H      -1.845251     3.306354    -2.738807      28.75
 C      -0.752208     0.705179     0.175828      38.08
 O       0.378468     1.133357     0.875632     191.69
 C      -1.502478    -0.366755     0.697393      30.57
 H      -1.190731    -0.717601     1.635530      15.37
 C      -2.823115    -0.460644    -1.380945      49.59
 C      -3.874479    -1.219028    -2.240640      44.57
 H      -3.961799    -0.660239    -3.285830      27.00
 O      -3.415931    -2.642779    -2.206854     208.59
 H      -2.300887    -2.611455    -2.461299      21.08
 C      -5.312511    -1.075998    -1.594751      88.53
 H      -5.253635    -1.353744    -0.555905      29.55
 O      -5.782313     0.286426    -1.644314     228.08
 H      -5.380119     0.868251    -0.846870      24.85
 C      -6.358715    -1.958827    -2.406541      99.21
 O      -6.171803    -3.372596    -2.248745     270.04
 H      -5.199850    -3.532972    -2.365083      32.00
 H      -6.343041    -1.698997    -3.519042      29.33
 H      -7.402007    -1.765030    -1.937632      26.15
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name = lig-ACN-frame_128
 C       3.275748     3.494622    -0.000866      47.53
 H       2.400254     4.107963    -0.339780      19.63
 C       4.173519     1.717527     1.335699      64.48
 H       4.131049     1.136060     2.273684      22.25
 C       5.306028     1.587752     0.529212      27.52
 O       6.305511     0.661153     0.666297     237.26
 C       6.224066    -0.337695     1.739776     118.10
 H       6.112083     0.208839     2.698508      26.36
 H       7.063246    -0.927735     1.786489      26.94
 H       5.366626    -0.915933     1.445861      27.53
 C       5.405480     2.420944    -0.678993      16.84
 O       6.415515     2.348627    -1.508509     140.21
 H       7.125326     1.787513    -1.251053      25.89
 C       4.328768     3.364607    -0.890648      78.97
 H       4.447425     3.979371    -1.771327      26.98
 C       3.124666     2.644070     1.150078      35.45
 C       1.937618     2.666242     2.119864      94.68
 H       1.897802     3.588564     2.644970      24.80
 O       1.900704     1.674574     3.184316     287.09
 H       1.628400     0.872316     2.818219      27.45
 C       0.466471     2.537072     1.330589      93.17
 H       0.449556     3.242952     0.580316      23.02
 C      -0.630948     2.894801     2.333635      97.84
 O      -0.688296     4.337397     2.665325     301.09
 H      -0.282089     4.862555     1.969979      31.97
 H      -0.425658     2.398298     3.358468      24.01
 H      -1.645687     2.431170     2.179429      25.32
 C      -2.477525    -1.023396    -0.110480      53.65
 H      -3.145160    -1.787430     0.235203      20.94
 C      -2.065112     0.614448    -1.929557      62.90
 H      -2.439955     0.923312    -2.936959      22.93
 C      -1.128841     1.258338    -1.103477       9.74
 O      -0.325988     2.373967    -1.429480     223.39
 C      -0.685949     2.947925    -2.732790     126.11
 H      -0.312334     3.914366    -2.601952      25.21
 H      -0.743412     2.387040    -3.672165      25.64
 H      -1.781614     3.072082    -2.796519      27.18
 C      -0.784352     0.761702     0.170336      13.95
 O       0.357762     1.215144     0.866294     237.55
 C      -1.494371    -0.386945     0.658344      43.97
 H      -1.168597    -0.873750     1.455408      20.02
 C      -2.836647    -0.452440    -1.353577      57.19
 C      -3.859123    -1.152543    -2.153880      65.69
 H      -3.852815    -0.952738    -3.300853      25.52
 O      -3.426735    -2.637056    -2.245095     183.96
 H      -2.406855    -2.674943    -2.360008      26.09
 C      -5.296298    -1.141217    -1.575595      98.64
 H      -5.262596    -1.616101    -0.599620      28.96
 O      -5.791508     0.246752    -1.611024     233.65
 H      -5.135164     0.838118    -1.098887      26.72
 C      -6.376861    -1.910292    -2.310791     101.59
 O      -6.204664    -3.341183    -2.296733     259.20
 H      -5.203018    -3.525372    -2.445093      29.86
 H      -6.448442    -1.450845    -3.355872      28.64
 H      -7.414680    -1.685567    -1.834007      26.03
55
name = lig-ACN-frame_129
 C       3.162834     3.457515    -0.006207      58.83
 H       2.308678     4.114684    -0.309656      19.34
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 C       4.169712     1.744708     1.400979      60.53
 H       4.103972     1.039199     2.261187      21.59
 C       5.274348     1.639259     0.500757      20.40
 O       6.350196     0.656512     0.722082     215.55
 C       6.199163    -0.323997     1.758414     127.34
 H       6.193832     0.119712     2.756785      28.38
 H       7.170375    -0.802741     1.600649      25.88
 H       5.431096    -1.016321     1.757565      29.70
 C       5.363414     2.486394    -0.606747      21.75
 O       6.490514     2.330372    -1.558055     113.30
 H       7.116454     1.699874    -1.123324      21.33
 C       4.331889     3.400376    -0.915797      54.48
 H       4.382884     4.094575    -1.701715      27.80
 C       3.144856     2.662446     1.152732      32.59
 C       1.912984     2.636788     2.122420     110.99
 H       1.972906     3.532407     2.633244      25.75
 O       1.836670     1.633271     3.155642     259.31
 H       1.634113     0.702783     2.707812      20.74
 C       0.443481     2.654057     1.339660      68.34
 H       0.453292     3.279417     0.450142      21.07
 C      -0.738041     2.954294     2.374663     103.38
 O      -0.712315     4.331007     2.693035     243.18
 H      -0.466452     4.887763     1.744494      27.07
 H      -0.424158     2.375595     3.290248      23.82
 H      -1.712433     2.727421     1.897050      24.54
 C      -2.450778    -1.015749    -0.111900      68.97
 H      -2.907426    -1.856062     0.354293      21.01
 C      -2.131529     0.654289    -1.919887      58.82
 H      -2.227855     1.012598    -2.942911      18.56
 C      -1.106015     1.266316    -1.111074      15.57
 O      -0.344573     2.341005    -1.461286     241.72
 C      -0.713868     2.997518    -2.676004     121.93
 H      -0.230283     3.883823    -2.856740      26.42
 H      -0.098613     2.435959    -3.456141      24.71
 H      -1.760117     3.161068    -2.600472      27.65
 C      -0.815446     0.748130     0.200048      43.01
 O       0.330722     1.206769     0.845565     196.88
 C      -1.400189    -0.443017     0.654644      33.57
 H      -1.180999    -0.719086     1.607542      18.75
 C      -2.793915    -0.460896    -1.375296      27.88
 C      -3.828664    -1.264228    -2.180345      60.76
 H      -3.966199    -0.576005    -3.107934      25.18
 O      -3.499839    -2.614130    -2.271424     296.78
 H      -2.624032    -2.712203    -2.243196      31.67
 C      -5.267996    -1.153786    -1.520179      95.15
 H      -5.227277    -1.411420    -0.458449      28.35
 O      -5.761160     0.200189    -1.558778     259.68
 H      -5.079165     0.762270    -1.304460      32.29
 C      -6.399922    -1.879682    -2.297311     100.13
 O      -6.227718    -3.327537    -2.343821     272.41
 H      -5.343465    -3.451378    -2.703673      32.06
 H      -6.525676    -1.476399    -3.355921      27.92
 H      -7.326417    -1.711324    -1.680061      25.78
55
name = lig-ACN-frame_130
 C       3.162782     3.398280    -0.063974      53.29
 H       2.369530     4.129797    -0.255894      25.20
 C       4.214099     1.745841     1.453421      48.41
 H       4.067152     1.044127     2.301448      19.35
 C       5.282434     1.613834     0.552135      24.37
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 O       6.304359     0.747513     0.705711     214.55
 C       6.242088    -0.309936     1.826751     107.28
 H       6.214741     0.159392     2.780556      28.81
 H       7.120932    -1.068201     1.764350      25.05
 H       5.404555    -0.792949     1.595799      31.48
 C       5.409574     2.510398    -0.640614      18.69
 O       6.429515     2.345922    -1.545038     117.61
 H       7.333332     2.022818    -1.096905      22.03
 C       4.299767     3.422435    -0.844474      63.25
 H       4.364079     3.986613    -1.728955      22.60
 C       3.075918     2.599076     1.133934      33.65
 C       1.755044     2.682135     2.087685      99.68
 H       1.754784     3.530578     2.651561      22.89
 O       1.826306     1.586363     3.101761     236.36
 H       1.640434     0.630072     2.605692      18.20
 C       0.449532     2.644101     1.410509      85.23
 H       0.364868     3.431435     0.580901      18.86
 C      -0.739119     2.989809     2.304962     104.15
 O      -0.747704     4.389421     2.745265     245.22
 H      -0.407674     4.999005     1.887105      27.67
 H      -0.950085     2.401774     3.207310      24.53
 H      -1.618271     2.725751     1.698487      24.19
 C      -2.396575    -0.995609    -0.085806      51.14
 H      -2.799749    -1.961435     0.149907      22.02
 C      -2.138239     0.682950    -1.841047      75.81
 H      -2.312097     0.938987    -2.856661      18.04
 C      -1.124138     1.247486    -1.087236      14.43
 O      -0.338762     2.345469    -1.483085     231.78
 C      -0.686650     3.101852    -2.697225     124.20
 H      -0.242948     3.991754    -2.429579      26.25
 H      -0.519305     2.447830    -3.666192      25.05
 H      -1.673166     3.216900    -3.024680      28.73
 C      -0.748538     0.732819     0.173278      29.84
 O       0.320516     1.251725     0.877091     207.53
 C      -1.352432    -0.442440     0.681017      30.26
 H      -1.053465    -0.897942     1.645872      18.36
 C      -2.757752    -0.541544    -1.380575      52.15
 C      -3.880442    -1.211387    -2.191084      67.91
 H      -3.948627    -0.982706    -3.288729      23.29
 O      -3.564575    -2.678651    -2.324520     275.09
 H      -2.605843    -2.726352    -2.407787      26.17
 C      -5.244901    -1.137138    -1.482674      94.77
 H      -5.138981    -1.657193    -0.507807      29.15
 O      -5.706831     0.215222    -1.526131     254.55
 H      -5.122364     0.836859    -0.982304      28.47
 C      -6.385893    -1.927332    -2.264157     104.21
 O      -6.259849    -3.325147    -2.403554     280.52
 H      -5.466786    -3.534289    -2.909122      33.12
 H      -6.462663    -1.350871    -3.244015      29.02
 H      -7.331101    -1.789317    -1.778457      27.73
55
name = lig-ACN-frame_131
 C       3.152756     3.351079    -0.006579      59.92
 H       2.340985     3.934534    -0.407144      17.41
 C       4.125483     1.772361     1.445991      49.55
 H       4.206974     1.248167     2.402497      19.92
 C       5.267941     1.684482     0.583756      37.12
 O       6.359007     0.738278     0.747500     239.82
 C       6.201334    -0.198547     1.795772     126.79
 H       6.272115     0.251828     2.754154      27.37
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 H       7.186536    -0.844342     1.624221      23.71
 H       5.395674    -0.796257     1.800294      28.96
 C       5.359465     2.467092    -0.555780      32.52
 O       6.359433     2.394420    -1.535014     118.45
 H       7.234086     2.092471    -1.095201      23.19
 C       4.363822     3.364707    -0.851692      58.67
 H       4.401962     4.053867    -1.693922      22.64
 C       2.980462     2.547731     1.123580      49.74
 C       1.813728     2.634990     2.112257     123.54
 H       1.887527     3.534436     2.611131      28.13
 O       1.832008     1.594464     3.048143     300.33
 H       1.529045     0.755361     2.608132      22.60
 C       0.380768     2.604111     1.398865      89.50
 H       0.515747     3.325019     0.477669      21.00
 C      -0.842481     3.044575     2.237208     107.56
 O      -0.775252     4.434487     2.776076     319.20
 H      -0.245038     4.990224     2.281376      34.14
 H      -0.852017     2.422321     3.111728      27.00
 H      -1.730396     2.968084     1.641246      27.05
 C      -2.338430    -1.096398    -0.108952      58.30
 H      -2.814804    -1.975378     0.360647      21.37
 C      -2.144679     0.625053    -1.830871      27.41
 H      -2.515945     1.124133    -2.691212      20.60
 C      -1.102086     1.284467    -1.074392      15.28
 O      -0.373733     2.369369    -1.523199     211.43
 C      -0.695186     3.179987    -2.740785     114.95
 H      -0.150663     4.114834    -2.745128      24.69
 H      -0.128330     2.876462    -3.744503      23.21
 H      -1.656320     3.358030    -2.545060      27.46
 C      -0.665361     0.738417     0.190125      28.10
 O       0.355878     1.297699     0.931847     229.41
 C      -1.363046    -0.416692     0.658786      54.45
 H      -0.881525    -0.972959     1.593365      16.82
 C      -2.764921    -0.549969    -1.363028      39.88
 C      -3.848022    -1.261226    -2.199157      54.84
 H      -3.947093    -0.608075    -3.080161      27.64
 O      -3.613809    -2.748250    -2.362492     194.94
 H      -2.521173    -2.907248    -2.590231      23.91
 C      -5.246842    -1.184853    -1.508238      89.66
 H      -5.150760    -1.450712    -0.419477      27.34
 O      -5.671219     0.270290    -1.466341     175.90
 H      -5.139131     0.701527    -0.643574      24.66
 C      -6.362179    -1.890705    -2.254095     108.12
 O      -6.293478    -3.373410    -2.470517     241.68
 H      -5.373961    -3.504962    -2.912207      29.73
 H      -6.472394    -1.441233    -3.274312      28.88
 H      -7.224072    -1.726999    -1.703688      28.65
55
name = lig-ACN-frame_132
 C       3.108863     3.362297    -0.059991      41.34
 H       2.299774     3.993190    -0.343628      23.26
 C       4.112802     1.740236     1.466423      50.45
 H       4.006066     1.230679     2.412581      20.01
 C       5.272947     1.672215     0.650749      46.79
 O       6.332056     0.811834     0.760897     251.57
 C       6.227798    -0.140615     1.844014     119.55
 H       6.270140     0.360486     2.776642      27.70
 H       7.114417    -0.889318     1.764877      24.45
 H       5.345870    -0.656189     1.727489      28.86
 C       5.333054     2.459636    -0.544581      30.01
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 O       6.351008     2.422167    -1.499255     143.88
 H       7.045090     1.846085    -1.220484      29.61
 C       4.255369     3.335817    -0.798091      91.16
 H       4.439911     4.014647    -1.683935      22.32
 C       3.004928     2.530994     1.087895      48.62
 C       1.814639     2.647350     2.100228     104.84
 H       2.018056     3.496292     2.691345      24.96
 O       1.850782     1.591034     3.098518     287.62
 H       1.607760     0.785983     2.747211      25.03
 C       0.421518     2.737789     1.335675      69.38
 H       0.376521     3.368774     0.313817      19.07
 C      -0.911968     3.128242     2.235894     108.58
 O      -0.783153     4.435335     2.797759     321.38
 H      -0.120080     4.868839     2.287844      32.82
 H      -0.963728     2.416977     3.019470      26.76
 H      -1.831581     2.999097     1.701100      26.90
 C      -2.282736    -1.149641    -0.117367      54.06
 H      -2.712487    -2.085409     0.341178      20.65
 C      -2.117658     0.630616    -1.802793      57.77
 H      -2.484920     1.073910    -2.730567      21.57
 C      -1.084490     1.294891    -1.126246      13.06
 O      -0.349101     2.436620    -1.584370     238.45
 C      -0.715775     3.261764    -2.702758     124.26
 H      -0.117748     4.149924    -2.470175      24.14
 H      -0.620686     2.490047    -3.603821      23.85
 H      -1.640628     3.506683    -3.034960      29.10
 C      -0.708597     0.749639     0.159326      52.06
 O       0.366445     1.209482     0.957007     154.95
 C      -1.300446    -0.428050     0.599041      33.75
 H      -1.086751    -0.754280     1.765772      17.11
 C      -2.753707    -0.621811    -1.306262      56.69
 C      -3.813801    -1.331276    -2.157505      51.15
 H      -3.855053    -0.972252    -3.168615      28.80
 O      -3.631935    -2.727819    -2.416095     207.96
 H      -2.510147    -2.934837    -2.521051      23.49
 C      -5.215617    -1.140511    -1.494035      85.77
 H      -5.210007    -1.702667    -0.486322      27.36
 O      -5.638423     0.244057    -1.419560     227.15
 H      -5.043292     0.788580    -0.823220      26.74
 C      -6.410475    -1.918758    -2.301532     104.62
 O      -6.303377    -3.350824    -2.512466     269.95
 H      -5.364993    -3.561345    -2.699599      30.55
 H      -6.531960    -1.331920    -3.232889      28.91
 H      -7.292763    -1.821613    -1.757597      27.63
55
name = lig-ACN-frame_133
 C       2.999785     3.367172    -0.061015      81.67
 H       2.271930     4.136916    -0.243180      27.49
 C       4.124136     1.698476     1.481125      46.54
 H       4.001759     0.999759     2.285625      19.74
 C       5.227323     1.675660     0.633038      27.65
 O       6.350484     0.859798     0.800873     229.77
 C       6.250216    -0.117012     1.930338     120.36
 H       6.258105     0.368440     2.902598      28.97
 H       7.082307    -0.804181     1.822954      26.21
 H       5.344358    -0.683180     1.829790      28.99
 C       5.282610     2.488358    -0.550031      26.95
 O       6.353235     2.423754    -1.437887     168.33
 H       7.049313     1.816810    -1.084975      28.36
 C       4.214978     3.348703    -0.859261      84.44
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 H       4.232727     3.994787    -1.825038      14.57
 C       3.008204     2.559583     1.107361      42.82
 C       1.807038     2.698571     2.068195     103.07
 H       1.833966     3.645735     2.600961      22.98
 O       1.847746     1.631835     3.173163     241.14
 H       1.692664     0.756039     2.716231      21.66
 C       0.399965     2.704870     1.369321      79.54
 H       0.525154     3.429584     0.409567      18.67
 C      -0.824428     3.103350     2.205695     105.75
 O      -0.765970     4.451546     2.815755     256.79
 H      -0.244517     5.225529     2.186811      27.56
 H      -0.994821     2.462272     3.016359      26.07
 H      -1.665874     3.045954     1.545838      25.61
 C      -2.224062    -1.167075    -0.087194      54.53
 H      -2.587803    -2.183660     0.228366      21.45
 C      -2.145393     0.595144    -1.807876      92.51
 H      -2.393478     0.813423    -2.882249      21.57
 C      -1.060344     1.305269    -1.155366      19.80
 O      -0.386773     2.461264    -1.543442     231.04
 C      -0.769726     3.242978    -2.764008     119.02
 H       0.013866     4.085058    -2.923505      24.73
 H      -0.407228     2.825888    -3.782195      24.97
 H      -1.663888     3.569125    -2.470340      28.96
 C      -0.688589     0.780176     0.111209      32.85
 O       0.295215     1.225555     0.938262     162.13
 C      -1.270503    -0.460893     0.609356      31.35
 H      -0.909911    -0.776919     1.733853      17.10
 C      -2.655304    -0.624796    -1.358703      35.60
 C      -3.823487    -1.293313    -2.177100      67.85
 H      -3.860658    -0.691741    -3.048919      27.01
 O      -3.588662    -2.757247    -2.415411     265.84
 H      -2.586634    -2.892435    -2.380985      25.86
 C      -5.264837    -1.212890    -1.516001      92.35
 H      -5.122779    -1.607860    -0.431753      26.75
 O      -5.617597     0.186768    -1.390577     248.46
 H      -4.871406     0.649375    -1.116744      32.76
 C      -6.430233    -1.875171    -2.329438     111.62
 O      -6.294071    -3.304351    -2.532360     282.99
 H      -5.361962    -3.471170    -2.642214      31.15
 H      -6.538650    -1.413218    -3.303875      28.13
 H      -7.335236    -1.708917    -1.778898      26.79
55
name = lig-ACN-frame_134
 C       3.061426     3.359197    -0.016681      54.04
 H       2.168572     3.928615    -0.299113      17.73
 C       4.026161     1.719217     1.414769      62.00
 H       4.042896     1.122596     2.326561      22.56
 C       5.197855     1.689147     0.573225      20.97
 O       6.369540     0.856106     0.898191     241.43
 C       6.267639    -0.067733     1.967018     126.57
 H       6.326710     0.456747     2.937632      27.92
 H       7.134923    -0.608558     1.861392      27.33
 H       5.431756    -0.811274     1.962936      27.27
 C       5.221824     2.521437    -0.569906      31.45
 O       6.361810     2.414146    -1.379266     110.88
 H       7.163331     2.104079    -0.771426      22.00
 C       4.116264     3.348957    -0.935736      62.26
 H       4.228628     3.998684    -1.894199      29.22
 C       2.972837     2.590427     1.178574      39.93
 C       1.776483     2.663089     2.148220     114.61
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 H       1.844404     3.682680     2.622272      21.17
 O       1.834817     1.769068     3.184059     281.74
 H       1.609095     0.757694     2.821322      20.50
 C       0.463438     2.594609     1.395810      84.32
 H       0.483908     3.322538     0.439854      18.61
 C      -0.745205     3.116749     2.206591     103.92
 O      -0.722172     4.449298     2.809989     257.73
 H      -0.485962     5.120205     1.950945      26.54
 H      -0.812853     2.459596     3.048401      25.95
 H      -1.611782     2.995052     1.570052      25.85
 C      -2.187289    -1.174512    -0.151275      56.29
 H      -2.576095    -2.084123     0.328453      21.43
 C      -2.066462     0.584843    -1.903080      47.66
 H      -2.382178     1.034011    -2.913550      20.29
 C      -1.110761     1.279716    -1.165938      14.96
 O      -0.410210     2.464738    -1.548491     220.85
 C      -0.783508     3.198280    -2.782461     119.43
 H      -0.095401     4.126814    -2.707379      22.35
 H      -1.042448     2.493039    -3.639667      24.23
 H      -1.778637     3.577026    -2.858551      27.65
 C      -0.705010     0.729540     0.120693      30.76
 O       0.249011     1.344055     0.925281     230.14
 C      -1.225893    -0.435515     0.614544      50.87
 H      -0.721525    -0.950078     1.492187      16.73
 C      -2.662540    -0.671666    -1.371715      59.12
 C      -3.804904    -1.283724    -2.192494      61.41
 H      -3.936250    -0.849300    -3.132081      30.52
 O      -3.521480    -2.730488    -2.394987     284.21
 H      -2.656967    -2.868784    -2.451405      32.26
 C      -5.244618    -1.256027    -1.531391      88.30
 H      -5.314109    -1.870130    -0.533991      26.49
 O      -5.623201     0.143119    -1.388981     209.03
 H      -4.839004     0.672126    -0.967312      26.99
 C      -6.403118    -1.827462    -2.356247     107.69
 O      -6.291671    -3.268067    -2.527708     250.76
 H      -5.322305    -3.409777    -2.799143      28.70
 H      -6.412688    -1.261392    -3.262050      29.29
 H      -7.359370    -1.657027    -1.816856      26.51
55
name = lig-ACN-frame_135
 C       3.020387     3.393953    -0.011682      37.80
 H       2.172845     4.041495    -0.340872      17.48
 C       4.036577     1.707157     1.402473      55.48
 H       3.971453     1.183007     2.370888      20.58
 C       5.140068     1.655563     0.616410      34.64
 O       6.275754     0.946043     0.899533     236.37
 C       6.341193    -0.042052     2.053640     109.10
 H       6.186170     0.460511     3.044428      28.07
 H       7.178764    -0.578526     2.014299      27.75
 H       5.405037    -0.671607     1.843110      26.41
 C       5.250052     2.482517    -0.602073      16.95
 O       6.381613     2.439441    -1.347377     130.77
 H       7.179166     2.146801    -0.818368      22.33
 C       4.117272     3.272179    -0.921793      85.64
 H       4.042671     3.960203    -1.812919      32.45
 C       2.970789     2.614403     1.159252      43.91
 C       1.794428     2.740464     2.136876     102.30
 H       1.765926     3.771968     2.673522      22.11
 O       1.820998     1.802474     3.278775     267.19
 H       1.594951     0.840439     2.922605      20.63
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 C       0.453541     2.762490     1.346539      67.91
 H       0.633866     3.501971     0.475735      17.93
 C      -0.756527     3.089203     2.288296     108.28
 O      -0.644616     4.430560     2.741947     331.94
 H      -0.440147     5.050515     2.101730      34.34
 H      -0.815406     2.445871     3.183099      24.69
 H      -1.712851     2.924192     1.761841      24.79
 C      -2.178949    -1.153559    -0.203930      75.80
 H      -2.647947    -2.046191     0.152087      21.77
 C      -2.028575     0.513321    -1.955884      58.25
 H      -2.475977     0.970557    -2.902774      21.70
 C      -1.108241     1.278851    -1.147090      26.56
 O      -0.478916     2.446558    -1.559618     248.38
 C      -0.901032     3.087888    -2.769464     129.44
 H      -0.017985     3.744990    -3.141229      23.54
 H      -0.664373     2.496867    -3.557598      27.16
 H      -1.839004     3.614145    -2.664605      26.48
 C      -0.726181     0.815930     0.117515      25.01
 O       0.273303     1.281650     0.919603     181.18
 C      -1.205567    -0.515208     0.541580      32.21
 H      -0.963976    -0.822882     1.516361      19.78
 C      -2.682477    -0.578112    -1.442387      45.48
 C      -3.789367    -1.369768    -2.197401      81.31
 H      -3.819628    -0.866794    -3.106176      29.78
 O      -3.473000    -2.720741    -2.376360     284.29
 H      -2.528303    -2.796713    -2.533193      30.54
 C      -5.194085    -1.224018    -1.523203      89.56
 H      -5.037803    -1.770269    -0.493990      26.60
 O      -5.621781     0.128649    -1.367151     221.34
 H      -5.112591     0.657187    -0.593071      25.30
 C      -6.345797    -1.813956    -2.419184     105.16
 O      -6.291534    -3.231764    -2.539616     255.89
 H      -5.431347    -3.504502    -2.958646      30.83
 H      -6.419563    -1.356165    -3.370483      29.10
 H      -7.337362    -1.609089    -1.876181      26.18
55
name = lig-ACN-frame_136
 C       2.997550     3.391267    -0.066417      79.98
 H       2.311784     4.255264    -0.241633      26.87
 C       3.974691     1.729703     1.499305      56.61
 H       3.948951     1.024194     2.357078      19.65
 C       5.126286     1.663008     0.603586      30.34
 O       6.292903     0.965570     0.938283     214.56
 C       6.289194     0.043458     2.048019     130.69
 H       6.268580     0.557125     3.062189      29.66
 H       7.243534    -0.339226     1.922169      27.85
 H       5.585980    -0.912120     2.034004      26.47
 C       5.212561     2.400169    -0.540070      19.69
 O       6.424612     2.486747    -1.369561     212.96
 H       7.044868     1.890246    -0.996764      31.58
 C       4.146863     3.228100    -0.884797      74.22
 H       4.311780     3.753432    -1.813037      18.62
 C       2.950165     2.630222     1.139955      47.53
 C       1.793157     2.835264     2.122391      93.60
 H       2.022194     3.870018     2.662384      21.16
 O       1.796327     1.822166     3.314397     217.46
 H       1.679015     0.995941     2.919649      24.37
 C       0.376433     2.768844     1.380504      89.67
 H       0.206931     3.392885     0.483109      19.07
 C      -0.763813     3.070101     2.290774     104.50
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 O      -0.587527     4.464815     2.742515     310.91
 H      -0.147533     4.915691     2.065567      33.74
 H      -0.547910     2.437807     3.198926      23.21
 H      -1.745696     2.901798     1.789794      24.54
 C      -2.245659    -1.142799    -0.273184      58.88
 H      -2.569763    -2.085042     0.070017      20.92
 C      -2.043236     0.576182    -1.960582      61.22
 H      -2.178251     0.855441    -3.027830      20.38
 C      -1.119063     1.260900    -1.185389      18.61
 O      -0.535372     2.443395    -1.545400     223.86
 C      -0.924948     2.993930    -2.848757     127.88
 H      -0.298223     3.913299    -2.867654      24.82
 H      -1.229624     2.391118    -3.571574      29.29
 H      -1.969855     3.404714    -2.642076      27.09
 C      -0.731364     0.748745     0.140760      35.65
 O       0.349710     1.310564     0.929582     172.85
 C      -1.221676    -0.473008     0.490571      37.43
 H      -0.966370    -0.846754     1.368254      21.45
 C      -2.668019    -0.617420    -1.457951      39.70
 C      -3.741536    -1.265510    -2.250495      70.20
 H      -3.918853    -0.879389    -3.192371      28.21
 O      -3.442320    -2.787238    -2.359806     189.40
 H      -2.341442    -2.922491    -2.430159      22.27
 C      -5.152875    -1.214142    -1.549627      82.51
 H      -5.233935    -1.747008    -0.524752      26.69
 O      -5.618391     0.177395    -1.319718     226.77
 H      -5.118660     0.509518    -0.593447      29.62
 C      -6.274728    -1.812475    -2.424901     102.33
 O      -6.302730    -3.262613    -2.573840     254.20
 H      -5.464917    -3.457643    -2.979350      33.21
 H      -6.168008    -1.302277    -3.354842      28.81
 H      -7.297597    -1.528587    -1.950074      25.82
55
name = lig-ACN-frame_137
 C       3.063860     3.355773    -0.061268      40.47
 H       2.255001     4.039713    -0.398121      18.23
 C       3.968350     1.753308     1.468405      47.37
 H       3.807039     1.240958     2.431304      19.59
 C       5.122155     1.623022     0.720813      45.95
 O       6.297768     0.948765     0.962581     269.87
 C       6.340241     0.080763     2.067646     121.91
 H       6.080167     0.640599     3.024168      28.71
 H       7.311607    -0.423966     2.209597      25.88
 H       5.440169    -0.703364     1.902334      25.27
 C       5.251260     2.384618    -0.577926      19.70
 O       6.366709     2.486845    -1.343458     185.22
 H       7.117732     1.864990    -1.078275      27.26
 C       4.168102     3.253980    -0.932872      66.61
 H       4.265672     3.901826    -1.749701      26.11
 C       2.902543     2.631193     1.145430      47.12
 C       1.745974     2.813709     2.149990     100.59
 H       1.736284     3.905366     2.666262      19.69
 O       1.769388     1.926847     3.213918     314.59
 H       1.662927     1.021804     2.873446      23.47
 C       0.365281     2.658328     1.373974      89.74
 H       0.441577     3.338980     0.571304      19.26
 C      -0.748713     3.109974     2.372840      95.51
 O      -0.579319     4.482068     2.757875     296.00
 H       0.085515     5.112962     2.156995      26.98
 H      -0.870174     2.457075     3.315613      23.22
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 H      -1.781929     3.020874     1.904160      23.03
 C      -2.241342    -1.153050    -0.234984      68.58
 H      -2.657622    -2.084071     0.119822      19.81
 C      -2.079527     0.600721    -1.957179      29.53
 H      -2.220782     0.899078    -2.978228      17.32
 C      -1.100143     1.257355    -1.124978      21.09
 O      -0.531626     2.450357    -1.592719     229.53
 C      -1.065716     3.005081    -2.841123     122.80
 H      -0.367025     3.686176    -3.299663      24.89
 H      -0.865634     2.394960    -3.522805      29.97
 H      -2.163008     3.416979    -2.820869      26.36
 C      -0.643192     0.779269     0.103995      26.61
 O       0.352702     1.332930     0.894564     233.65
 C      -1.290604    -0.493878     0.548175      44.42
 H      -0.851226    -1.003612     1.287897      16.95
 C      -2.632183    -0.599265    -1.542147      43.74
 C      -3.739890    -1.325483    -2.299495      56.57
 H      -3.712574    -0.944147    -3.276879      26.33
 O      -3.477126    -2.768066    -2.351009     215.64
 H      -2.309206    -2.865820    -2.411138      21.59
 C      -5.155902    -1.192594    -1.544534      84.77
 H      -4.918953    -1.839701    -0.633224      26.60
 O      -5.591117     0.195167    -1.287773     226.19
 H      -4.926325     0.723517    -0.851393      28.32
 C      -6.236660    -1.812497    -2.462659     101.87
 O      -6.296123    -3.273433    -2.615231     242.81
 H      -5.374518    -3.617775    -2.832784      31.15
 H      -6.210004    -1.382964    -3.465092      28.37
 H      -7.280868    -1.544090    -2.030811      25.65
55
name = lig-ACN-frame_138
 C       3.048102     3.354300    -0.089171      49.05
 H       2.189724     3.920688    -0.452441      20.59
 C       3.974806     1.748228     1.498609      77.73
 H       4.030412     1.278277     2.473936      26.59
 C       5.150996     1.683895     0.637236      29.81
 O       6.342967     0.939497     0.960303     226.10
 C       6.305344     0.035404     2.170947     103.07
 H       6.073769     0.520028     3.175978      26.87
 H       7.386385    -0.471066     2.158018      24.24
 H       5.549707    -0.880373     1.957117      23.81
 C       5.201032     2.422301    -0.511630      28.33
 O       6.361445     2.427688    -1.346838     164.74
 H       7.133154     2.020953    -0.752904      25.16
 C       4.194858     3.257293    -0.911712      24.95
 H       4.261766     3.863219    -1.766809      22.77
 C       2.933428     2.642937     1.122843      58.63
 C       1.682783     2.795723     2.027694     121.11
 H       1.695772     3.920536     2.453086      18.69
 O       1.764936     1.944686     3.200204     244.10
 H       1.589082     0.924762     2.847528      14.78
 C       0.377784     2.695906     1.390495      94.35
 H       0.283675     3.348338     0.609063      20.45
 C      -0.801122     3.159005     2.379247      96.00
 O      -0.586864     4.518650     2.835156     239.57
 H      -0.003945     5.043334     1.987473      26.28
 H      -0.737753     2.560113     3.358653      22.13
 H      -1.766480     3.071047     1.766309      22.75
 C      -2.229642    -1.108404    -0.247992      66.42
 H      -2.697758    -2.044139     0.135403      20.24
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 C      -2.053116     0.592269    -1.911104      80.60
 H      -2.496825     1.094501    -2.725927      21.67
 C      -1.108384     1.328769    -1.171844      16.82
 O      -0.531339     2.512909    -1.651287     219.03
 C      -1.098936     2.998064    -2.895103     131.56
 H      -0.645784     3.931892    -2.896715      24.69
 H      -1.207393     2.388543    -3.601947      30.88
 H      -2.273307     3.262594    -2.691883      26.63
 C      -0.683212     0.707215     0.113827      34.87
 O       0.342088     1.260332     0.856197     175.68
 C      -1.236129    -0.461216     0.573480      17.57
 H      -1.052484    -0.774411     1.586771      17.76
 C      -2.632774    -0.639473    -1.476593      59.08
 C      -3.720917    -1.351174    -2.320387      50.53
 H      -3.899087    -0.950364    -3.299043      28.70
 O      -3.532194    -2.753171    -2.341300     230.60
 H      -2.448064    -2.988868    -2.592076      22.42
 C      -5.089727    -1.180293    -1.613197      87.35
 H      -5.130731    -1.654711    -0.604689      26.39
 O      -5.550941     0.154202    -1.292014     235.98
 H      -4.700235     0.722010    -1.004318      25.68
 C      -6.277539    -1.834603    -2.512646      96.72
 O      -6.266213    -3.271221    -2.631309     237.37
 H      -5.278060    -3.500152    -2.673084      30.18
 H      -6.165598    -1.306088    -3.503886      28.01
 H      -7.280141    -1.569002    -2.047921      25.72
55
name = lig-ACN-frame_139
 C       2.963826     3.351653    -0.126566      59.07
 H       2.207038     4.075194    -0.391687      23.39
 C       4.062217     1.788262     1.487800      51.91
 H       3.906460     1.174150     2.352982      19.77
 C       5.176120     1.658361     0.700847      24.15
 O       6.333135     0.913969     1.026645     227.19
 C       6.268491    -0.014978     2.158928     107.93
 H       6.121196     0.589538     3.092459      28.57
 H       7.462563    -0.378609     2.218138      24.68
 H       5.501131    -0.927605     2.112727      25.55
 C       5.287749     2.480845    -0.535727      13.23
 O       6.379259     2.342622    -1.326448     131.38
 H       7.183207     2.061134    -0.843593      22.55
 C       4.139268     3.310920    -0.897057      66.17
 H       4.303631     3.764591    -1.875134      22.41
 C       2.966985     2.598560     1.082572      34.27
 C       1.771348     2.815174     1.985251      85.88
 H       1.932770     3.856362     2.516528      21.47
 O       1.758620     1.912411     3.207195     238.08
 H       1.658878     0.907391     2.878648      20.00
 C       0.252162     2.727234     1.300699      85.29
 H       0.176389     3.242401     0.446671      21.12
 C      -0.809305     3.170950     2.329836      92.95
 O      -0.596045     4.533432     2.888287     276.11
 H      -0.377193     5.265575     2.176144      29.08
 H      -0.850888     2.438644     3.208914      23.43
 H      -1.897683     3.102920     1.909509      22.78
 C      -2.203543    -1.154793    -0.171207      71.58
 H      -2.655032    -2.098592     0.280063      20.37
 C      -2.104692     0.612106    -1.887510      48.00
 H      -2.463106     0.949709    -2.850688      18.13
 C      -1.094983     1.300706    -1.182451      10.49
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 O      -0.535540     2.508239    -1.677307     235.31
 C      -1.191696     3.088838    -2.891703     119.35
 H      -0.773577     3.941039    -3.244221      26.59
 H      -0.944284     2.556574    -3.651807      29.66
 H      -2.353257     3.178632    -2.580983      24.86
 C      -0.694021     0.803601     0.052445      50.22
 O       0.330816     1.252199     0.883500     168.13
 C      -1.278792    -0.448792     0.543565      50.71
 H      -0.972837    -0.779919     1.627188      17.73
 C      -2.617234    -0.613669    -1.444053      63.37
 C      -3.725412    -1.274768    -2.248043      42.76
 H      -3.564942    -0.865591    -3.268088      25.85
 O      -3.553987    -2.817944    -2.358487     228.20
 H      -2.633731    -2.945713    -2.651950      27.26
 C      -5.176913    -1.244491    -1.645864      98.18
 H      -5.039674    -1.961264    -0.816109      27.94
 O      -5.493674     0.139675    -1.376333     227.95
 H      -4.808819     0.606519    -0.742362      26.03
 C      -6.276063    -1.793767    -2.515274     110.62
 O      -6.212821    -3.264154    -2.632897     232.34
 H      -5.286807    -3.481937    -2.740297      31.30
 H      -6.313900    -1.359098    -3.582774      27.99
 H      -7.247438    -1.539738    -2.056039      27.17
55
name = lig-ACN-frame_140
 C       3.007884     3.336552    -0.148305      37.69
 H       2.133203     3.932253    -0.385198      17.82
 C       4.044873     1.807432     1.467702      45.69
 H       3.903710     1.226249     2.368204      15.76
 C       5.245752     1.710462     0.718356      27.77
 O       6.296135     0.869298     1.061437     262.52
 C       6.274109     0.007404     2.163224     102.46
 H       5.971798     0.466170     3.131701      28.54
 H       7.322989    -0.708760     2.263026      22.96
 H       5.442906    -0.772392     1.881365      25.82
 C       5.300245     2.472035    -0.460759      25.97
 O       6.419444     2.296492    -1.363803     166.24
 H       7.095441     1.807851    -0.923455      23.73
 C       4.207841     3.285935    -0.932059      55.92
 H       4.162140     3.983073    -1.810774      26.75
 C       2.918802     2.574359     1.039478      43.91
 C       1.750126     2.783032     2.072575     112.22
 H       1.795159     3.837615     2.506902      25.70
 O       1.752539     1.897947     3.146099     331.72
 H       1.729242     1.028891     2.816349      25.33
 C       0.354869     2.740676     1.242810      92.28
 H       0.310611     3.352641     0.418831      21.17
 C      -0.847057     3.201040     2.283937      95.35
 O      -0.627995     4.475023     2.938180     335.07
 H      -0.354628     5.029929     2.324209      36.52
 H      -0.759105     2.509193     3.162636      23.97
 H      -1.887310     3.216015     1.733191      22.38
 C      -2.223484    -1.182541    -0.152992      46.33
 H      -2.597651    -2.184425     0.223330      19.48
 C      -2.148664     0.594028    -1.899788      64.78
 H      -2.267553     0.800309    -2.981856      17.81
 C      -1.106004     1.332054    -1.240537      16.68
 O      -0.548221     2.511490    -1.712992     220.34
 C      -1.236283     3.130805    -2.871631     116.51
 H      -0.823412     4.049591    -2.792791      27.25
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 H      -1.149093     2.532810    -3.633546      30.54
 H      -2.417105     3.278709    -2.962162      27.18
 C      -0.686879     0.796454     0.090810      28.42
 O       0.251707     1.352097     0.930392     211.47
 C      -1.260726    -0.370976     0.533634      44.92
 H      -0.624262    -0.895995     1.433003      15.87
 C      -2.674619    -0.645488    -1.354858      38.80
 C      -3.714468    -1.376466    -2.227542      54.47
 H      -3.860922    -0.862422    -3.253365      27.22
 O      -3.519368    -2.804147    -2.381798     301.13
 H      -2.678503    -2.930625    -2.574236      32.29
 C      -5.151371    -1.237929    -1.657486      95.88
 H      -5.280503    -1.702100    -0.684790      28.13
 O      -5.481977     0.142188    -1.437488     252.29
 H      -5.108820     0.385325    -0.638954      29.56
 C      -6.303503    -1.823336    -2.557207     104.11
 O      -6.183988    -3.238789    -2.632723     247.22
 H      -5.271342    -3.386569    -2.939680      31.10
 H      -6.261997    -1.226579    -3.569137      28.40
 H      -7.232866    -1.647237    -2.064591      28.11
55
name = lig-ACN-frame_141
 C       3.090652     3.291738    -0.151621      62.65
 H       2.360284     3.896211    -0.711751      22.85
 C       3.982818     1.790121     1.479042      69.27
 H       4.038190     1.340588     2.474591      25.77
 C       5.207527     1.774852     0.747518      14.74
 O       6.344989     0.900340     1.017890     225.17
 C       6.151065    -0.064030     2.189808      99.31
 H       6.116403     0.490815     3.154786      25.73
 H       7.333988    -0.497124     2.131672      23.06
 H       5.356893    -0.880811     2.099104      24.79
 C       5.358158     2.444299    -0.528715      16.11
 O       6.412390     2.280526    -1.378422     146.47
 H       7.140353     1.713504    -0.924923      25.16
 C       4.284693     3.237702    -0.893287      52.93
 H       4.591831     3.795327    -1.839160      21.08
 C       2.911719     2.598298     1.081736      39.56
 C       1.705013     2.798016     2.003227     107.09
 H       1.846750     3.760840     2.520669      19.36
 O       1.745446     1.847950     3.129070     330.73
 H       1.676201     0.958481     2.786370      22.78
 C       0.401090     2.834711     1.351641      96.47
 H       0.574241     3.449808     0.493123      20.66
 C      -0.796596     3.190702     2.207272      96.14
 O      -0.663654     4.412149     2.966463     326.17
 H      -0.064854     5.046403     2.523255      30.22
 H      -0.999967     2.357874     2.877852      24.72
 H      -1.733507     3.184434     1.490109      22.91
 C      -2.202256    -1.109341    -0.141469      77.06
 H      -2.443041    -2.099264     0.276441      20.43
 C      -2.106371     0.492236    -1.891836      41.03
 H      -2.513113     0.849686    -2.872559      20.11
 C      -1.186459     1.306378    -1.203112      15.63
 O      -0.623871     2.495886    -1.742527     256.42
 C      -1.232450     3.169396    -2.867211     125.29
 H      -0.813109     4.113725    -3.043821      25.77
 H      -1.031808     2.862023    -3.794301      28.22
 H      -2.265998     3.193475    -2.407084      24.21
 C      -0.749616     0.865960     0.046266      31.01
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 O       0.181008     1.424238     0.942960     183.12
 C      -1.186875    -0.448221     0.536669      43.55
 H      -0.838285    -0.770661     1.688236      18.04
 C      -2.743935    -0.648448    -1.389797      42.24
 C      -3.772084    -1.432908    -2.209822      59.82
 H      -3.685545    -0.946224    -3.281650      25.94
 O      -3.432467    -2.821058    -2.401584     247.78
 H      -2.426331    -2.837942    -2.592491      26.09
 C      -5.201961    -1.228324    -1.592394      99.45
 H      -5.180342    -1.784050    -0.676472      28.11
 O      -5.510725     0.192361    -1.512365     258.08
 H      -5.094039     0.684130    -0.739223      26.30
 C      -6.286818    -1.815677    -2.534707     105.92
 O      -6.173132    -3.259779    -2.687333     224.36
 H      -5.243864    -3.495293    -3.028337      30.14
 H      -6.261176    -1.374249    -3.615052      27.55
 H      -7.249047    -1.608823    -2.169619      28.50
55
name = lig-ACN-frame_142
 C       3.138578     3.293030    -0.199149      73.63
 H       2.278090     3.959798    -0.452903      25.59
 C       4.049373     1.812797     1.517721      48.01
 H       3.827308     1.254804     2.452541      21.45
 C       5.223265     1.689546     0.737433      17.53
 O       6.285068     0.917222     1.054803     259.92
 C       6.149326    -0.042446     2.143628     104.80
 H       5.963596     0.527638     3.087325      26.94
 H       7.088348    -0.842488     2.234802      23.09
 H       5.225048    -0.642886     1.967215      26.84
 C       5.382216     2.360344    -0.488779      31.14
 O       6.443119     2.253735    -1.394096     225.23
 H       7.337220     1.872647    -0.955291      23.05
 C       4.360550     3.225271    -0.908933      61.14
 H       4.227467     3.719711    -1.907756      20.18
 C       2.965918     2.636851     1.057740      21.69
 C       1.799135     2.792812     2.067734      94.25
 H       1.942551     3.713260     2.565289      20.16
 O       1.732207     1.815850     3.125182     290.45
 H       1.632754     0.823417     2.710479      17.47
 C       0.381505     2.863850     1.292101      91.38
 H       0.269978     3.597716     0.451678      20.56
 C      -0.825722     3.224674     2.151359     100.75
 O      -0.696610     4.361665     3.008643     258.09
 H      -0.008488     5.097853     2.484299      27.06
 H      -1.008333     2.450178     2.843839      24.56
 H      -1.685268     3.453153     1.403206      22.98
 C      -2.187434    -1.135102    -0.137427      59.32
 H      -2.662026    -1.967353     0.321111      19.97
 C      -2.139724     0.484525    -1.955736      42.31
 H      -2.469870     0.887348    -2.941999      18.43
 C      -1.241822     1.301074    -1.212273      22.46
 O      -0.630978     2.445176    -1.733400     222.83
 C      -1.289931     3.219609    -2.838251     120.73
 H      -0.765108     4.168788    -2.692979      24.61
 H      -1.165720     2.575235    -3.575847      28.08
 H      -2.361193     3.437841    -2.957933      27.96
 C      -0.775282     0.872252     0.125726      41.81
 O       0.142425     1.465055     0.906873     191.26
 C      -1.169426    -0.391100     0.502361      40.62
 H      -0.872751    -0.797512     1.611897      18.93
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 C      -2.692694    -0.694276    -1.373931      41.99
 C      -3.775600    -1.366206    -2.196757      38.22
 H      -3.912254    -0.860262    -3.276504      25.67
 O      -3.347855    -2.874045    -2.390521     138.27
 H      -2.233609    -2.782522    -2.658882      20.77
 C      -5.232102    -1.238407    -1.580739      94.28
 H      -5.314723    -1.605214    -0.588032      27.76
 O      -5.563445     0.236225    -1.572371     207.98
 H      -4.773990     0.647972    -0.964069      24.71
 C      -6.275341    -1.842733    -2.524561     104.93
 O      -6.182251    -3.301098    -2.740817     238.48
 H      -5.232967    -3.441213    -2.940154      31.78
 H      -6.072662    -1.209350    -3.464244      27.97
 H      -7.265074    -1.683517    -2.188344      27.64
55
name = lig-ACN-frame_143
 C       3.131944     3.339498    -0.138914      56.85
 H       2.375662     4.016336    -0.607698      19.23
 C       4.103407     1.847798     1.523480      56.10
 H       4.030654     1.230070     2.440181      19.40
 C       5.233175     1.602088     0.705823      21.93
 O       6.334284     0.863457     1.117253     246.17
 C       6.059092    -0.032873     2.127109     120.18
 H       6.077001     0.362181     3.191462      28.14
 H       7.005648    -0.747179     2.023800      24.30
 H       5.161684    -0.630075     1.927704      28.27
 C       5.365471     2.362246    -0.516999      -2.76
 O       6.492558     2.217110    -1.393549     132.05
 H       7.280368     1.811599    -0.895234      23.27
 C       4.299909     3.192888    -0.962428      56.40
 H       4.602005     3.684883    -1.897712      24.43
 C       3.066920     2.632579     1.076212      34.58
 C       1.797738     2.811643     2.050779     104.91
 H       1.893115     3.673622     2.588245      25.03
 O       1.722104     1.820201     3.106259     304.50
 H       1.764565     0.809733     2.714012      19.78
 C       0.388917     2.867062     1.219510      61.07
 H       0.677000     3.408204     0.231657      18.09
 C      -0.926698     3.290387     2.155707      89.42
 O      -0.681807     4.377551     3.063695     261.70
 H      -0.351793     5.245344     2.448700      27.37
 H      -1.088661     2.428314     2.752073      25.73
 H      -1.891170     3.380058     1.525104      22.53
 C      -2.204941    -1.178971    -0.153130      58.21
 H      -2.545322    -2.034898     0.347064      19.81
 C      -2.166649     0.539796    -1.954565      64.47
 H      -2.316308     0.683540    -3.027109      19.94
 C      -1.244253     1.305368    -1.219762      21.74
 O      -0.698491     2.454109    -1.683112     239.27
 C      -1.287418     3.181581    -2.827311     119.04
 H      -0.659441     4.129654    -2.994349      24.48
 H      -1.111397     2.909328    -3.813112      27.93
 H      -2.255405     3.334137    -2.511205      29.23
 C      -0.827572     0.885719     0.053560      28.39
 O       0.198423     1.489879     0.867739     187.91
 C      -1.257529    -0.392074     0.559571      59.46
 H      -0.620470    -0.789214     1.442024      15.94
 C      -2.640016    -0.676474    -1.425232      49.80
 C      -3.731076    -1.441590    -2.140426      35.20
 H      -3.794056    -0.933596    -3.239960      24.96
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 O      -3.345271    -2.815655    -2.362062     166.17
 H      -2.232537    -2.799882    -2.695952      20.11
 C      -5.217812    -1.211438    -1.573849      95.12
 H      -5.295774    -1.568204    -0.574363      28.98
 O      -5.580880     0.197522    -1.618320     230.63
 H      -4.960948     0.749260    -1.055683      28.14
 C      -6.287016    -1.893763    -2.544993     109.18
 O      -6.169092    -3.297409    -2.782546     251.37
 H      -5.246396    -3.544117    -2.861452      33.69
 H      -6.278198    -1.395950    -3.550451      28.29
 H      -7.277321    -1.698887    -2.124395      27.36
55
name = lig-ACN-frame_144
 C       3.191567     3.370671    -0.135912      29.15
 H       2.337123     4.012407    -0.421857      19.37
 C       4.163733     1.810589     1.503164      49.67
 H       4.150141     1.486950     2.545351      24.41
 C       5.275555     1.651258     0.651472      16.63
 O       6.382828     0.877152     1.089467     206.73
 C       6.029181    -0.199295     2.205180     102.87
 H       6.030934     0.418599     3.144044      25.82
 H       6.873174    -0.945617     2.189095      24.80
 H       5.069244    -0.684236     2.102777      27.24
 C       5.381813     2.312770    -0.597996      22.08
 O       6.477701     2.201360    -1.355159     169.61
 H       7.146189     1.684281    -0.942480      26.25
 C       4.304028     3.135959    -0.970446      67.04
 H       4.319398     3.812461    -1.792223      29.02
 C       3.006818     2.694153     1.142277      25.73
 C       1.729743     2.818251     1.987348     113.88
 H       1.773440     3.728173     2.434972      22.31
 O       1.724197     1.857234     3.079717     303.78
 H       1.839854     0.965256     2.726473      22.21
 C       0.372858     2.864916     1.237288      81.56
 H       0.323018     3.690589     0.358511      19.22
 C      -0.868446     3.309761     2.108061      98.21
 O      -0.679911     4.424816     3.090564     306.84
 H      -0.500784     5.182668     2.619391      34.22
 H      -1.086991     2.472792     2.777045      24.81
 H      -1.740864     3.590438     1.472144      24.22
 C      -2.186280    -1.143199    -0.157029      48.70
 H      -2.396172    -2.166814     0.005776      20.46
 C      -2.161137     0.526101    -1.955267      48.77
 H      -2.435411     0.859464    -2.943268      16.85
 C      -1.263966     1.328321    -1.232614      27.25
 O      -0.684119     2.542073    -1.677702     248.20
 C      -1.270741     3.170030    -2.808907     131.32
 H      -0.845236     4.245005    -2.710156      22.41
 H      -1.301133     2.480533    -3.579673      27.92
 H      -2.273239     3.363473    -2.701997      29.91
 C      -0.808523     0.868723     0.085727      44.95
 O       0.232012     1.408123     0.764840     163.09
 C      -1.285597    -0.377116     0.566060      37.19
 H      -0.962962    -0.735997     1.530129      20.38
 C      -2.669389    -0.689385    -1.387463      46.53
 C      -3.698192    -1.411172    -2.192016      56.38
 H      -3.736041    -0.937323    -3.298363      27.02
 O      -3.385837    -2.816160    -2.306553     260.15
 H      -2.400517    -2.816573    -2.636662      25.48
 C      -5.179058    -1.260681    -1.630961      93.20
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 H      -5.237477    -1.712611    -0.664283      29.33
 O      -5.582539     0.142595    -1.659888     243.74
 H      -5.260053     0.539616    -0.900570      30.61
 C      -6.283339    -1.889035    -2.544767     104.70
 O      -6.148073    -3.339440    -2.794540     220.71
 H      -5.142749    -3.446415    -2.924139      30.83
 H      -6.257150    -1.274215    -3.437241      29.35
 H      -7.295689    -1.810893    -2.056753      26.69
55
name = lig-ACN-frame_145
 C       3.187655     3.335278    -0.073767      65.91
 H       2.511523     4.074100    -0.465634      24.16
 C       4.098183     1.898602     1.487648      63.92
 H       4.105307     1.381370     2.421883      23.97
 C       5.287480     1.664971     0.724769      -1.82
 O       6.363892     0.792552     1.105488     240.85
 C       6.060700    -0.220437     2.199892     108.89
 H       6.031973     0.207147     3.246467      26.32
 H       6.777104    -0.962967     2.159841      26.25
 H       5.111550    -0.592929     1.871210      26.73
 C       5.326083     2.255716    -0.587508      13.73
 O       6.506211     2.186278    -1.406029     203.83
 H       7.216392     1.688328    -0.940340      25.84
 C       4.290547     3.174467    -0.968952      51.11
 H       4.333021     3.554556    -1.951188      22.44
 C       3.055162     2.676901     1.097381      42.09
 C       1.718957     2.861589     1.984285     108.22
 H       1.753076     3.746522     2.529481      23.04
 O       1.716034     1.918100     3.053779     334.66
 H       1.765684     1.065361     2.726097      27.61
 C       0.352269     2.814010     1.238366      78.65
 H       0.438073     3.423889     0.191000      18.13
 C      -0.803015     3.318946     2.150304     101.44
 O      -0.678368     4.421958     3.069686     328.87
 H      -0.188427     5.077690     2.616268      32.82
 H      -1.266190     2.488923     2.741987      25.79
 H      -1.558081     3.544944     1.382538      24.69
 C      -2.189480    -1.171285    -0.199384      68.77
 H      -2.491163    -2.086195     0.336970      20.02
 C      -2.160709     0.567466    -1.929951      47.50
 H      -2.680945     0.919021    -2.796611      22.56
 C      -1.232748     1.359124    -1.186088       7.74
 O      -0.662701     2.571038    -1.602395     226.72
 C      -1.348078     3.179577    -2.812129     121.82
 H      -0.672439     4.007794    -3.244551      23.93
 H      -1.019707     2.666971    -3.659022      27.17
 H      -2.315820     3.319519    -2.701995      29.39
 C      -0.810795     0.846950     0.055104      17.29
 O       0.294797     1.424089     0.709209     203.71
 C      -1.284223    -0.362739     0.591795      39.39
 H      -0.964012    -0.670303     1.492213      17.21
 C      -2.695659    -0.615685    -1.419892      70.79
 C      -3.736409    -1.360030    -2.281307      50.38
 H      -3.726689    -0.924532    -3.372072      28.85
 O      -3.418403    -2.878839    -2.259821     232.83
 H      -2.608366    -2.963847    -2.554331      32.87
 C      -5.153358    -1.328284    -1.713824      98.27
 H      -5.101690    -1.704379    -0.690265      28.04
 O      -5.584577     0.076351    -1.642370     225.53
 H      -5.211208     0.484902    -0.786552      26.42
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 C      -6.257773    -1.941717    -2.545655     113.50
 O      -6.103897    -3.347039    -2.814677     229.18
 H      -5.155680    -3.516026    -3.076112      31.72
 H      -6.312473    -1.408350    -3.453151      30.45
 H      -7.253360    -1.737306    -1.990747      26.96
55
name = lig-ACN-frame_146
 C       3.156196     3.409344    -0.205668      34.84
 H       2.351868     4.033491    -0.491397      19.91
 C       4.130290     1.855707     1.585729      48.74
 H       3.871766     1.284276     2.440752      18.70
 C       5.271086     1.630494     0.761977      18.43
 O       6.295502     0.751545     1.142378     239.75
 C       6.050104    -0.202394     2.101464     141.01
 H       6.102408     0.264339     3.117295      28.71
 H       6.837829    -0.774230     1.985475      27.64
 H       5.168564    -0.813563     2.086290      28.92
 C       5.384929     2.266705    -0.534467      16.29
 O       6.437643     2.164913    -1.441699     135.81
 H       7.304086     1.754566    -1.002989      23.31
 C       4.332252     3.113498    -0.948652      53.11
 H       4.444742     3.594701    -1.901705      26.19
 C       2.999510     2.698957     1.095672       9.51
 C       1.802718     2.875972     1.988862     110.28
 H       1.880616     3.869492     2.401803      25.38
 O       1.707751     1.946075     3.072249     276.42
 H       1.657708     0.973076     2.682832      20.52
 C       0.456804     2.797648     1.199956      81.83
 H       0.493867     3.642831     0.337857      19.30
 C      -0.889124     3.266103     2.111649      90.20
 O      -0.616105     4.401727     3.027825     256.57
 H       0.115479     5.064787     2.521070      28.00
 H      -1.099002     2.386257     2.808339      24.21
 H      -1.740295     3.532149     1.525205      25.17
 C      -2.222116    -1.126588    -0.183291      67.37
 H      -2.785089    -2.035220     0.190667      20.60
 C      -2.214512     0.679960    -1.887742      60.25
 H      -2.403483     1.073800    -2.887665      19.18
 C      -1.225693     1.386027    -1.184525      11.07
 O      -0.718718     2.615059    -1.586595     226.22
 C      -1.268383     3.133584    -2.860899     128.13
 H      -0.960384     4.194862    -2.762871      24.24
 H      -1.357557     2.442697    -3.620875      29.38
 H      -2.236520     3.303799    -2.645145      31.04
 C      -0.734249     0.869849     0.064635      24.04
 O       0.342349     1.434414     0.731564     196.14
 C      -1.278694    -0.393083     0.537679      41.77
 H      -0.809032    -0.776636     1.317894      20.33
 C      -2.691725    -0.631863    -1.459181      53.71
 C      -3.700198    -1.463652    -2.304920      56.50
 H      -3.640979    -1.171304    -3.401213      25.83
 O      -3.455141    -2.869898    -2.248459     259.93
 H      -2.509219    -2.938671    -2.530297      28.92
 C      -5.140586    -1.295264    -1.715672      94.31
 H      -5.107882    -1.914560    -0.796091      29.41
 O      -5.599485     0.033304    -1.587666     211.14
 H      -4.941922     0.589489    -0.919361      24.66
 C      -6.241671    -2.004708    -2.599407     107.69
 O      -6.081073    -3.399401    -2.840726     242.11
 H      -5.160122    -3.495842    -3.045690      33.13
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 H      -6.339691    -1.427926    -3.454192      30.45
 H      -7.255409    -1.967515    -2.019647      25.85
55
name = lig-ACN-frame_147
 C       3.173599     3.333506    -0.197494      60.78
 H       2.478419     3.931116    -0.713165      21.24
 C       4.056591     1.862170     1.543688      76.28
 H       4.042971     1.418852     2.525567      23.79
 C       5.199158     1.618769     0.772273      19.02
 O       6.235956     0.791938     1.057656     223.52
 C       6.085774    -0.276166     2.153026     116.89
 H       6.036301     0.236226     3.111442      29.12
 H       6.834322    -0.888620     2.159904      28.48
 H       5.157786    -0.751517     1.910339      28.32
 C       5.393374     2.325666    -0.436147      12.16
 O       6.373526     2.123188    -1.432802     106.47
 H       7.235897     1.686311    -1.046205      22.18
 C       4.340906     3.109443    -0.940241      52.08
 H       4.559913     3.670280    -1.869482      24.54
 C       3.094069     2.711132     1.039620      35.07
 C       1.795711     2.864615     1.980006      98.40
 H       1.888278     3.803525     2.620952      22.90
 O       1.725586     1.953566     3.118717     251.00
 H       1.733472     0.931665     2.742383      21.41
 C       0.414744     2.903978     1.219999      70.26
 H       0.441021     3.514873     0.215463      19.89
 C      -0.825891     3.206211     2.076686     100.19
 O      -0.536016     4.340863     2.951900     240.39
 H      -0.094085     5.183052     2.278499      26.26
 H      -1.001296     2.336396     2.809863      24.05
 H      -1.668200     3.271099     1.450627      26.12
 C      -2.302592    -1.027705    -0.229301      49.59
 H      -2.437488    -2.096390     0.156141      20.16
 C      -2.252359     0.675712    -1.883625      54.82
 H      -2.563123     0.930057    -2.922351      19.10
 C      -1.260888     1.409616    -1.145640       7.02
 O      -0.751661     2.629269    -1.614741     232.78
 C      -1.306242     3.157467    -2.793772     135.63
 H      -0.684206     3.968428    -3.175994      25.19
 H      -0.853532     2.631437    -3.599480      27.58
 H      -2.311113     3.273267    -2.830474      29.89
 C      -0.689873     0.862056     0.073316      19.87
 O       0.394472     1.408294     0.769524     171.56
 C      -1.186368    -0.376948     0.475084      51.82
 H      -0.953437    -0.788983     1.402783      21.40
 C      -2.668858    -0.602950    -1.494267      34.43
 C      -3.668528    -1.454089    -2.291608      87.94
 H      -3.683537    -1.070848    -3.311278      25.40
 O      -3.421907    -2.904624    -2.240388     205.95
 H      -2.340308    -3.130793    -2.545390      23.67
 C      -5.163175    -1.366646    -1.729174      88.44
 H      -5.156380    -1.746209    -0.684043      27.72
 O      -5.620137     0.023032    -1.550238     233.04
 H      -4.988915     0.500324    -0.886472      26.83
 C      -6.251155    -2.003254    -2.622826     106.19
 O      -6.046107    -3.487950    -2.886238     207.02
 H      -5.061635    -3.645871    -2.991710      31.16
 H      -6.258633    -1.482675    -3.520224      29.52
 H      -7.275415    -1.883640    -2.108969      25.93
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name = lig-ACN-frame_148
 C       3.177925     3.263572    -0.201186      70.43
 H       2.351390     3.887919    -0.495998      26.22
 C       4.042778     1.866003     1.520617      57.36
 H       3.886376     1.458952     2.545627      23.80
 C       5.200974     1.627813     0.731944      12.59
 O       6.272390     0.710410     1.053595     229.60
 C       6.060577    -0.238066     2.142265     128.82
 H       5.939115     0.165892     3.114306      28.38
 H       6.932056    -0.766415     2.038713      26.83
 H       5.229022    -0.899445     1.970865      28.34
 C       5.356865     2.352487    -0.488640      23.47
 O       6.372643     2.059224    -1.361503     189.43
 H       7.064980     1.587340    -0.911004      24.49
 C       4.369857     3.205854    -0.942507      53.42
 H       4.405820     3.556897    -2.026812      21.85
 C       2.965319     2.705427     1.105986      21.82
 C       1.778438     2.903149     1.999850      90.08
 H       1.861979     3.993321     2.446646      20.37
 O       1.763487     1.933234     3.110630     279.34
 H       1.882314     1.028703     2.772178      24.39
 C       0.459177     2.813848     1.189754     101.98
 H       0.466952     3.533019     0.318576      21.20
 C      -0.715262     3.155596     2.090104     106.95
 O      -0.505383     4.300974     2.856071     295.24
 H      -0.319597     5.097797     2.232385      30.30
 H      -0.880877     2.257742     2.791179      23.85
 H      -1.597408     3.305923     1.545933      25.26
 C      -2.174783    -1.033736    -0.215670      59.49
 H      -2.596913    -2.010795     0.163690      21.86
 C      -2.218320     0.666643    -1.935175      77.81
 H      -2.633109     1.237092    -2.804782      23.43
 C      -1.303204     1.416944    -1.142291      22.81
 O      -0.780493     2.635620    -1.556488     206.00
 C      -1.241477     3.194828    -2.907593     116.42
 H      -0.925005     4.186648    -2.788824      25.24
 H      -1.130631     2.431387    -3.628030      26.67
 H      -2.306978     3.356052    -2.916558      28.00
 C      -0.677558     0.894698     0.017021      14.64
 O       0.396979     1.413857     0.781131     185.58
 C      -1.209985    -0.360191     0.472064      48.30
 H      -0.735338    -0.770391     1.407943      17.82
 C      -2.727087    -0.585971    -1.465246      55.47
 C      -3.720207    -1.418125    -2.277672      69.21
 H      -3.699231    -1.171457    -3.284470      31.17
 O      -3.340145    -2.936229    -2.234400     185.57
 H      -2.282429    -2.905179    -2.665933      23.27
 C      -5.172200    -1.382251    -1.687150      92.49
 H      -5.131313    -2.051027    -0.773887      28.45
 O      -5.648965    -0.015858    -1.591549     245.69
 H      -5.359931     0.364761    -0.789491      29.09
 C      -6.198631    -2.098252    -2.666181     111.53
 O      -6.041879    -3.497884    -2.912543     232.35
 H      -5.012963    -3.582659    -2.898443      31.29
 H      -6.137186    -1.554492    -3.585465      30.37
 H      -7.235187    -1.946239    -2.273680      27.71
55
name = lig-ACN-frame_149
 C       3.068695     3.338013    -0.165697      56.75
 H       2.287630     3.952014    -0.651436      23.69
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 C       4.079424     1.847026     1.555566      65.78
 H       4.036718     1.168145     2.453844      22.23
 C       5.216607     1.625868     0.744427       6.54
 O       6.236570     0.700749     1.038626     248.61
 C       6.056607    -0.221365     2.104145     130.33
 H       5.933922     0.366577     2.949487      29.17
 H       6.965929    -0.793925     2.333603      26.29
 H       5.230893    -0.892918     1.960298      27.70
 C       5.333378     2.284058    -0.529498       9.70
 O       6.452510     1.992544    -1.313827     144.66
 H       7.159878     1.533467    -0.845735      24.04
 C       4.289839     3.243735    -0.934636      37.60
 H       4.323958     3.769136    -1.960764      22.19
 C       3.002228     2.651107     1.079085      30.17
 C       1.781468     2.857158     2.005599     104.76
 H       1.680304     3.895717     2.606904      21.08
 O       1.804641     1.950203     3.080634     299.38
 H       1.897591     1.111647     2.719499      30.23
 C       0.522985     2.722210     1.168390     101.73
 H       0.579753     3.398604     0.321722      22.64
 C      -0.724930     3.063009     2.081834      98.36
 O      -0.496309     4.337711     2.841198     312.89
 H      -0.161852     4.927251     2.293550      35.49
 H      -0.759616     2.308276     2.939785      24.45
 H      -1.598986     3.003683     1.503939      26.56
 C      -2.146576    -1.125267    -0.258535      52.00
 H      -2.543804    -2.001673     0.254037      21.83
 C      -2.215668     0.683340    -1.920138      53.34
 H      -2.693606     1.046847    -2.857311      23.39
 C      -1.270301     1.433704    -1.211053      11.35
 O      -0.839422     2.706584    -1.580130     223.65
 C      -1.220294     3.215839    -2.879293     125.02
 H      -0.698732     4.064794    -3.112439      26.83
 H      -0.777386     2.779597    -3.788940      27.09
 H      -2.316263     3.290696    -2.852431      26.33
 C      -0.706076     0.890088     0.023856      24.34
 O       0.361727     1.383445     0.705533     209.98
 C      -1.181359    -0.293716     0.522641      42.00
 H      -0.638953    -0.776220     1.473109      18.59
 C      -2.723654    -0.557445    -1.418146      38.51
 C      -3.734346    -1.486783    -2.224446      79.17
 H      -3.793960    -1.096391    -3.164409      29.40
 O      -3.263291    -2.851916    -2.239557     246.38
 H      -2.338458    -2.859837    -2.629534      27.87
 C      -5.198117    -1.460446    -1.710417      95.92
 H      -5.285872    -1.792663    -0.625319      27.57
 O      -5.709824    -0.095997    -1.641156     230.23
 H      -5.302349     0.345592    -0.884501      28.79
 C      -6.159244    -2.103962    -2.721650     114.22
 O      -5.994271    -3.530541    -2.910697     236.82
 H      -5.074096    -3.784563    -3.006191      33.18
 H      -6.020318    -1.544131    -3.653075      29.30
 H      -7.172642    -1.990410    -2.368618      27.71
55
name = lig-ACN-frame_150
 C       3.117799     3.376848    -0.126981      54.44
 H       2.273485     4.071417    -0.391100      19.91
 C       4.097295     1.818360     1.534769      73.16
 H       3.898804     1.360934     2.539721      21.92
 C       5.209084     1.609378     0.710064      19.83
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 O       6.220795     0.733583     0.963741     208.99
 C       6.035351    -0.181372     2.170717     108.60
 H       5.755911     0.251513     3.053691      29.27
 H       7.048612    -0.758505     2.129002      24.63
 H       5.253358    -0.860440     1.868211      28.02
 C       5.276406     2.269633    -0.522411       8.11
 O       6.486147     1.987175    -1.328334      53.77
 H       7.210588     1.560023    -0.704389      24.20
 C       4.253698     3.130810    -0.906559      65.96
 H       4.505541     3.828910    -1.743063      26.62
 C       3.072044     2.667098     1.080650      30.41
 C       1.834101     2.756933     1.944436      99.32
 H       1.951825     3.865949     2.354933      23.39
 O       1.838358     1.910837     3.119680     256.56
 H       1.805811     0.889519     2.863544      21.80
 C       0.437557     2.745116     1.188487      87.98
 H       0.424625     3.423028     0.389408      21.94
 C      -0.698728     3.039283     2.125321     105.14
 O      -0.538675     4.332646     2.796022     298.98
 H      -0.018442     4.962454     2.235843      30.60
 H      -0.740931     2.223906     2.879663      24.82
 H      -1.660562     3.058313     1.641112      25.62
 C      -2.137331    -1.096769    -0.176148      45.58
 H      -2.256625    -2.113743     0.030573      20.32
 C      -2.288419     0.652905    -1.890620      50.97
 H      -2.550681     0.938435    -2.913065      20.41
 C      -1.237672     1.442749    -1.245835      11.57
 O      -0.844501     2.767369    -1.607401     202.48
 C      -1.183024     3.276640    -2.903159     120.86
 H      -0.820925     4.196245    -2.834270      26.90
 H      -0.917021     2.377499    -3.457442      26.53
 H      -2.256740     3.484591    -3.232098      26.56
 C      -0.779591     0.912933    -0.022285      18.74
 O       0.415083     1.323539     0.627251     158.96
 C      -1.228631    -0.376959     0.481101      42.72
 H      -0.838182    -0.681326     1.591226      18.98
 C      -2.684377    -0.615009    -1.388490      39.62
 C      -3.678643    -1.431564    -2.163700      79.50
 H      -3.732849    -1.064618    -3.126164      27.16
 O      -3.216657    -2.800550    -2.250182     305.68
 H      -2.371099    -2.760708    -2.480741      31.79
 C      -5.231091    -1.493648    -1.691018      88.91
 H      -5.339139    -2.167254    -0.755898      27.94
 O      -5.766945    -0.145597    -1.700357     217.66
 H      -5.123937     0.473850    -1.104417      26.31
 C      -6.135173    -2.139168    -2.759565     106.84
 O      -5.952471    -3.599719    -2.916813     231.47
 H      -5.015436    -3.602573    -3.140729      33.50
 H      -5.930619    -1.609636    -3.745340      28.51
 H      -7.131845    -1.938421    -2.520220      28.64
55
name = lig-ACN-frame_151
 C       3.239480     3.360368    -0.090298      42.18
 H       2.548013     4.202077    -0.380683      19.93
 C       4.091456     1.799235     1.514257      71.78
 H       4.061553     1.328759     2.504216      22.91
 C       5.167718     1.559260     0.683972      22.47
 O       6.256546     0.711615     1.011995     241.01
 C       6.021613    -0.144808     2.101341     124.38
 H       5.920442     0.429131     2.962742      29.27
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 H       7.107732    -0.675338     2.337282      24.67
 H       5.245505    -0.910885     1.997190      26.90
 C       5.351981     2.219952    -0.565900      17.72
 O       6.395763     2.062311    -1.335631      91.32
 H       7.181820     1.603785    -0.835164      23.06
 C       4.319768     3.118986    -0.974391      62.95
 H       4.345486     3.588467    -1.954018      25.96
 C       3.037167     2.637622     1.108283      39.80
 C       1.823824     2.754853     1.947070     101.82
 H       1.804747     3.753633     2.531117      23.76
 O       1.852115     1.858491     3.162172     210.59
 H       1.870611     0.833293     2.770615      21.63
 C       0.478773     2.690529     1.173919      80.31
 H       0.437101     3.426772     0.436778      22.87
 C      -0.738613     3.033016     2.207132     100.30
 O      -0.585235     4.316176     2.770478     257.10
 H      -0.044070     5.024283     2.053365      26.38
 H      -0.746294     2.363767     3.062744      25.20
 H      -1.656283     2.940734     1.608259      25.45
 C      -2.192786    -1.172004    -0.158521      47.03
 H      -2.492927    -2.109510     0.206417      20.34
 C      -2.267064     0.671468    -1.885076      50.40
 H      -2.771615     0.970605    -2.788065      22.90
 C      -1.349779     1.449062    -1.233873       9.59
 O      -0.883382     2.742477    -1.545821     178.58
 C      -1.152505     3.295563    -2.989528     108.65
 H      -0.608933     4.106152    -3.149823      26.85
 H      -0.717658     2.894130    -3.931277      26.35
 H      -2.277034     3.374655    -2.872716      24.46
 C      -0.729076     0.873250    -0.021799      25.28
 O       0.418697     1.363224     0.571991     185.64
 C      -1.213361    -0.307367     0.500208      45.09
 H      -0.666234    -0.730044     1.484144      18.78
 C      -2.688102    -0.606584    -1.368201      33.53
 C      -3.700315    -1.399344    -2.185911      77.66
 H      -3.700442    -0.925000    -3.148125      28.95
 O      -3.212281    -2.809655    -2.250416     257.14
 H      -2.354863    -2.870131    -2.598903      28.55
 C      -5.191788    -1.485879    -1.743258      89.17
 H      -5.283629    -1.922390    -0.672115      27.19
 O      -5.802075    -0.177806    -1.713672     218.12
 H      -5.314896     0.466824    -1.024635      25.73
 C      -6.103332    -2.228941    -2.832618     107.70
 O      -5.898754    -3.617622    -2.942166     220.62
 H      -4.930472    -3.860629    -3.142124      31.05
 H      -5.845104    -1.703797    -3.839278      28.25
 H      -7.103842    -2.112286    -2.588190      28.79
55
name = lig-ACN-frame_152
 C       3.299416     3.373174    -0.114228      51.52
 H       2.536092     4.084384    -0.499890      18.86
 C       4.080875     1.730797     1.518950      61.30
 H       3.999156     1.125587     2.403066      22.32
 C       5.215279     1.499455     0.654708      26.55
 O       6.282600     0.710020     1.008815     226.05
 C       6.089235    -0.147514     2.159142     114.17
 H       5.813647     0.371521     3.042414      29.17
 H       7.081376    -0.896269     2.271372      23.73
 H       5.187562    -0.767486     1.933750      26.81
 C       5.297872     2.205140    -0.560800      19.13
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 O       6.439306     2.107679    -1.438578     206.38
 H       7.121342     1.548997    -1.092791      26.49
 C       4.361641     3.118548    -1.000845      56.28
 H       4.423730     3.500547    -1.974813      26.38
 C       3.073114     2.629930     1.100956      29.48
 C       1.758152     2.774871     2.106976     106.54
 H       1.678750     3.803153     2.535616      24.48
 O       1.843014     1.818864     3.131983     280.80
 H       2.024138     0.904526     2.784087      24.37
 C       0.472191     2.674269     1.257544      91.56
 H       0.587147     3.436286     0.536406      23.09
 C      -0.728784     2.955617     2.188628     100.49
 O      -0.624562     4.359376     2.761765     241.58
 H      -0.321495     5.036871     1.945727      27.92
 H      -0.714039     2.294476     3.015075      26.08
 H      -1.746334     2.783200     1.722166      25.24
 C      -2.193279    -1.085886    -0.139193      59.66
 H      -2.635199    -1.922200     0.382035      22.37
 C      -2.322703     0.638145    -1.882745      62.10
 H      -2.807699     1.115488    -2.718276      24.05
 C      -1.362482     1.480673    -1.126577      10.61
 O      -0.900003     2.708673    -1.615728     187.03
 C      -1.134775     3.310323    -2.928258     107.09
 H      -0.749319     4.219776    -2.742445      24.89
 H      -0.910141     2.379205    -3.554648      23.21
 H      -2.236885     3.646994    -3.298576      24.26
 C      -0.719687     0.875926    -0.057703      20.28
 O       0.429626     1.421217     0.534639     202.73
 C      -1.211575    -0.364913     0.526070      41.31
 H      -0.620858    -0.745044     1.430259      18.87
 C      -2.756766    -0.588243    -1.357510      31.54
 C      -3.681937    -1.446364    -2.259290      77.64
 H      -3.674573    -1.081862    -3.325887      27.23
 O      -3.296065    -2.825432    -2.264414     250.59
 H      -2.284299    -2.770508    -2.613694      24.47
 C      -5.182512    -1.465021    -1.823327      91.17
 H      -5.197008    -2.028318    -0.804293      27.82
 O      -5.833736    -0.154878    -1.716841     230.48
 H      -5.575121     0.177862    -0.885619      30.23
 C      -6.008649    -2.254577    -2.854179     107.65
 O      -5.829854    -3.709523    -2.995912     230.44
 H      -4.844106    -3.753654    -2.989190      32.22
 H      -5.889469    -1.695707    -3.888461      28.50
 H      -7.022246    -2.096631    -2.600892      28.56
55
name = lig-ACN-frame_153
 C       3.200572     3.371574    -0.109982      51.14
 H       2.395354     4.055640    -0.378558      23.23
 C       4.074007     1.663917     1.440173      63.47
 H       3.898996     1.167578     2.371114      24.44
 C       5.231668     1.495661     0.657133      13.94
 O       6.358021     0.691873     1.009627     216.00
 C       6.098112    -0.195908     2.204247     107.06
 H       6.132816     0.347154     3.167196      26.85
 H       7.162280    -0.819316     2.181854      24.14
 H       5.240163    -0.919663     2.024782      25.77
 C       5.408500     2.177061    -0.642160      10.22
 O       6.469966     2.109037    -1.520361     154.87
 H       7.200968     1.593028    -1.131392      25.62
 C       4.340619     3.101020    -0.956052      47.63
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 H       4.521688     3.752015    -1.764055      25.39
 C       3.097978     2.681730     1.140097      26.30
 C       1.844886     2.765474     2.078429      95.73
 H       1.940840     3.658802     2.638947      22.57
 O       1.824406     1.772872     3.161016     302.25
 H       1.889979     0.944332     2.795395      27.60
 C       0.449915     2.760965     1.304325      84.06
 H       0.386933     3.584227     0.619103      22.74
 C      -0.743957     2.964658     2.212058     106.76
 O      -0.688200     4.321023     2.722152     322.85
 H      -0.525122     4.900327     2.065155      34.79
 H      -0.665948     2.327663     3.045082      25.58
 H      -1.719401     2.851237     1.592005      23.93
 C      -2.276984    -0.988726    -0.130003      45.97
 H      -2.480191    -2.051455     0.195378      19.86
 C      -2.370876     0.722737    -1.805895      60.79
 H      -2.683761     0.975651    -2.816334      20.90
 C      -1.417167     1.436624    -1.199534       9.63
 O      -0.934106     2.692347    -1.572492     217.26
 C      -1.162867     3.252743    -2.853471     123.26
 H      -0.465134     3.997885    -3.046992      25.70
 H      -0.644327     2.801198    -3.760629      26.35
 H      -2.346069     3.480043    -3.018391      24.23
 C      -0.716940     0.898535     0.024878      14.68
 O       0.468419     1.428729     0.525936     171.76
 C      -1.153577    -0.345560     0.493460      53.63
 H      -0.860154    -0.728333     1.431040      20.92
 C      -2.798822    -0.594708    -1.380812      28.09
 C      -3.688866    -1.426750    -2.285941      78.85
 H      -3.500717    -0.981860    -3.355173      23.33
 O      -3.363767    -2.868409    -2.285008     214.86
 H      -2.245259    -3.129278    -2.419096      22.61
 C      -5.180485    -1.485541    -1.872449      89.60
 H      -5.252553    -2.095126    -0.893711      27.28
 O      -5.833850    -0.162566    -1.722021     246.71
 H      -5.576312     0.297652    -0.914720      28.64
 C      -6.023551    -2.275339    -2.912954     101.48
 O      -5.726880    -3.739270    -3.040770     216.11
 H      -4.792705    -3.872400    -2.937675      33.64
 H      -5.767559    -1.825154    -3.972727      28.21
 H      -7.084940    -2.194798    -2.638891      27.61
55
name = lig-ACN-frame_154
 C       3.180078     3.307461    -0.080520      76.36
 H       2.598799     4.142369    -0.412092      27.18
 C       4.108241     1.686348     1.356637      60.41
 H       4.149018     1.098582     2.261127      24.62
 C       5.308393     1.498861     0.579811      19.91
 O       6.352338     0.653716     1.072531     252.90
 C       6.219507    -0.229887     2.161186     114.13
 H       6.100523     0.429636     3.093914      26.18
 H       7.137608    -0.978568     2.246882      24.46
 H       5.218642    -0.810591     2.192347      25.28
 C       5.385384     2.221253    -0.623807      19.51
 O       6.495184     2.077797    -1.559077     113.46
 H       7.348509     1.704511    -1.052108      24.44
 C       4.319870     3.132424    -0.881671      47.01
 H       4.379088     3.742735    -1.781866      21.59
 C       3.092306     2.604155     1.112874      41.34
 C       1.901060     2.764904     2.047485      98.25
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 H       1.914201     3.673586     2.520301      22.76
 O       1.812700     1.757292     3.172230     269.14
 H       1.752950     0.807794     2.814818      22.52
 C       0.527230     2.794796     1.268497      74.98
 H       0.516749     3.536404     0.441670      21.05
 C      -0.772301     2.976401     2.248139      95.86
 O      -0.777090     4.291133     2.733252     311.28
 H      -0.455381     4.895685     2.059113      30.40
 H      -0.856035     2.324987     3.095372      24.79
 H      -1.707332     2.621011     1.621587      23.62
 C      -2.285336    -1.022036    -0.143977      43.51
 H      -2.554677    -2.083757     0.224555      17.63
 C      -2.472118     0.722916    -1.862486      43.42
 H      -2.778056     1.110651    -2.848787      18.80
 C      -1.330616     1.429696    -1.126316       9.43
 O      -0.927103     2.684882    -1.474503     174.02
 C      -1.145141     3.225545    -2.862093     103.95
 H      -0.842250     4.241272    -2.706759      24.03
 H      -1.114923     2.327871    -3.546326      25.43
 H      -2.354502     3.542118    -2.885693      24.58
 C      -0.742816     0.949427     0.021908      22.11
 O       0.476922     1.491212     0.561405     181.50
 C      -1.226551    -0.293945     0.491207      46.81
 H      -0.690086    -0.718744     1.242180      21.03
 C      -2.801013    -0.524407    -1.366142      37.58
 C      -3.687643    -1.443481    -2.263880      63.19
 H      -3.692309    -1.024473    -3.386573      23.17
 O      -3.385365    -2.904331    -2.279801     209.94
 H      -2.274352    -2.935874    -2.486407      21.53
 C      -5.226209    -1.491767    -1.890679      87.05
 H      -5.218495    -1.977770    -0.848340      27.77
 O      -5.822721    -0.210045    -1.762619     223.12
 H      -5.209648     0.283375    -1.031314      26.25
 C      -6.023099    -2.346324    -3.018562     105.22
 O      -5.671135    -3.708665    -3.081559     229.95
 H      -4.655607    -3.631754    -2.985258      28.87
 H      -5.910929    -1.723542    -4.019683      28.33
 H      -7.150922    -2.303190    -2.811851      26.47
55
name = lig-ACN-frame_155
 C       3.235253     3.314182    -0.085895      39.34
 H       2.422622     3.994609    -0.270268      18.51
 C       4.223210     1.649943     1.396187      66.53
 H       4.017572     1.065974     2.304248      21.95
 C       5.328104     1.470042     0.601298      27.93
 O       6.366381     0.660798     0.995920     199.44
 C       6.240209    -0.218930     2.193401     105.13
 H       6.367148     0.221594     3.287605      25.80
 H       7.145350    -0.828757     2.048644      25.53
 H       5.341449    -0.920110     1.992144      25.99
 C       5.440476     2.250928    -0.627764      13.17
 O       6.452242     2.080379    -1.528898     118.65
 H       7.250037     1.620714    -1.036743      21.64
 C       4.388739     3.161693    -0.927471      55.99
 H       4.416998     3.673747    -1.942237      24.93
 C       3.070453     2.460513     1.065044      24.39
 C       1.843725     2.714652     2.091956     108.95
 H       2.002846     3.615831     2.523400      27.59
 O       1.816520     1.808914     3.138228     273.20
 H       1.938211     0.819424     2.671272      21.77
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 C       0.511273     2.737309     1.289916      93.03
 H       0.593553     3.689499     0.675104      21.75
 C      -0.706367     2.932821     2.171086      92.92
 O      -0.890326     4.328339     2.780018     234.65
 H      -0.254099     5.036992     2.143035      26.12
 H      -0.512545     2.223252     2.973605      24.42
 H      -1.696532     2.854350     1.576088      23.50
 C      -2.225482    -1.028478    -0.189215      55.53
 H      -2.588243    -1.994510     0.317462      21.41
 C      -2.356879     0.773171    -1.827866      69.88
 H      -2.945776     1.233103    -2.640051      24.63
 C      -1.425192     1.486215    -1.158066       7.36
 O      -0.874948     2.755067    -1.455123     213.98
 C      -1.278288     3.200560    -2.722771     122.05
 H      -0.496560     3.879552    -3.170325      23.14
 H      -0.800456     2.576227    -3.529480      25.15
 H      -2.478335     3.357760    -2.988779      23.53
 C      -0.742942     0.933524     0.042244       8.67
 O       0.419536     1.480554     0.580870     179.39
 C      -1.274890    -0.298708     0.548822      44.93
 H      -0.802719    -0.746163     1.363029      20.17
 C      -2.858307    -0.567502    -1.381263      37.93
 C      -3.776703    -1.482091    -2.246633      70.30
 H      -3.595393    -1.095576    -3.369401      24.79
 O      -3.300639    -2.853649    -2.244573     246.53
 H      -2.421013    -2.944653    -2.645503      26.38
 C      -5.268519    -1.566388    -1.920888     102.89
 H      -5.483856    -2.222044    -1.026238      28.46
 O      -5.811584    -0.220624    -1.824958     241.22
 H      -5.338945     0.411141    -1.148872      26.36
 C      -6.039677    -2.288544    -3.034959     101.35
 O      -5.619055    -3.689484    -3.168518     213.41
 H      -4.594583    -3.737651    -3.128465      29.99
 H      -5.792944    -1.788249    -4.047395      28.42
 H      -7.188489    -2.277277    -2.760075      26.39
55
name = lig-ACN-frame_156
 C       3.297646     3.258808    -0.094455      57.55
 H       2.533617     3.920179    -0.491908      17.00
 C       4.147333     1.596168     1.499437      57.59
 H       4.248108     1.018216     2.428801      21.00
 C       5.309737     1.511078     0.639513       8.52
 O       6.432358     0.654613     0.930105     213.16
 C       6.302032    -0.241624     2.096987     109.68
 H       6.238960     0.553151     3.029650      25.90
 H       7.153228    -0.805167     2.116596      27.28
 H       5.356893    -0.905859     2.214794      24.92
 C       5.432608     2.244951    -0.571416      14.61
 O       6.463085     2.084407    -1.499653     155.29
 H       7.164391     1.504082    -1.225219      22.61
 C       4.421211     3.155942    -0.958072      69.82
 H       4.597822     3.831907    -1.889315      27.05
 C       3.105610     2.444590     1.050314      39.39
 C       1.889193     2.682010     1.979271     109.41
 H       1.968772     3.609770     2.430415      28.70
 O       1.837361     1.776343     3.159220     258.79
 H       1.989894     0.791628     2.934033      23.26
 C       0.500712     2.785439     1.287110      68.47
 H       0.488136     3.454512     0.334356      20.06
 C      -0.714977     3.010361     2.192806      95.76
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 O      -0.941490     4.292950     2.788412     279.46
 H      -0.209505     5.047729     2.459683      27.14
 H      -0.803658     2.301478     3.062803      24.51
 H      -1.590952     2.595260     1.546361      25.29
 C      -2.238976    -1.041082    -0.189907      68.52
 H      -2.489308    -2.092366     0.087185      19.86
 C      -2.395050     0.719765    -1.802459      64.36
 H      -2.824457     1.167305    -2.707780      21.47
 C      -1.382288     1.546297    -1.030456      12.00
 O      -0.887519     2.797441    -1.443446     193.32
 C      -1.256627     3.191927    -2.798474     101.94
 H      -0.971232     4.326732    -2.792347      21.52
 H      -1.289503     2.272382    -3.407495      24.06
 H      -2.480154     3.520068    -2.677427      23.94
 C      -0.815215     0.910432     0.048888      31.06
 O       0.361394     1.414778     0.582157     178.02
 C      -1.255040    -0.301146     0.550163      45.90
 H      -1.005954    -0.579316     1.584689      19.36
 C      -2.811206    -0.534272    -1.381594      24.07
 C      -3.750320    -1.475910    -2.249213      53.67
 H      -3.851874    -0.957295    -3.309781      26.66
 O      -3.192207    -2.821793    -2.205718     296.59
 H      -2.358578    -2.777730    -2.451633      31.28
 C      -5.301206    -1.576335    -1.921870      95.83
 H      -5.423012    -2.017314    -0.906789      28.68
 O      -5.835680    -0.217771    -1.896802     259.76
 H      -5.542121     0.064367    -1.080431      30.98
 C      -6.018846    -2.272895    -3.090407     106.55
 O      -5.628656    -3.674460    -3.261592     241.93
 H      -4.677729    -3.616491    -3.125225      33.16
 H      -5.914728    -1.593770    -4.000674      28.93
 H      -7.201576    -2.293656    -2.864622      25.99
55
name = lig-ACN-frame_157
 C       3.281490     3.193433    -0.141203      73.21
 H       2.540475     3.978650    -0.343518      26.94
 C       4.160374     1.579037     1.478933      69.48
 H       3.908223     1.116213     2.434082      23.70
 C       5.335849     1.487283     0.704234      22.61
 O       6.426919     0.635049     0.871409     250.69
 C       6.371627    -0.179176     2.013531     109.18
 H       6.257153     0.424823     3.114930      24.85
 H       7.185380    -0.752096     2.123510      26.92
 H       5.446134    -0.817166     1.810900      25.79
 C       5.438941     2.219171    -0.554489      18.31
 O       6.502949     2.082832    -1.463103     183.39
 H       7.191301     1.575569    -1.014973      25.37
 C       4.466851     3.118545    -0.888324      51.93
 H       4.555098     3.821454    -1.798607      18.93
 C       3.151396     2.483552     1.078779      36.85
 C       1.905989     2.669265     1.936356      97.49
 H       2.074972     3.618351     2.386300      22.54
 O       1.869313     1.757129     3.154810     279.68
 H       1.826419     0.921951     2.801767      27.68
 C       0.516990     2.713537     1.197566      89.00
 H       0.515170     3.684249     0.487028      19.67
 C      -0.791345     3.001687     2.237480      87.36
 O      -0.963340     4.309919     2.791669     339.89
 H      -0.321039     4.843341     2.510966      33.96
 H      -0.621630     2.186885     3.033543      23.17
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 H      -1.731122     2.947291     1.593356      22.99
 C      -2.256738    -1.099563    -0.152785      46.81
 H      -2.480393    -2.083099     0.198919      19.97
 C      -2.403846     0.820938    -1.771228      68.43
 H      -2.699532     1.079308    -2.771626      21.10
 C      -1.463932     1.510860    -1.077903      13.44
 O      -0.907982     2.765825    -1.438066     186.69
 C      -1.384635     3.264666    -2.771300     100.30
 H      -0.605064     4.081079    -3.235778      22.70
 H      -1.076179     2.679976    -3.644672      26.57
 H      -2.618265     3.383245    -2.757418      23.29
 C      -0.835300     0.954637     0.117576      26.13
 O       0.355876     1.377772     0.667868     171.50
 C      -1.330331    -0.342654     0.546213      51.00
 H      -0.726709    -0.798769     1.443347      17.37
 C      -2.773479    -0.534349    -1.361081      44.65
 C      -3.670488    -1.396798    -2.230467      57.97
 H      -3.524407    -1.132147    -3.337019      24.41
 O      -3.140131    -2.780653    -2.193571     240.28
 H      -2.166942    -2.823933    -2.390203      25.71
 C      -5.256234    -1.518286    -1.906979      88.91
 H      -5.457299    -2.105134    -0.998916      29.12
 O      -5.862633    -0.217619    -1.933844     248.16
 H      -5.890310     0.325980    -1.108798      27.98
 C      -6.034565    -2.296341    -3.104983     102.70
 O      -5.644424    -3.629066    -3.363095     260.01
 H      -4.710519    -3.726376    -3.182823      34.60
 H      -5.785518    -1.702930    -4.016491      29.15
 H      -7.221637    -2.282168    -2.881807      26.71
55
name = lig-ACN-frame_158
 C       3.237885     3.220719    -0.121507      59.81
 H       2.457474     3.944624    -0.429501      25.89
 C       4.210705     1.598991     1.448601      68.31
 H       4.148433     0.919963     2.283731      22.80
 C       5.355077     1.461951     0.636125      26.92
 O       6.441272     0.662417     0.848094     235.18
 C       6.391552    -0.227799     1.989332     112.26
 H       6.232185     0.415400     3.063521      25.91
 H       7.365393    -0.613252     1.919763      26.89
 H       5.646118    -1.058202     1.989569      26.91
 C       5.498934     2.188280    -0.532539      17.33
 O       6.555679     2.071508    -1.372599     138.22
 H       7.443228     1.629946    -1.025857      21.40
 C       4.442432     3.118135    -0.866755      70.99
 H       4.630713     3.625245    -1.848086      19.49
 C       3.133531     2.468758     1.065948      36.29
 C       1.874295     2.695918     2.037998     104.57
 H       1.870667     3.684037     2.527065      23.99
 O       1.897769     1.778869     3.066218     289.83
 H       1.689007     0.850040     2.768072      24.83
 C       0.448558     2.699103     1.294968      83.82
 H       0.536046     3.330587     0.264251      19.33
 C      -0.757423     2.941313     2.157259      85.02
 O      -0.939489     4.348204     2.822810     281.47
 H      -0.268761     4.948881     2.423654      29.04
 H      -0.753956     2.242161     3.105747      23.51
 H      -1.678660     2.554891     1.659889      24.70
 C      -2.278072    -1.083189    -0.140295      57.52
 H      -2.617875    -2.043656     0.132329      21.00
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 C      -2.448680     0.767518    -1.771765      52.37
 H      -2.860747     1.195564    -2.663583      20.78
 C      -1.444608     1.542726    -1.041841      10.90
 O      -0.971352     2.734560    -1.528195     184.72
 C      -1.403446     3.292275    -2.760091     103.32
 H      -0.938152     4.426385    -2.610455      21.50
 H      -1.264782     2.479794    -3.429837      25.24
 H      -2.586016     3.694692    -2.912205      24.14
 C      -0.910695     0.910870     0.142131      35.01
 O       0.340513     1.356507     0.739996     169.44
 C      -1.299974    -0.326678     0.577845      40.95
 H      -0.633749    -0.927075     1.356640      17.77
 C      -2.810294    -0.510641    -1.324420      22.18
 C      -3.598333    -1.388498    -2.261388      76.51
 H      -3.577427    -0.847114    -3.236172      26.35
 O      -3.163715    -2.760849    -2.173238     205.24
 H      -2.138009    -2.801012    -2.670559      21.39
 C      -5.179437    -1.486955    -1.978477      87.13
 H      -5.242645    -1.931861    -0.990441      28.91
 O      -5.915596    -0.184515    -1.968990     196.44
 H      -5.611130     0.183016    -0.991099      25.06
 C      -5.963684    -2.209149    -3.095144     103.34
 O      -5.656562    -3.649883    -3.434579     211.14
 H      -4.632309    -3.658840    -3.274100      31.40
 H      -5.931550    -1.568238    -3.979758      28.84
 H      -7.100200    -2.211945    -2.746696      26.28
55
name = lig-ACN-frame_159
 C       3.281123     3.253696    -0.095153      39.46
 H       2.496714     3.883101    -0.555079      15.94
 C       4.186004     1.612400     1.426705      59.95
 H       4.147879     1.027373     2.328813      22.84
 C       5.320407     1.454851     0.581021      10.52
 O       6.452725     0.628206     0.900403     235.72
 C       6.485453    -0.310529     1.983924     106.94
 H       6.247228     0.343762     3.036473      25.56
 H       7.489434    -0.785446     2.189879      25.14
 H       5.733532    -1.067877     1.842065      27.65
 C       5.475984     2.279697    -0.564893       8.23
 O       6.626505     2.112639    -1.353359     154.23
 H       7.237585     1.420519    -0.826752      17.31
 C       4.435095     3.089291    -0.932532      67.74
 H       4.458447     3.703927    -1.807704      29.95
 C       3.066893     2.483719     1.101181      31.25
 C       1.844310     2.739540     2.017014     103.19
 H       2.046169     3.727590     2.539029      25.02
 O       1.898356     1.737956     3.097967     238.50
 H       1.856402     0.789664     2.542245      20.77
 C       0.470094     2.697384     1.331156      74.68
 H       0.371324     3.600596     0.531300      19.73
 C      -0.764768     2.999498     2.245548      95.62
 O      -0.874285     4.273145     2.775369     276.87
 H      -0.374088     5.076925     2.124800      26.27
 H      -0.672635     2.223742     3.142696      23.09
 H      -1.628439     2.882337     1.603234      24.01
 C      -2.316391    -1.036299    -0.121242      59.82
 H      -2.442786    -2.080700     0.168041      20.14
 C      -2.446424     0.768761    -1.714604      56.82
 H      -2.956546     1.179532    -2.566961      22.84
 C      -1.508151     1.484871    -1.021600      17.79
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 O      -1.007521     2.720485    -1.506118     205.99
 C      -1.459237     3.345693    -2.757100     102.41
 H      -0.781150     4.343363    -3.025853      21.71
 H      -1.218496     2.997590    -3.728228      26.18
 H      -2.653510     3.401040    -2.522872      22.93
 C      -0.843442     0.934006     0.133755      26.46
 O       0.273549     1.288478     0.785970     172.80
 C      -1.279817    -0.379952     0.575897      53.93
 H      -0.886739    -0.670025     1.635670      18.28
 C      -2.856547    -0.493707    -1.296374      41.66
 C      -3.660418    -1.343311    -2.323155      89.48
 H      -3.430409    -1.099794    -3.333778      27.10
 O      -3.201844    -2.746508    -2.218187     187.78
 H      -2.130265    -2.849901    -2.651825      21.94
 C      -5.121625    -1.441102    -2.040272     101.15
 H      -5.255051    -1.980662    -1.120932      28.85
 O      -5.872287    -0.177165    -1.953288     244.64
 H      -5.591021     0.401186    -1.175907      27.77
 C      -5.928162    -2.203096    -3.111298     111.59
 O      -5.646444    -3.579988    -3.457439     233.83
 H      -4.657910    -3.734745    -3.430238      32.59
 H      -5.899841    -1.577198    -3.992621      29.40
 H      -6.989447    -2.237085    -2.680721      27.00
55
name = lig-ACN-frame_160
 C       3.287288     3.251628    -0.123672      43.69
 H       2.514752     4.014707    -0.288147      20.62
 C       4.106911     1.608576     1.424147      65.28
 H       3.973847     1.144946     2.394829      23.43
 C       5.292759     1.444832     0.644230      13.46
 O       6.457150     0.625044     0.913003     228.48
 C       6.487113    -0.352369     2.027711     100.32
 H       6.163757     0.012584     3.141083      26.30
 H       7.622489    -0.698357     1.876401      24.93
 H       5.886501    -1.189870     1.779465      28.27
 C       5.500690     2.248541    -0.598811       2.01
 O       6.627882     2.205309    -1.347465     210.66
 H       7.294104     1.516667    -1.111258      22.70
 C       4.384087     3.138551    -0.994934      65.90
 H       4.486361     3.718540    -1.850926      28.70
 C       3.122361     2.532809     1.060554      42.57
 C       1.893602     2.667887     2.014796      93.36
 H       1.881685     3.714030     2.559972      21.54
 O       1.872635     1.700178     3.134305     265.54
 H       2.020449     0.737303     2.825845      22.92
 C       0.449210     2.706357     1.341114      68.72
 H       0.533746     3.402421     0.374191      17.75
 C      -0.769029     2.960198     2.279383      91.24
 O      -0.773672     4.319766     2.783131     276.60
 H      -0.423177     4.926143     1.925850      26.08
 H      -0.906149     2.236007     3.206792      22.97
 H      -1.648105     2.687248     1.713118      24.84
 C      -2.317397    -1.081004    -0.105616      49.73
 H      -2.686144    -2.101268     0.252418      20.80
 C      -2.516803     0.814061    -1.686799      55.18
 H      -2.772689     1.186655    -2.692840      19.07
 C      -1.460762     1.511202    -1.024579      13.05
 O      -0.963296     2.726363    -1.471888     165.64
 C      -1.542034     3.369938    -2.732815      95.83
 H      -1.048405     4.428778    -2.547874      22.15
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 H      -1.334091     2.617864    -3.415464      26.45
 H      -2.713344     3.721092    -2.882156      24.25
 C      -0.833598     0.859461     0.108868      20.94
 O       0.303416     1.363956     0.848953     176.33
 C      -1.358277    -0.328917     0.573182      41.05
 H      -0.943918    -0.773472     1.487466      19.09
 C      -2.891127    -0.542408    -1.321113      28.54
 C      -3.622383    -1.343668    -2.348903      84.09
 H      -3.526688    -0.815968    -3.240762      26.88
 O      -3.238756    -2.748888    -2.293281     251.12
 H      -2.225533    -2.741459    -2.406453      26.53
 C      -5.186950    -1.437463    -2.027499      94.81
 H      -5.212384    -1.999906    -1.116438      29.35
 O      -5.791368    -0.155819    -1.958769     278.40
 H      -5.531266     0.232509    -1.173260      30.85
 C      -5.979241    -2.174975    -3.180379     114.83
 O      -5.611697    -3.528874    -3.453422     257.87
 H      -4.673401    -3.514376    -3.443300      33.25
 H      -5.880193    -1.575556    -4.072144      29.75
 H      -7.044716    -2.167930    -2.904133      28.47
55
name = lig-ACN-frame_161
 C       3.236025     3.327726    -0.181767      78.05
 H       2.593379     4.157611    -0.497402      29.61
 C       4.151903     1.567002     1.424700      66.36
 H       4.087490     0.890346     2.292312      23.43
 C       5.321030     1.467920     0.642689      30.79
 O       6.390337     0.674691     0.972681     257.50
 C       6.454299    -0.393013     1.967384     107.16
 H       6.258963     0.147732     2.993366      26.36
 H       7.649144    -0.693867     2.136051      23.88
 H       5.854974    -1.268331     1.833511      27.27
 C       5.388007     2.190137    -0.544072      20.21
 O       6.618663     2.304962    -1.380385     214.01
 H       7.262307     1.723972    -1.024501      25.63
 C       4.443521     3.108035    -0.963711      31.66
 H       4.622256     3.645237    -1.847715      16.04
 C       3.122729     2.521163     1.067747      21.71
 C       1.874360     2.610661     2.065439      98.31
 H       2.061504     3.645827     2.651065      20.36
 O       1.872634     1.688198     3.153017     292.61
 H       1.811073     0.856160     2.800035      28.08
 C       0.457937     2.654107     1.360555      94.10
 H       0.366599     3.507664     0.575865      19.65
 C      -0.748790     2.952297     2.265314      95.15
 O      -0.687305     4.381104     2.799267     320.20
 H      -0.277250     4.970814     2.215071      33.22
 H      -0.520712     2.338438     3.213883      23.43
 H      -1.666094     2.765606     1.784427      25.74
 C      -2.389580    -1.104901    -0.167206      55.61
 H      -2.739567    -2.120398     0.279071      20.77
 C      -2.500230     0.793547    -1.673090      49.31
 H      -2.976672     1.186547    -2.611982      20.88
 C      -1.431918     1.508240    -1.023633      11.18
 O      -0.977525     2.784214    -1.445229     203.80
 C      -1.550429     3.341996    -2.622582     112.56
 H      -0.964238     4.255177    -3.014361      24.20
 H      -1.358063     2.854754    -3.560232      27.23
 H      -2.751376     3.383484    -2.399149      24.25
 C      -0.814796     0.923221     0.131526      12.80
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 O       0.301338     1.322124     0.806869     186.36
 C      -1.406705    -0.344649     0.618963      40.12
 H      -0.894277    -0.782971     1.415658      18.82
 C      -2.834008    -0.498324    -1.326770      35.17
 C      -3.704960    -1.366415    -2.321282      81.54
 H      -3.589955    -1.016725    -3.273021      27.64
 O      -3.226944    -2.743562    -2.402609     274.22
 H      -2.376012    -2.838154    -2.438447      33.50
 C      -5.238681    -1.488281    -2.056193     100.29
 H      -5.486894    -1.981284    -1.150098      29.20
 O      -5.728705    -0.100296    -1.965302     246.23
 H      -5.651048     0.259444    -0.987899      26.19
 C      -6.039771    -2.084231    -3.244377     114.41
 O      -5.576202    -3.511418    -3.446904     203.74
 H      -4.575587    -3.472558    -3.345568      29.21
 H      -5.846871    -1.430512    -4.080136      29.42
 H      -7.060642    -2.114170    -3.048990      29.71
55
name = lig-ACN-frame_162
 C       3.271591     3.284003    -0.096690      42.39
 H       2.476550     3.930996    -0.455841      18.16
 C       4.126356     1.594217     1.387217      60.33
 H       3.908855     0.930882     2.250971      19.76
 C       5.299693     1.439405     0.638496      27.56
 O       6.421339     0.679616     0.995039     255.36
 C       6.391293    -0.333771     1.979654     111.05
 H       6.025983    -0.053887     2.991321      27.63
 H       7.520210    -0.828158     1.896340      24.05
 H       5.724448    -1.099028     1.561261      27.45
 C       5.478961     2.222396    -0.600771      14.03
 O       6.536050     2.344900    -1.344546     211.55
 H       7.324662     1.760205    -1.065509      22.46
 C       4.383028     3.103108    -0.883713      92.15
 H       4.586179     3.714308    -1.773825      28.58
 C       3.061682     2.487964     1.035943      40.75
 C       1.865123     2.650594     2.059673      93.06
 H       1.935044     3.741068     2.588581      23.81
 O       1.892450     1.644215     3.162535     267.99
 H       1.610545     0.759349     2.762602      22.79
 C       0.486776     2.664842     1.357874      78.51
 H       0.632821     3.336766     0.479282      19.94
 C      -0.642821     3.068868     2.368668     107.14
 O      -0.627800     4.366502     2.814698     383.81
 H      -0.006350     4.807111     2.370643      34.19
 H      -0.717843     2.320165     3.215593      24.74
 H      -1.563560     2.917421     1.879614      26.20
 C      -2.360653    -1.027380    -0.118935      48.15
 H      -2.586621    -2.135066     0.066864      20.69
 C      -2.402520     0.818784    -1.720741      70.67
 H      -3.000730     1.366089    -2.504947      21.23
 C      -1.445048     1.521200    -1.012573      11.01
 O      -0.948225     2.785882    -1.384248     197.71
 C      -1.576063     3.306955    -2.599234     108.12
 H      -1.200978     4.325462    -2.618378      23.91
 H      -1.619143     2.530471    -3.352834      24.67
 H      -2.774033     3.606112    -2.384092      24.11
 C      -0.927121     0.871308     0.171281      25.68
 O       0.320228     1.246155     0.728255     168.06
 C      -1.392873    -0.359817     0.585317      51.49
 H      -1.090929    -0.684914     1.513867      21.97
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 C      -2.894701    -0.558247    -1.363042      32.91
 C      -3.762576    -1.386024    -2.329405      84.76
 H      -3.747240    -0.834182    -3.191588      29.41
 O      -3.210610    -2.776560    -2.474339     227.19
 H      -2.274221    -2.569404    -2.826308      26.43
 C      -5.321250    -1.419902    -2.052029     104.26
 H      -5.523625    -2.085012    -1.242238      30.44
 O      -5.689250    -0.037084    -1.978910     253.29
 H      -5.886215     0.272891    -0.942804      24.72
 C      -6.002022    -2.094604    -3.291125     122.68
 O      -5.600809    -3.432835    -3.463940     229.05
 H      -4.606206    -3.488027    -3.214520      28.41
 H      -5.806826    -1.563188    -4.212743      30.39
 H      -6.992171    -2.101162    -3.081984      31.73
55
name = lig-ACN-frame_163
 C       3.211497     3.221019    -0.029941      46.76
 H       2.476250     3.984934    -0.280897      16.16
 C       4.078184     1.556073     1.381422      60.17
 H       4.043800     1.034590     2.356060      22.07
 C       5.281830     1.444305     0.590823      17.24
 O       6.493710     0.750532     0.970730     243.56
 C       6.264679    -0.363559     1.945487     115.43
 H       6.067434     0.050057     2.900202      29.06
 H       7.352797    -0.854425     2.106501      24.42
 H       5.485539    -1.169619     1.708276      25.32
 C       5.402141     2.289414    -0.484740       5.79
 O       6.594863     2.343742    -1.372984     164.39
 H       7.251329     1.549846    -1.122802      23.04
 C       4.370535     3.139013    -0.870933      56.02
 H       4.360369     3.854849    -1.755881      23.43
 C       3.032587     2.429293     1.109749      41.27
 C       1.888992     2.591710     2.029099     109.06
 H       2.009964     3.604059     2.661659      23.13
 O       1.911033     1.648377     3.121070     255.64
 H       1.703891     0.649915     2.695074      18.38
 C       0.526610     2.617521     1.329961      92.11
 H       0.392104     3.345834     0.571479      18.45
 C      -0.628005     3.010335     2.350115      91.88
 O      -0.540542     4.429363     2.900175     310.17
 H       0.052834     5.062106     2.322353      29.45
 H      -0.565625     2.397090     3.233140      24.57
 H      -1.526921     2.861849     1.831689      25.60
 C      -2.398704    -1.087099    -0.191686      58.97
 H      -2.651590    -2.063981     0.250481      20.82
 C      -2.450869     0.748184    -1.780372      49.47
 H      -2.796010     1.161566    -2.754314      19.12
 C      -1.477796     1.487217    -0.961895       7.24
 O      -0.949091     2.734782    -1.328126     190.21
 C      -1.640691     3.335322    -2.514543     106.69
 H      -1.010409     4.068952    -2.934908      24.45
 H      -1.402137     2.683208    -3.383044      24.31
 H      -2.835675     3.551986    -2.413231      24.40
 C      -0.890048     0.889346     0.178288      20.13
 O       0.325831     1.277744     0.734314     193.46
 C      -1.400113    -0.350995     0.630189      41.43
 H      -0.917864    -0.874100     1.470519      16.22
 C      -2.879055    -0.494064    -1.367045      32.43
 C      -3.760044    -1.343157    -2.339157      64.86
 H      -3.658919    -0.942286    -3.290389      27.45
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 O      -3.199493    -2.713009    -2.532953     156.82
 H      -2.177662    -2.790719    -3.084128      21.30
 C      -5.301439    -1.384951    -2.074679     101.81
 H      -5.604671    -1.739558    -1.115131      28.34
 O      -5.720507     0.022329    -2.006001     250.39
 H      -5.725022     0.286185    -1.031145      26.28
 C      -6.011280    -2.034592    -3.315645     120.09
 O      -5.633836    -3.441638    -3.482593     234.74
 H      -4.675972    -3.456040    -3.299147      31.62
 H      -5.717140    -1.369900    -4.126811      30.29
 H      -7.030116    -2.000989    -3.288997      30.38
55
name = lig-ACN-frame_164
 C       3.134589     3.233356    -0.048698      51.31
 H       2.395668     4.015250    -0.247031      25.17
 C       4.159305     1.419612     1.448952      61.46
 H       4.134056     0.826466     2.364089      23.09
 C       5.303073     1.474948     0.631228       3.40
 O       6.448746     0.757957     0.961918     226.57
 C       6.206818    -0.330221     1.931931     109.84
 H       5.931797     0.090222     2.832007      29.25
 H       7.132703    -0.975155     2.001451      25.62
 H       5.309989    -0.952017     1.485684      25.40
 C       5.443470     2.369975    -0.566520      13.15
 O       6.581002     2.305122    -1.332664     246.31
 H       7.131116     1.575342    -1.016062      25.29
 C       4.307276     3.205343    -0.820784      93.85
 H       4.516852     3.812538    -1.773797      23.82
 C       3.108542     2.369652     1.098667      17.24
 C       1.882357     2.537466     2.058257      96.36
 H       1.996320     3.614383     2.508971      20.58
 O       1.910946     1.602239     3.097689     291.82
 H       1.989996     0.659945     2.728101      23.32
 C       0.466368     2.652539     1.338495      90.54
 H       0.621266     3.322273     0.582750      20.37
 C      -0.607136     3.007145     2.352908     104.64
 O      -0.466548     4.390249     2.970164     278.81
 H      -0.122525     5.017690     2.084010      26.15
 H      -0.526375     2.339967     3.144124      25.51
 H      -1.591119     2.952443     1.975555      25.58
 C      -2.383064    -1.089814    -0.152192      55.37
 H      -2.837216    -2.000840     0.082799      23.14
 C      -2.426944     0.772724    -1.771439      61.46
 H      -2.632967     1.027773    -2.797023      19.14
 C      -1.521601     1.450776    -0.985129      12.63
 O      -1.030414     2.704574    -1.335831     211.29
 C      -1.551905     3.322611    -2.490036     118.52
 H      -1.154533     4.249084    -2.531175      26.28
 H      -1.786680     2.650856    -3.364234      24.92
 H      -2.684543     3.616680    -2.122049      25.38
 C      -0.864134     0.841895     0.181861      17.68
 O       0.319283     1.331370     0.774640     192.00
 C      -1.433343    -0.400835     0.591238      46.30
 H      -0.890089    -0.941685     1.460972      17.75
 C      -2.886792    -0.562952    -1.360513      24.87
 C      -3.675032    -1.285459    -2.406318      78.70
 H      -3.653760    -0.675487    -3.297389      26.56
 O      -3.233514    -2.656431    -2.563024     198.59
 H      -2.112235    -2.495600    -2.744553      22.72
 C      -5.266695    -1.319475    -2.081842      94.30
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 H      -5.417839    -2.015810    -1.249696      29.18
 O      -5.769753     0.064669    -2.084590     264.36
 H      -5.633736     0.448323    -1.271348      31.04
 C      -6.005355    -1.960554    -3.312463     105.35
 O      -5.689133    -3.432971    -3.508028     202.78
 H      -4.736626    -3.468993    -3.434517      32.08
 H      -5.633728    -1.487440    -4.221391      29.78
 H      -7.062717    -1.871536    -3.171369      29.91
55
name = lig-ACN-frame_165
 C       3.213473     3.182488    -0.010042      40.36
 H       2.318024     3.773120    -0.233493      20.30
 C       4.168730     1.478735     1.390329      64.92
 H       3.999660     0.766478     2.174406      21.24
 C       5.345120     1.558894     0.641931      26.65
 O       6.429032     0.723098     0.947956     261.89
 C       6.148512    -0.292272     1.880896     124.81
 H       6.005534    -0.040879     2.863274      29.22
 H       7.027070    -0.888661     1.819615      26.85
 H       5.227613    -0.999039     1.561252      25.87
 C       5.391271     2.331538    -0.494242      21.18
 O       6.543236     2.282172    -1.296001     232.81
 H       7.204111     1.709871    -0.929501      25.20
 C       4.354556     3.241618    -0.854597      37.14
 H       4.311728     3.970483    -1.692478      15.74
 C       3.094648     2.321775     1.084917      37.29
 C       1.904456     2.545767     2.037700     100.42
 H       2.065586     3.457168     2.696196      24.96
 O       1.903012     1.502113     3.139763     269.14
 H       1.861048     0.683327     2.748590      26.61
 C       0.511672     2.700629     1.346304      89.24
 H       0.414007     3.389698     0.607140      21.97
 C      -0.640170     3.065999     2.429690     109.69
 O      -0.407119     4.262413     3.001679     299.25
 H      -0.056363     5.077712     2.306097      28.13
 H      -0.630431     2.357983     3.161518      26.70
 H      -1.576137     2.936440     1.898480      25.58
 C      -2.442461    -1.108902    -0.133764      55.82
 H      -2.567549    -2.049561     0.233202      21.15
 C      -2.403634     0.703836    -1.733612      56.55
 H      -2.810560     1.217450    -2.557201      20.59
 C      -1.464239     1.423270    -0.963139      13.62
 O      -1.027285     2.669203    -1.327086     216.33
 C      -1.616603     3.399809    -2.438444     113.84
 H      -0.960257     4.125537    -2.607917      26.44
 H      -1.325136     2.865102    -3.415638      24.56
 H      -2.759259     3.703203    -2.326985      24.54
 C      -0.917023     0.810013     0.157989      26.20
 O       0.235895     1.295933     0.783248     188.26
 C      -1.357277    -0.450894     0.572174      61.83
 H      -1.067781    -0.842829     1.656871      18.54
 C      -2.836275    -0.528302    -1.393796      34.27
 C      -3.713032    -1.215924    -2.426704      81.85
 H      -3.472811    -0.736781    -3.421418      25.27
 O      -3.239323    -2.598191    -2.602013     250.51
 H      -2.294248    -2.714958    -2.489157      27.98
 C      -5.187227    -1.268841    -2.201695      99.95
 H      -5.428280    -1.646427    -1.184438      27.80
 O      -5.804401     0.050223    -2.161716     247.10
 H      -5.729497     0.403308    -1.216135      27.50
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 C      -5.940931    -1.979670    -3.336409     115.59
 O      -5.784675    -3.357010    -3.508289     218.28
 H      -4.779310    -3.520990    -3.523185      30.58
 H      -5.836016    -1.338660    -4.236738      29.77
 H      -7.034659    -1.846387    -3.084053      28.39
55
name = lig-ACN-frame_166
 C       3.235209     3.184663    -0.026191      62.94
 H       2.496927     3.924960    -0.372898      23.30
 C       4.105490     1.537001     1.391018      61.63
 H       4.080400     0.873357     2.232283      21.77
 C       5.326093     1.561592     0.675280      12.93
 O       6.422215     0.736284     0.900341     264.35
 C       6.164959    -0.398884     1.865379     116.23
 H       6.127660     0.123393     2.760509      29.71
 H       6.937226    -1.026861     1.857985      28.19
 H       5.134149    -0.955048     1.626465      24.51
 C       5.437094     2.371398    -0.507130      18.20
 O       6.524183     2.292411    -1.295383     208.97
 H       7.206506     1.607227    -0.894916      21.80
 C       4.396671     3.195140    -0.827433      58.78
 H       4.548495     3.776558    -1.709877      21.73
 C       3.035157     2.348495     1.082054      46.79
 C       1.912029     2.458943     2.098959     103.15
 H       2.120355     3.423210     2.568866      23.02
 O       1.881832     1.453145     3.123391     301.97
 H       1.507035     0.596764     2.734631      21.86
 C       0.452225     2.616070     1.410194      90.10
 H       0.562495     3.318947     0.648680      20.83
 C      -0.635941     2.939513     2.378063     107.47
 O      -0.349933     4.274330     3.121172     306.74
 H       0.055000     4.858468     2.450493      31.60
 H      -0.753082     2.268521     3.140374      26.67
 H      -1.565363     3.142554     1.839175      24.67
 C      -2.379767    -1.153265    -0.147994      40.15
 H      -2.843468    -2.050339     0.073070      21.73
 C      -2.404786     0.760898    -1.739692      79.29
 H      -2.899876     1.210479    -2.561075      20.76
 C      -1.431623     1.418194    -0.983614      12.11
 O      -0.991767     2.712205    -1.290794     198.85
 C      -1.562872     3.467088    -2.460796     113.60
 H      -1.196445     4.375575    -2.403104      26.70
 H      -1.568151     2.805273    -3.415508      24.41
 H      -2.719814     3.682583    -2.340962      25.61
 C      -0.887018     0.803759     0.197692      34.11
 O       0.208931     1.287394     0.838306     195.08
 C      -1.405730    -0.468847     0.584588      48.43
 H      -0.905195    -0.953833     1.531697      17.12
 C      -2.843173    -0.576570    -1.347600      50.09
 C      -3.628180    -1.198024    -2.472676      76.20
 H      -3.515361    -0.539557    -3.433893      27.58
 O      -3.282786    -2.607130    -2.633727     272.95
 H      -2.412856    -2.568934    -2.671221      31.21
 C      -5.199381    -1.227871    -2.245148      94.03
 H      -5.314954    -1.904236    -1.325100      28.31
 O      -5.812623     0.080543    -2.241773     224.76
 H      -5.896245     0.378814    -1.194459      24.82
 C      -6.002505    -1.910117    -3.360128     104.78
 O      -5.840519    -3.356325    -3.525417     188.76
 H      -4.867594    -3.541503    -3.524597      32.06
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 H      -5.721412    -1.432371    -4.328834      29.99
 H      -7.134284    -1.774261    -3.058199      28.32
55
name = lig-ACN-frame_167
 C       3.154512     3.284516    -0.101227       2.70
 H       2.401050     4.068339    -0.296617      18.05
 C       4.126850     1.511016     1.466783      50.30
 H       3.954816     1.003245     2.411805      20.04
 C       5.290914     1.512135     0.668436      10.84
 O       6.412946     0.663208     0.885728     214.23
 C       6.218095    -0.409088     1.852143     122.05
 H       6.129641    -0.198178     2.913550      28.22
 H       6.926111    -1.064172     1.666170      28.00
 H       5.202119    -0.902886     1.575229      25.82
 C       5.511042     2.348994    -0.450501      10.44
 O       6.600203     2.296043    -1.340167     239.58
 H       7.216806     1.512096    -1.090033      23.53
 C       4.384675     3.182479    -0.824863     106.03
 H       4.475912     3.760959    -1.698389      27.98
 C       3.025384     2.395910     1.059154      13.32
 C       1.800744     2.438963     2.126990     109.04
 H       1.857246     3.295201     2.735597      24.04
 O       1.859338     1.406347     3.109450     284.69
 H       1.571750     0.448307     2.643523      18.47
 C       0.493407     2.518104     1.455679     100.99
 H       0.527792     3.271588     0.662455      19.08
 C      -0.672527     2.994876     2.435380     101.61
 O      -0.304354     4.197998     3.195748     345.71
 H       0.056351     4.767136     2.647920      37.33
 H      -0.852697     2.157934     3.066890      27.07
 H      -1.636977     3.071014     1.841248      24.87
 C      -2.345393    -1.190721    -0.221309      67.26
 H      -2.615961    -2.181578     0.158036      21.34
 C      -2.425741     0.784147    -1.705503      38.73
 H      -2.699729     1.148530    -2.696878      18.64
 C      -1.426892     1.492002    -0.986274       6.83
 O      -0.945362     2.801271    -1.284579     214.13
 C      -1.550050     3.463555    -2.398261     110.74
 H      -1.089085     4.326996    -2.467301      26.51
 H      -1.278248     3.042829    -3.445259      25.40
 H      -2.689691     3.436304    -2.121029      25.37
 C      -0.906641     0.794122     0.186701      20.01
 O       0.257408     1.217046     0.923482     193.82
 C      -1.428433    -0.469465     0.622392      44.07
 H      -0.911832    -1.008048     1.458883      15.43
 C      -2.836092    -0.505991    -1.395254      33.41
 C      -3.676884    -1.230822    -2.480282      55.41
 H      -3.337028    -0.695305    -3.489129      23.83
 O      -3.301044    -2.619200    -2.684625     229.45
 H      -2.357942    -2.813169    -2.983328      25.87
 C      -5.227935    -1.236846    -2.275209      90.98
 H      -5.502624    -1.733591    -1.262477      27.12
 O      -5.788872     0.136403    -2.251654     218.31
 H      -5.824852     0.515635    -1.321049      26.91
 C      -6.056972    -1.897389    -3.440873      99.98
 O      -5.894149    -3.368731    -3.537950     210.97
 H      -4.948674    -3.406953    -3.434408      33.86
 H      -5.795708    -1.349754    -4.399630      29.66
 H      -7.231072    -1.624761    -3.308442      27.69
55
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name = lig-ACN-frame_168
 C       3.173521     3.248569    -0.034099      44.15
 H       2.382261     3.896836    -0.437834      16.83
 C       4.099080     1.604165     1.435658      63.03
 H       4.043608     0.935149     2.302675      22.37
 C       5.322914     1.432531     0.674743       4.44
 O       6.394262     0.603346     0.926842     257.88
 C       6.240014    -0.495733     1.811664     128.41
 H       6.436013    -0.041843     2.811288      27.82
 H       7.046230    -1.097433     1.655994      27.46
 H       5.292496    -1.067593     1.666106      26.09
 C       5.432506     2.330127    -0.467571      -6.28
 O       6.645248     2.287353    -1.343866     221.39
 H       7.235308     1.596819    -1.103018      26.73
 C       4.372674     3.212416    -0.839651      63.13
 H       4.506336     3.842300    -1.697260      25.83
 C       3.038888     2.453450     1.121364      37.29
 C       1.853325     2.476603     2.124156     105.89
 H       1.979125     3.335345     2.680076      26.21
 O       1.837983     1.325941     3.115817     248.73
 H       1.865038     0.414165     2.625181      21.72
 C       0.410651     2.533480     1.450472      76.47
 H       0.435288     3.240372     0.550443      20.17
 C      -0.694306     3.000622     2.480662     106.20
 O      -0.272159     4.086152     3.258924     269.52
 H      -0.081739     4.925834     2.650065      29.47
 H      -0.924669     2.319923     3.310066      24.55
 H      -1.621455     3.358199     1.890691      23.83
 C      -2.325211    -1.131339    -0.265097      54.24
 H      -2.478745    -2.264200    -0.198688      19.37
 C      -2.382035     0.839721    -1.719563      78.17
 H      -2.728692     1.346675    -2.675237      17.53
 C      -1.415381     1.533158    -0.881768      16.69
 O      -0.880588     2.789011    -1.237715     216.74
 C      -1.533084     3.479263    -2.361230     110.07
 H      -1.263332     4.492431    -2.323039      25.21
 H      -1.268297     2.856477    -3.263406      24.69
 H      -2.712591     3.597095    -2.443967      25.82
 C      -0.886875     0.826547     0.225802      29.34
 O       0.233763     1.068067     0.949645     160.61
 C      -1.413019    -0.449330     0.539879      44.69
 H      -1.138560    -0.815729     1.486675      20.36
 C      -2.836520    -0.526281    -1.440367      55.00
 C      -3.723551    -1.254179    -2.500500      52.38
 H      -3.705235    -0.661513    -3.527295      27.98
 O      -3.343008    -2.691386    -2.728769     197.42
 H      -2.207326    -2.498150    -2.759277      20.70
 C      -5.323149    -1.197423    -2.319329      88.70
 H      -5.584242    -1.745276    -1.315191      28.60
 O      -5.735821     0.189658    -2.248855     264.84
 H      -5.550635     0.416774    -1.393386      31.65
 C      -6.063325    -1.907730    -3.510475     106.24
 O      -5.945264    -3.316947    -3.548862     206.45
 H      -5.007153    -3.595234    -3.337327      31.98
 H      -5.674100    -1.444284    -4.482342      29.68
 H      -7.242544    -1.756633    -3.322885      27.61
55
name = lig-ACN-frame_169
 C       3.224676     3.225757    -0.016113      51.24
 H       2.374618     3.840613    -0.322828      27.05
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 C       4.183140     1.581108     1.436225      69.11
 H       4.036309     0.931524     2.312449      24.19
 C       5.269443     1.500599     0.607896      21.43
 O       6.369391     0.594787     0.901153     198.61
 C       6.304052    -0.604131     1.864454     109.01
 H       6.276460    -0.303466     2.982857      26.15
 H       7.082472    -1.292612     1.562573      26.17
 H       5.374122    -1.098406     1.803153      28.76
 C       5.454856     2.270426    -0.574491      29.67
 O       6.554382     2.301695    -1.272397     224.28
 H       7.187759     1.641570    -0.911363      22.17
 C       4.397372     3.177748    -0.782804      74.84
 H       4.458523     3.833803    -1.679943      22.30
 C       3.081825     2.458034     1.177200      26.01
 C       1.857736     2.438890     2.147985     102.47
 H       1.934987     3.249001     2.780666      22.82
 O       1.859232     1.350222     3.080125     311.10
 H       1.736356     0.554279     2.649695      27.62
 C       0.401174     2.472757     1.482726      82.15
 H       0.336292     3.135797     0.494921      19.23
 C      -0.722974     2.934178     2.468478      88.17
 O      -0.194430     4.079913     3.346808     196.87
 H      -0.273284     5.000202     2.659446      26.41
 H      -1.023068     1.958916     3.001708      25.19
 H      -1.711580     3.221893     1.912313      24.48
 C      -2.327506    -1.116392    -0.380260      87.49
 H      -2.698968    -2.172373    -0.000217      22.62
 C      -2.356351     0.846608    -1.710845      45.38
 H      -2.854315     1.454515    -2.544758      22.22
 C      -1.444232     1.510624    -0.871996      20.53
 O      -0.891098     2.775446    -1.180590     213.60
 C      -1.482976     3.476016    -2.355188      95.00
 H      -0.976534     4.505542    -2.297418      24.12
 H      -1.216280     3.136962    -3.360884      26.24
 H      -2.646830     3.414199    -2.081017      25.53
 C      -0.893521     0.797526     0.244441      19.09
 O       0.224000     1.112584     1.022262     181.67
 C      -1.441937    -0.475750     0.501414      35.46
 H      -1.048512    -0.985906     1.288926      17.43
 C      -2.832231    -0.469626    -1.534950      53.53
 C      -3.801956    -1.254979    -2.540897      52.51
 H      -3.504777    -0.712421    -3.519478      27.42
 O      -3.370618    -2.669121    -2.733771     178.61
 H      -2.247317    -2.911371    -2.588867      23.67
 C      -5.345249    -1.204894    -2.329646      97.20
 H      -5.723011    -1.829084    -1.416188      28.39
 O      -5.687595     0.216498    -2.253685     245.68
 H      -5.577016     0.606609    -1.306181      26.27
 C      -6.055917    -1.848903    -3.536230     104.02
 O      -5.990927    -3.331129    -3.549873     172.08
 H      -4.985769    -3.475031    -3.357928      30.69
 H      -5.651187    -1.415952    -4.526455      29.72
 H      -7.184626    -1.529702    -3.551533      28.83
55
name = lig-ACN-frame_170
 C       3.219981     3.224226     0.040521      69.30
 H       2.541315     4.038278    -0.192815      24.46
 C       4.186443     1.528616     1.508020      57.14
 H       4.257714     0.908742     2.406626      22.17
 C       5.311030     1.401335     0.633196       8.96
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 O       6.373766     0.551770     0.886737     217.67
 C       6.262185    -0.596810     1.855434     111.03
 H       6.557949    -0.301478     2.947259      25.44
 H       7.215478    -1.177634     1.512430      24.15
 H       5.435395    -1.133689     1.640835      27.86
 C       5.350883     2.243177    -0.495099       9.74
 O       6.581837     2.303378    -1.290170     195.52
 H       7.262939     1.556892    -0.968259      21.10
 C       4.363199     3.174739    -0.812626      52.39
 H       4.505719     3.875097    -1.701426      18.91
 C       3.117128     2.399123     1.184824      25.92
 C       1.816114     2.449917     2.158195     118.44
 H       1.834153     3.366972     2.681049      24.84
 O       1.919728     1.363693     3.084209     282.82
 H       1.472053     0.582421     2.668091      23.21
 C       0.475819     2.492900     1.492888      88.92
 H       0.596782     3.369957     0.653798      19.84
 C      -0.654419     2.919029     2.486773      99.04
 O      -0.194981     3.988813     3.356955     261.71
 H      -0.216979     4.847743     2.861124      31.30
 H      -0.880548     2.174191     3.376858      23.64
 H      -1.588730     3.298525     1.888536      23.52
 C      -2.388525    -1.138309    -0.433933      81.44
 H      -2.870172    -2.180993    -0.161564      20.01
 C      -2.431461     0.866982    -1.767941      49.03
 H      -2.728931     1.440547    -2.699201      14.55
 C      -1.410865     1.474204    -0.897339      24.96
 O      -0.912957     2.749647    -1.165081     225.89
 C      -1.416140     3.474755    -2.267508     101.77
 H      -0.947488     4.620301    -2.213779      22.79
 H      -1.218386     2.917534    -3.148504      28.28
 H      -2.637985     3.715228    -2.279584      25.67
 C      -0.901821     0.747190     0.240974      26.10
 O       0.157222     1.153079     1.064726     181.74
 C      -1.432384    -0.564507     0.478419      25.00
 H      -1.049907    -1.166610     1.232145      18.07
 C      -2.865194    -0.473489    -1.575138      51.52
 C      -3.720027    -1.217228    -2.585281      45.62
 H      -3.731901    -0.761885    -3.612033      26.93
 O      -3.437958    -2.640616    -2.696467     211.75
 H      -2.367423    -2.619764    -2.668260      25.18
 C      -5.295620    -1.183678    -2.337420      86.05
 H      -5.552536    -1.657928    -1.310662      28.55
 O      -5.674344     0.223784    -2.272610     226.34
 H      -5.773293     0.381718    -1.196536      23.67
 C      -6.070594    -1.804370    -3.589623     100.48
 O      -6.021768    -3.285620    -3.540104     195.20
 H      -5.091913    -3.504089    -3.449406      33.88
 H      -5.491822    -1.397936    -4.513654      30.31
 H      -7.150288    -1.540321    -3.574641      29.96
55
name = lig-ACN-frame_171
 C       3.221084     3.255430     0.099046      51.58
 H       2.427530     3.976500    -0.030480      19.49
 C       4.174130     1.457803     1.561059      72.24
 H       3.968926     0.934123     2.489439      22.11
 C       5.284052     1.316561     0.712384       8.58
 O       6.412912     0.498088     0.875109     222.76
 C       6.289441    -0.547360     1.756851     121.03
 H       6.212381    -0.084264     2.847748      24.87
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 H       7.161741    -1.373434     1.631816      24.26
 H       5.417778    -1.049917     1.793874      28.13
 C       5.420594     2.225414    -0.471122      -0.03
 O       6.556214     2.278490    -1.293505     179.86
 H       7.180703     1.512296    -1.096975      23.40
 C       4.323267     3.127505    -0.786348      62.10
 H       4.502802     3.875896    -1.621973      24.73
 C       3.087427     2.345352     1.198854      20.12
 C       1.946885     2.450258     2.145232      96.80
 H       2.088383     3.330626     2.769127      25.13
 O       1.958125     1.371875     3.157674     228.90
 H       1.564246     0.468326     2.662254      20.71
 C       0.476190     2.563547     1.502760      63.23
 H       0.423494     3.186726     0.464558      18.32
 C      -0.554376     2.945492     2.525926     104.85
 O      -0.200733     3.973451     3.388637     307.29
 H      -0.031727     4.689326     2.898237      35.04
 H      -0.826038     1.876047     3.020020      24.30
 H      -1.568609     3.122430     1.949345      24.74
 C      -2.446803    -1.159445    -0.405555      53.36
 H      -2.625738    -2.283424    -0.392528      19.85
 C      -2.421831     0.875522    -1.810641      47.80
 H      -2.715186     1.366331    -2.744681      19.16
 C      -1.453584     1.395943    -0.959205       9.45
 O      -0.933354     2.710180    -1.078752     218.77
 C      -1.378545     3.490061    -2.245890      84.41
 H      -0.460077     4.404816    -2.280003      21.46
 H      -1.166195     3.012278    -3.153716      27.84
 H      -2.571081     3.843432    -2.187197      23.61
 C      -0.943882     0.689672     0.191879      20.29
 O       0.079464     1.129667     1.036360     163.44
 C      -1.426369    -0.642216     0.395137      68.37
 H      -1.156310    -1.083543     1.361527      21.49
 C      -2.876280    -0.455997    -1.578468      32.69
 C      -3.755801    -1.161021    -2.652579      84.92
 H      -3.416216    -0.684977    -3.560755      27.68
 O      -3.438898    -2.608970    -2.652557     252.54
 H      -2.565142    -2.767948    -2.814275      32.16
 C      -5.241951    -1.109016    -2.388248     102.32
 H      -5.448309    -1.812666    -1.511213      30.13
 O      -5.700834     0.232909    -2.267880     263.34
 H      -5.848724     0.551286    -1.344622      28.67
 C      -6.010656    -1.807716    -3.544158     110.78
 O      -6.066367    -3.213501    -3.552107     206.18
 H      -5.141145    -3.483578    -3.454833      33.13
 H      -5.648139    -1.422765    -4.582134      30.38
 H      -7.026146    -1.491674    -3.509829      31.57
55
name = lig-ACN-frame_172
 C       3.250254     3.197039     0.137076      62.99
 H       2.482897     3.873336    -0.197150      18.91
 C       4.139521     1.387287     1.527880      77.87
 H       4.044979     0.679531     2.340662      23.62
 C       5.296665     1.370416     0.663898      -1.35
 O       6.437702     0.511162     0.790973     170.84
 C       6.250394    -0.580872     1.842292     103.11
 H       6.380929    -0.192294     2.944632      24.36
 H       7.242237    -1.304694     1.646892      23.99
 H       5.439270    -1.065798     1.485622      26.90
 C       5.406326     2.198361    -0.411842      35.88
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 O       6.487763     2.234560    -1.273095     202.95
 H       7.136436     1.595967    -1.065124      26.29
 C       4.380157     3.072379    -0.664361      70.15
 H       4.459352     3.710324    -1.549444      25.38
 C       3.143667     2.309358     1.201644      16.37
 C       1.964576     2.390719     2.191830      87.74
 H       2.092968     3.371296     2.739795      26.50
 O       1.959823     1.391351     3.208455     229.00
 H       1.845041     0.451762     2.769708      24.62
 C       0.505424     2.496912     1.427566      68.58
 H       0.514342     3.312320     0.558930      21.96
 C      -0.579553     2.868534     2.481042      88.94
 O      -0.170783     4.023466     3.470677     174.25
 H       0.095480     4.865111     2.810409      28.59
 H      -0.613079     2.030120     3.302407      25.26
 H      -1.578700     3.223634     2.026130      25.17
 C      -2.440901    -1.206367    -0.466147      91.21
 H      -2.806046    -2.189115    -0.205640      24.35
 C      -2.405015     0.798662    -1.860296      74.91
 H      -2.797680     1.392089    -2.644414      24.21
 C      -1.457500     1.421973    -0.946259      21.13
 O      -0.966007     2.674312    -1.033250     220.60
 C      -1.263302     3.487471    -2.236908      97.39
 H      -0.514874     4.576896    -2.144662      20.70
 H      -1.351752     2.943856    -3.147727      26.87
 H      -2.322494     3.930420    -1.979489      25.08
 C      -0.971549     0.655918     0.133412      26.13
 O       0.054939     1.110929     1.020518     180.12
 C      -1.458079    -0.625658     0.395139      39.96
 H      -0.992751    -1.294769     1.217729      17.59
 C      -2.901041    -0.461666    -1.570388      48.45
 C      -3.670322    -1.125673    -2.647089      68.31
 H      -3.593076    -0.760676    -3.616842      34.22
 O      -3.446527    -2.597316    -2.651758     251.52
 H      -2.564919    -2.628096    -2.613774      33.53
 C      -5.219869    -1.093897    -2.439777      93.11
 H      -5.422975    -1.566010    -1.450097      28.88
 O      -5.765080     0.283832    -2.273950     243.45
 H      -5.553622     0.404877    -1.401228      30.86
 C      -6.042603    -1.710176    -3.561831     108.64
 O      -6.083642    -3.212284    -3.551128     172.16
 H      -5.117762    -3.510365    -3.381655      30.85
 H      -5.612336    -1.304222    -4.557876      29.10
 H      -6.997203    -1.401861    -3.407031      31.61
55
name = lig-ACN-frame_173
 C       3.251004     3.107487     0.153215      57.01
 H       2.499116     3.866385    -0.069457      25.90
 C       4.194204     1.295099     1.426048      70.94
 H       4.144969     0.568371     2.241105      23.85
 C       5.373199     1.303302     0.706789      22.59
 O       6.418808     0.496184     0.841442     227.75
 C       6.270391    -0.588131     1.809961     113.33
 H       6.120258    -0.151476     2.873566      25.72
 H       7.303425    -1.239575     1.664552      24.33
 H       5.410070    -1.245081     1.827654      26.55
 C       5.414854     2.215548    -0.414918      10.65
 O       6.458817     2.191871    -1.279098     181.66
 H       7.168707     1.558373    -0.959424      21.09
 C       4.422235     3.153358    -0.664077      56.64
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 H       4.554796     3.763042    -1.518497      23.46
 C       3.123919     2.251721     1.298191      21.05
 C       1.851986     2.328420     2.158619      96.36
 H       1.788063     3.362965     2.690502      22.32
 O       1.954787     1.379591     3.257900     288.44
 H       1.778882     0.563139     2.886912      29.90
 C       0.496350     2.388691     1.475696      77.39
 H       0.667162     3.076974     0.583526      20.77
 C      -0.537453     2.940952     2.568752     105.33
 O      -0.130441     4.016120     3.405040     210.85
 H      -0.022816     5.035022     2.886842      25.56
 H      -0.802214     2.068556     3.210725      26.45
 H      -1.524799     3.092502     2.019245      25.77
 C      -2.422858    -1.221287    -0.465365      73.90
 H      -2.909748    -2.095915    -0.236356      25.50
 C      -2.366926     0.834708    -1.838325      62.65
 H      -2.734239     1.304426    -2.709032      23.26
 C      -1.497655     1.396406    -0.943781      12.59
 O      -0.945239     2.720202    -1.049508     234.58
 C      -1.250413     3.512183    -2.150971      95.45
 H      -0.140158     4.240630    -2.323222      21.73
 H      -1.042521     2.876376    -3.033025      25.31
 H      -2.210820     4.072949    -2.225044      25.38
 C      -0.928948     0.681990     0.171831      25.96
 O       0.093417     1.085677     0.989004     206.04
 C      -1.479747    -0.634463     0.385906      47.30
 H      -0.969455    -1.246183     1.269155      17.15
 C      -2.859393    -0.512058    -1.606513      44.16
 C      -3.746999    -1.181057    -2.672148      65.23
 H      -3.407379    -0.688444    -3.504442      30.57
 O      -3.418199    -2.584021    -2.681999     240.71
 H      -2.443400    -2.790702    -2.488340      28.92
 C      -5.274164    -1.032685    -2.398198      99.76
 H      -5.489273    -1.691818    -1.544366      28.79
 O      -5.769208     0.305645    -2.293353     262.74
 H      -5.658949     0.804866    -1.411515      27.15
 C      -6.097116    -1.703853    -3.594702     108.92
 O      -6.077348    -3.155424    -3.555773     208.13
 H      -5.146292    -3.374139    -3.352304      33.59
 H      -5.709077    -1.334626    -4.609258      29.95
 H      -7.099245    -1.487696    -3.562159      31.81
55
name = lig-ACN-frame_174
 C       3.249346     3.112645     0.191593      58.37
 H       2.411080     3.828144     0.124270      23.08
 C       4.147628     1.227062     1.488079      64.82
 H       3.985394     0.506838     2.311644      22.61
 C       5.310582     1.326604     0.660994     -10.21
 O       6.454985     0.397655     0.897896     182.68
 C       6.310129    -0.610412     1.852530     112.26
 H       6.291914    -0.139146     2.898496      25.22
 H       7.320502    -1.260872     1.877437      25.01
 H       5.481911    -1.247185     1.427318      25.03
 C       5.469320     2.239639    -0.419006       9.03
 O       6.521224     2.154632    -1.330373      92.38
 H       7.301602     1.480386    -1.036151      21.25
 C       4.389393     3.191078    -0.640340      53.38
 H       4.452768     3.975473    -1.335474      22.02
 C       3.123659     2.169005     1.229962      -4.47
 C       1.861539     2.254083     2.182056      86.07
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 H       2.065511     3.297288     2.697157      23.22
 O       1.920693     1.336635     3.301039     247.34
 H       1.530522     0.473083     3.009818      25.83
 C       0.438030     2.352688     1.532913      98.23
 H       0.393165     3.071227     0.727472      22.55
 C      -0.567207     2.935634     2.540147     113.40
 O      -0.068468     4.052868     3.317196     281.99
 H      -0.214472     4.782820     2.723461      31.41
 H      -0.808964     2.207060     3.269261      27.24
 H      -1.443038     3.357624     2.001273      25.64
 C      -2.434703    -1.186138    -0.431865      50.63
 H      -2.601510    -2.188530    -0.291265      20.24
 C      -2.388037     0.810648    -1.823831      46.78
 H      -2.573644     1.375306    -2.721920      19.31
 C      -1.436286     1.461213    -0.891783       5.61
 O      -0.941220     2.725456    -0.981202     220.57
 C      -1.143935     3.525090    -2.253748      88.33
 H      -0.308110     4.530103    -2.086208      21.32
 H      -1.274028     2.963671    -3.264934      25.70
 H      -2.053390     3.997945    -2.114208      27.01
 C      -0.969563     0.671317     0.197811      28.09
 O       0.169471     1.006340     0.993912     196.89
 C      -1.423516    -0.623010     0.406569      66.65
 H      -1.229591    -1.129977     1.440516      20.51
 C      -2.815991    -0.500267    -1.645818      34.48
 C      -3.755494    -1.159740    -2.644585      74.77
 H      -3.787261    -0.803855    -3.614529      28.86
 O      -3.445073    -2.637266    -2.738919     184.72
 H      -2.315058    -2.543036    -2.780489      21.76
 C      -5.394725    -1.059146    -2.413633      89.30
 H      -5.669305    -1.501656    -1.467764      30.49
 O      -5.747986     0.354368    -2.350094     234.73
 H      -5.681631     0.446155    -1.249729      24.41
 C      -6.140001    -1.692984    -3.607490     119.37
 O      -6.041982    -3.111873    -3.555264     214.95
 H      -5.123369    -3.318378    -3.425103      33.86
 H      -5.691474    -1.270143    -4.552352      30.12
 H      -7.175518    -1.398266    -3.561991      31.00
55
name = lig-ACN-frame_175
 C       3.243396     3.134796     0.248244      50.32
 H       2.517164     3.931127    -0.055747      21.02
 C       4.131865     1.225385     1.485406      63.89
 H       4.066946     0.468604     2.289585      23.72
 C       5.313408     1.230597     0.671861      -3.59
 O       6.459395     0.453608     0.849875     138.21
 C       6.342685    -0.688592     1.941146      99.91
 H       6.048547    -0.410363     2.980802      24.83
 H       7.333643    -1.210925     1.790673      24.83
 H       5.461992    -1.481808     1.786900      24.16
 C       5.452871     2.226481    -0.410603       4.06
 O       6.556798     2.171748    -1.365966     123.80
 H       7.259667     1.501200    -1.017816      22.18
 C       4.420876     3.165660    -0.576875      51.69
 H       4.515469     3.928356    -1.336918      21.71
 C       3.038574     2.057616     1.179680      11.35
 C       1.946135     2.219400     2.223591      84.93
 H       2.092393     3.261826     2.771137      23.44
 O       1.864607     1.260583     3.324093     238.84
 H       1.439757     0.364174     2.848941      23.18
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 C       0.473006     2.357202     1.532699      77.25
 H       0.605261     3.004373     0.749843      23.67
 C      -0.680531     2.882701     2.516753     104.43
 O       0.000780     4.121316     3.207241     283.96
 H       0.012219     4.868752     2.720908      33.62
 H      -0.999057     2.230715     3.252239      28.57
 H      -1.562009     3.115168     1.935691      27.10
 C      -2.390117    -1.178586    -0.465633      69.73
 H      -2.780148    -2.171943    -0.290917      25.35
 C      -2.319619     0.875982    -1.791985      71.28
 H      -2.733339     1.407667    -2.669558      22.89
 C      -1.435186     1.427745    -0.882139      12.88
 O      -0.912259     2.774185    -1.004353     222.03
 C      -1.133950     3.552547    -2.237785      92.50
 H      -0.177606     4.423631    -2.364462      21.72
 H      -0.820340     2.855462    -3.183971      23.61
 H      -2.043212     3.965659    -2.260742      26.30
 C      -0.922169     0.686781     0.252296      31.88
 O       0.196721     0.959108     1.023630     182.78
 C      -1.482902    -0.607006     0.460758      40.00
 H      -1.021550    -1.234096     1.266860      17.50
 C      -2.840648    -0.494620    -1.597772      54.20
 C      -3.847229    -1.198356    -2.643613      50.35
 H      -3.556557    -0.601636    -3.467890      28.94
 O      -3.490947    -2.627319    -2.802362     173.11
 H      -2.383087    -2.937406    -2.937619      23.91
 C      -5.405748    -1.058145    -2.400759     105.38
 H      -5.762641    -1.590621    -1.552386      29.67
 O      -5.718201     0.380660    -2.371942     252.58
 H      -5.715503     0.754559    -1.409880      26.60
 C      -6.151671    -1.652223    -3.600093     109.04
 O      -6.018500    -3.131391    -3.575086     184.96
 H      -5.005706    -3.265822    -3.515107      30.91
 H      -5.766481    -1.205566    -4.535247      30.93
 H      -7.271600    -1.529622    -3.544309      29.84
55
name = lig-ACN-frame_176
 C       3.267494     3.084489     0.237045      57.86
 H       2.452434     3.851841     0.174583      23.31
 C       4.161968     1.183019     1.387388      68.57
 H       4.066681     0.535300     2.264723      23.86
 C       5.324338     1.216860     0.638142      23.12
 O       6.425015     0.400094     0.941550     212.09
 C       6.367508    -0.681193     1.912793     115.90
 H       6.305514    -0.119464     2.825296      26.87
 H       7.326476    -1.125109     1.949066      27.51
 H       5.510691    -1.481946     1.533774      24.02
 C       5.466893     2.117364    -0.414934      22.33
 O       6.467834     2.237319    -1.298829     198.79
 H       7.199709     1.663648    -1.135215      22.73
 C       4.463500     3.124226    -0.511593      46.97
 H       4.609450     3.847052    -1.351723      25.72
 C       3.038690     2.074826     1.207662      -7.83
 C       1.839786     2.188192     2.272447      91.47
 H       2.085686     3.182476     2.856488      22.86
 O       1.823876     1.170547     3.290497     253.47
 H       1.627628     0.204106     2.848028      22.02
 C       0.531643     2.327523     1.560563      95.17
 H       0.596616     2.931231     0.760440      24.43
 C      -0.594182     2.965892     2.458489     118.64
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 O      -0.029428     4.100407     3.085982     274.09
 H       0.072959     4.772325     2.225009      27.85
 H      -0.794352     2.280607     3.252694      26.99
 H      -1.448587     3.238096     1.925300      27.22
 C      -2.395611    -1.193881    -0.461420      84.03
 H      -2.853142    -2.207335    -0.189744      25.06
 C      -2.348292     0.836105    -1.768106      58.32
 H      -2.709498     1.537886    -2.563005      22.21
 C      -1.380848     1.466844    -0.866277       5.33
 O      -0.888962     2.798611    -1.021287     220.47
 C      -1.073238     3.498123    -2.249711      90.61
 H      -0.304086     4.456732    -2.031110      22.33
 H      -0.875715     2.738951    -3.216690      24.10
 H      -1.990149     3.901847    -2.457434      26.81
 C      -0.892008     0.670292     0.256758      13.60
 O       0.204960     0.997000     1.070391     199.19
 C      -1.492520    -0.607811     0.475541      35.95
 H      -1.052443    -1.216919     1.220860      19.81
 C      -2.904123    -0.441935    -1.555443      42.16
 C      -3.787850    -1.146190    -2.605817      65.85
 H      -3.715781    -0.777155    -3.625043      28.37
 O      -3.571727    -2.608486    -2.864504     237.53
 H      -2.521297    -2.570141    -2.654993      26.42
 C      -5.355369    -1.006816    -2.390392      99.57
 H      -5.581742    -1.459527    -1.453832      29.56
 O      -5.696877     0.391958    -2.387652     279.14
 H      -5.530470     0.608601    -1.520079      32.26
 C      -6.166861    -1.707277    -3.596305     109.77
 O      -6.000824    -3.127890    -3.626621     194.99
 H      -4.995816    -3.306941    -3.538284      28.59
 H      -5.883473    -1.253456    -4.538318      30.01
 H      -7.297918    -1.453099    -3.433630      28.77
55
name = lig-ACN-frame_177
 C       3.259241     3.039042     0.251496      63.05
 H       2.621628     3.918272     0.014770      23.31
 C       4.080958     1.115771     1.400555      62.14
 H       4.056983     0.372070     2.179496      24.27
 C       5.328964     1.132584     0.666120       6.35
 O       6.456915     0.367885     0.939545     217.10
 C       6.391258    -0.621560     1.927188     128.81
 H       6.123874    -0.452528     2.934792      27.93
 H       7.254300    -1.125656     1.790349      28.40
 H       5.475005    -1.461406     1.729567      24.48
 C       5.396748     2.104255    -0.387325      18.80
 O       6.477328     2.292241    -1.280180     188.06
 H       7.176872     1.670398    -1.031328      22.93
 C       4.430551     3.074896    -0.508697      51.53
 H       4.606488     3.961038    -1.204216      23.70
 C       3.118873     2.111144     1.301805      22.12
 C       1.878803     2.117067     2.266457      92.05
 H       1.933428     3.081811     2.909282      21.46
 O       1.809002     1.079850     3.250831     302.14
 H       1.636678     0.232551     2.803893      25.61
 C       0.503693     2.340695     1.488235      94.81
 H       0.720863     2.984294     0.737911      23.80
 C      -0.496356     2.956081     2.397100     110.95
 O      -0.068527     4.185799     2.971342     287.21
 H       0.325682     5.082684     2.329903      24.27
 H      -0.829033     2.299096     3.227160      25.61
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 H      -1.338014     3.079367     1.791190      26.96
 C      -2.472471    -1.156087    -0.383967      46.25
 H      -2.707240    -2.314200    -0.246146      18.21
 C      -2.367095     0.893285    -1.694892      50.03
 H      -2.677218     1.359906    -2.659027      17.75
 C      -1.373962     1.446795    -0.859390      15.26
 O      -0.883914     2.733896    -0.976700     237.14
 C      -1.024154     3.450620    -2.302745      92.91
 H      -0.382965     4.444144    -2.326875      23.48
 H      -0.533200     2.860047    -3.290546      24.73
 H      -2.056868     3.629940    -2.307088      25.75
 C      -0.885695     0.685714     0.216792      24.55
 O       0.160175     0.994258     1.096268     206.72
 C      -1.416944    -0.619619     0.435176      78.64
 H      -1.300913    -1.057301     1.357525      22.88
 C      -2.886472    -0.460544    -1.542307      34.57
 C      -3.805841    -1.063022    -2.679685      68.48
 H      -3.492148    -0.365606    -3.507137      25.06
 O      -3.551451    -2.534560    -2.832729     258.94
 H      -2.740285    -2.896289    -2.720735      31.30
 C      -5.305340    -1.013083    -2.430286     105.71
 H      -5.576917    -1.447179    -1.500720      30.69
 O      -5.676358     0.413095    -2.395040     255.27
 H      -5.613340     0.776170    -1.466150      28.75
 C      -6.135311    -1.713283    -3.519804     111.66
 O      -6.011209    -3.155758    -3.690123     224.62
 H      -5.073845    -3.287328    -3.558429      33.46
 H      -5.907740    -1.196999    -4.429787      31.40
 H      -7.289337    -1.622443    -3.255232      28.46
55
name = lig-ACN-frame_178
 C       3.234572     3.080066     0.318401      64.95
 H       2.405703     3.792929     0.229940      23.56
 C       4.113393     1.012735     1.497132      71.39
 H       3.832693     0.254441     2.189774      22.36
 C       5.256777     1.108150     0.669173      -0.75
 O       6.473917     0.416560     0.875790     152.45
 C       6.380960    -0.727603     1.999224     105.42
 H       6.329940    -0.154154     2.841667      28.37
 H       7.262160    -1.202244     1.980946      28.71
 H       5.460617    -1.439897     1.601021      23.99
 C       5.423321     2.114763    -0.370027       4.41
 O       6.527879     2.288828    -1.225503     118.92
 H       7.352775     1.656722    -1.010339      23.14
 C       4.352017     3.049696    -0.545718      41.74
 H       4.537078     3.876725    -1.305699      20.19
 C       3.125113     2.077085     1.355928      -5.07
 C       1.929536     2.110611     2.240309      94.48
 H       2.036244     3.043011     2.883110      21.82
 O       1.824646     1.027740     3.208160     301.93
 H       1.502971     0.255911     2.825111      26.90
 C       0.643275     2.316246     1.428839      70.34
 H       0.709572     2.818352     0.497988      21.47
 C      -0.557027     2.983951     2.305017      98.43
 O      -0.092819     4.314755     2.948317     276.61
 H       0.106917     4.963129     2.085728      26.35
 H      -0.628992     2.326193     3.231001      24.29
 H      -1.468815     3.069631     1.805301      26.62
 C      -2.465611    -1.135493    -0.362285      72.07
 H      -2.942106    -2.202962    -0.113463      18.62
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 C      -2.403401     0.874834    -1.697131      29.90
 H      -2.643124     1.477300    -2.573715      13.44
 C      -1.405170     1.421537    -0.871311      30.89
 O      -0.830971     2.714021    -1.010350     234.91
 C      -1.005335     3.377002    -2.294773     106.08
 H      -0.489975     4.291016    -2.075236      25.53
 H      -0.522556     2.540356    -3.067167      25.42
 H      -2.022374     3.653854    -2.767259      27.19
 C      -0.884553     0.645671     0.217313      21.59
 O       0.092836     0.982770     1.081136     185.93
 C      -1.462581    -0.633348     0.451501      53.13
 H      -0.976249    -1.125884     1.254341      19.63
 C      -2.854999    -0.436728    -1.525495      60.17
 C      -3.701465    -1.023235    -2.660538      67.30
 H      -3.517291    -0.664994    -3.740864      26.00
 O      -3.508503    -2.451508    -2.813051     267.85
 H      -2.630186    -2.438418    -2.803691      31.27
 C      -5.276765    -0.983866    -2.400368      82.95
 H      -5.366714    -1.498362    -1.454753      30.07
 O      -5.680812     0.426922    -2.424522     221.14
 H      -5.671341     0.644816    -1.333302      24.51
 C      -6.164815    -1.694123    -3.498661     105.56
 O      -6.004455    -3.174403    -3.733646     214.73
 H      -5.064806    -3.354018    -3.612982      33.39
 H      -6.082311    -1.186736    -4.431878      30.88
 H      -7.271335    -1.499072    -3.142161      28.79
55
name = lig-ACN-frame_179
 C       3.286749     3.031206     0.408358      67.92
 H       2.532980     3.791260     0.309199      23.16
 C       4.138203     1.039273     1.504849      66.72
 H       4.100923     0.272110     2.247946      21.76
 C       5.297997     1.127893     0.661675       8.13
 O       6.450436     0.323465     0.898141     211.80
 C       6.396450    -0.636354     1.921107     130.30
 H       6.221451    -0.292165     2.873358      28.58
 H       7.279875    -1.206207     1.851831      27.42
 H       5.468059    -1.408045     1.911619      24.62
 C       5.392988     2.140843    -0.344511      11.36
 O       6.549683     2.256508    -1.127365     159.58
 H       7.230038     1.518808    -0.813672      22.61
 C       4.313906     3.036078    -0.554085      52.52
 H       4.318530     3.687005    -1.434369      21.55
 C       3.160186     1.996572     1.312122      19.37
 C       1.919128     2.113450     2.256105      94.79
 H       2.026820     3.041734     2.837826      24.27
 O       1.850076     1.082629     3.186653     317.15
 H       1.567568     0.229736     2.776372      24.59
 C       0.545067     2.325081     1.411276      73.50
 H       0.939618     2.894884     0.511285      21.25
 C      -0.460861     3.093141     2.286040     112.65
 O      -0.183049     4.297782     2.883803     369.56
 H      -0.036674     5.039236     2.367695      32.99
 H      -0.734765     2.354956     3.141447      24.97
 H      -1.375093     3.186607     1.722686      25.85
 C      -2.478077    -1.170809    -0.406886     104.36
 H      -3.009992    -2.167884    -0.138133      25.62
 C      -2.364904     0.899916    -1.753309      55.90
 H      -2.833894     1.450602    -2.538894      21.52
 C      -1.407056     1.442862    -0.844386      20.38
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 O      -0.843671     2.675990    -1.036856     239.75
 C      -0.939945     3.296056    -2.331022      92.14
 H      -0.454338     4.200041    -2.310797      25.63
 H      -0.352114     2.747943    -3.237163      24.24
 H      -2.126862     3.402694    -2.453425      21.97
 C      -0.939210     0.625880     0.211935      27.83
 O       0.125587     0.952438     1.110809     203.61
 C      -1.488152    -0.636943     0.513463      29.48
 H      -1.121126    -1.369425     1.285407      16.83
 C      -2.872318    -0.399132    -1.546324      53.48
 C      -3.731600    -1.041620    -2.648378      47.52
 H      -3.488727    -0.280364    -3.513542      25.59
 O      -3.374643    -2.426487    -2.787348     236.33
 H      -2.412245    -2.842944    -2.827446      26.17
 C      -5.214221    -0.951778    -2.415426     102.19
 H      -5.496612    -1.300493    -1.425811      28.00
 O      -5.710585     0.411287    -2.401424     223.98
 H      -5.627957     0.767237    -1.405939      25.79
 C      -6.186409    -1.708095    -3.493476     104.47
 O      -6.004641    -3.117316    -3.738943     214.47
 H      -4.973142    -3.224999    -3.690636      31.29
 H      -6.081548    -1.131359    -4.390225      30.73
 H      -7.257655    -1.693979    -3.085204      28.84
55
name = lig-ACN-frame_180
 C       3.311924     2.999330     0.370653      53.84
 H       2.624145     3.818878     0.302995      23.86
 C       4.210152     1.059956     1.464588      65.09
 H       4.176317     0.388275     2.326102      22.16
 C       5.360642     1.153478     0.717125      26.29
 O       6.402734     0.309186     0.843223     225.57
 C       6.386417    -0.632053     1.944289     121.03
 H       6.445549    -0.137468     2.850352      27.88
 H       7.342790    -1.169364     1.768536      25.60
 H       5.534774    -1.361687     1.657526      24.33
 C       5.411187     2.105280    -0.330575      19.69
 O       6.551845     2.215677    -1.035169     189.90
 H       7.206565     1.563986    -0.802088      26.19
 C       4.373679     2.996384    -0.541158      65.62
 H       4.466259     3.817620    -1.217721      22.34
 C       3.101018     1.984710     1.355361      10.62
 C       1.887743     2.146531     2.205324     105.56
 H       2.017765     3.055270     2.753403      23.85
 O       1.859282     1.128666     3.243984     262.94
 H       1.625737     0.172903     2.776467      20.78
 C       0.590928     2.337013     1.458909      75.37
 H       0.557234     2.903899     0.414290      18.29
 C      -0.544366     3.051638     2.215881     104.22
 O      -0.215029     4.340781     2.911450     341.75
 H       0.099105     4.904942     2.292172      33.50
 H      -0.869028     2.407233     3.109884      24.89
 H      -1.385518     3.135347     1.516588      26.07
 C      -2.491090    -1.153856    -0.428261      51.72
 H      -2.777600    -2.206999    -0.413586      18.97
 C      -2.340803     0.899904    -1.755092      39.81
 H      -2.554132     1.457017    -2.636865      17.40
 C      -1.412114     1.405808    -0.856537      15.10
 O      -0.800976     2.661802    -1.032686     219.51
 C      -0.910164     3.272347    -2.397757      98.87
 H      -0.490785     4.199968    -2.305097      26.54
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 H      -0.504863     2.484052    -3.145349      25.34
 H      -2.081752     3.522100    -2.838682      23.77
 C      -0.945967     0.625063     0.320047      32.12
 O       0.140899     0.956688     1.112243     174.36
 C      -1.571735    -0.666014     0.467811      72.10
 H      -1.365411    -1.056422     1.541621      20.19
 C      -2.879085    -0.404697    -1.530359      47.40
 C      -3.685385    -1.005022    -2.636800      52.45
 H      -3.479268    -0.624445    -3.734817      24.73
 O      -3.301839    -2.485820    -2.817277     162.26
 H      -2.204337    -2.292751    -2.586993      21.12
 C      -5.326117    -1.013600    -2.395595      86.66
 H      -5.411522    -1.601076    -1.455249      28.57
 O      -5.730076     0.423004    -2.391149     255.97
 H      -5.483016     0.676485    -1.538416      31.26
 C      -6.177514    -1.654534    -3.449833     116.16
 O      -5.947570    -3.064109    -3.728941     232.75
 H      -4.973674    -3.217844    -3.782261      33.27
 H      -6.182198    -1.090790    -4.381539      30.21
 H      -7.214440    -1.519779    -3.079853      29.84
55
name = lig-ACN-frame_181
 C       3.262468     2.989003     0.276450      69.09
 H       2.482702     3.724906     0.162555      22.66
 C       4.139170     1.089922     1.570461      68.33
 H       3.996653     0.290419     2.340886      20.56
 C       5.299484     1.167287     0.758574       9.33
 O       6.445486     0.306204     0.769943     216.09
 C       6.422354    -0.678936     1.927382     123.11
 H       6.382517    -0.114842     2.834068      27.94
 H       7.384147    -1.340316     1.873409      25.35
 H       5.540099    -1.295207     2.073916      26.60
 C       5.477671     2.059424    -0.307037       8.76
 O       6.642542     2.199067    -1.051784     174.99
 H       7.307224     1.565074    -0.774612      24.47
 C       4.451287     3.028411    -0.488491      49.96
 H       4.763311     3.838171    -1.105978      22.36
 C       3.151908     2.045018     1.283638      20.18
 C       1.918158     2.165264     2.267359      92.02
 H       2.013693     3.076351     2.763345      24.36
 O       1.832284     1.171984     3.302401     278.31
 H       1.544057     0.232319     2.892394      21.99
 C       0.533356     2.325423     1.450331      62.16
 H       1.006769     2.936608     0.509899      18.40
 C      -0.669755     3.012668     2.252022      90.04
 O      -0.243366     4.314372     2.903621     294.37
 H       0.239252     5.037749     2.253920      26.38
 H      -1.051809     2.316248     3.046671      24.15
 H      -1.521397     3.272254     1.538700      23.44
 C      -2.502097    -1.176260    -0.452348     108.21
 H      -2.840042    -2.143648    -0.273714      25.70
 C      -2.318794     0.867079    -1.724400      48.52
 H      -2.438361     1.351398    -2.687674      15.01
 C      -1.331558     1.395885    -0.812646      25.34
 O      -0.775802     2.663605    -1.082687     222.72
 C      -0.894557     3.232622    -2.424849      95.40
 H      -0.249172     4.061630    -2.428765      25.71
 H      -0.392616     2.562424    -3.180007      26.55
 H      -2.114996     3.521909    -2.725920      22.56
 C      -0.992126     0.669390     0.313986      39.56
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 O       0.123626     0.943280     1.120293     187.11
 C      -1.613447    -0.574496     0.552082      37.59
 H      -1.321696    -1.343697     1.389785      15.81
 C      -2.882149    -0.395131    -1.614260      47.63
 C      -3.755313    -1.124309    -2.701385      36.87
 H      -3.625370    -0.401258    -3.647382      24.23
 O      -3.300882    -2.455166    -2.828368     201.99
 H      -2.194095    -2.818806    -2.776178      20.46
 C      -5.269808    -1.012484    -2.374917     102.87
 H      -5.570182    -1.383318    -1.357926      27.88
 O      -5.729277     0.372817    -2.341699     236.51
 H      -5.570690     0.752182    -1.482537      29.01
 C      -6.218059    -1.616817    -3.481891     108.54
 O      -5.889808    -3.023277    -3.710290     237.39
 H      -4.945879    -3.046366    -3.727510      33.82
 H      -6.021938    -0.971562    -4.363263      29.92
 H      -7.227720    -1.667122    -3.159233      30.05
55
name = lig-ACN-frame_182
 C       3.274493     2.993489     0.166600      44.52
 H       2.558754     3.741742    -0.211422      22.39
 C       4.135528     1.129087     1.598345      56.26
 H       3.895771     0.393163     2.420319      20.99
 C       5.325765     1.050676     0.751838       4.12
 O       6.432990     0.205607     0.827284     223.10
 C       6.455667    -0.626818     1.905873     124.48
 H       6.655795    -0.155268     2.891851      26.57
 H       7.351443    -1.384263     1.648854      24.49
 H       5.608877    -1.200777     1.790423      28.10
 C       5.518164     2.127306    -0.260527       4.39
 O       6.700766     2.187787    -1.085032     178.54
 H       7.454455     1.546054    -0.746330      20.13
 C       4.559049     3.114291    -0.473832      55.24
 H       4.552173     3.812814    -1.299955      24.27
 C       3.069580     2.085112     1.319725       8.06
 C       1.875809     2.195826     2.305178      98.74
 H       2.021562     3.066192     2.840485      24.67
 O       1.808367     1.199492     3.344783     289.97
 H       1.439864     0.439392     2.955303      28.42
 C       0.464184     2.307397     1.526242      71.69
 H       0.455846     2.924737     0.472177      17.65
 C      -0.651266     3.068290     2.266001     105.61
 O      -0.287474     4.203654     2.899827     255.52
 H      -0.019034     5.031214     2.112940      24.38
 H      -0.956620     2.446662     3.107390      25.48
 H      -1.615268     3.111280     1.566959      24.15
 C      -2.514989    -1.115611    -0.407472      75.05
 H      -2.970995    -1.996481    -0.196981      26.38
 C      -2.260867     0.839746    -1.767691      52.48
 H      -2.596598     1.476716    -2.610745      21.01
 C      -1.360914     1.439323    -0.891069      14.82
 O      -0.737152     2.652590    -1.121756     229.69
 C      -0.822087     3.177756    -2.446205      99.87
 H      -0.299974     4.171072    -2.439516      24.03
 H      -0.659637     2.477912    -3.234436      26.64
 H      -2.053744     3.578341    -2.590469      23.42
 C      -0.986873     0.674664     0.335305      26.22
 O       0.112933     0.948514     1.138766     183.69
 C      -1.679857    -0.553489     0.539060      43.62
 H      -1.185665    -1.125251     1.392779      16.94
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 C      -2.845104    -0.488502    -1.605720      46.90
 C      -3.727872    -1.073915    -2.692219      46.91
 H      -3.591807    -0.608606    -3.779387      25.85
 O      -3.401284    -2.514700    -2.881320     211.92
 H      -2.347732    -2.562761    -2.941390      24.27
 C      -5.314827    -1.012020    -2.348497      94.30
 H      -5.384909    -1.660782    -1.398022      27.74
 O      -5.702142     0.362997    -2.299966     253.47
 H      -5.504103     0.623126    -1.250684      24.08
 C      -6.180944    -1.638291    -3.476627     116.55
 O      -5.841291    -2.993773    -3.724293     236.36
 H      -4.839570    -3.086017    -3.591319      28.93
 H      -6.132971    -1.041233    -4.436761      29.49
 H      -7.179182    -1.524703    -3.234016      31.08
55
name = lig-ACN-frame_183
 C       3.322086     2.984714     0.193432      64.19
 H       2.422933     3.576953    -0.088526      22.21
 C       4.150969     1.199494     1.507635      58.68
 H       4.185500     0.582995     2.428885      21.48
 C       5.316346     1.139923     0.690749      18.50
 O       6.375079     0.225059     0.830360     219.47
 C       6.491190    -0.759458     1.960899     111.08
 H       6.734674    -0.119268     2.894337      26.03
 H       7.410139    -1.441515     1.680758      25.18
 H       5.678430    -1.258826     2.213706      30.10
 C       5.635893     2.146631    -0.210696       7.13
 O       6.673198     2.177552    -1.065062     120.89
 H       7.460816     1.523870    -0.778205      22.09
 C       4.553811     3.093059    -0.483880      43.87
 H       4.820995     3.775505    -1.319472      20.64
 C       3.090359     2.108462     1.268891      18.33
 C       1.773434     2.272421     2.261577      87.46
 H       1.855137     3.207507     2.736029      24.41
 O       1.777930     1.218239     3.347449     280.32
 H       1.465652     0.386599     3.003246      26.69
 C       0.463770     2.343324     1.539846      82.23
 H       0.800820     2.969181     0.578740      20.00
 C      -0.708329     2.908188     2.339543      98.29
 O      -0.290749     4.249772     2.916088     274.43
 H      -0.145400     5.004167     2.185557      27.78
 H      -1.028664     2.247027     3.123372      25.90
 H      -1.577182     3.157414     1.557696      23.46
 C      -2.595113    -1.124881    -0.337395      58.73
 H      -2.946105    -2.104175    -0.145651      16.00
 C      -2.263573     0.803241    -1.863381      39.53
 H      -2.627398     1.334289    -2.766366      15.71
 C      -1.370444     1.391028    -0.886790      20.61
 O      -0.668975     2.607314    -1.139023     213.94
 C      -0.848359     3.213495    -2.491348      82.82
 H       0.004106     3.999829    -2.576621      23.72
 H      -0.535202     2.493304    -3.191235      26.93
 H      -2.035870     3.633815    -2.784819      22.42
 C      -0.989957     0.712746     0.257750      38.21
 O       0.069641     0.944837     1.174961     169.22
 C      -1.628155    -0.516365     0.553917      62.49
 H      -1.601741    -0.949330     1.540412      24.68
 C      -2.771256    -0.449132    -1.609567      37.85
 C      -3.741110    -1.056418    -2.667607      65.86
 H      -3.476268    -0.436496    -3.627519      24.08
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 O      -3.486640    -2.560444    -2.924879     247.33
 H      -2.627357    -2.773609    -2.937815      30.91
 C      -5.265357    -1.028028    -2.393754      99.77
 H      -5.534000    -1.558190    -1.400813      28.61
 O      -5.688450     0.372844    -2.206386     254.92
 H      -5.409015     0.704049    -1.171055      23.89
 C      -6.137964    -1.633850    -3.480321     116.16
 O      -5.826281    -3.034729    -3.760180     215.68
 H      -4.820534    -3.147824    -3.575096      27.44
 H      -5.953010    -0.960633    -4.379343      29.75
 H      -7.094068    -1.685278    -3.121844      30.59
55
name = lig-ACN-frame_184
 C       3.320576     3.041530     0.213553      54.11
 H       2.657907     3.878205    -0.134700      22.18
 C       4.165887     1.226820     1.499531      67.05
 H       4.066967     0.508829     2.311611      22.98
 C       5.366239     1.206354     0.758843      13.56
 O       6.327258     0.187824     0.839671     187.50
 C       6.496284    -0.771301     2.021685     104.97
 H       6.960255    -0.233679     2.980871      24.97
 H       7.242118    -1.510291     1.599237      25.85
 H       5.670182    -1.233963     2.147120      29.98
 C       5.576286     2.202771    -0.248525      19.99
 O       6.722188     2.174118    -1.065498     101.10
 H       7.337734     1.510069    -0.699348      23.82
 C       4.546233     3.032391    -0.507607      60.85
 H       4.637345     3.894238    -1.214038      21.86
 C       3.099832     2.114719     1.268602      20.67
 C       1.851627     2.217034     2.244893      98.29
 H       1.940699     3.165404     2.751116      25.02
 O       1.750567     1.299869     3.297687     265.06
 H       1.606549     0.351642     2.795018      23.69
 C       0.444688     2.317239     1.490993      82.20
 H       0.443798     3.012206     0.577221      21.17
 C      -0.710581     2.930386     2.391342      94.74
 O      -0.329092     4.247741     2.945571     325.02
 H      -0.166433     4.741130     2.267249      35.45
 H      -0.895782     2.306274     3.259509      26.28
 H      -1.749135     2.931168     1.761989      24.86
 C      -2.560187    -1.082971    -0.338092      66.16
 H      -3.105882    -2.014224    -0.036408      24.74
 C      -2.223162     0.792970    -1.857829      58.03
 H      -2.244438     1.218186    -2.855393      17.31
 C      -1.306541     1.411326    -0.988890      18.14
 O      -0.655409     2.589498    -1.204236     225.19
 C      -0.791771     3.176080    -2.527140      96.37
 H      -0.080113     4.165860    -2.462102      22.89
 H      -0.697664     2.514034    -3.335623      27.95
 H      -1.952406     3.746197    -2.580655      24.98
 C      -0.981995     0.649115     0.261011      20.23
 O       0.022184     0.989907     1.155829     193.60
 C      -1.700822    -0.516948     0.594414      34.86
 H      -1.441155    -0.929359     1.500798      19.51
 C      -2.837939    -0.520015    -1.581557      58.67
 C      -3.690061    -1.128617    -2.657236      54.70
 H      -3.614527    -0.558041    -3.658966      28.01
 O      -3.525604    -2.535256    -2.936043     241.13
 H      -2.560308    -2.817210    -2.824430      27.19
 C      -5.212931    -0.975359    -2.323978      81.76
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 H      -5.351728    -1.619680    -1.360653      27.26
 O      -5.682794     0.371429    -2.160912     246.57
 H      -5.427640     0.621764    -1.181461      25.65
 C      -6.102282    -1.664239    -3.509424     106.43
 O      -5.853302    -3.075637    -3.813518     220.63
 H      -4.898914    -3.121606    -3.740005      30.60
 H      -6.092628    -1.054348    -4.484763      28.97
 H      -7.107608    -1.527272    -3.248141      30.75
55
name = lig-ACN-frame_185
 C       3.304728     3.120256     0.231056      59.28
 H       2.517933     3.915292     0.164770      23.41
 C       4.150790     1.193074     1.574576      57.22
 H       3.907878     0.369474     2.214875      22.09
 C       5.410536     1.211094     0.848390       3.82
 O       6.334167     0.142976     0.880885     238.34
 C       6.448821    -0.702759     1.959051     125.97
 H       6.949241    -0.200038     2.951041      24.12
 H       7.085642    -1.483304     1.613938      25.81
 H       5.611343    -1.065731     2.304567      29.80
 C       5.582365     2.106980    -0.291681      -3.33
 O       6.751532     2.179649    -1.046834     186.99
 H       7.454077     1.620221    -0.756972      25.29
 C       4.467000     3.128164    -0.566082      42.17
 H       4.613620     3.821675    -1.428491      22.82
 C       3.111955     2.144838     1.272988      23.20
 C       1.874090     2.260693     2.138438      88.77
 H       2.071971     3.234260     2.658033      24.51
 O       1.760002     1.296637     3.243724     254.14
 H       1.573039     0.314256     2.944661      24.47
 C       0.380811     2.379299     1.475597      78.68
 H       0.501500     2.932638     0.559382      22.68
 C      -0.626821     2.958167     2.475604     102.18
 O      -0.393620     4.226552     2.952036     310.36
 H      -0.006676     4.928560     2.338660      29.07
 H      -0.658908     2.291854     3.356961      25.49
 H      -1.704046     2.952083     1.932802      24.25
 C      -2.600107    -1.113913    -0.324813      82.01
 H      -3.192739    -2.087308    -0.033447      24.41
 C      -2.152881     0.695579    -1.865238      33.50
 H      -2.318524     1.079678    -2.842711      21.36
 C      -1.250272     1.294342    -0.975043      13.36
 O      -0.623191     2.560289    -1.279735     222.61
 C      -0.782527     3.221562    -2.545052      77.83
 H       0.104845     4.110999    -2.608882      23.05
 H      -0.556309     2.595157    -3.405892      26.17
 H      -1.991411     3.657840    -2.654376      23.04
 C      -0.990639     0.692699     0.240005      25.86
 O       0.013409     0.987357     1.120164     199.04
 C      -1.728306    -0.493803     0.616415      41.50
 H      -1.397699    -1.042580     1.417139      19.66
 C      -2.807339    -0.473720    -1.589921      45.55
 C      -3.704663    -1.106988    -2.689592      54.83
 H      -3.361252    -0.565264    -3.623256      26.85
 O      -3.481875    -2.553380    -2.899734     177.50
 H      -2.333381    -2.708870    -2.818215      22.81
 C      -5.244922    -1.047970    -2.332042      91.67
 H      -5.421034    -1.620628    -1.341399      27.27
 O      -5.668435     0.349132    -2.151553     269.83
 H      -5.486750     0.666283    -1.307373      30.21
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 C      -6.097811    -1.654083    -3.497349     104.07
 O      -5.916033    -3.073100    -3.848889     215.54
 H      -4.974594    -3.259594    -3.906275      31.96
 H      -5.752198    -1.008667    -4.380109      28.34
 H      -7.140110    -1.637839    -3.220719      29.37
55
name = lig-ACN-frame_186
 C       3.348574     3.139134     0.268276      62.49
 H       2.515775     3.808333    -0.004876      22.54
 C       4.146178     1.185884     1.555104      74.70
 H       3.986984     0.518367     2.379881      22.50
 C       5.325673     1.190735     0.810021       6.61
 O       6.345795     0.216029     0.825260     184.03
 C       6.404935    -0.711160     2.034664     114.49
 H       6.979373    -0.017531     2.806885      23.92
 H       6.946342    -1.531657     1.772804      27.35
 H       5.477334    -0.986054     2.337105      28.16
 C       5.481298     2.133147    -0.264006      10.98
 O       6.713395     2.187564    -1.033790     138.12
 H       7.387250     1.526007    -0.623496      23.45
 C       4.536582     3.065564    -0.560669      60.08
 H       4.701051     3.723616    -1.415450      23.37
 C       3.169758     2.160735     1.244617      16.62
 C       1.788036     2.294349     2.116513      90.17
 H       1.806490     3.305576     2.668002      24.39
 O       1.805125     1.280029     3.186088     284.83
 H       1.431793     0.578535     2.744479      28.60
 C       0.467911     2.426886     1.441827      90.41
 H       0.412642     3.086700     0.659249      24.39
 C      -0.597094     2.882328     2.501214      88.64
 O      -0.410608     4.333466     3.019841     179.71
 H       0.126531     4.847075     2.118122      25.55
 H      -0.545756     2.222277     3.408135      25.54
 H      -1.667982     2.759326     2.027775      25.27
 C      -2.661115    -1.102067    -0.304787      57.10
 H      -3.063387    -2.194877    -0.049315      19.81
 C      -2.073570     0.641986    -1.950226      59.95
 H      -2.305714     1.213307    -2.826426      21.50
 C      -1.203643     1.312775    -1.037037      12.18
 O      -0.562251     2.479950    -1.304045     194.68
 C      -0.786981     3.225903    -2.605458      74.27
 H      -0.052901     4.237436    -2.378121      22.11
 H      -0.524335     2.513253    -3.454473      24.43
 H      -1.937187     3.754714    -2.807184      23.75
 C      -1.028608     0.670722     0.281657      28.49
 O       0.064037     1.018325     1.131262     167.39
 C      -1.712677    -0.515279     0.566176      53.18
 H      -1.622012    -0.871537     1.571616      24.45
 C      -2.818647    -0.559740    -1.579191      43.36
 C      -3.725513    -1.098585    -2.661100      68.43
 H      -3.748735    -0.505562    -3.608239      29.27
 O      -3.367629    -2.565853    -2.833687     156.32
 H      -2.258161    -2.906611    -3.011194      21.85
 C      -5.239571    -1.103633    -2.351928      97.57
 H      -5.440738    -1.696681    -1.400903      28.88
 O      -5.675178     0.295038    -2.198613     286.08
 H      -5.379031     0.497048    -1.326208      31.61
 C      -6.091759    -1.646225    -3.505217     105.77
 O      -5.987668    -3.047889    -3.861359     197.88
 H      -4.952218    -3.196302    -3.872250      29.66
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 H      -5.984745    -0.959347    -4.425859      28.52
 H      -7.174862    -1.424842    -3.282133      28.88
55
name = lig-ACN-frame_187
 C       3.401597     3.107328     0.202620      63.96
 H       2.739106     3.897724    -0.134126      23.51
 C       4.105787     1.229440     1.534680      54.11
 H       4.025242     0.632070     2.450968      22.30
 C       5.261896     1.118042     0.676953      20.18
 O       6.342144     0.252733     0.820296     214.73
 C       6.374995    -0.621012     2.070048     112.67
 H       6.887247    -0.269072     3.045105      26.03
 H       6.879438    -1.420329     1.697337      28.52
 H       5.367957    -0.922019     2.330429      27.70
 C       5.547127     2.136234    -0.249301      24.09
 O       6.620746     2.160999    -0.988685     134.32
 H       7.310114     1.440883    -0.615610      22.56
 C       4.538782     3.062566    -0.535926      64.61
 H       4.701934     3.828466    -1.264369      22.49
 C       3.079915     2.219552     1.292150      26.20
 C       1.918312     2.330842     2.172832      93.89
 H       2.081453     3.305660     2.811855      23.71
 O       1.822637     1.276372     3.093699     293.07
 H       1.388725     0.451179     2.769714      25.70
 C       0.431813     2.419093     1.463623      86.33
 H       0.506522     2.947520     0.629652      25.66
 C      -0.566782     2.940044     2.546901      96.91
 O      -0.412961     4.327551     3.014546     249.61
 H      -0.026105     4.969617     2.222428      27.09
 H      -0.454800     2.339960     3.515749      25.39
 H      -1.623853     2.801147     2.124472      26.16
 C      -2.636782    -1.096765    -0.319408      77.20
 H      -3.277444    -2.019028     0.024078      24.19
 C      -2.061507     0.609055    -1.958113      24.05
 H      -2.162951     0.915479    -3.013293      21.30
 C      -1.214168     1.248626    -1.056178      17.59
 O      -0.499423     2.465189    -1.358163     211.59
 C      -0.759066     3.173953    -2.578491      87.61
 H      -0.052377     4.271035    -2.578459      22.17
 H      -0.445218     2.731309    -3.634123      24.66
 H      -1.998696     3.361237    -2.557421      25.08
 C      -0.974869     0.693466     0.223505      32.02
 O       0.088773     1.054194     1.106837     185.71
 C      -1.736108    -0.511646     0.592466      44.05
 H      -1.550975    -0.955919     1.628984      19.76
 C      -2.793629    -0.522053    -1.627465      54.35
 C      -3.710750    -1.230447    -2.635548      60.95
 H      -3.438072    -0.720090    -3.582702      27.91
 O      -3.308598    -2.576742    -2.811201     211.47
 H      -2.313575    -2.431232    -2.921052      25.72
 C      -5.248873    -1.143562    -2.349018      97.39
 H      -5.504860    -1.763909    -1.448989      28.35
 O      -5.670188     0.211396    -2.231741     247.47
 H      -5.452635     0.739887    -1.314816      25.17
 C      -6.167361    -1.613126    -3.562323     102.36
 O      -6.020212    -3.015602    -3.851649     205.37
 H      -5.057039    -3.253537    -3.727926      30.79
 H      -5.899307    -0.998187    -4.476320      27.74
 H      -7.230964    -1.517595    -3.114349      27.46
55
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name = lig-ACN-frame_188
 C       3.277807     3.134882     0.170531      57.45
 H       2.540293     3.915781     0.122470      23.93
 C       4.089530     1.265733     1.490589      80.11
 H       3.880693     0.545071     2.314347      22.71
 C       5.192717     1.093685     0.697402      13.06
 O       6.328172     0.237323     0.918590     213.50
 C       6.334087    -0.574995     2.007285     127.13
 H       6.776908     0.096757     2.789742      26.13
 H       6.932376    -1.427973     1.880724      27.69
 H       5.300525    -0.946821     2.367924      26.59
 C       5.486393     2.096223    -0.267698       0.90
 O       6.703638     2.095956    -1.028464     131.63
 H       7.403834     1.498356    -0.713046      24.28
 C       4.556167     3.146752    -0.544197      50.84
 H       4.843953     3.868788    -1.284669      23.62
 C       3.147760     2.241292     1.211142      25.19
 C       1.896143     2.355575     2.203689      84.61
 H       2.020261     3.323336     2.879076      24.28
 O       1.856657     1.216927     3.121208     227.33
 H       1.550801     0.443444     2.404636      23.07
 C       0.470550     2.489017     1.529033      82.15
 H       0.429394     3.123106     0.744951      25.23
 C      -0.573875     3.013320     2.561781     108.22
 O      -0.381671     4.327287     2.989273     330.11
 H      -0.258764     4.870522     2.328989      35.91
 H      -0.460292     2.346073     3.489685      25.59
 H      -1.627042     2.853318     2.199958      26.62
 C      -2.600623    -1.042888    -0.311951      64.65
 H      -3.291906    -1.847572     0.018572      25.70
 C      -2.058303     0.608013    -2.011798      55.61
 H      -1.946655     0.925927    -3.075346      20.56
 C      -1.153128     1.268767    -1.081425       7.17
 O      -0.408649     2.386929    -1.392856     203.33
 C      -0.780806     3.134262    -2.563161      78.04
 H      -0.308405     4.312283    -2.344667      22.48
 H      -0.376352     2.440363    -3.473667      23.51
 H      -1.987327     3.363868    -2.737773      25.93
 C      -0.925001     0.651388     0.206760      24.55
 O       0.081604     1.052825     1.072483     185.39
 C      -1.707315    -0.425778     0.599072      50.28
 H      -1.418790    -1.015101     1.581088      21.09
 C      -2.812404    -0.551278    -1.579489      40.70
 C      -3.675290    -1.242686    -2.674153      60.39
 H      -3.639177    -0.684648    -3.630966      28.56
 O      -3.284294    -2.660988    -2.796840     250.37
 H      -2.440294    -2.939079    -2.792405      30.60
 C      -5.277078    -1.173735    -2.396964      95.46
 H      -5.508361    -1.732205    -1.481253      28.19
 O      -5.676140     0.211652    -2.238914     224.77
 H      -5.311349     0.477547    -1.250957      25.14
 C      -6.179912    -1.620210    -3.525455     107.33
 O      -6.041395    -3.032198    -3.846428     227.19
 H      -5.132703    -3.207494    -3.701292      32.89
 H      -6.005652    -0.895050    -4.387246      27.75
 H      -7.332304    -1.449487    -3.369962      26.87
55
name = lig-ACN-frame_189
 C       3.286804     3.232201     0.124017      62.24
 H       2.571002     3.977887    -0.224037      23.97
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 C       4.052399     1.199461     1.484501      54.88
 H       3.820676     0.518657     2.342139      21.61
 C       5.283517     1.159236     0.712900       2.73
 O       6.257067     0.255279     0.861391     187.22
 C       6.309378    -0.582390     2.147167     104.47
 H       6.585099    -0.077597     3.046606      27.14
 H       7.098354    -1.306389     1.834223      25.61
 H       5.241156    -1.118672     2.268544      24.72
 C       5.468385     2.098729    -0.390117      10.34
 O       6.728119     2.031062    -1.070256     174.15
 H       7.272419     1.510609    -0.503229      22.40
 C       4.527524     3.167872    -0.544065      53.38
 H       4.722863     3.951289    -1.283615      24.33
 C       3.062529     2.253653     1.202803       7.98
 C       1.860010     2.302476     2.181500      88.03
 H       2.015980     3.270839     2.874969      23.41
 O       1.885333     1.179405     3.123496     262.16
 H       1.641975     0.292454     2.694021      25.27
 C       0.469339     2.528364     1.546067      84.66
 H       0.566743     3.174046     0.712344      24.25
 C      -0.613026     2.934846     2.566647     100.16
 O      -0.327728     4.407546     2.999258     242.76
 H      -0.269958     4.941314     2.146780      29.81
 H      -0.634437     2.375197     3.540177      25.85
 H      -1.562360     2.841822     2.040925      26.98
 C      -2.641275    -1.005266    -0.250123      56.12
 H      -2.991755    -1.926384     0.105626      22.53
 C      -1.995249     0.610699    -2.000433      49.11
 H      -2.223690     1.015351    -2.997693      22.50
 C      -1.124190     1.213350    -1.119862      19.01
 O      -0.331698     2.325527    -1.389836     216.70
 C      -0.788686     3.091846    -2.568010      84.64
 H      -0.176877     4.241850    -2.529562      22.56
 H      -0.353306     2.778546    -3.685132      23.92
 H      -1.966145     3.094932    -2.599491      25.21
 C      -0.883565     0.722391     0.182177      19.79
 O       0.139578     1.110185     1.088846     158.03
 C      -1.662288    -0.428157     0.582292      48.14
 H      -1.504794    -0.756204     1.718437      21.53
 C      -2.794997    -0.510797    -1.651950      45.32
 C      -3.663354    -1.247249    -2.689953      68.46
 H      -3.408126    -0.809794    -3.658212      28.91
 O      -3.374058    -2.776482    -2.796357     223.95
 H      -2.486489    -2.802359    -2.793538      31.01
 C      -5.272137    -1.165555    -2.375160      91.59
 H      -5.452715    -1.787202    -1.512862      28.81
 O      -5.649776     0.237258    -2.194964     281.55
 H      -5.351103     0.588474    -1.380508      31.30
 C      -6.185720    -1.666732    -3.552448     106.54
 O      -6.050372    -3.062928    -3.846656     200.22
 H      -5.066707    -3.284556    -3.787949      29.71
 H      -5.945045    -1.118045    -4.492682      27.65
 H      -7.239787    -1.477201    -3.080722      27.53
55
name = lig-ACN-frame_190
 C       3.349623     3.183794     0.184201      58.54
 H       2.627342     3.969543    -0.105548      23.97
 C       4.015802     1.292019     1.381432      67.37
 H       3.990217     0.597404     2.220903      22.13
 C       5.198751     1.298031     0.695305      -5.40
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 O       6.254864     0.198147     0.891498     182.22
 C       6.281958    -0.581518     2.171909     106.04
 H       6.376795     0.006278     3.002060      27.84
 H       7.222524    -1.281032     2.073567      24.91
 H       5.319714    -1.368108     2.271967      24.22
 C       5.502102     2.122458    -0.397074      20.05
 O       6.646666     1.980995    -1.103363     120.12
 H       7.378772     1.431539    -0.608378      22.27
 C       4.535460     3.142778    -0.630853      57.43
 H       4.710447     3.908698    -1.430392      22.68
 C       3.021829     2.225949     1.162171      29.85
 C       1.870206     2.243217     2.182694      95.61
 H       2.106832     3.172557     2.885852      23.83
 O       1.894370     1.170876     3.135950     297.73
 H       1.501369     0.457278     2.731724      29.22
 C       0.448187     2.439379     1.555766      89.21
 H       0.477529     3.212298     0.747265      24.44
 C      -0.617124     3.036661     2.553656     108.93
 O      -0.315804     4.371915     2.978915     216.80
 H      -0.068480     5.069941     2.081301      26.03
 H      -0.615479     2.394168     3.438522      27.17
 H      -1.605973     3.012930     2.157070      27.58
 C      -2.611462    -0.985639    -0.290697      47.63
 H      -3.177053    -1.788874    -0.058777      23.43
 C      -2.020129     0.590115    -2.015722      79.97
 H      -2.105203     1.053287    -2.987675      20.43
 C      -1.014113     1.200758    -1.106508       5.39
 O      -0.268711     2.323003    -1.481965     213.93
 C      -0.723552     3.089778    -2.566003      83.61
 H      -0.468183     4.276922    -2.290116      23.03
 H      -0.481184     2.463817    -3.636217      22.58
 H      -1.873852     3.179774    -2.531601      26.65
 C      -0.865169     0.730693     0.236234      31.26
 O       0.163316     1.161987     1.061679     216.08
 C      -1.646029    -0.369443     0.580766      52.55
 H      -1.547516    -0.833634     1.637150      22.77
 C      -2.751192    -0.573733    -1.578440      28.32
 C      -3.695277    -1.338620    -2.681055      75.40
 H      -3.471979    -0.912562    -3.645131      28.98
 O      -3.496592    -2.763066    -2.769470     222.34
 H      -2.522698    -3.070010    -2.986549      25.91
 C      -5.180846    -1.113263    -2.381423     100.65
 H      -5.379885    -1.673207    -1.500569      28.83
 O      -5.626929     0.248039    -2.166181     281.72
 H      -5.321053     0.554016    -1.324400      31.42
 C      -6.147545    -1.693256    -3.534597      98.76
 O      -6.049437    -3.132802    -3.833721     186.05
 H      -5.037799    -3.334853    -3.857966      29.81
 H      -6.063220    -0.990344    -4.395352      28.53
 H      -7.265491    -1.623460    -3.273521      27.46
55
name = lig-ACN-frame_191
 C       3.360180     3.185612     0.142072      55.44
 H       2.670621     4.059249     0.097903      22.97
 C       4.046751     1.281827     1.394240      59.01
 H       3.760332     0.555813     2.123408      23.58
 C       5.289468     1.164018     0.691251      18.78
 O       6.189800     0.217024     0.939806     222.09
 C       6.236297    -0.539252     2.122420     109.15
 H       6.112313     0.075645     2.907600      28.70
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 H       7.340322    -0.999267     2.232447      24.58
 H       5.307675    -1.381558     2.228265      24.53
 C       5.502299     2.166004    -0.334563      14.27
 O       6.615087     1.966278    -1.196345     128.21
 H       7.208796     1.264262    -0.696907      23.04
 C       4.518194     3.100001    -0.677656      61.90
 H       4.679506     3.817808    -1.539863      20.59
 C       3.029090     2.213643     1.127080      17.26
 C       1.856090     2.302010     2.206626      88.00
 H       1.995397     3.294150     2.800957      23.95
 O       1.883639     1.157717     3.139414     266.69
 H       1.441336     0.348676     2.677669      24.47
 C       0.444413     2.486213     1.562817      75.66
 H       0.608120     3.135132     0.623621      22.53
 C      -0.627659     3.065018     2.536325     114.17
 O      -0.277313     4.376909     2.964979     253.27
 H       0.145102     4.928642     2.125631      27.70
 H      -0.667862     2.534339     3.464004      27.36
 H      -1.564529     2.989222     2.063405      28.23
 C      -2.555276    -1.030236    -0.269179      58.56
 H      -3.114544    -1.707303     0.262046      24.68
 C      -1.945589     0.586000    -1.967363      55.60
 H      -1.965717     0.803963    -3.012101      23.08
 C      -1.014168     1.210273    -1.158611      13.10
 O      -0.193507     2.275859    -1.508327     221.25
 C      -0.759036     3.131235    -2.582040      95.33
 H      -0.021917     4.101763    -2.644235      23.27
 H      -0.298375     2.745537    -3.695204      23.42
 H      -1.842342     3.203730    -2.605385      27.75
 C      -0.868916     0.728537     0.190489      16.48
 O       0.159098     1.094260     1.037485     174.25
 C      -1.697198    -0.369720     0.640106      42.20
 H      -1.443556    -0.820539     1.608024      22.19
 C      -2.722078    -0.596369    -1.674243      42.05
 C      -3.631989    -1.286391    -2.652686      69.21
 H      -3.453617    -0.835423    -3.609246      29.33
 O      -3.604200    -2.770850    -2.722684     147.33
 H      -2.463104    -2.974211    -2.903888      23.41
 C      -5.225439    -1.153299    -2.352941      91.13
 H      -5.425691    -1.700292    -1.469165      29.18
 O      -5.581282     0.256630    -2.181244     225.84
 H      -5.255533     0.548500    -1.177346      25.50
 C      -6.119213    -1.710818    -3.478440     109.19
 O      -6.013271    -3.156697    -3.816768     199.31
 H      -5.081869    -3.334591    -3.776893      31.60
 H      -5.906136    -1.203316    -4.426403      28.30
 H      -7.139988    -1.496506    -3.073360      28.76
55
name = lig-ACN-frame_192
 C       3.290152     3.219159     0.092038      50.24
 H       2.652961     4.037020    -0.325888      21.01
 C       4.051505     1.156222     1.452082      70.57
 H       3.891420     0.415877     2.193910      22.30
 C       5.203150     1.176109     0.696286       9.61
 O       6.244733     0.204106     0.881549     196.94
 C       6.160941    -0.476911     2.191048     104.14
 H       5.899806     0.045492     3.040323      28.43
 H       7.276680    -0.937209     2.203778      24.93
 H       5.497657    -1.512396     1.963995      24.49
 C       5.521926     2.074122    -0.356344      18.46
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 O       6.580844     1.967298    -1.259780     123.80
 H       7.272796     1.409463    -0.941835      26.91
 C       4.497807     3.056235    -0.638485      53.68
 H       4.708445     3.769529    -1.487622      21.80
 C       3.099380     2.256993     1.173819      -4.34
 C       1.872460     2.334527     2.171579      96.00
 H       2.098677     3.139318     2.912887      24.35
 O       1.852546     1.208429     3.110985     236.32
 H       1.503942     0.309982     2.592430      21.92
 C       0.478153     2.479093     1.517309      77.67
 H       0.444340     3.268485     0.608313      22.31
 C      -0.627690     2.995864     2.491011     103.38
 O      -0.220123     4.448533     2.940652     284.11
 H       0.128576     4.871123     2.251757      35.30
 H      -0.752326     2.369540     3.329505      27.77
 H      -1.529316     3.102958     1.995167      28.19
 C      -2.564958    -1.064545    -0.240281      49.00
 H      -3.070609    -2.018013    -0.124986      22.45
 C      -1.884073     0.493879    -2.077035      48.45
 H      -1.921577     0.898138    -3.072887      20.89
 C      -1.034397     1.213302    -1.128469      18.92
 O      -0.175258     2.253353    -1.559139     210.05
 C      -0.635818     3.164496    -2.651402     106.61
 H      -0.269278     4.177383    -2.330520      23.89
 H      -0.672927     2.594195    -3.800177      22.32
 H      -1.660909     3.358706    -2.469418      28.90
 C      -0.887042     0.703927     0.171330      26.16
 O       0.155348     1.048656     1.062578     178.04
 C      -1.682660    -0.359521     0.607436      47.96
 H      -1.610219    -0.593809     1.613943      23.42
 C      -2.642041    -0.612987    -1.568080      36.47
 C      -3.697220    -1.237703    -2.632897      60.99
 H      -3.454331    -0.903234    -3.625712      29.01
 O      -3.576004    -2.755755    -2.675186     181.42
 H      -2.500570    -3.134548    -2.633861      23.50
 C      -5.192554    -1.147091    -2.276006      97.67
 H      -5.380254    -1.701780    -1.385821      28.39
 O      -5.542244     0.239765    -2.204798     269.74
 H      -5.333483     0.724399    -1.277366      25.97
 C      -6.100692    -1.739787    -3.464693     109.12
 O      -5.987015    -3.132390    -3.757860     233.20
 H      -5.062607    -3.350099    -3.541018      29.79
 H      -5.880527    -1.055991    -4.299557      28.79
 H      -7.160176    -1.612925    -3.245929      29.01
55
name = lig-ACN-frame_193
 C       3.319896     3.083758     0.118510      65.85
 H       2.427632     3.678293    -0.102462      24.49
 C       3.980560     1.236290     1.416027      58.81
 H       3.811726     0.602320     2.278703      23.31
 C       5.230519     1.119752     0.658013       2.87
 O       6.278423     0.210550     0.885668     198.78
 C       6.177615    -0.532055     2.160559     101.56
 H       5.760249     0.216436     2.818247      27.27
 H       7.195003    -0.807140     2.673105      25.10
 H       5.335734    -1.438684     2.201167      24.99
 C       5.409419     2.018665    -0.433149      24.98
 O       6.547838     1.970553    -1.290848     177.46
 H       7.258386     1.611450    -0.746979      25.62
 C       4.525527     3.040007    -0.632743      57.60
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 H       4.731421     3.717554    -1.471019      23.90
 C       3.111759     2.267468     1.241145      30.27
 C       1.918963     2.321839     2.144354     104.49
 H       1.946754     3.280819     2.642881      24.55
 O       1.819966     1.256167     3.074274     306.26
 H       1.544873     0.470506     2.553330      26.78
 C       0.469398     2.427081     1.459753      78.33
 H       0.565108     3.040923     0.397557      21.02
 C      -0.569437     3.087332     2.428870     113.79
 O      -0.201646     4.384297     2.911804     305.46
 H       0.083660     4.939097     2.180977      31.81
 H      -0.617123     2.538348     3.335929      27.41
 H      -1.505036     3.055341     1.970784      28.32
 C      -2.553990    -1.084158    -0.294966      50.78
 H      -3.063308    -2.006608     0.214059      21.50
 C      -1.829662     0.454536    -2.067003      40.55
 H      -2.029792     0.708962    -3.113635      23.63
 C      -1.005247     1.196428    -1.230598      16.18
 O      -0.175943     2.235200    -1.612027     228.55
 C      -0.622524     3.171314    -2.593357     118.10
 H       0.104436     3.964706    -2.647795      25.89
 H      -0.206473     2.738870    -3.742334      23.22
 H      -1.633140     3.409142    -2.556817      28.35
 C      -0.864418     0.716615     0.196099      10.96
 O       0.138716     1.082987     1.091215     191.68
 C      -1.695442    -0.404307     0.628326      34.76
 H      -1.583301    -0.718741     1.596891      22.28
 C      -2.682762    -0.624967    -1.636105      47.85
 C      -3.646252    -1.332360    -2.538214      81.25
 H      -3.585688    -0.803513    -3.490633      28.27
 O      -3.479129    -2.738884    -2.607382     236.55
 H      -2.495869    -2.873949    -2.680247      27.92
 C      -5.177959    -1.115048    -2.235148      96.11
 H      -5.382722    -1.539491    -1.257867      28.02
 O      -5.551954     0.272986    -2.227998     311.87
 H      -5.294473     0.597559    -1.416204      31.96
 C      -6.095581    -1.688952    -3.413427     104.16
 O      -5.938083    -3.125052    -3.693004     210.40
 H      -4.968938    -3.373580    -3.424284      28.47
 H      -5.861666    -1.155261    -4.340294      28.24
 H      -7.105993    -1.482748    -3.151016      29.48
55
name = lig-ACN-frame_194
 C       3.302255     3.060898     0.121925      57.06
 H       2.718026     3.931527    -0.137573      24.73
 C       4.133830     1.220500     1.436703      66.16
 H       3.904892     0.533911     2.281514      22.71
 C       5.220426     1.043770     0.614509      15.46
 O       6.280056     0.176166     0.923935     196.51
 C       6.147511    -0.483835     2.175567     110.21
 H       5.727901     0.089769     3.100124      25.56
 H       7.211207    -0.835452     2.334947      26.11
 H       5.525004    -1.502749     1.968906      25.28
 C       5.400942     1.959107    -0.491810      14.69
 O       6.525476     1.956515    -1.265887     107.27
 H       7.343159     1.507042    -0.762753      23.54
 C       4.437244     3.036001    -0.682874      47.53
 H       4.524519     3.789935    -1.433241      23.36
 C       3.086521     2.203039     1.202622      19.60
 C       1.818582     2.386199     2.113631     105.32
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 H       1.960302     3.196866     2.756741      24.95
 O       1.815283     1.283061     3.086429     294.08
 H       1.477632     0.530721     2.697549      29.01
 C       0.517797     2.461066     1.369103      78.03
 H       0.628088     3.154513     0.350788      21.03
 C      -0.530253     3.084189     2.364648     107.81
 O      -0.157742     4.369454     2.866711     223.80
 H      -0.042140     5.167739     2.043021      26.24
 H      -0.557745     2.432519     3.224501      26.95
 H      -1.487173     3.132635     1.941434      27.21
 C      -2.504201    -1.051860    -0.275081      54.02
 H      -3.339068    -1.861028     0.085683      22.74
 C      -1.888269     0.426939    -2.077890      61.17
 H      -1.773034     0.764813    -3.132059      19.32
 C      -0.942174     1.091966    -1.181560      12.51
 O      -0.166796     2.200430    -1.593518     222.29
 C      -0.528479     3.183537    -2.648932     105.10
 H      -0.038220     3.993822    -2.330664      27.62
 H      -0.497135     2.628128    -3.818250      22.29
 H      -1.533948     3.502124    -2.589290      28.79
 C      -0.885047     0.696074     0.137791      28.91
 O       0.076062     1.080877     1.102218     184.86
 C      -1.649833    -0.399925     0.582836      47.08
 H      -1.422082    -0.841175     1.510471      22.78
 C      -2.681494    -0.646397    -1.609070      48.62
 C      -3.653644    -1.309898    -2.553261      56.96
 H      -3.436850    -1.058310    -3.590499      29.32
 O      -3.333197    -2.779668    -2.533532     222.93
 H      -2.515306    -2.928327    -2.801303      30.74
 C      -5.204949    -1.101474    -2.221268      97.91
 H      -5.560674    -1.620682    -1.314174      27.79
 O      -5.551389     0.336226    -2.240277     261.12
 H      -5.284721     0.805551    -1.442773      29.05
 C      -6.048337    -1.677164    -3.335498     112.11
 O      -5.903423    -3.105543    -3.608309     227.20
 H      -4.928086    -3.261253    -3.461240      30.15
 H      -5.800545    -1.080952    -4.216873      29.00
 H      -7.060740    -1.541525    -3.044540      29.99
55
name = lig-ACN-frame_195
 C       3.265091     3.143013     0.095204      53.70
 H       2.555834     3.940414     0.036091      21.06
 C       4.106183     1.193984     1.489589      53.58
 H       4.115472     0.461608     2.340981      21.30
 C       5.206128     1.066374     0.562649      11.86
 O       6.253535     0.195699     0.914431     201.27
 C       6.194465    -0.564795     2.187749     103.69
 H       5.927528     0.135756     3.159310      25.42
 H       7.181021    -0.922749     2.411306      27.01
 H       5.415418    -1.455792     2.135337      25.67
 C       5.386395     1.959948    -0.500369      22.34
 O       6.571491     1.930194    -1.271156     169.12
 H       7.218612     1.279380    -0.784811      22.11
 C       4.405185     2.917140    -0.752195      56.54
 H       4.728259     3.620697    -1.477751      25.67
 C       3.092810     2.125396     1.153788      11.84
 C       1.898131     2.322962     2.111136      97.55
 H       1.973717     3.252933     2.526896      25.31
 O       1.791361     1.316325     3.132848     287.24
 H       1.396294     0.469127     2.646914      23.75
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 C       0.478019     2.527526     1.323352      67.32
 H       0.556773     3.132364     0.268061      18.96
 C      -0.541479     3.058724     2.261107     102.65
 O      -0.102970     4.422253     2.838519     206.10
 H      -0.072484     5.020400     1.869028      25.85
 H      -0.607844     2.394645     3.159452      25.69
 H      -1.503150     3.110113     1.792580      26.53
 C      -2.582720    -1.031127    -0.264346      50.24
 H      -3.120513    -2.072976     0.161332      20.67
 C      -1.850117     0.456527    -2.071098      48.46
 H      -2.008891     0.720348    -3.146148      20.62
 C      -0.962898     1.087092    -1.252585      22.17
 O      -0.135527     2.154616    -1.563460     214.02
 C      -0.515146     3.138995    -2.639281     108.88
 H       0.074822     3.907479    -2.556259      28.03
 H      -0.169607     2.800791    -3.824537      23.13
 H      -1.561820     3.349142    -2.502355      27.14
 C      -0.817793     0.657607     0.158034      26.36
 O       0.037253     1.103176     1.086346     180.29
 C      -1.582691    -0.456536     0.565008      48.54
 H      -1.450098    -0.680787     1.658141      20.99
 C      -2.663238    -0.592003    -1.609168      40.28
 C      -3.633880    -1.335785    -2.568204      63.49
 H      -3.565168    -0.855699    -3.578144      27.56
 O      -3.298676    -2.829965    -2.464794     232.68
 H      -2.413743    -2.884687    -2.538402      29.81
 C      -5.166980    -1.056215    -2.209154      91.94
 H      -5.238154    -1.442940    -1.158344      27.17
 O      -5.528381     0.359117    -2.252971     272.48
 H      -5.190562     0.751922    -1.284433      24.51
 C      -6.076950    -1.682424    -3.327831     110.86
 O      -5.844522    -3.077024    -3.511054     256.35
 H      -4.941078    -3.287403    -3.495463      33.71
 H      -5.940909    -1.094043    -4.248239      29.16
 H      -7.138297    -1.564663    -3.145412      28.88
55
name = lig-ACN-frame_196
 C       3.309906     3.011884     0.097285      55.52
 H       2.571632     3.730278    -0.208030      22.30
 C       4.019575     1.183058     1.384916      75.55
 H       3.742117     0.697943     2.341719      22.28
 C       5.204468     1.061159     0.689338      11.56
 O       6.248469     0.185922     0.907288     190.69
 C       6.252765    -0.622592     2.168673     105.47
 H       6.117921     0.279012     3.034510      23.65
 H       7.158953    -1.128258     2.192409      26.87
 H       5.388035    -1.337682     2.221030      25.99
 C       5.397048     1.922193    -0.502834      11.25
 O       6.590000     1.885498    -1.269455     133.20
 H       7.240424     1.377552    -0.814215      27.97
 C       4.399078     2.908996    -0.815056      62.62
 H       4.483931     3.599034    -1.648377      24.36
 C       3.089712     2.159059     1.125895      41.16
 C       1.922775     2.316028     2.055441     112.20
 H       2.152466     3.121397     2.638756      25.51
 O       1.753392     1.354290     3.152255     273.31
 H       1.496969     0.378676     2.758179      22.23
 C       0.516098     2.450684     1.327418      78.34
 H       0.660764     3.063872     0.332599      20.66
 C      -0.572679     3.196256     2.256476     101.10
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 O      -0.111380     4.402815     2.740486     333.68
 H       0.225670     5.038681     2.115873      31.96
 H      -0.727149     2.530866     3.197840      24.60
 H      -1.527944     3.257672     1.720516      25.93
 C      -2.556794    -1.030894    -0.259443      51.87
 H      -3.180338    -2.028510     0.121930      20.18
 C      -1.874713     0.467985    -2.118136      66.64
 H      -1.986868     0.895756    -3.142636      23.21
 C      -0.927160     1.140977    -1.200986      30.36
 O      -0.067919     2.165587    -1.595088     247.00
 C      -0.482311     3.052495    -2.589549     123.35
 H      -0.006470     3.875011    -2.403803      27.36
 H      -0.296623     2.407626    -3.658340      22.92
 H      -1.551533     3.329460    -2.673317      28.68
 C      -0.803148     0.602709     0.074614      21.84
 O       0.078351     1.156198     1.078997     203.00
 C      -1.604954    -0.494879     0.576388      35.91
 H      -1.510713    -0.906096     1.663661      19.07
 C      -2.714944    -0.602232    -1.616622      56.83
 C      -3.587435    -1.336854    -2.528775      64.62
 H      -3.280029    -1.172783    -3.607561      29.16
 O      -3.388600    -2.778091    -2.418563     227.37
 H      -2.414784    -2.996373    -2.513488      26.06
 C      -5.122716    -1.034185    -2.231507      92.05
 H      -5.491613    -1.514893    -1.260456      25.70
 O      -5.456408     0.352066    -2.251202     286.08
 H      -5.214280     0.927852    -1.339130      22.80
 C      -6.097035    -1.672409    -3.285014     105.06
 O      -5.810114    -3.107459    -3.445719     232.58
 H      -4.811207    -3.105642    -3.362068      29.17
 H      -5.875994    -1.179801    -4.233249      28.81
 H      -7.115529    -1.561763    -2.869343      28.45
55
name = lig-ACN-frame_197
 C       3.294751     2.970739    -0.083953      53.70
 H       2.569780     3.749283    -0.353343      24.78
 C       3.986597     1.089137     1.403483      53.54
 H       3.897894     0.324169     2.164040      21.85
 C       5.238401     1.097521     0.663897      15.18
 O       6.258976     0.117705     0.915605     229.64
 C       6.275407    -0.585274     2.106073     124.93
 H       6.558213    -0.119169     3.250159      24.45
 H       7.054474    -1.258486     1.974529      27.69
 H       5.388374    -1.202793     2.211221      26.54
 C       5.440181     1.896919    -0.461322      28.42
 O       6.565635     1.821585    -1.249670     185.76
 H       7.281641     1.486477    -0.688035      27.07
 C       4.464468     2.841664    -0.807743      50.32
 H       4.562876     3.469326    -1.736558      22.03
 C       3.044080     2.159863     1.119457      12.47
 C       1.822004     2.360433     2.113598     102.63
 H       1.889171     3.330936     2.518043      22.17
 O       1.757455     1.354699     3.142569     310.71
 H       1.503777     0.544676     2.708287      26.07
 C       0.514064     2.501333     1.371900      81.31
 H       0.675466     3.101724     0.436372      20.67
 C      -0.567328     3.211700     2.185994     101.72
 O      -0.091368     4.502928     2.704602     329.69
 H       0.294347     4.874530     2.030670      36.42
 H      -0.928303     2.597544     3.114968      24.41
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 H      -1.453212     3.384141     1.539551      25.36
 C      -2.524359    -1.069435    -0.319462      66.19
 H      -3.337208    -1.836911     0.041899      21.97
 C      -1.884631     0.524183    -2.048430      29.25
 H      -1.933355     0.760995    -3.111258      19.70
 C      -0.953024     1.086918    -1.220839      20.61
 O      -0.021910     2.124290    -1.535588     211.97
 C      -0.471475     3.006086    -2.666367     110.24
 H      -0.036427     3.864498    -2.568951      28.30
 H      -0.166358     2.668358    -3.809860      24.21
 H      -1.569962     3.104662    -2.443542      26.82
 C      -0.779382     0.614620     0.159732      28.92
 O       0.106369     1.050552     1.038756     195.81
 C      -1.593316    -0.438295     0.558807      55.98
 H      -1.270599    -0.897514     1.589326      19.56
 C      -2.632819    -0.543899    -1.589426      50.93
 C      -3.617492    -1.329980    -2.551463      38.11
 H      -3.452389    -0.899052    -3.620115      25.81
 O      -3.493466    -2.768474    -2.339045     164.83
 H      -2.482065    -3.003260    -2.797098      22.05
 C      -5.127015    -1.052466    -2.271105      96.09
 H      -5.202657    -1.516214    -1.209091      26.35
 O      -5.379881     0.373970    -2.290998     287.81
 H      -5.079094     0.695488    -1.391773      25.42
 C      -6.044033    -1.705150    -3.243599     110.84
 O      -5.811952    -3.121088    -3.397557     239.48
 H      -4.837735    -3.400286    -3.171101      28.07
 H      -6.149519    -1.132538    -4.183071      29.01
 H      -7.132878    -1.629859    -2.914115      27.17
55
name = lig-ACN-frame_198
 C       3.213086     2.905102    -0.094113      59.85
 H       2.530386     3.720236    -0.430380      21.93
 C       4.025009     1.112442     1.377135      73.42
 H       3.764990     0.411185     2.131304      23.11
 C       5.213836     1.006075     0.684724      21.72
 O       6.244916     0.149549     0.870380     202.26
 C       6.311817    -0.716495     2.117495     107.26
 H       6.673717     0.199233     2.879788      24.35
 H       6.981967    -1.522167     1.913922      27.47
 H       5.391067    -1.062417     2.429244      28.61
 C       5.478517     1.909734    -0.413499      18.32
 O       6.600038     1.751375    -1.239466      41.26
 H       7.403707     1.257239    -0.760843      21.48
 C       4.497065     2.783139    -0.838877      59.07
 H       4.923934     3.415646    -1.693121      22.06
 C       3.023302     2.102277     1.083752      15.94
 C       1.825361     2.404118     2.114226      95.74
 H       2.069034     3.266406     2.737897      22.83
 O       1.773602     1.361864     3.131062     314.18
 H       1.386302     0.632875     2.714339      25.89
 C       0.456439     2.478044     1.341319      95.61
 H       0.582100     2.951384     0.417041      21.75
 C      -0.627414     3.235987     2.132722      89.66
 O      -0.076989     4.576688     2.668496     286.99
 H       0.138108     5.191954     1.953033      30.13
 H      -0.963422     2.622372     3.056609      24.22
 H      -1.526377     3.384980     1.437774      24.16
 C      -2.484208    -1.048931    -0.286105      53.29
 H      -2.949892    -1.973438     0.075639      20.88
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 C      -1.867939     0.561337    -2.044498      82.08
 H      -1.902285     0.898694    -3.063858      18.09
 C      -0.858153     1.116164    -1.151378      11.16
 O      -0.012545     2.088397    -1.555376     226.73
 C      -0.466209     2.972644    -2.681592      97.36
 H       0.014403     3.843716    -2.530840      26.91
 H      -0.242718     2.362388    -3.664914      22.97
 H      -1.599719     3.157267    -2.768953      25.08
 C      -0.840901     0.656882     0.151629      35.50
 O       0.225288     1.030152     1.073359     185.84
 C      -1.588883    -0.468732     0.567636      42.86
 H      -1.513962    -0.802039     1.652610      19.94
 C      -2.676161    -0.599830    -1.666836      37.30
 C      -3.634347    -1.246550    -2.560204      69.61
 H      -3.407905    -1.127125    -3.704062      24.52
 O      -3.512246    -2.768802    -2.315411     153.42
 H      -2.444558    -3.140117    -2.626459      21.71
 C      -5.075409    -1.017855    -2.221193      96.68
 H      -5.408874    -1.341763    -1.158131      27.58
 O      -5.325736     0.378544    -2.358088     317.19
 H      -5.114472     0.809215    -1.592398      32.91
 C      -6.095090    -1.776163    -3.238232      98.41
 O      -5.858359    -3.174184    -3.397812     263.27
 H      -4.924471    -3.229270    -3.033036      29.43
 H      -5.874018    -1.304698    -4.217287      29.48
 H      -7.110104    -1.599093    -2.730295      27.75
55
name = lig-ACN-frame_199
 C       3.285956     2.845718    -0.105327      46.97
 H       2.469497     3.541963    -0.407931      21.13
 C       3.977429     1.152225     1.410922      58.74
 H       3.816576     0.676866     2.356924      22.32
 C       5.189950     0.981559     0.652969      14.66
 O       6.259264     0.034956     0.875362     208.45
 C       6.316467    -0.717849     2.088737     120.05
 H       7.011856    -0.260906     3.041485      25.23
 H       6.925405    -1.624140     1.800962      26.76
 H       5.436723    -1.034686     2.432411      29.26
 C       5.489876     1.856040    -0.417291      23.82
 O       6.633323     1.703612    -1.234799      69.02
 H       7.349833     1.174788    -0.633939      21.44
 C       4.433693     2.780058    -0.802843      64.20
 H       4.393980     3.564586    -1.621084      24.15
 C       3.013646     2.091802     1.021102      33.70
 C       1.908871     2.351504     2.042151     100.69
 H       2.150632     3.382194     2.488081      23.36
 O       1.779966     1.377684     3.126613     281.76
 H       1.369684     0.475030     2.736858      21.06
 C       0.505323     2.467962     1.315404      87.80
 H       0.628592     2.934988     0.435214      22.79
 C      -0.656851     3.341018     2.133604      97.62
 O      -0.168287     4.515602     2.642154     283.55
 H       0.221654     5.122894     1.785856      25.96
 H      -0.953541     2.812165     3.086075      24.11
 H      -1.667422     3.515779     1.547875      23.78
 C      -2.488347    -1.091838    -0.347422      61.71
 H      -2.920069    -1.988268    -0.124797      21.12
 C      -1.840460     0.519081    -2.033325      14.32
 H      -1.981369     0.958868    -2.989244      20.54
 C      -0.922595     1.104255    -1.159367      29.48
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 O      -0.013563     2.132907    -1.619624     232.49
 C      -0.421711     2.890887    -2.700303     125.50
 H      -0.019024     3.807843    -2.571766      26.95
 H      -0.060751     2.503712    -3.715697      25.55
 H      -1.555696     3.113463    -2.620376      27.20
 C      -0.751281     0.666196     0.256661      45.07
 O       0.239395     1.060899     1.082875     206.70
 C      -1.587504    -0.434070     0.618667      47.67
 H      -1.501504    -0.844071     1.615310      19.81
 C      -2.591007    -0.546719    -1.604065      32.47
 C      -3.597265    -1.374141    -2.550255      47.64
 H      -3.415474    -1.021221    -3.678804      25.06
 O      -3.475978    -2.761557    -2.318845     228.26
 H      -2.443644    -2.947547    -2.441083      25.64
 C      -5.154039    -1.003475    -2.227492      87.25
 H      -5.209157    -1.342947    -1.111525      26.21
 O      -5.329838     0.426234    -2.476403     295.18
 H      -5.117096     0.883113    -1.645499      26.85
 C      -6.088704    -1.754732    -3.193157     100.81
 O      -5.912134    -3.245126    -3.379451     253.15
 H      -5.022710    -3.493762    -3.192850      32.78
 H      -6.057006    -1.213903    -4.177662      28.47
 H      -7.232437    -1.606534    -3.029914      26.45
55
name = lig-ACN-frame_200
 C       3.210828     2.859556    -0.095593      64.34
 H       2.521699     3.614787    -0.519414      22.55
 C       4.066196     1.115718     1.463014      68.20
 H       4.019558     0.602326     2.432343      21.98
 C       5.206731     0.973589     0.654429       8.53
 O       6.215330    -0.038120     0.874183     202.52
 C       6.334956    -0.806277     2.084705     108.67
 H       6.944841    -0.142333     2.951499      23.86
 H       6.802309    -1.826083     1.790064      24.80
 H       5.431112    -0.985423     2.505897      27.34
 C       5.422509     1.802483    -0.516746      19.60
 O       6.609310     1.677046    -1.210177     100.60
 H       7.350443     1.304128    -0.648856      25.23
 C       4.501555     2.777570    -0.832983      58.45
 H       4.823058     3.329994    -1.754920      20.20
 C       3.043726     2.013097     1.066988      20.15
 C       1.864961     2.328255     1.996213     102.87
 H       2.115238     3.343150     2.550929      21.51
 O       1.814573     1.422048     3.113513     270.95
 H       1.544014     0.478675     2.635665      20.68
 C       0.531088     2.562136     1.323537      85.12
 H       0.640279     3.042193     0.453358      21.57
 C      -0.639418     3.218108     2.136659      91.63
 O      -0.249310     4.544466     2.655960     247.64
 H       0.439899     5.080211     1.860020      24.44
 H      -0.988757     2.559964     2.922553      25.19
 H      -1.431724     3.301939     1.261284      22.76
 C      -2.393274    -1.096603    -0.255456      63.76
 H      -3.020686    -1.825615     0.027008      21.94
 C      -1.821659     0.528441    -2.025932      37.18
 H      -1.891453     0.796034    -3.074375      19.76
 C      -0.893370     1.142620    -1.116828      19.27
 O      -0.019826     2.089407    -1.574562     218.17
 C      -0.401537     2.929356    -2.797389     107.07
 H       0.058039     3.829158    -2.726290      26.67
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 H      -0.209267     2.403167    -3.734857      25.05
 H      -1.549502     3.028430    -2.787431      26.05
 C      -0.767625     0.615042     0.172609      22.13
 O       0.190555     1.102327     1.100823     197.42
 C      -1.590575    -0.432089     0.639376      51.36
 H      -1.333644    -0.853276     1.543386      21.29
 C      -2.628991    -0.621914    -1.632586      45.39
 C      -3.611042    -1.344622    -2.501422      55.10
 H      -3.352729    -1.118106    -3.651490      23.38
 O      -3.378043    -2.816629    -2.333076     253.09
 H      -2.531505    -2.990054    -2.489440      30.39
 C      -5.104505    -1.014376    -2.286038      91.68
 H      -5.517032    -1.104912    -1.208305      24.30
 O      -5.366172     0.432691    -2.590335     236.40
 H      -5.061053     0.929360    -1.660153      21.87
 C      -6.113057    -1.792443    -3.225713      95.45
 O      -5.993802    -3.237181    -3.341073     251.06
 H      -5.001034    -3.369445    -3.409379      31.39
 H      -5.905280    -1.324159    -4.222443      29.20
 H      -7.134938    -1.672520    -2.708871      27.09
55
name = lig-ACN-frame_201
 C       3.299336     2.820596    -0.115970      50.61
 H       2.498473     3.535092    -0.247427      22.54
 C       4.144066     1.113372     1.474973      64.07
 H       3.938071     0.435877     2.347032      21.63
 C       5.251785     0.894773     0.674619      25.61
 O       6.175644    -0.072121     0.810973     189.06
 C       6.270183    -0.870978     2.108995     105.55
 H       7.046858    -0.213003     2.780696      24.10
 H       6.916312    -1.827513     1.845707      24.36
 H       5.390260    -1.131487     2.618677      26.46
 C       5.402440     1.695257    -0.478087      20.65
 O       6.586170     1.661839    -1.240603     153.20
 H       7.242198     1.229969    -0.738906      27.42
 C       4.475961     2.745744    -0.855798      44.23
 H       4.709704     3.479219    -1.622836      23.16
 C       3.091699     2.050839     1.046698      10.03
 C       1.899064     2.394919     2.068388      95.32
 H       2.209282     3.438110     2.592708      22.91
 O       1.834273     1.428300     3.106724     291.78
 H       1.570439     0.554329     2.790785      25.68
 C       0.521385     2.518593     1.297894     103.16
 H       0.651986     3.079852     0.433345      23.39
 C      -0.579901     3.127136     2.079581      97.63
 O      -0.347734     4.517453     2.697546     205.78
 H       0.060216     5.183055     1.803247      25.30
 H      -0.827747     2.604025     2.954655      26.09
 H      -1.606426     3.209117     1.458646      23.87
 C      -2.459610    -1.106592    -0.237524      49.65
 H      -2.912216    -1.937854     0.238822      19.70
 C      -1.853424     0.448320    -2.016583      51.98
 H      -1.808468     0.779729    -3.067630      15.60
 C      -0.925797     1.101435    -1.196855      24.27
 O      -0.001208     2.147304    -1.592390     234.14
 C      -0.406504     2.883844    -2.821455     123.60
 H       0.071887     3.730014    -2.731537      29.18
 H      -0.029586     2.320545    -3.655407      27.53
 H      -1.478141     3.201952    -2.876191      28.41
 C      -0.758836     0.680178     0.162030      28.61
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 O       0.099855     1.147788     1.076981     200.36
 C      -1.485074    -0.459641     0.642540      47.75
 H      -1.428397    -0.691943     1.653603      19.98
 C      -2.577915    -0.629729    -1.535095      32.98
 C      -3.575868    -1.343066    -2.505788      44.91
 H      -3.356801    -1.011766    -3.632568      25.56
 O      -3.325120    -2.870626    -2.359366     235.34
 H      -2.473673    -2.926298    -2.681454      26.93
 C      -5.113389    -0.995775    -2.335237      89.44
 H      -5.295700    -1.318587    -1.238806      26.83
 O      -5.374404     0.373422    -2.694474     253.57
 H      -5.091096     1.003739    -1.838550      24.76
 C      -6.122097    -1.796417    -3.253059     106.51
 O      -6.035322    -3.217328    -3.289418     246.32
 H      -5.063283    -3.486002    -3.452467      31.81
 H      -6.222972    -1.365944    -4.293810      29.59
 H      -7.157157    -1.465468    -2.921352      28.57
55
name = lig-ACN-frame_202
 C       3.330318     2.817576    -0.048692      56.95
 H       2.754974     3.613931    -0.461898      22.62
 C       4.056746     1.116938     1.463201      68.22
 H       3.841556     0.556938     2.415527      22.43
 C       5.204933     0.867425     0.633715       4.58
 O       6.199238    -0.231041     0.819394     187.25
 C       6.280482    -0.860122     2.057706     110.96
 H       6.786852    -0.303087     2.979584      25.36
 H       6.772693    -1.897183     1.746910      24.76
 H       5.233143    -1.121014     2.370381      26.03
 C       5.459741     1.729932    -0.499822      25.09
 O       6.553912     1.627105    -1.301614      62.42
 H       7.314955     1.153484    -0.865994      24.69
 C       4.486209     2.636281    -0.844305      65.46
 H       4.644435     3.333315    -1.622123      25.91
 C       3.162836     2.096630     1.140418      38.63
 C       1.999820     2.386206     2.038764     102.82
 H       2.032289     3.490758     2.529188      22.96
 O       1.845399     1.431118     3.158958     324.65
 H       1.507849     0.702968     2.712609      27.06
 C       0.587517     2.513571     1.253957      72.41
 H       0.759757     2.921663     0.241933      21.26
 C      -0.632066     3.204874     2.188892      96.90
 O      -0.438566     4.433338     2.673892     290.03
 H      -0.370248     5.135493     1.959779      29.51
 H      -0.610101     2.521909     2.984173      26.04
 H      -1.648323     3.025421     1.545989      23.45
 C      -2.443058    -1.100833    -0.128569      42.52
 H      -3.029886    -2.058837     0.014621      20.38
 C      -1.826214     0.399429    -2.044623      66.41
 H      -2.143488     0.603208    -3.096444      19.18
 C      -0.871165     1.104765    -1.224241      14.87
 O      -0.082281     2.185140    -1.633875     245.19
 C      -0.336919     2.844707    -2.826916     133.95
 H       0.148045     3.675738    -2.877189      29.11
 H      -0.172605     2.308952    -3.720636      27.79
 H      -1.436404     3.030488    -2.810858      26.54
 C      -0.811610     0.687151     0.134679      31.44
 O       0.101351     1.186277     1.089178     199.55
 C      -1.477980    -0.457327     0.586789      51.17
 H      -1.279066    -0.716604     1.620281      20.36
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 C      -2.638592    -0.677869    -1.517414      41.54
 C      -3.516392    -1.425736    -2.540854      70.41
 H      -3.120765    -1.056610    -3.585380      25.37
 O      -3.327304    -2.825327    -2.433137     257.36
 H      -2.314307    -3.109051    -2.637368      24.42
 C      -5.101774    -1.068014    -2.386617      94.29
 H      -5.434767    -1.121715    -1.306502      26.33
 O      -5.358959     0.330367    -2.754224     276.54
 H      -5.101344     0.842962    -1.998188      29.63
 C      -6.152268    -1.738699    -3.286728     102.14
 O      -6.065017    -3.229030    -3.232086     259.19
 H      -5.136242    -3.437711    -3.254340      33.17
 H      -5.878062    -1.285259    -4.281504      29.37
 H      -7.152423    -1.625325    -2.875118      28.07
55
name = lig-ACN-frame_203
 C       3.369888     2.896202    -0.028785      47.11
 H       2.593767     3.602050    -0.228257      22.89
 C       4.092985     1.022874     1.442825      60.15
 H       4.015034     0.472342     2.397348      24.37
 C       5.230915     0.779281     0.621858      20.75
 O       6.163247    -0.227172     0.748643     198.10
 C       6.205411    -0.954697     2.052808     106.73
 H       6.628576    -0.175372     2.821700      26.08
 H       6.951465    -1.834652     2.081311      25.54
 H       5.161913    -1.322845     2.422170      24.90
 C       5.501707     1.666278    -0.458920      16.95
 O       6.590460     1.566776    -1.392774     104.59
 H       7.381723     1.120041    -0.829743      23.13
 C       4.497906     2.617500    -0.844686      45.73
 H       4.683238     3.014570    -1.807002      24.11
 C       3.174529     2.160785     1.183387      12.29
 C       1.900901     2.397370     2.066160     101.61
 H       2.230054     3.389191     2.643569      19.87
 O       1.858332     1.487109     3.164378     295.57
 H       1.556128     0.519092     2.941351      21.68
 C       0.584115     2.578466     1.295041      82.64
 H       0.658976     3.283629     0.363694      19.89
 C      -0.564226     3.051192     2.182743      90.55
 O      -0.522115     4.510604     2.700728     294.23
 H      -0.378793     4.982464     2.004299      35.35
 H      -0.702534     2.505760     3.103383      25.05
 H      -1.601224     2.963279     1.574220      23.09
 C      -2.461208    -1.136616    -0.226954      60.56
 H      -2.908812    -1.976227     0.469117      17.88
 C      -1.839655     0.352938    -2.034068      33.14
 H      -1.819345     0.738257    -3.072880      18.19
 C      -0.919931     1.063697    -1.246305      11.75
 O      -0.102840     2.167149    -1.603138     222.36
 C      -0.384036     2.852729    -2.948280     123.71
 H       0.186314     3.593273    -2.867505      29.23
 H      -0.110032     2.127531    -3.700469      26.29
 H      -1.375482     3.241643    -3.060363      28.80
 C      -0.763958     0.701582     0.115985      17.02
 O       0.129830     1.137406     1.090893     175.51
 C      -1.516851    -0.432535     0.625769      49.31
 H      -1.090039    -0.913779     1.572334      18.82
 C      -2.643892    -0.688741    -1.534818      49.87
 C      -3.530050    -1.412578    -2.558928      40.55
 H      -3.308007    -1.058000    -3.628629      25.50
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 O      -3.364440    -2.870395    -2.506000     195.05
 H      -2.192051    -2.953468    -2.570445      20.44
 C      -5.074405    -1.077585    -2.403546      95.52
 H      -5.310744    -1.351545    -1.338995      26.10
 O      -5.294329     0.318577    -2.781875     289.06
 H      -5.042953     0.858344    -2.075534      29.70
 C      -6.108888    -1.817670    -3.293265     112.03
 O      -6.086260    -3.216782    -3.201180     284.43
 H      -5.148644    -3.445243    -3.049004      32.77
 H      -6.037110    -1.541980    -4.391510      29.88
 H      -7.023406    -1.320688    -3.089456      29.78
55
name = lig-ACN-frame_204
 C       3.442727     2.914662     0.029076      43.31
 H       2.772656     3.665315    -0.381185      19.45
 C       4.121820     1.032633     1.424309      72.91
 H       3.829117     0.341099     2.199236      22.54
 C       5.247758     0.780169     0.597770      12.72
 O       6.139834    -0.304893     0.728466     176.69
 C       6.146064    -0.968201     2.058007     104.90
 H       6.342067    -0.259559     2.875895      26.31
 H       6.952101    -1.671260     1.800162      25.27
 H       5.137420    -1.656250     2.260537      24.22
 C       5.484807     1.622749    -0.531944      19.47
 O       6.604587     1.470216    -1.392105      98.39
 H       7.426350     1.100131    -0.941321      24.91
 C       4.539513     2.634027    -0.821971      58.01
 H       4.586195     3.249382    -1.715770      25.48
 C       3.218442     2.074572     1.134939      15.66
 C       1.936276     2.444141     2.123644      98.49
 H       1.950186     3.536293     2.550977      24.40
 O       1.842029     1.529117     3.215002     262.24
 H       1.726698     0.590293     2.639592      20.16
 C       0.537381     2.539973     1.409629      73.93
 H       0.635325     3.149003     0.369201      19.59
 C      -0.596202     3.067519     2.265448      91.66
 O      -0.592860     4.505849     2.679539     261.50
 H      -0.017765     5.055777     2.008042      28.55
 H      -0.572257     2.401808     3.184332      24.11
 H      -1.548407     2.853645     1.581620      24.16
 C      -2.416286    -1.114024    -0.232357      46.84
 H      -3.105783    -2.055317    -0.028671      21.95
 C      -1.838792     0.364414    -2.060598      62.04
 H      -1.904517     0.504597    -3.141587      14.49
 C      -0.944933     1.078860    -1.154188      18.80
 O      -0.168469     2.181535    -1.663932     198.46
 C      -0.387183     2.802514    -2.978967     130.94
 H       0.242497     3.526170    -3.060237      28.60
 H      -0.134242     2.147939    -3.825617      26.05
 H      -1.361685     3.162610    -3.118338      29.38
 C      -0.750347     0.622512     0.185731      30.67
 O       0.222091     1.135901     1.024713     206.82
 C      -1.526910    -0.433470     0.572005      47.51
 H      -1.472589    -0.773023     1.693704      19.54
 C      -2.626201    -0.731033    -1.606464      78.91
 C      -3.595782    -1.394594    -2.625083      51.07
 H      -3.273333    -0.995294    -3.615276      27.84
 O      -3.403158    -2.912609    -2.553342     210.09
 H      -2.297362    -3.178342    -2.844508      21.14
 C      -5.056366    -1.068211    -2.417148     100.58
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 H      -5.375699    -1.201338    -1.374251      25.82
 O      -5.214335     0.320169    -2.769804     238.54
 H      -4.936034     0.890694    -1.884120      23.52
 C      -6.043176    -1.820640    -3.354470     105.62
 O      -6.115480    -3.275798    -3.134725     235.92
 H      -5.147788    -3.637141    -3.031306      29.62
 H      -5.742990    -1.488718    -4.380312      31.40
 H      -7.007142    -1.618996    -3.052911      29.70
55
name = lig-ACN-frame_205
 C       3.517600     2.877545     0.038818      48.38
 H       2.889314     3.782687    -0.100559      21.96
 C       4.095374     1.022014     1.391393      48.47
 H       3.945549     0.313389     2.183497      21.05
 C       5.235070     0.791938     0.540423       9.79
 O       6.086019    -0.348140     0.755670     212.65
 C       6.129913    -1.034411     1.988243     114.70
 H       6.062228    -0.426017     2.864046      28.30
 H       6.987168    -1.634209     2.128274      26.65
 H       5.112572    -1.782815     1.957944      23.56
 C       5.486383     1.603892    -0.615642      19.51
 O       6.590784     1.370524    -1.374053     102.57
 H       7.224528     1.011797    -0.802774      27.23
 C       4.624201     2.685001    -0.822484      56.15
 H       4.980210     3.473714    -1.538088      22.31
 C       3.146059     2.086026     1.166147      21.29
 C       2.010361     2.453875     2.096894      97.51
 H       2.399071     3.419369     2.549220      23.65
 O       1.847915     1.567369     3.260542     260.23
 H       1.567673     0.600291     3.003381      21.36
 C       0.565924     2.470442     1.398310      63.41
 H       0.622713     3.227410     0.433816      20.12
 C      -0.696863     3.106983     2.374234      90.72
 O      -0.620576     4.461587     2.629844     209.74
 H       0.157714     4.933638     1.867541      24.91
 H      -0.728940     2.643987     3.448665      23.08
 H      -1.757314     2.857121     1.917810      23.43
 C      -2.467591    -1.139770    -0.336373      52.90
 H      -2.967084    -2.037880     0.167567      19.06
 C      -1.814527     0.387229    -2.054432      39.54
 H      -1.844292     0.805229    -3.041019      17.44
 C      -0.962418     1.117956    -1.220183      16.51
 O      -0.227864     2.182324    -1.683591     237.99
 C      -0.406248     2.714745    -2.998103     134.83
 H       0.124407     3.487444    -3.003642      29.25
 H      -0.276398     1.922234    -3.809015      24.83
 H      -1.368388     3.059458    -3.059174      29.67
 C      -0.744441     0.674252     0.146311      23.47
 O       0.346690     1.104635     0.995575     171.88
 C      -1.577623    -0.514526     0.616536      42.33
 H      -1.604757    -0.718011     1.771490      18.13
 C      -2.566751    -0.736228    -1.679506      32.99
 C      -3.507174    -1.491751    -2.639913      53.07
 H      -3.348641    -1.199519    -3.664963      24.41
 O      -3.464010    -2.905820    -2.612716     264.58
 H      -2.492024    -3.083360    -2.940168      25.01
 C      -5.085532    -1.056991    -2.399017      91.85
 H      -5.381486    -1.251082    -1.376616      28.28
 O      -5.152786     0.373851    -2.741253     294.42
 H      -4.878288     0.894989    -1.787355      21.69
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 C      -6.012685    -1.864502    -3.345436     113.78
 O      -6.100035    -3.329141    -3.084776     261.71
 H      -5.159838    -3.599356    -3.196875      32.31
 H      -5.663575    -1.630371    -4.358051      32.24
 H      -6.928652    -1.383073    -3.375009      30.49
55
name = lig-ACN-frame_206
 C       3.527693     2.935034     0.038481      52.47
 H       2.981322     3.897270    -0.088486      24.78
 C       4.063948     0.958821     1.356833      77.09
 H       3.920409     0.441258     2.307773      22.91
 C       5.140095     0.714702     0.544715      17.55
 O       6.076369    -0.294759     0.692693     174.21
 C       6.029530    -1.129568     1.989154     106.42
 H       5.862663    -0.471016     2.750168      28.21
 H       6.974104    -1.510442     1.965877      27.10
 H       5.198716    -2.102608     2.072004      23.49
 C       5.471755     1.547362    -0.562656      19.38
 O       6.612487     1.281372    -1.385334     104.30
 H       7.323717     0.750770    -0.912152      25.63
 C       4.706700     2.750160    -0.775766      59.96
 H       4.995935     3.558359    -1.536964      19.47
 C       3.213735     2.048744     1.102503      16.01
 C       1.972045     2.376609     2.113280      96.70
 H       2.082260     3.414400     2.460468      22.26
 O       1.901695     1.624920     3.314257     311.27
 H       1.601868     0.819387     3.011717      26.87
 C       0.516491     2.518529     1.451843      58.58
 H       0.466938     3.234570     0.468069      18.62
 C      -0.676307     2.967717     2.400433      82.57
 O      -0.586851     4.519606     2.569526     169.30
 H      -0.154918     4.972910     1.598840      24.66
 H      -0.578454     2.444165     3.462017      22.85
 H      -1.620680     2.708400     1.825134      23.53
 C      -2.438574    -1.164292    -0.311784      51.10
 H      -3.065952    -1.993703    -0.030669      19.53
 C      -1.841862     0.404341    -2.123273      67.54
 H      -2.010056     0.768185    -3.123408      11.44
 C      -0.934778     1.095022    -1.178354      10.12
 O      -0.215871     2.200217    -1.634702     186.83
 C      -0.513482     2.651948    -3.025043     125.94
 H       0.136873     3.338854    -3.179740      28.88
 H      -0.111110     1.856922    -3.752030      24.35
 H      -1.440661     2.970557    -3.242727      29.04
 C      -0.772313     0.639189     0.156362      27.94
 O       0.370464     1.035141     0.929192     151.42
 C      -1.572690    -0.401729     0.532539      53.31
 H      -1.312766    -0.957693     1.482629      20.16
 C      -2.520363    -0.782692    -1.691598      42.28
 C      -3.540656    -1.453922    -2.679575      73.07
 H      -3.283667    -1.087119    -3.628077      26.81
 O      -3.466165    -2.962470    -2.652782     316.51
 H      -2.641575    -3.208113    -2.722195      32.59
 C      -4.995348    -1.056099    -2.378559      90.63
 H      -5.228089    -1.252304    -1.361523      28.60
 O      -5.125555     0.382400    -2.696199     292.72
 H      -4.940775     0.938267    -1.865017      26.15
 C      -5.979973    -1.887897    -3.350393     109.57
 O      -6.079543    -3.286002    -3.047914     267.94
 H      -5.212567    -3.632869    -3.162318      33.08
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 H      -5.470569    -1.807446    -4.300674      32.66
 H      -6.997895    -1.591424    -3.322313      29.68
55
name = lig-ACN-frame_207
 C       3.578200     2.992959     0.048137      56.30
 H       2.865464     3.748578    -0.334537      21.13
 C       3.978587     0.918889     1.382644      48.30
 H       3.692778     0.232438     2.227111      18.48
 C       5.115904     0.629700     0.487669       7.47
 O       6.063989    -0.361857     0.718588     204.32
 C       5.987813    -1.126149     1.909768     114.08
 H       5.799911    -0.675157     2.804920      29.94
 H       6.896410    -1.634692     2.012874      27.21
 H       5.115852    -2.030406     1.613143      23.80
 C       5.498823     1.571917    -0.539672      19.50
 O       6.570123     1.225314    -1.368750     113.41
 H       7.252870     0.678400    -0.759908      22.16
 C       4.748727     2.724745    -0.682011      53.55
 H       5.020887     3.382560    -1.566631      22.54
 C       3.163006     2.071702     1.072191      10.88
 C       1.914232     2.453428     2.071939      96.10
 H       2.139121     3.436016     2.391767      26.35
 O       1.965094     1.649464     3.335318     262.09
 H       1.863747     0.707242     3.178752      25.43
 C       0.525426     2.397863     1.455374      82.27
 H       0.611231     3.120281     0.507309      21.08
 C      -0.546191     2.970601     2.330835     104.12
 O      -0.557153     4.439875     2.498429     278.36
 H      -0.454578     4.791468     1.630634      32.41
 H      -0.479229     2.617885     3.459838      24.23
 H      -1.524322     2.636554     1.971881      26.18
 C      -2.395846    -1.144307    -0.342757      71.48
 H      -2.815138    -1.962415     0.070296      20.41
 C      -1.843153     0.357236    -2.062588      48.53
 H      -1.908563     0.641331    -3.120219      16.52
 C      -0.963525     1.082222    -1.244397      18.61
 O      -0.237390     2.243727    -1.621866     230.68
 C      -0.496906     2.601900    -3.024278     134.93
 H      -0.094572     3.409187    -3.234289      29.57
 H      -0.371594     1.691685    -3.745045      25.01
 H      -1.510485     2.761215    -3.042553      30.74
 C      -0.725502     0.660237     0.092260      24.80
 O       0.296887     1.034572     0.885445     179.87
 C      -1.548121    -0.469936     0.542134      49.19
 H      -1.286889    -0.813010     1.529256      19.83
 C      -2.550631    -0.778307    -1.700505      37.15
 C      -3.484200    -1.431775    -2.689663      50.52
 H      -3.299575    -1.170077    -3.664611      27.97
 O      -3.445864    -2.981147    -2.661690     281.95
 H      -2.499230    -3.116532    -2.736101      28.62
 C      -4.960598    -1.052741    -2.398961      97.31
 H      -5.210916    -1.269726    -1.396756      28.50
 O      -5.137013     0.340415    -2.673107     322.64
 H      -4.965331     0.810724    -1.919837      30.98
 C      -5.893716    -1.854898    -3.346412     113.04
 O      -6.071205    -3.268418    -2.995047     243.05
 H      -5.126670    -3.651163    -2.946478      30.47
 H      -5.702132    -1.621237    -4.376984      32.26
 H      -6.860337    -1.341490    -3.199285      29.50
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name = lig-ACN-frame_208
 C       3.572966     2.943370     0.089105      47.27
 H       2.995587     3.829502    -0.193101      23.34
 C       3.926082     0.935836     1.264139      57.70
 H       3.676364     0.133692     2.029380      20.28
 C       5.063897     0.644578     0.551453      20.16
 O       6.062752    -0.384986     0.710254     207.95
 C       5.929124    -1.243320     1.846260     113.47
 H       5.707629    -0.596987     2.620775      30.16
 H       6.852061    -1.807983     1.978283      26.24
 H       4.909117    -2.037661     1.812504      23.69
 C       5.500300     1.506382    -0.458558      19.73
 O       6.521596     1.201295    -1.322394      72.26
 H       7.275650     0.760362    -0.866424      21.81
 C       4.764870     2.713853    -0.696276      53.43
 H       5.098038     3.443289    -1.459412      21.20
 C       3.103589     2.098548     1.123130      28.62
 C       2.001621     2.417703     2.052556     112.09
 H       2.012350     3.408387     2.319630      25.47
 O       2.036653     1.702911     3.305814     241.64
 H       1.903909     0.678492     2.961404      19.98
 C       0.607637     2.360084     1.293513      77.29
 H       0.635161     3.084193     0.381943      22.03
 C      -0.534088     2.953267     2.335086     101.61
 O      -0.511969     4.339885     2.413137     316.73
 H      -0.325893     4.745899     1.638700      33.52
 H      -0.267727     2.538050     3.385869      23.79
 H      -1.485839     2.580577     2.007213      25.91
 C      -2.381517    -1.215465    -0.300326      43.83
 H      -2.836230    -2.057414    -0.014374      21.07
 C      -1.817917     0.346208    -2.118584      93.44
 H      -1.840717     0.627461    -3.174649      15.22
 C      -0.943633     1.134441    -1.243205      14.88
 O      -0.259797     2.245603    -1.668181     225.99
 C      -0.568205     2.591356    -3.000153     130.66
 H      -0.017763     3.347058    -3.198389      29.28
 H      -0.147987     1.822657    -3.771822      24.97
 H      -1.556745     2.796490    -3.154461      30.06
 C      -0.774650     0.608704     0.049126      31.89
 O       0.266562     1.047514     0.936333     200.89
 C      -1.439511    -0.500138     0.539337      40.15
 H      -1.485872    -0.729441     1.535106      18.92
 C      -2.558099    -0.770142    -1.643837      30.21
 C      -3.440767    -1.521360    -2.691049      75.80
 H      -3.146718    -1.154300    -3.607534      28.75
 O      -3.363019    -2.909264    -2.633970     282.75
 H      -2.377543    -3.297442    -2.974499      23.83
 C      -4.917094    -1.099760    -2.427224     102.72
 H      -5.178143    -1.406822    -1.444846      26.85
 O      -5.179079     0.320345    -2.684045     286.19
 H      -4.880566     0.836285    -1.874262      25.26
 C      -5.929033    -1.800283    -3.310318     104.89
 O      -6.053890    -3.218775    -2.963392     251.74
 H      -5.086477    -3.513569    -2.862000      30.88
 H      -5.584669    -1.770740    -4.317468      32.29
 H      -6.969169    -1.374822    -3.144696      28.81
55
name = lig-ACN-frame_209
 C       3.580124     2.961861     0.073527      67.13
 H       3.198523     3.954264     0.087001      24.89
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 C       3.866925     0.844197     1.258569      68.08
 H       3.557005     0.251616     2.143872      22.35
 C       5.139945     0.644843     0.585303       9.51
 O       5.993663    -0.409069     0.675687     180.34
 C       5.818304    -1.332272     1.877638      98.56
 H       5.868664    -0.898068     2.836751      26.86
 H       6.774016    -1.982238     1.770657      23.98
 H       4.843773    -2.130640     1.745017      23.05
 C       5.462660     1.546989    -0.465950      23.18
 O       6.530529     1.201642    -1.303852     167.01
 H       7.225551     0.786123    -0.838469      27.65
 C       4.706614     2.670081    -0.670359      59.33
 H       5.080302     3.403882    -1.338253      22.93
 C       3.234822     2.062776     1.076244      24.83
 C       2.003651     2.435667     1.997786      93.23
 H       2.176488     3.405984     2.300047      24.24
 O       2.091650     1.713050     3.227950     273.48
 H       1.760494     0.698757     3.181060      22.37
 C       0.574194     2.440837     1.263980      73.10
 H       0.662761     3.004632     0.318394      20.69
 C      -0.461181     2.805854     2.226057     104.71
 O      -0.471478     4.350296     2.374228     213.23
 H       0.069496     4.675291     1.464543      25.24
 H      -0.231280     2.391585     3.228515      24.20
 H      -1.389233     2.461263     1.934858      26.35
 C      -2.346268    -1.269146    -0.288998      63.23
 H      -2.917928    -2.065385     0.101463      19.66
 C      -1.794732     0.344766    -2.119134      37.10
 H      -1.966197     0.560526    -3.163200      17.78
 C      -0.983052     1.060354    -1.244114       8.97
 O      -0.282236     2.226973    -1.689069     195.92
 C      -0.568470     2.688541    -3.082567     124.64
 H      -0.156565     3.524772    -3.119699      28.92
 H      -0.245806     1.875410    -3.801332      23.85
 H      -1.617054     2.848305    -3.276098      27.68
 C      -0.722469     0.622468     0.115068      18.34
 O       0.260340     0.977750     0.976524     177.31
 C      -1.462075    -0.567181     0.527902      46.00
 H      -1.096667    -0.884555     1.442790      20.69
 C      -2.483367    -0.772113    -1.630549      60.80
 C      -3.391796    -1.441178    -2.666665      57.51
 H      -3.144064    -1.170788    -3.661088      28.26
 O      -3.282271    -2.948723    -2.590302     199.82
 H      -2.144668    -3.033425    -2.949406      20.34
 C      -4.931882    -1.098417    -2.417757      95.96
 H      -5.076761    -1.269918    -1.373966      26.75
 O      -5.191088     0.288916    -2.692523     261.21
 H      -4.864848     0.920808    -1.833630      21.80
 C      -5.982699    -1.841240    -3.325775     107.37
 O      -6.046220    -3.189130    -2.923133     276.13
 H      -5.154514    -3.506622    -2.968324      34.87
 H      -5.713780    -1.605988    -4.346812      31.84
 H      -7.044691    -1.353639    -3.248703      28.33
55
name = lig-ACN-frame_210
 C       3.616800     3.010949     0.109585      44.64
 H       2.980948     3.865956    -0.105117      20.62
 C       3.959110     0.783522     1.305370      56.79
 H       3.742704     0.090890     2.084623      20.15
 C       5.093721     0.622934     0.584337      17.06
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 O       5.918601    -0.523384     0.761999     226.14
 C       5.780958    -1.413234     1.807827     100.25
 H       5.792426    -0.891455     2.801163      25.92
 H       6.566298    -2.297689     1.675777      22.55
 H       4.619775    -1.859067     1.702456      23.08
 C       5.475565     1.516225    -0.486325      11.13
 O       6.562851     1.247702    -1.305957     122.39
 H       7.221932     0.670038    -0.741907      23.46
 C       4.726869     2.724306    -0.753891      50.79
 H       5.026215     3.349017    -1.542190      24.25
 C       3.180815     2.019325     1.048673      20.76
 C       2.064313     2.461889     1.892166     104.19
 H       2.189730     3.473436     2.155480      26.30
 O       2.088624     1.696568     3.181442     260.26
 H       1.743022     0.866577     2.936159      25.52
 C       0.656119     2.338092     1.246217      86.96
 H       0.559717     2.914184     0.368697      24.06
 C      -0.468390     2.895850     2.176726     107.72
 O      -0.441667     4.261082     2.337564     241.58
 H       0.185373     4.957237     1.618849      24.35
 H      -0.345341     2.441578     3.133261      26.20
 H      -1.375969     2.618364     1.755437      26.31
 C      -2.317031    -1.249800    -0.336214      48.44
 H      -2.789374    -2.218350     0.038363      19.02
 C      -1.805091     0.309138    -2.058150      85.07
 H      -1.889552     0.758381    -3.040410      13.58
 C      -0.917110     1.079175    -1.219312      14.53
 O      -0.317968     2.220357    -1.731069     207.41
 C      -0.573861     2.767117    -3.097471     121.65
 H      -0.114328     3.605417    -3.192641      29.64
 H      -0.219188     2.183967    -3.969956      27.26
 H      -1.650697     2.909224    -3.073275      27.96
 C      -0.734187     0.545264     0.099031      27.16
 O       0.329738     0.955680     1.002852     184.78
 C      -1.405156    -0.590302     0.565462      36.90
 H      -1.160799    -1.152006     1.448028      19.54
 C      -2.481189    -0.853961    -1.667853      36.58
 C      -3.437344    -1.448003    -2.638979      65.32
 H      -3.194992    -1.049625    -3.639616      26.89
 O      -3.215483    -2.945826    -2.562723     248.11
 H      -2.102146    -3.238220    -2.591720      21.45
 C      -4.968353    -1.055704    -2.395155      91.70
 H      -5.320550    -1.378824    -1.420664      27.00
 O      -5.184138     0.313765    -2.709553     270.63
 H      -4.930485     0.955004    -1.867248      23.98
 C      -5.950609    -1.822738    -3.309311      99.36
 O      -6.063087    -3.247143    -2.907203     244.69
 H      -5.163349    -3.611153    -3.107506      32.44
 H      -5.775955    -1.816337    -4.381860      30.29
 H      -6.980468    -1.377952    -2.977642      27.96
55
name = lig-ACN-frame_211
 C       3.669258     2.915413     0.053497      61.69
 H       2.932961     3.682036    -0.238795      22.77
 C       3.970479     0.909009     1.337377      66.88
 H       3.635603     0.234637     2.062481      20.25
 C       5.107848     0.540687     0.504813      14.10
 O       5.933112    -0.544555     0.715958     191.91
 C       5.616936    -1.520143     1.811064     101.41
 H       6.028070    -1.060796     2.753403      26.22
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 H       6.434807    -2.390086     1.646829      23.63
 H       4.532430    -1.994253     1.971979      25.27
 C       5.489067     1.503245    -0.509839      15.85
 O       6.620266     1.289419    -1.287599     145.25
 H       7.281014     0.515926    -1.008280      21.20
 C       4.771793     2.698180    -0.771355      56.49
 H       5.024972     3.329079    -1.593899      23.98
 C       3.233564     1.996108     1.003760      29.77
 C       2.037879     2.400480     1.925337     105.48
 H       2.131687     3.462418     2.135916      25.77
 O       2.047157     1.703197     3.104496     297.38
 H       1.897353     0.790237     2.968904      28.82
 C       0.670349     2.294156     1.208264      88.19
 H       0.798492     2.761398     0.304874      24.62
 C      -0.500295     2.887242     2.110398     111.42
 O      -0.411566     4.333885     2.370955     243.54
 H       0.070632     4.681881     1.412624      25.14
 H      -0.579551     2.442500     3.028216      27.15
 H      -1.374440     2.672491     1.576257      26.70
 C      -2.269725    -1.293792    -0.327247      56.32
 H      -2.757120    -2.356884    -0.025395      20.18
 C      -1.789105     0.351518    -2.048826      23.27
 H      -2.023416     0.601274    -3.084591      19.58
 C      -0.909021     1.044845    -1.224257      12.24
 O      -0.272605     2.241904    -1.751600     193.18
 C      -0.629326     2.817394    -3.021502     129.35
 H      -0.177878     3.607357    -2.912380      29.98
 H      -0.270196     2.143752    -3.778893      26.69
 H      -1.684420     3.108470    -3.343903      26.86
 C      -0.604220     0.540180     0.141544      24.39
 O       0.396303     0.886157     0.978782     191.21
 C      -1.372766    -0.641761     0.504636      46.81
 H      -1.259459    -0.840734     1.617898      19.10
 C      -2.499840    -0.800745    -1.655221      53.68
 C      -3.486296    -1.553745    -2.624769      62.20
 H      -3.267203    -1.242995    -3.710561      24.45
 O      -3.258795    -2.930451    -2.539464     286.35
 H      -2.274375    -2.956809    -2.813238      27.09
 C      -4.969867    -1.102679    -2.387536      90.89
 H      -5.175637    -1.164229    -1.304683      26.81
 O      -5.170972     0.379181    -2.717421     273.72
 H      -4.925366     0.862148    -1.942960      27.78
 C      -5.959913    -1.890421    -3.249158     106.14
 O      -6.068868    -3.295877    -2.912594     242.16
 H      -5.149978    -3.719810    -3.100602      31.89
 H      -5.635802    -1.649113    -4.295416      30.71
 H      -7.027715    -1.447792    -3.188319      28.10
55
name = lig-ACN-frame_212
 C       3.602634     2.866110    -0.110355      56.32
 H       3.205796     3.906969    -0.265442      25.13
 C       4.054509     0.892306     1.293561      64.02
 H       3.836455     0.352726     2.197109      22.25
 C       5.108209     0.552426     0.476479      14.95
 O       5.921844    -0.604880     0.654104     180.22
 C       5.564330    -1.577707     1.813236      86.72
 H       5.810314    -1.191215     2.936441      24.11
 H       6.062850    -2.535871     1.410637      23.71
 H       4.452628    -1.673063     1.724958      25.77
 C       5.573161     1.441233    -0.533604      28.60
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 O       6.700960     1.315326    -1.310534     125.71
 H       7.222441     0.638605    -0.867237      24.63
 C       4.833284     2.573975    -0.756534      50.83
 H       5.243970     3.342667    -1.446020      22.62
 C       3.251243     2.087627     1.034434       2.22
 C       2.013188     2.380148     1.874573      97.35
 H       2.160811     3.405547     2.281652      23.23
 O       2.003682     1.651037     3.159804     233.17
 H       1.817106     0.613056     2.946095      22.85
 C       0.645624     2.326616     1.190148      93.06
 H       0.628461     2.832256     0.314709      23.76
 C      -0.545500     2.857803     1.987826     101.05
 O      -0.363768     4.377165     2.377102     248.62
 H      -0.164372     4.935801     1.633233      30.38
 H      -0.559976     2.372224     2.868099      27.39
 H      -1.470783     2.757681     1.466072      26.14
 C      -2.232228    -1.337889    -0.366330      41.82
 H      -2.852618    -2.241740     0.175431      19.60
 C      -1.833399     0.376006    -2.079618      40.11
 H      -1.928091     0.842737    -3.061338      19.33
 C      -0.865679     1.045424    -1.244942      10.59
 O      -0.247842     2.215449    -1.659852     200.24
 C      -0.634822     2.860825    -2.970492     117.86
 H      -0.220341     3.677028    -3.103171      30.15
 H      -0.313037     2.319306    -3.832392      27.12
 H      -1.776091     2.932115    -2.791983      25.82
 C      -0.574709     0.477611     0.015887      20.86
 O       0.465990     0.837733     0.958237     178.72
 C      -1.315720    -0.604177     0.493728      41.68
 H      -1.124224    -1.047311     1.571284      20.28
 C      -2.538043    -0.787958    -1.628312      50.09
 C      -3.468367    -1.455247    -2.617455      71.92
 H      -3.237483    -1.119798    -3.714571      25.56
 O      -3.328724    -2.997408    -2.520890     257.88
 H      -2.615836    -3.270480    -2.912082      33.50
 C      -4.980015    -1.068673    -2.315445      91.99
 H      -5.207551    -1.264949    -1.221772      26.71
 O      -5.138674     0.330101    -2.730167     274.94
 H      -4.887896     0.865737    -2.022518      29.60
 C      -5.977160    -1.932239    -3.233655      99.57
 O      -6.064776    -3.342876    -2.930499     252.40
 H      -5.146603    -3.625768    -2.991895      33.05
 H      -5.635446    -1.877653    -4.320776      30.00
 H      -7.024692    -1.529937    -3.117003      28.26
55
name = lig-ACN-frame_213
 C       3.602091     2.852428    -0.157220      56.79
 H       3.045959     3.800673    -0.447571      24.41
 C       4.057114     0.946007     1.264858      56.45
 H       3.886317     0.340886     2.184402      21.60
 C       5.216768     0.500581     0.485117      13.75
 O       5.898315    -0.691985     0.666746     217.56
 C       5.462065    -1.553009     1.648247     113.61
 H       6.002287    -1.143673     2.695838      23.19
 H       5.894785    -2.571554     1.576907      24.74
 H       4.405769    -1.650613     1.772322      26.24
 C       5.630392     1.375859    -0.554416      12.64
 O       6.821528     1.277481    -1.321236     120.82
 H       7.533944     0.765991    -0.980144      27.77
 C       4.822538     2.569247    -0.808632      35.81
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 H       5.349537     3.287945    -1.522926      22.32
 C       3.254640     2.068795     0.992342      24.91
 C       2.040313     2.430635     1.952008      79.86
 H       2.023540     3.551015     2.206173      23.80
 O       1.960347     1.569530     3.192306     232.86
 H       1.584850     0.600677     2.841346      20.85
 C       0.644132     2.315775     1.105506      79.91
 H       0.810445     2.801445     0.203456      22.77
 C      -0.563458     2.987543     1.955004     114.95
 O      -0.358090     4.283909     2.379460     314.92
 H       0.032347     4.698195     1.740086      35.83
 H      -0.754571     2.439130     2.812745      27.14
 H      -1.447669     2.877676     1.298400      26.14
 C      -2.231763    -1.264991    -0.360632      57.14
 H      -2.782901    -2.262182    -0.028758      20.16
 C      -1.851178     0.400469    -2.066484      35.52
 H      -2.200456     0.700348    -3.059436      17.11
 C      -0.862602     1.017254    -1.296861      17.07
 O      -0.166941     2.232075    -1.613184     203.77
 C      -0.666015     2.854742    -2.836678     124.95
 H      -0.276103     3.680079    -2.789460      29.91
 H      -0.542227     2.150502    -3.658471      26.93
 H      -1.824918     3.113878    -2.889990      26.86
 C      -0.510404     0.421236    -0.005668      20.79
 O       0.463293     0.884710     0.848413     202.37
 C      -1.279821    -0.662017     0.441946      57.64
 H      -0.860174    -1.150603     1.435973      19.90
 C      -2.487372    -0.789492    -1.647913      45.96
 C      -3.489647    -1.458869    -2.572355      56.20
 H      -3.249713    -1.083300    -3.683646      23.46
 O      -3.439412    -2.996365    -2.525639     253.43
 H      -2.481313    -3.157404    -2.836500      27.48
 C      -4.981806    -1.103744    -2.342883      96.53
 H      -5.323319    -1.238382    -1.257162      27.36
 O      -5.134739     0.247552    -2.730636     275.53
 H      -4.830213     0.923232    -1.976225      24.89
 C      -5.964671    -1.935548    -3.220698     104.11
 O      -6.046177    -3.383855    -2.920023     249.76
 H      -5.133194    -3.644625    -2.822825      32.63
 H      -5.718567    -1.685683    -4.323363      30.08
 H      -6.965214    -1.512166    -3.032704      28.57
55
name = lig-ACN-frame_214
 C       3.672673     2.826491    -0.136678      47.12
 H       2.926945     3.529529    -0.585295      21.46
 C       4.113615     0.931214     1.261368      69.62
 H       3.646429     0.330553     2.102326      20.77
 C       5.231921     0.529467     0.482790      12.02
 O       5.892470    -0.704729     0.577129     186.72
 C       5.374473    -1.611097     1.643404      99.25
 H       5.745635    -1.264167     2.814710      23.99
 H       5.821984    -2.486756     1.301487      26.06
 H       4.349534    -1.635802     1.675183      29.24
 C       5.693658     1.415219    -0.581624      13.24
 O       6.893255     1.246822    -1.324589      99.96
 H       7.411062     0.490822    -0.844769      22.94
 C       4.864290     2.518353    -0.878885      52.22
 H       4.982119     3.182573    -1.803415      23.96
 C       3.268241     2.033241     0.954583      -0.66
 C       1.989736     2.357598     1.969306      94.09
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 H       2.311769     3.349387     2.517745      22.89
 O       1.926024     1.568416     3.113368     279.19
 H       1.644647     0.648752     2.907496      25.53
 C       0.722475     2.357747     1.127772      91.66
 H       0.866890     2.979738     0.245205      23.01
 C      -0.589122     2.906333     1.844103     104.58
 O      -0.321930     4.283410     2.394143     251.22
 H       0.268600     4.739142     1.744991      30.52
 H      -0.861457     2.262168     2.657256      26.41
 H      -1.429883     3.038775     1.134049      25.88
 C      -2.251859    -1.284067    -0.359865      46.45
 H      -2.639353    -2.284887    -0.040870      21.81
 C      -1.848289     0.424081    -2.103013      67.15
 H      -2.118348     0.922200    -3.039226      18.00
 C      -0.835159     1.002126    -1.277215      11.48
 O      -0.164083     2.187657    -1.600360     224.61
 C      -0.690523     2.885546    -2.721841     123.63
 H      -0.180754     3.639754    -2.890093      29.93
 H      -0.405283     2.380675    -3.667974      26.28
 H      -1.838079     3.117252    -2.518246      24.70
 C      -0.511876     0.445352    -0.039367      23.98
 O       0.479663     0.965494     0.751177     205.24
 C      -1.160677    -0.741837     0.424395      48.99
 H      -1.004303    -1.145617     1.499387      19.89
 C      -2.486022    -0.804842    -1.668609      23.80
 C      -3.536159    -1.559174    -2.560477      80.83
 H      -3.312450    -1.266492    -3.704325      23.01
 O      -3.464268    -2.926635    -2.539077     221.64
 H      -2.385035    -3.340067    -2.589517      22.99
 C      -4.984518    -1.176720    -2.344919      92.46
 H      -5.190855    -1.338891    -1.214711      27.78
 O      -5.175558     0.242991    -2.745946     230.31
 H      -4.826465     0.816074    -1.856583      23.61
 C      -5.979189    -1.957104    -3.203865     111.74
 O      -6.027723    -3.357712    -2.912984     223.55
 H      -5.047142    -3.675739    -2.886343      29.56
 H      -5.747050    -1.788186    -4.341908      29.02
 H      -6.961861    -1.601291    -2.988971      28.89
55
name = lig-ACN-frame_215
 C       3.704599     2.766951    -0.161329      56.06
 H       3.159703     3.656916    -0.491788      22.65
 C       4.125867     0.870879     1.263000      64.27
 H       3.983624     0.081595     2.041826      20.03
 C       5.235255     0.605839     0.436509       9.87
 O       5.855856    -0.674585     0.530197     178.28
 C       5.336186    -1.683743     1.580312      92.65
 H       5.651226    -1.325987     2.779841      24.17
 H       5.709861    -2.626146     1.467884      26.67
 H       4.335558    -1.758056     1.455086      28.99
 C       5.745041     1.461115    -0.566748      17.01
 O       6.863023     1.221227    -1.293884     142.87
 H       7.440245     0.343470    -1.068756      22.35
 C       4.842903     2.493894    -0.954769      46.66
 H       5.135327     2.980814    -1.922587      21.35
 C       3.303192     1.995392     1.001096      26.13
 C       2.088290     2.296332     1.861759      92.15
 H       2.153540     3.478400     2.105665      23.14
 O       1.897990     1.504735     3.081858     293.97
 H       1.755947     0.637998     2.837102      29.17
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 C       0.699904     2.447072     1.120357      80.35
 H       0.925435     3.106258     0.215902      21.50
 C      -0.551657     2.894247     1.739444     101.11
 O      -0.283216     4.233884     2.400726     180.16
 H       0.154747     4.898149     1.580708      25.26
 H      -0.919389     2.251837     2.590302      24.89
 H      -1.321668     2.869678     0.897426      24.90
 C      -2.159251    -1.360815    -0.406539      64.14
 H      -2.716986    -2.116220     0.039507      21.54
 C      -1.842262     0.381882    -2.115980      71.97
 H      -2.040017     0.800893    -3.108030      20.06
 C      -0.886648     0.977978    -1.296978      11.99
 O      -0.159509     2.131946    -1.589703     210.91
 C      -0.667153     2.983182    -2.697356     119.16
 H      -0.210813     3.795940    -2.618852      27.96
 H      -0.878244     2.325973    -3.616719      23.77
 H      -1.776297     3.295858    -2.453644      25.49
 C      -0.531318     0.441405    -0.008909      28.65
 O       0.574267     1.004614     0.704999     158.25
 C      -1.125639    -0.742687     0.402328      37.66
 H      -0.848388    -1.138482     1.394335      18.39
 C      -2.543123    -0.801248    -1.667096      58.04
 C      -3.483609    -1.484544    -2.663448      24.29
 H      -3.274598    -1.061805    -3.754759      25.29
 O      -3.409812    -3.024095    -2.502033     171.59
 H      -2.294253    -3.191054    -2.659492      23.78
 C      -5.020812    -1.137739    -2.322442      91.09
 H      -5.334136    -1.361204    -1.220419      26.31
 O      -5.224334     0.220802    -2.708269     250.69
 H      -4.892122     0.882929    -2.017774      25.82
 C      -6.024943    -1.974506    -3.205134     103.43
 O      -6.020286    -3.376521    -2.896401     238.09
 H      -5.068767    -3.649187    -3.088544      31.93
 H      -5.707775    -1.795493    -4.326396      30.76
 H      -7.004801    -1.592325    -3.052120      30.45
55
name = lig-ACN-frame_216
 C       3.690503     2.743663    -0.166835      58.19
 H       3.127719     3.639965    -0.275416      23.88
 C       4.127456     0.835669     1.241690      74.74
 H       3.792195     0.287680     2.127449      22.03
 C       5.261794     0.509451     0.471125      16.46
 O       5.845547    -0.705367     0.550961     200.13
 C       5.315820    -1.669683     1.414749     107.74
 H       5.546479    -1.198015     2.601909      23.66
 H       6.022849    -2.395832     1.198091      25.10
 H       4.313000    -1.893455     1.416832      28.60
 C       5.690990     1.448438    -0.554822       9.59
 O       6.848169     1.210318    -1.326743     103.94
 H       7.344888     0.466259    -0.838212      24.48
 C       4.845131     2.472454    -0.968315      59.52
 H       5.088236     3.227616    -1.703135      22.38
 C       3.380581     1.955665     0.957521      27.95
 C       2.100309     2.373269     1.830761      83.51
 H       2.404107     3.341231     2.462454      21.84
 O       1.924384     1.483845     3.024127     254.57
 H       1.663461     0.531769     2.722200      22.71
 C       0.817555     2.344784     0.959307      77.48
 H       0.911244     2.980486    -0.021856      19.15
 C      -0.505775     2.975916     1.750861      93.43
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 O      -0.278695     4.151377     2.335934     173.77
 H       0.073996     4.961714     1.527570      23.30
 H      -0.835394     2.187533     2.566300      23.54
 H      -1.375221     3.125975     1.004649      23.00
 C      -2.113403    -1.397802    -0.447581      55.99
 H      -2.563760    -2.246105    -0.136895      20.95
 C      -1.843005     0.317176    -2.124047      33.67
 H      -2.071049     0.584075    -3.160076      22.88
 C      -0.920310     0.980008    -1.279986      11.37
 O      -0.167246     2.129420    -1.663144     216.17
 C      -0.716143     3.058233    -2.615297     123.81
 H      -0.032826     3.718881    -2.725395      27.96
 H      -0.526866     2.693954    -3.735988      24.24
 H      -1.742897     3.465403    -2.328265      26.06
 C      -0.474926     0.488445    -0.010167      20.78
 O       0.605175     0.971181     0.626642     218.47
 C      -1.130888    -0.740176     0.405775      48.87
 H      -0.763920    -1.275502     1.241410      21.63
 C      -2.519410    -0.826494    -1.677606      50.04
 C      -3.532463    -1.497098    -2.610702      57.16
 H      -3.286839    -1.319630    -3.722035      25.21
 O      -3.290345    -3.020225    -2.519002     230.74
 H      -2.367547    -3.230728    -2.800944      28.49
 C      -5.024300    -1.136981    -2.371265      95.99
 H      -5.111412    -1.298194    -1.214585      25.61
 O      -5.310509     0.255771    -2.668766     277.22
 H      -4.867705     0.714558    -2.032145      30.44
 C      -6.016840    -1.960371    -3.214739     107.44
 O      -6.023121    -3.409232    -2.888558     242.37
 H      -5.158576    -3.734619    -3.052391      34.45
 H      -5.797610    -1.736819    -4.346921      29.81
 H      -7.042870    -1.658983    -3.034076      29.01
55
name = lig-ACN-frame_217
 C       3.677790     2.793443    -0.167732      55.09
 H       3.064823     3.572358    -0.542855      23.82
 C       4.110440     0.806532     1.271073      67.73
 H       3.790657     0.146120     2.040694      20.48
 C       5.199346     0.494851     0.458390       8.14
 O       5.920166    -0.714630     0.480321     222.20
 C       5.376184    -1.725164     1.362976      99.85
 H       5.313053    -1.464024     2.614859      23.95
 H       5.865224    -2.691855     1.305451      25.37
 H       4.429345    -1.918745     0.925373      28.00
 C       5.636009     1.346403    -0.606625      11.34
 O       6.825093     1.188240    -1.332509     162.70
 H       7.433163     0.574535    -0.987431      28.43
 C       4.839209     2.525797    -0.880235      43.33
 H       5.223913     3.157839    -1.625794      24.91
 C       3.331129     1.986500     0.946552      17.14
 C       2.151822     2.319660     1.841943     100.37
 H       2.172973     3.477650     2.109352      22.96
 O       1.972863     1.497560     2.933212     263.97
 H       1.539343     0.538402     2.605231      19.82
 C       0.836105     2.346082     0.898630      74.70
 H       1.123995     2.904938    -0.112940      20.13
 C      -0.411663     2.844957     1.612328      82.75
 O      -0.227348     4.232091     2.328285     170.63
 H       0.337050     4.830928     1.532210      24.60
 H      -0.619072     2.137449     2.579377      22.44
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 H      -1.357109     2.813837     0.939314      24.19
 C      -2.101743    -1.409814    -0.433581      57.72
 H      -2.207798    -2.426181    -0.161263      20.34
 C      -1.826165     0.332449    -2.137543      69.38
 H      -1.957897     0.875707    -3.075376      17.78
 C      -0.907691     1.034056    -1.319989      24.75
 O      -0.196718     2.116521    -1.758453     245.23
 C      -0.673801     3.158362    -2.611560     121.45
 H      -0.113406     3.937694    -2.431762      27.19
 H      -1.038417     2.645923    -3.668944      23.48
 H      -1.675464     3.515534    -2.269585      27.33
 C      -0.549033     0.431839    -0.095658      27.96
 O       0.664338     0.881429     0.590972     173.30
 C      -1.097389    -0.742645     0.375099      42.73
 H      -0.795553    -1.192717     1.284070      18.48
 C      -2.478968    -0.881382    -1.685490      58.04
 C      -3.488033    -1.609885    -2.598916      59.89
 H      -3.313310    -1.114621    -3.601356      28.49
 O      -3.256819    -2.973212    -2.550599     321.93
 H      -2.378817    -3.063568    -2.666494      31.86
 C      -5.017613    -1.181878    -2.354485      82.19
 H      -5.433680    -1.446013    -1.294573      26.88
 O      -5.369739     0.277848    -2.636657     212.87
 H      -4.938717     0.920451    -2.003279      26.23
 C      -6.007041    -2.013703    -3.206143     109.89
 O      -6.028507    -3.395475    -2.906362     239.55
 H      -5.065365    -3.663200    -2.902474      32.26
 H      -5.814808    -1.883577    -4.339379      29.73
 H      -6.989661    -1.590952    -2.901343      28.95
55
name = lig-ACN-frame_218
 C       3.684519     2.825240    -0.154644      63.85
 H       3.078298     3.685673    -0.416619      24.73
 C       4.067071     0.834426     1.234989      67.28
 H       3.781850     0.182406     2.015030      21.68
 C       5.176577     0.440068     0.367691      -2.81
 O       6.029541    -0.725268     0.467085     195.26
 C       5.370319    -1.856698     1.279282      98.29
 H       5.209461    -1.355434     2.400052      23.93
 H       6.212205    -2.648288     1.255058      22.87
 H       4.324717    -2.084804     0.988658      25.83
 C       5.597557     1.348499    -0.639239      19.89
 O       6.780555     1.171467    -1.346179     198.90
 H       7.177222     0.332120    -1.009332      22.11
 C       4.919126     2.527886    -0.835275      53.22
 H       5.197025     3.103245    -1.666321      26.12
 C       3.335058     1.977698     0.958240      34.85
 C       2.080261     2.323063     1.710473     103.24
 H       2.260869     3.349049     2.214241      22.33
 O       2.005687     1.491552     2.920270     253.77
 H       1.687547     0.576952     2.646479      24.78
 C       0.890544     2.278345     0.890124      89.64
 H       1.016800     2.944013    -0.075294      18.79
 C      -0.316189     2.825938     1.605109      85.30
 O      -0.173474     4.197448     2.219263     245.82
 H       0.428443     4.770771     1.649367      28.93
 H      -0.535510     2.041865     2.543839      22.01
 H      -1.204732     2.827281     0.842235      23.35
 C      -2.038783    -1.447954    -0.432595      76.00
 H      -2.611480    -2.378064    -0.086914      18.15
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 C      -1.887583     0.362709    -2.144362     -18.04
 H      -2.322402     0.595313    -3.109606      17.44
 C      -0.917200     1.012822    -1.392835      22.15
 O      -0.138432     2.127652    -1.823703     213.82
 C      -0.772647     3.240604    -2.593835     112.97
 H      -0.054280     3.956326    -2.683385      26.23
 H      -0.800920     3.080694    -3.850332      23.96
 H      -1.709273     3.486918    -2.128646      26.22
 C      -0.459707     0.448671    -0.121576      38.48
 O       0.657243     0.819193     0.544125     178.69
 C      -1.105490    -0.774579     0.334119      45.77
 H      -0.695215    -1.092764     1.311780      18.28
 C      -2.420064    -0.848961    -1.694984      68.74
 C      -3.451768    -1.467676    -2.621667      55.68
 H      -3.313197    -1.241522    -3.678991      28.71
 O      -3.311461    -3.015956    -2.586352     277.98
 H      -2.453384    -3.206472    -2.561241      34.52
 C      -5.045114    -1.190563    -2.295921      83.68
 H      -5.139724    -1.400225    -1.150468      25.54
 O      -5.377127     0.189469    -2.610015     219.73
 H      -4.850986     0.774297    -1.822841      22.40
 C      -6.007781    -1.996703    -3.230102     106.86
 O      -6.015040    -3.423469    -2.900470     232.19
 H      -5.030110    -3.718085    -2.837871      29.79
 H      -5.739112    -1.753276    -4.305144      30.62
 H      -7.096087    -1.661874    -3.131071      28.00
55
name = lig-ACN-frame_219
 C       3.793154     2.838795    -0.115624      52.28
 H       3.294157     3.826166    -0.233545      23.48
 C       4.121432     0.756881     1.114252      66.07
 H       3.782837     0.253009     2.001659      21.02
 C       5.181634     0.369784     0.332677      22.21
 O       5.986172    -0.743846     0.512563     235.11
 C       5.429198    -1.839012     1.189886     109.57
 H       5.262118    -1.629493     2.370809      25.10
 H       6.205276    -2.754517     1.196436      23.39
 H       4.534328    -2.347278     0.643826      25.77
 C       5.617398     1.360486    -0.626199       7.93
 O       6.744415     1.119648    -1.377301     115.60
 H       7.187129     0.177908    -1.158004      23.29
 C       4.890342     2.587613    -0.886856      62.16
 H       5.251913     3.333533    -1.582654      22.79
 C       3.380416     1.971958     0.874537      28.78
 C       2.160486     2.284906     1.753604     100.05
 H       2.143343     3.365065     2.051004      23.47
 O       2.003701     1.481002     2.930211     309.35
 H       1.854317     0.608728     2.734053      28.16
 C       0.847407     2.208659     0.818831      78.70
 H       1.039880     2.741907    -0.182592      20.06
 C      -0.336193     2.844886     1.651094      93.89
 O      -0.099920     4.097690     2.102076     306.27
 H       0.235966     4.604473     1.476655      33.66
 H      -0.723890     2.168156     2.631279      21.97
 H      -1.291338     2.873639     0.928394      22.87
 C      -2.051910    -1.424376    -0.494827      73.45
 H      -2.685477    -2.326280     0.026802      16.46
 C      -1.939737     0.383894    -2.164852      67.02
 H      -2.179948     0.929475    -3.073719      14.53
 C      -0.832481     1.039134    -1.444559      13.74
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 O      -0.115832     2.158483    -1.915411     242.78
 C      -0.804632     3.277356    -2.581210     106.31
 H      -0.216855     4.113057    -2.347377      25.83
 H      -1.119690     2.773652    -3.731281      23.06
 H      -1.732932     3.583153    -2.210494      29.26
 C      -0.447702     0.395996    -0.241024      32.37
 O       0.683890     0.844858     0.530151     217.04
 C      -1.040472    -0.739716     0.310086      44.03
 H      -0.777447    -1.260429     1.300726      19.86
 C      -2.462511    -0.869016    -1.705524      35.56
 C      -3.513143    -1.503918    -2.641668      66.61
 H      -3.322395    -1.070049    -3.574714      27.65
 O      -3.423553    -2.990849    -2.603416     274.37
 H      -2.474133    -3.226694    -2.756926      30.79
 C      -4.986417    -1.201378    -2.288481      95.94
 H      -5.214276    -1.515123    -1.187792      26.76
 O      -5.358429     0.123037    -2.545525     225.54
 H      -4.865542     0.855015    -1.891130      22.53
 C      -5.961113    -2.025578    -3.199047     103.71
 O      -6.002252    -3.434149    -2.914487     246.17
 H      -5.067805    -3.664551    -2.932969      32.15
 H      -5.529503    -1.863943    -4.220526      31.33
 H      -7.029625    -1.626142    -3.112389      28.32
55
name = lig-ACN-frame_220
 C       3.867608     2.935922    -0.082462      49.87
 H       3.332453     3.936010    -0.168671      21.20
 C       4.067433     0.687497     1.069193      73.90
 H       3.849700    -0.119741     1.788806      20.37
 C       5.210667     0.427353     0.283415      20.02
 O       5.969375    -0.715212     0.502344     226.73
 C       5.455626    -1.918311     1.160457      93.57
 H       4.935088    -1.745816     2.176450      24.73
 H       6.325094    -2.679104     1.134889      23.39
 H       4.511805    -2.153637     0.506164      25.93
 C       5.655883     1.349090    -0.686784      19.09
 O       6.759078     1.060355    -1.461870     161.27
 H       7.281112     0.339978    -0.992995      25.66
 C       4.971786     2.559641    -0.933024      47.49
 H       5.509895     3.266657    -1.626362      21.74
 C       3.413497     1.900091     0.902490      18.72
 C       2.195079     2.239421     1.734316      97.66
 H       2.344910     3.231971     2.077725      25.06
 O       2.021371     1.479873     2.954741     281.22
 H       1.740362     0.527720     2.677872      23.74
 C       0.826979     2.220403     0.875391      81.40
 H       0.997653     2.921287     0.036743      20.86
 C      -0.446560     2.702063     1.551406      84.98
 O      -0.011497     4.119359     2.076579     238.55
 H       0.309842     4.638095     1.372786      30.81
 H      -0.481133     2.053356     2.588353      21.95
 H      -1.450495     2.630252     0.913347      23.22
 C      -2.090562    -1.327914    -0.500379      82.81
 H      -2.318167    -2.490899    -0.158025      20.56
 C      -1.873703     0.418361    -2.168547      49.99
 H      -2.302751     0.817337    -3.079001      22.34
 C      -0.818181     1.001999    -1.509626      19.45
 O      -0.125229     2.169549    -1.971908     228.28
 C      -0.875730     3.238659    -2.546526     104.16
 H      -0.221206     4.155224    -2.658584      23.68
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 H      -1.128149     3.217685    -3.839515      22.98
 H      -1.741173     3.241269    -1.987557      26.92
 C      -0.345469     0.387276    -0.280767      24.46
 O       0.685474     0.798079     0.486998     188.29
 C      -1.054220    -0.766933     0.179214      56.95
 H      -0.617673    -1.057507     1.208639      16.61
 C      -2.523907    -0.798288    -1.772649      66.89
 C      -3.556008    -1.560209    -2.627470      68.81
 H      -3.515702    -1.307629    -3.632643      28.05
 O      -3.491098    -2.955949    -2.635879     207.68
 H      -2.393752    -3.270503    -2.764710      23.77
 C      -4.995317    -1.282537    -2.254578      94.25
 H      -5.208469    -1.587463    -1.164874      28.30
 O      -5.353005     0.161448    -2.486250     246.87
 H      -4.780836     0.686776    -1.902947      28.38
 C      -5.869493    -2.059605    -3.203725     115.28
 O      -6.010424    -3.449396    -2.921423     249.65
 H      -5.135069    -3.848718    -2.996887      33.30
 H      -5.666044    -1.865099    -4.269694      31.38
 H      -6.892054    -1.578833    -3.041599      28.64
55
name = lig-ACN-frame_221
 C       3.966433     2.836386    -0.013699      63.73
 H       3.483456     3.848699    -0.153190      24.38
 C       4.032885     0.647054     0.999819      50.12
 H       3.443801    -0.055677     1.637468      18.77
 C       5.220219     0.426557     0.287694       4.34
 O       6.049490    -0.685045     0.466041     191.67
 C       5.350440    -1.909000     1.087259     109.81
 H       5.076139    -1.632456     2.100914      26.74
 H       6.162378    -2.598468     1.193975      25.06
 H       4.553089    -2.574129     0.467135      26.04
 C       5.688759     1.326930    -0.772522      11.21
 O       6.825318     1.001755    -1.560263     184.86
 H       7.425534     0.454683    -1.111583      25.28
 C       5.049810     2.560631    -0.870206      52.14
 H       5.268920     3.271192    -1.753040      24.58
 C       3.409638     1.941451     0.851413      18.88
 C       2.120298     2.253358     1.748028     103.46
 H       2.228465     3.206021     2.096856      25.07
 O       2.055287     1.444893     2.953809     264.11
 H       1.652513     0.428983     2.836303      20.26
 C       0.877074     2.219384     0.881577      87.85
 H       1.033104     2.737026    -0.023894      22.13
 C      -0.363703     2.714074     1.605557      96.80
 O      -0.069800     4.019527     2.064367     254.11
 H       0.567728     4.565055     1.391443      26.31
 H      -0.779553     2.090399     2.528673      22.24
 H      -1.249396     2.812076     0.799963      22.87
 C      -2.116557    -1.321976    -0.581545      60.93
 H      -2.652442    -2.362476    -0.297693      15.75
 C      -1.906280     0.387973    -2.289199      85.75
 H      -2.158407     0.858685    -3.239267      15.48
 C      -0.754868     1.007475    -1.538198      26.46
 O      -0.103552     2.120544    -2.017138     221.24
 C      -0.983579     3.227171    -2.541912      84.20
 H      -0.319399     4.124750    -2.232021      23.80
 H      -1.267804     2.835829    -3.764004      22.24
 H      -1.881617     3.497653    -2.099839      28.85
 C      -0.337536     0.401772    -0.361956      40.21
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 O       0.760762     0.776583     0.452266     209.59
 C      -0.996459    -0.736118     0.096220      40.90
 H      -0.685209    -1.341592     0.984158      19.60
 C      -2.528358    -0.759734    -1.770984      24.01
 C      -3.551953    -1.458097    -2.667345      60.05
 H      -3.381899    -1.060665    -3.602901      31.10
 O      -3.441597    -3.045337    -2.628905     190.61
 H      -2.267256    -3.262282    -2.571929      21.36
 C      -5.042681    -1.241725    -2.231289      92.40
 H      -5.204979    -1.591788    -1.168766      26.97
 O      -5.335443     0.136893    -2.415646     278.21
 H      -4.871209     0.690902    -1.854249      31.23
 C      -5.942375    -2.059400    -3.233177     104.00
 O      -6.051163    -3.499336    -2.928703     212.39
 H      -5.088583    -3.879009    -3.000970      29.34
 H      -5.482244    -1.833051    -4.199607      31.38
 H      -7.013172    -1.765343    -3.162100      28.39
55
name = lig-ACN-frame_222
 C       4.013737     2.843765    -0.011169      50.66
 H       3.581368     3.858228    -0.087626      23.44
 C       3.998437     0.669399     0.897679      48.78
 H       3.670092    -0.157670     1.558683      22.19
 C       5.259093     0.386659     0.225722       9.57
 O       6.048950    -0.761878     0.436804     235.02
 C       5.377621    -1.821501     1.049209     112.47
 H       4.850044    -1.591377     1.924758      27.44
 H       6.004539    -2.614259     1.223836      26.18
 H       4.428383    -1.888337     0.267617      24.48
 C       5.775511     1.257088    -0.752556       8.31
 O       6.841888     0.986327    -1.638874     114.69
 H       7.424695     0.252271    -1.262910      23.18
 C       5.107970     2.542466    -0.845975      37.79
 H       5.377467     3.354236    -1.625859      23.23
 C       3.366380     1.912296     0.898754      23.07
 C       2.172145     2.235891     1.751198     110.28
 H       2.163707     3.210930     2.049767      25.04
 O       2.079988     1.408467     2.943950     309.45
 H       1.781817     0.530757     2.597373      24.27
 C       0.927618     2.108318     0.832454      96.66
 H       1.088893     2.794584     0.077203      23.38
 C      -0.321202     2.719690     1.570050      94.20
 O      -0.156235     4.015096     2.143144     210.17
 H       0.520255     4.673291     1.423880      23.64
 H      -0.654446     2.039832     2.409359      23.66
 H      -1.175059     2.717196     0.729747      22.77
 C      -2.090020    -1.318741    -0.631478      83.00
 H      -2.637037    -2.089465    -0.012815      19.72
 C      -1.825694     0.400205    -2.355959      42.03
 H      -2.074321     0.785429    -3.352406      22.72
 C      -0.808649     0.975503    -1.638700      13.55
 O      -0.136894     2.132252    -2.052840     226.70
 C      -1.016618     3.182370    -2.514013      89.71
 H      -0.419427     4.257843    -2.677369      21.58
 H      -1.280413     3.089638    -3.798547      22.52
 H      -1.885588     3.044076    -1.935956      25.24
 C      -0.337712     0.370783    -0.369086      22.31
 O       0.824125     0.778187     0.398344     199.73
 C      -0.995211    -0.825299     0.064575      28.39
 H      -0.555801    -1.232919     0.943789      17.65
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 C      -2.533863    -0.735473    -1.867759      64.48
 C      -3.565060    -1.507131    -2.664090      50.50
 H      -3.581732    -1.270926    -3.699593      28.81
 O      -3.332414    -2.999584    -2.614464     170.84
 H      -2.233377    -3.281732    -2.560556      23.76
 C      -5.051384    -1.253848    -2.260356      92.80
 H      -5.211477    -1.612136    -1.223249      28.25
 O      -5.390246     0.146956    -2.380185     248.62
 H      -4.828030     0.694176    -1.684463      23.75
 C      -6.035306    -2.085179    -3.228010     111.10
 O      -6.073745    -3.499202    -2.955610     257.67
 H      -5.112819    -3.717559    -2.894667      32.27
 H      -5.670157    -2.027541    -4.249240      31.01
 H      -7.003868    -1.587316    -3.313287      29.22
55
name = lig-ACN-frame_223
 C       4.003231     2.896211    -0.004270      68.12
 H       3.665486     3.908387    -0.067980      23.87
 C       4.101892     0.588846     0.847967      62.50
 H       3.711482    -0.099260     1.586939      22.80
 C       5.282356     0.350855     0.147811      10.76
 O       6.073667    -0.757063     0.397924     206.11
 C       5.260213    -1.813744     1.045065     115.64
 H       5.094941    -1.468988     1.988057      27.40
 H       5.920383    -2.627560     0.955697      25.76
 H       4.269675    -2.282479     0.493859      25.05
 C       5.815110     1.307475    -0.756929      19.83
 O       6.824107     0.984578    -1.661259      73.37
 H       7.402420     0.169433    -1.281845      23.79
 C       5.153467     2.483702    -0.815705      49.86
 H       5.727859     3.212290    -1.446998      20.11
 C       3.505779     1.904909     0.832748       9.52
 C       2.225420     2.182079     1.723227      96.55
 H       2.369146     3.164380     2.098458      23.98
 O       2.095885     1.369207     2.905376     327.18
 H       1.958761     0.487844     2.756914      27.72
 C       0.960329     2.187866     0.812365      78.85
 H       1.207685     2.690752    -0.032853      23.58
 C      -0.342741     2.606679     1.481726      85.49
 O      -0.197389     4.067494     2.224292     153.83
 H       0.169281     4.822195     1.457445      25.11
 H      -0.504336     1.999318     2.339400      24.10
 H      -1.300112     2.665233     0.831788      23.70
 C      -2.097632    -1.291212    -0.636719      47.20
 H      -2.600210    -2.179016    -0.412819      20.06
 C      -1.818692     0.334645    -2.443896      51.07
 H      -2.103491     0.777908    -3.427390      18.39
 C      -0.728871     0.966255    -1.601212       7.77
 O      -0.142120     2.146799    -2.082434     226.27
 C      -1.066912     3.143246    -2.563727      79.00
 H      -0.444924     4.180703    -2.193107      21.66
 H      -1.481580     2.865006    -3.759524      21.93
 H      -2.015055     3.368084    -1.995097      25.98
 C      -0.307897     0.349584    -0.420937      32.12
 O       0.789793     0.715593     0.281615     192.91
 C      -0.942413    -0.829472     0.049347      36.79
 H      -0.752247    -1.239974     0.963371      18.63
 C      -2.490034    -0.790949    -1.917248      26.17
 C      -3.583568    -1.589714    -2.730326      74.62
 H      -3.457450    -1.225838    -3.769405      27.19
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 O      -3.255661    -2.928765    -2.580505     307.22
 H      -2.281214    -3.033390    -2.597291      27.88
 C      -5.102944    -1.330278    -2.292616      91.17
 H      -5.272903    -1.689145    -1.287675      28.52
 O      -5.474737     0.132156    -2.384204     216.55
 H      -4.783852     0.720667    -1.704936      22.70
 C      -6.041699    -2.047001    -3.261508     116.21
 O      -6.083747    -3.461599    -2.953671     257.19
 H      -5.228466    -3.835019    -2.823962      32.88
 H      -5.767049    -1.746221    -4.255058      30.66
 H      -7.039387    -1.800702    -2.941310      28.02
55
name = lig-ACN-frame_224
 C       4.116366     2.872835    -0.049343      63.01
 H       3.647058     3.810804    -0.039144      24.90
 C       4.182818     0.614680     0.868333      64.52
 H       3.719571    -0.133818     1.464491      20.82
 C       5.322051     0.320517     0.122424      23.27
 O       6.026698    -0.818850     0.313291     190.34
 C       5.261618    -1.919730     1.089214     101.89
 H       5.157782    -1.729774     2.113695      27.86
 H       5.912532    -2.830251     1.085236      24.60
 H       4.167213    -1.910158     0.636083      25.42
 C       5.798032     1.284187    -0.779802       9.32
 O       6.824483     0.998263    -1.653942     130.65
 H       7.512403     0.395259    -1.216769      22.58
 C       5.196845     2.642639    -0.823468      39.93
 H       5.461026     3.386872    -1.567150      25.85
 C       3.557791     1.847670     0.788001      23.72
 C       2.301018     2.107969     1.639571     104.69
 H       2.300948     3.183695     1.996305      24.37
 O       2.125348     1.336720     2.879028     268.24
 H       1.895953     0.367115     2.607609      23.36
 C       0.988837     2.213897     0.712157      71.44
 H       1.092776     2.901204    -0.071001      22.69
 C      -0.313273     2.702409     1.565508     105.19
 O      -0.248285     3.966827     2.189487     305.80
 H       0.034669     4.568627     1.541566      32.43
 H      -0.568224     1.996375     2.252594      26.88
 H      -1.083602     2.682654     0.714509      24.14
 C      -2.102831    -1.350463    -0.699234      62.31
 H      -2.431105    -2.178031    -0.270543      19.82
 C      -1.759844     0.293506    -2.413327      28.13
 H      -2.016915     0.779926    -3.385803      22.54
 C      -0.768700     0.915672    -1.718741      22.31
 O      -0.152647     2.124247    -2.067282     213.88
 C      -1.124302     3.173566    -2.558321      82.87
 H      -0.436376     4.261010    -2.766080      21.25
 H      -1.270672     2.997946    -3.818794      23.24
 H      -2.115621     3.079723    -1.968254      24.11
 C      -0.294307     0.310962    -0.488884      12.49
 O       0.834437     0.753062     0.258163     171.02
 C      -1.015456    -0.804537     0.029146      45.74
 H      -0.624978    -1.248082     0.878291      20.12
 C      -2.468787    -0.799879    -1.950454      52.43
 C      -3.541000    -1.470881    -2.749684      59.21
 H      -3.544302    -1.187689    -3.867631      28.18
 O      -3.246690    -2.986553    -2.561359     228.33
 H      -2.396339    -3.168089    -2.589419      31.76
 C      -5.071892    -1.288633    -2.320987      97.74
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 H      -5.191252    -1.712253    -1.352921      28.78
 O      -5.529628     0.032346    -2.395229     247.09
 H      -4.895997     0.715843    -1.901342      25.45
 C      -6.097012    -2.015508    -3.210882     114.68
 O      -6.060707    -3.439974    -2.987623     233.99
 H      -5.068254    -3.704096    -3.053768      29.92
 H      -5.971280    -1.816547    -4.271283      29.78
 H      -7.068809    -1.598115    -3.065781      29.17
55
name = lig-ACN-frame_225
 C       4.107570     2.869756    -0.010564      59.03
 H       3.614413     3.808568    -0.094620      23.58
 C       4.193806     0.612698     0.917216      57.40
 H       3.818085    -0.130790     1.589707      19.62
 C       5.337405     0.345732     0.140043     -12.49
 O       5.973469    -1.012685     0.243237     166.60
 C       5.336884    -1.905166     1.098767     105.41
 H       5.324987    -1.380949     2.104305      25.24
 H       5.887826    -2.929922     0.897145      23.00
 H       4.256344    -2.161646     0.728758      25.55
 C       5.807062     1.377032    -0.845593      10.03
 O       6.874064     1.030771    -1.663238     140.32
 H       7.540066     0.550976    -1.214906      24.38
 C       5.298703     2.646895    -0.902048      60.41
 H       5.665603     3.337217    -1.617588      25.98
 C       3.550834     1.854770     0.785738      28.12
 C       2.278647     2.142627     1.552417     107.48
 H       2.518381     3.209041     1.985493      23.57
 O       2.168651     1.312870     2.766765     256.43
 H       1.741394     0.311707     2.564549      19.69
 C       1.008097     2.160386     0.745366      88.41
 H       1.212489     2.788681    -0.108874      21.52
 C      -0.265163     2.632996     1.499907     105.04
 O      -0.257196     3.927997     2.159868     320.16
 H       0.206773     4.527763     1.715517      34.49
 H      -0.481425     2.013752     2.264110      26.66
 H      -1.133204     2.674765     0.767506      24.13
 C      -2.060452    -1.427388    -0.688226      54.60
 H      -2.698252    -2.162953    -0.356999      18.17
 C      -1.773543     0.317846    -2.485102      42.77
 H      -2.119717     0.672353    -3.497621      21.94
 C      -0.697037     0.911327    -1.712797       2.91
 O      -0.201735     2.155500    -2.072464     215.52
 C      -1.072469     3.121052    -2.651288      77.12
 H      -0.541451     4.244824    -2.334122      20.49
 H      -1.527229     2.802117    -3.766845      21.95
 H      -2.094849     3.238388    -1.929002      23.29
 C      -0.279110     0.338726    -0.509608      16.06
 O       0.837282     0.840523     0.220864     220.75
 C      -1.035621    -0.772018    -0.019578      39.77
 H      -0.705295    -1.192082     0.936271      22.22
 C      -2.484223    -0.817234    -1.933309      43.37
 C      -3.524284    -1.517345    -2.759944      71.06
 H      -3.341257    -1.285811    -3.908975      26.56
 O      -3.355932    -3.000341    -2.604596     249.28
 H      -2.464049    -3.196116    -2.552916      32.74
 C      -5.003804    -1.297281    -2.313478      95.40
 H      -5.006835    -1.618603    -1.311266      28.75
 O      -5.558725     0.056615    -2.401464     265.27
 H      -5.050693     0.623260    -1.918071      31.55
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 C      -6.115289    -2.029691    -3.210020     109.37
 O      -6.029905    -3.432627    -3.040131     226.87
 H      -5.046164    -3.650228    -3.205089      29.28
 H      -5.851089    -1.738943    -4.228113      29.49
 H      -7.068868    -1.730372    -2.840073      28.52
55
name = lig-ACN-frame_226
 C       4.144125     2.896094    -0.100154      52.36
 H       3.683857     3.888273    -0.108446      23.62
 C       4.223578     0.602905     0.913127      53.29
 H       3.820577    -0.038729     1.699869      19.87
 C       5.366057     0.309309     0.111486      16.64
 O       5.934701    -0.978579     0.060858     190.79
 C       5.369427    -1.906251     1.120514      99.98
 H       5.455428    -1.486371     2.218667      25.85
 H       6.207703    -2.716500     1.325076      24.12
 H       4.319543    -2.258197     1.030798      26.85
 C       5.897989     1.269921    -0.780353      14.88
 O       6.945583     1.083216    -1.698209     107.20
 H       7.530329     0.376583    -1.353793      25.93
 C       5.216931     2.587615    -0.851818      45.30
 H       5.711932     3.329578    -1.416288      23.71
 C       3.582164     1.887765     0.746010       7.59
 C       2.282864     2.168725     1.603949      98.02
 H       2.173459     3.315528     2.028643      22.05
 O       2.199938     1.307574     2.660485     309.60
 H       1.864275     0.412443     2.328420      22.83
 C       1.001587     2.205808     0.701698      85.34
 H       1.147141     2.960057    -0.116398      21.76
 C      -0.282945     2.520707     1.437245      93.54
 O      -0.221177     3.947582     2.148303     208.91
 H       0.507219     4.513609     1.571588      27.76
 H      -0.418665     1.816765     2.171209      25.52
 H      -1.084144     2.406321     0.704449      25.14
 C      -2.071218    -1.346482    -0.725256      68.35
 H      -2.418028    -2.298379    -0.229687      21.38
 C      -1.798887     0.292680    -2.457564      61.11
 H      -2.068999     0.790885    -3.415828      20.21
 C      -0.752655     0.948775    -1.765457      11.25
 O      -0.171601     2.168125    -2.087026     223.86
 C      -1.104453     3.094627    -2.655050      83.31
 H      -0.402188     4.168994    -2.781488      22.25
 H      -1.240911     2.947433    -3.870749      23.25
 H      -2.217229     3.203839    -2.092306      23.47
 C      -0.304116     0.392637    -0.503332      23.69
 O       0.814709     0.801542     0.176691     186.96
 C      -0.941943    -0.784397     0.027243      45.11
 H      -0.778643    -1.088476     1.127750      17.49
 C      -2.429803    -0.839011    -1.959487      27.19
 C      -3.548734    -1.615669    -2.780645      62.22
 H      -3.509606    -1.178943    -3.890070      25.42
 O      -3.475830    -3.009082    -2.668318     233.95
 H      -2.439329    -3.320380    -2.564821      24.83
 C      -5.042483    -1.284139    -2.300046      94.10
 H      -5.160680    -1.649562    -1.325495      29.47
 O      -5.525060     0.127788    -2.401041     245.04
 H      -5.024655     0.708609    -1.802333      28.49
 C      -6.008100    -2.029567    -3.159390     118.32
 O      -5.994093    -3.482398    -3.126712     246.83
 H      -5.129896    -3.851192    -3.103601      32.65
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 H      -6.103027    -1.574163    -4.159296      29.53
 H      -7.006809    -1.795523    -2.811379      28.21
55
name = lig-ACN-frame_227
 C       4.085730     2.866556    -0.125641      64.20
 H       3.756757     3.936952    -0.256162      23.52
 C       4.235298     0.701763     0.827366      69.61
 H       3.839454    -0.094400     1.485156      21.37
 C       5.332257     0.282563     0.061575      15.21
 O       5.866616    -0.977630    -0.013117     182.90
 C       5.518184    -1.887410     1.163447      93.04
 H       5.368620    -1.148991     2.103573      25.82
 H       6.179865    -2.811048     1.038946      23.63
 H       4.566645    -2.201910     0.823186      28.25
 C       5.927733     1.276100    -0.770147      30.12
 O       6.975552     1.119068    -1.680295     -23.74
 H       7.681490     0.377283    -1.365995      19.37
 C       5.313036     2.468803    -0.842455      53.98
 H       5.706465     3.191851    -1.544353      24.57
 C       3.568143     1.938715     0.771095      24.92
 C       2.310998     2.210801     1.509247     102.60
 H       2.536659     3.289879     2.039315      21.28
 O       2.186889     1.255056     2.665305     276.51
 H       2.011970     0.419292     2.365382      26.78
 C       1.000153     2.204352     0.612981      69.35
 H       1.093851     2.910666    -0.299335      19.49
 C      -0.286985     2.596381     1.495490     104.22
 O      -0.187505     3.832446     2.054374     237.89
 H       0.406339     4.565066     1.344543      24.54
 H      -0.462332     1.908859     2.299360      23.91
 H      -1.126872     2.677514     0.844121      24.12
 C      -1.975274    -1.294000    -0.657539      95.00
 H      -2.540909    -2.296943    -0.320075      25.18
 C      -1.818291     0.329512    -2.466094      99.37
 H      -2.178408     0.689616    -3.433965      20.09
 C      -0.809434     0.953561    -1.699048       2.85
 O      -0.168559     2.152316    -2.105871     219.46
 C      -1.054449     3.148697    -2.786043      76.99
 H      -0.580237     4.236759    -2.674100      22.33
 H      -1.348429     2.650616    -3.820536      22.13
 H      -2.170394     3.121526    -2.084582      23.48
 C      -0.347568     0.380211    -0.507903      25.54
 O       0.854767     0.800558     0.151796     164.02
 C      -0.965611    -0.738344     0.010098      36.04
 H      -0.441604    -1.201580     0.967609      17.55
 C      -2.433051    -0.918563    -2.016520      83.38
 C      -3.599112    -1.501754    -2.742665      65.37
 H      -3.605731    -1.310745    -3.864969      26.21
 O      -3.517956    -3.088697    -2.719219     126.53
 H      -2.358729    -3.358197    -2.647905      20.40
 C      -5.039273    -1.224785    -2.241550      97.56
 H      -5.099289    -1.505834    -1.225253      29.61
 O      -5.439452     0.137666    -2.394273     235.53
 H      -4.774538     0.735156    -1.727643      24.52
 C      -6.072309    -2.064361    -3.156175     109.47
 O      -5.976483    -3.525731    -3.222346     218.38
 H      -4.996785    -3.635701    -3.101459      29.55
 H      -5.838239    -1.730424    -4.182194      29.44
 H      -7.034519    -1.773832    -2.727525      28.62
55
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name = lig-ACN-frame_228
 C       4.178156     2.852065    -0.198137      60.19
 H       3.582078     3.794807    -0.417178      23.47
 C       4.180448     0.672791     0.785858      44.25
 H       3.642246    -0.098313     1.368264      19.12
 C       5.315716     0.325390    -0.018497      15.41
 O       5.841705    -1.018655     0.015290     226.67
 C       5.556840    -1.838453     1.047924     125.59
 H       5.809397    -1.367729     2.172624      26.85
 H       6.357605    -2.582710     1.115896      25.90
 H       4.660165    -2.361458     1.207789      29.23
 C       5.937210     1.277985    -0.821725      18.27
 O       7.012747     1.111615    -1.646509      64.96
 H       7.775727     0.561000    -1.122954      20.52
 C       5.307063     2.581192    -0.877772      42.72
 H       5.753534     3.224709    -1.663023      24.85
 C       3.601383     1.940007     0.701745      19.45
 C       2.271503     2.143450     1.493152     108.49
 H       2.212233     3.242865     1.928768      22.71
 O       2.158467     1.294139     2.657868     284.31
 H       1.903891     0.345458     2.397446      22.75
 C       0.972717     2.157676     0.641739      84.93
 H       1.130037     2.882922    -0.284944      19.92
 C      -0.262023     2.570407     1.405107     100.37
 O      -0.109001     3.897824     2.035583     267.14
 H       0.114222     4.637023     1.292374      27.94
 H      -0.377970     1.858540     2.277396      23.36
 H      -1.076109     2.415941     0.776006      25.66
 C      -2.054635    -1.406122    -0.734703      56.58
 H      -2.572095    -2.292313    -0.130093      14.85
 C      -1.856774     0.310387    -2.468992      16.19
 H      -2.094750     0.742110    -3.416762      18.30
 C      -0.851816     1.018518    -1.701464      10.36
 O      -0.209062     2.156941    -2.144662     214.77
 C      -1.020332     3.073267    -2.848061     104.80
 H      -0.386988     4.025407    -2.848310      23.53
 H      -1.242905     2.961045    -3.998495      24.95
 H      -2.150063     3.374579    -2.244880      23.31
 C      -0.271797     0.440424    -0.489044      14.41
 O       0.881956     0.824916     0.107961     209.82
 C      -0.948277    -0.719820     0.017844      49.62
 H      -0.540572    -1.317888     0.957907      19.89
 C      -2.405602    -0.844870    -1.925297      37.25
 C      -3.600898    -1.563475    -2.723185      60.41
 H      -3.565075    -1.034843    -3.690404      28.10
 O      -3.491396    -3.057665    -2.743209     187.90
 H      -2.364182    -3.311115    -2.674637      24.97
 C      -5.049907    -1.278406    -2.171947      88.13
 H      -5.109849    -1.545906    -1.137052      28.01
 O      -5.339289     0.145175    -2.386311     219.36
 H      -4.791010     0.902453    -1.796738      22.53
 C      -6.121124    -2.072775    -3.155230     104.30
 O      -5.962696    -3.496256    -3.278979     219.58
 H      -4.969136    -3.791393    -3.205627      27.62
 H      -6.019745    -1.475207    -4.095784      29.35
 H      -7.224049    -1.935458    -3.012989      27.15
55
name = lig-ACN-frame_229
 C       4.147378     2.924464    -0.225386      55.49
 H       3.641872     3.927849    -0.374174      22.76
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 C       4.150701     0.575730     0.711921      64.13
 H       3.749075    -0.175669     1.398548      21.03
 C       5.270690     0.296328    -0.014098      15.59
 O       5.840712    -0.924906    -0.061446     183.29
 C       5.624498    -1.929492     1.149720      89.20
 H       5.872613    -1.252602     2.138049      25.12
 H       6.235430    -2.701346     0.801705      25.02
 H       4.591246    -2.110430     1.091407      27.20
 C       5.900246     1.356477    -0.871985      21.50
 O       7.075783     1.088005    -1.623399      78.37
 H       7.722535     0.421548    -1.188903      21.01
 C       5.362481     2.646948    -1.012052      52.34
 H       5.801862     3.523089    -1.570071      24.53
 C       3.562994     1.887408     0.621481       9.64
 C       2.240355     2.152964     1.510629     110.20
 H       2.320828     3.195733     1.912438      24.53
 O       2.125885     1.345464     2.658066     287.59
 H       1.780095     0.336660     2.392774      19.66
 C       1.046257     2.149421     0.616180      83.74
 H       1.255743     3.025147    -0.172395      20.92
 C      -0.240248     2.551356     1.373430      94.48
 O      -0.072122     3.980951     1.997509     295.31
 H       0.194061     4.532448     1.373669      34.67
 H      -0.426695     1.870605     2.318638      22.27
 H      -1.026137     2.624722     0.745531      26.32
 C      -2.004340    -1.371397    -0.653664      89.96
 H      -2.468621    -2.330494    -0.344889      23.13
 C      -1.838398     0.346235    -2.389341      68.19
 H      -2.154138     0.679225    -3.345598      21.68
 C      -0.835844     0.990053    -1.702116      13.54
 O      -0.257585     2.147790    -2.182216     230.31
 C      -0.955147     3.140266    -2.956177      92.60
 H      -0.362959     4.000107    -3.002865      24.29
 H      -1.189460     2.544571    -3.917182      22.81
 H      -2.178391     3.393840    -2.403340      22.69
 C      -0.368239     0.368479    -0.541142      29.87
 O       0.898179     0.807945     0.054907     167.13
 C      -0.966544    -0.791570    -0.039145      25.91
 H      -0.667954    -1.005330     1.021652      18.34
 C      -2.558742    -0.851214    -1.905064      61.95
 C      -3.573461    -1.597989    -2.689845      72.59
 H      -3.619215    -1.328621    -3.722329      32.87
 O      -3.378863    -2.975677    -2.754201     233.55
 H      -2.401881    -3.238178    -2.609058      27.92
 C      -5.086550    -1.325344    -2.186137      92.86
 H      -5.305614    -1.651340    -1.159066      30.79
 O      -5.292508     0.108181    -2.387522     256.14
 H      -4.772931     0.512650    -1.717652      29.76
 C      -6.105710    -2.003481    -3.133895     111.06
 O      -5.976863    -3.450257    -3.331827     204.89
 H      -4.982704    -3.562888    -3.349805      30.39
 H      -6.009083    -1.540196    -4.134204      29.85
 H      -7.059136    -1.830980    -2.546582      27.61
55
name = lig-ACN-frame_230
 C       4.113189     2.884939    -0.233677      64.72
 H       3.794149     3.912417    -0.042519      24.40
 C       4.068479     0.625771     0.653143      55.48
 H       3.690081    -0.109499     1.346621      21.86
 C       5.303984     0.387876    -0.114768       5.06
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 O       5.920710    -0.941428    -0.070584     194.57
 C       5.633770    -1.870195     1.071297     109.03
 H       6.026983    -1.561811     2.177839      25.79
 H       6.123802    -2.802418     0.961152      26.70
 H       4.604503    -2.138357     1.213347      27.79
 C       5.905497     1.375993    -0.926047      15.67
 O       7.067044     1.074294    -1.596015     102.89
 H       7.494170     0.357281    -1.150540      26.12
 C       5.272429     2.646818    -0.993524      48.80
 H       5.909696     3.356806    -1.585198      22.96
 C       3.505836     1.876256     0.564257      30.35
 C       2.366867     2.210471     1.456763      99.92
 H       2.507341     3.166081     1.810259      25.98
 O       2.096192     1.347929     2.691279     270.54
 H       1.857260     0.424803     2.342237      22.69
 C       1.017003     2.193053     0.572307      66.23
 H       1.157718     2.770732    -0.459556      19.97
 C      -0.209012     2.736236     1.394824     108.28
 O      -0.071567     3.950983     1.936665     360.24
 H       0.500148     4.479821     1.453203      31.87
 H      -0.540811     1.945809     2.242061      22.79
 H      -0.988334     2.644216     0.739668      27.14
 C      -2.106839    -1.373491    -0.659690      45.78
 H      -2.478004    -2.212361    -0.277872      19.74
 C      -1.984693     0.320392    -2.376687      60.81
 H      -2.315762     0.745616    -3.305438      20.21
 C      -0.861764     0.958735    -1.756303      21.98
 O      -0.219599     2.164891    -2.146335     190.16
 C      -0.949648     3.098348    -3.089612     104.72
 H      -0.318457     3.882071    -3.222814      26.72
 H      -1.245693     2.761701    -4.098854      28.25
 H      -2.036526     3.545995    -2.432209      23.95
 C      -0.294919     0.376173    -0.539211      42.15
 O       0.850913     0.761482    -0.003027     195.03
 C      -0.929194    -0.781649     0.013372      50.21
 H      -0.525678    -1.274508     0.861553      19.40
 C      -2.543953    -0.814358    -1.834706       8.50
 C      -3.625062    -1.530122    -2.709885      57.69
 H      -3.551497    -1.018283    -3.615626      30.02
 O      -3.241838    -3.020712    -2.725873     242.25
 H      -2.320934    -3.091667    -2.585464      27.52
 C      -5.021906    -1.347240    -2.271970     105.07
 H      -5.098863    -1.682005    -1.203556      27.48
 O      -5.298646     0.035430    -2.361470     250.87
 H      -4.851285     0.611964    -1.797327      29.57
 C      -6.127395    -1.962363    -3.109609     117.74
 O      -5.981427    -3.371703    -3.361357     240.53
 H      -5.078850    -3.610771    -3.403166      34.59
 H      -6.228466    -1.314168    -4.019446      29.03
 H      -7.186842    -1.787474    -2.691643      26.77
55
name = lig-ACN-frame_231
 C       4.105528     2.893374    -0.204485      57.33
 H       3.741266     3.890228    -0.221645      24.24
 C       4.146777     0.610871     0.532218      72.50
 H       3.655942    -0.145444     1.116819      21.84
 C       5.269779     0.298077    -0.109048      21.44
 O       5.989512    -0.900249    -0.029258     219.26
 C       5.616523    -1.809237     0.981732     118.89
 H       6.038763    -1.295830     1.944821      25.57
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 H       6.216047    -2.637039     0.624360      25.04
 H       4.526312    -1.922351     1.081769      26.10
 C       5.860592     1.308759    -0.934690      21.45
 O       7.041702     1.101167    -1.604284     111.17
 H       7.589716     0.384910    -1.204775      24.47
 C       5.242201     2.596499    -0.959166      49.52
 H       5.530961     3.483867    -1.538964      25.11
 C       3.509933     1.894740     0.554899      22.60
 C       2.270525     2.199282     1.421784     113.30
 H       2.367529     3.123858     1.763740      25.57
 O       2.126801     1.401365     2.618798     330.54
 H       1.927592     0.552208     2.403407      28.30
 C       1.007176     2.219276     0.540147      77.46
 H       1.150897     3.018325    -0.329196      20.80
 C      -0.242595     2.685676     1.265167      91.66
 O      -0.046086     4.049192     1.964088     248.32
 H       0.479609     4.802214     1.331466      26.04
 H      -0.309386     2.006617     2.241695      21.30
 H      -1.057820     2.773606     0.671400      25.64
 C      -2.117941    -1.341291    -0.560895      57.42
 H      -2.567556    -2.144781    -0.133827      22.20
 C      -2.016961     0.426346    -2.380553     102.97
 H      -2.485025     0.845481    -3.289522      21.52
 C      -0.883611     0.982348    -1.759882       2.70
 O      -0.250286     2.158926    -2.176499     214.71
 C      -0.900809     3.012555    -3.104279     103.19
 H      -0.211943     3.773261    -3.217016      24.94
 H      -1.220786     2.381969    -3.886489      25.90
 H      -2.040058     3.593708    -2.587374      22.99
 C      -0.348605     0.330992    -0.591729      21.73
 O       0.898800     0.813336     0.059311     154.76
 C      -0.960574    -0.792213    -0.004987      28.58
 H      -0.467599    -1.271722     0.725542      20.55
 C      -2.598417    -0.802076    -1.823486      61.79
 C      -3.488049    -1.573671    -2.766752      67.80
 H      -3.419911    -1.307665    -3.759032      35.20
 O      -3.214953    -2.975022    -2.725214     242.82
 H      -2.352383    -3.169208    -2.657528      31.72
 C      -5.008214    -1.350953    -2.221728      79.30
 H      -5.043490    -1.802755    -1.171702      29.90
 O      -5.379322     0.070237    -2.344563     191.54
 H      -4.701067     0.609580    -1.686697      25.21
 C      -6.183028    -1.942776    -3.143378     112.27
 O      -6.004359    -3.329634    -3.399111     203.79
 H      -5.010498    -3.474951    -3.337833      31.46
 H      -6.149608    -1.356461    -4.082758      30.19
 H      -7.140026    -1.867665    -2.520663      27.78
55
name = lig-ACN-frame_232
 C       4.099427     2.928121    -0.187113      60.82
 H       3.576506     3.822512    -0.371708      24.20
 C       4.045451     0.556824     0.570562      54.03
 H       3.574918    -0.248360     1.128922      21.67
 C       5.310028     0.293339    -0.171596      12.95
 O       6.065612    -0.830611    -0.072278     211.10
 C       5.633286    -1.787209     0.946947     110.54
 H       5.797010    -1.541599     2.044082      27.27
 H       6.078442    -2.807314     0.867536      26.41
 H       4.531496    -2.036732     0.803423      26.62
 C       5.840545     1.307229    -0.936178      20.53
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 O       7.042310     1.144032    -1.658025     121.61
 H       7.657502     0.448851    -1.145929      23.52
 C       5.258497     2.564442    -0.978055      44.56
 H       5.888777     3.156396    -1.634102      24.21
 C       3.506888     1.871057     0.595413       1.65
 C       2.196252     2.216439     1.386370     109.05
 H       2.268376     3.192230     1.663251      25.98
 O       2.160158     1.439438     2.549004     307.57
 H       1.908358     0.480474     2.327565      24.00
 C       0.983363     2.236900     0.471099      80.59
 H       1.320872     2.880585    -0.436941      21.87
 C      -0.259245     2.744008     1.265968      96.85
 O      -0.058905     4.063988     1.979348     240.12
 H       0.237780     4.814058     1.126322      24.14
 H      -0.627732     1.969069     2.045851      23.47
 H      -1.060610     2.758620     0.586145      25.78
 C      -2.166492    -1.264404    -0.594556      62.66
 H      -2.637438    -2.217738    -0.179805      24.30
 C      -2.017855     0.454331    -2.294515      50.05
 H      -2.397891     0.881381    -3.250118      19.91
 C      -0.909066     1.025324    -1.696455      23.50
 O      -0.254415     2.115378    -2.139286     228.72
 C      -0.891786     2.916375    -3.129458     107.22
 H      -0.210135     3.683568    -3.520017      25.98
 H      -1.157225     2.490736    -4.025307      28.87
 H      -2.006491     3.464093    -2.559387      23.62
 C      -0.297026     0.385459    -0.582528      22.33
 O       0.846978     0.846489     0.060816     191.68
 C      -0.951855    -0.771821    -0.026124      54.65
 H      -0.682246    -0.988249     0.945583      19.26
 C      -2.558329    -0.741163    -1.842163      34.09
 C      -3.500526    -1.559138    -2.762047      83.90
 H      -3.395699    -1.124577    -3.698202      28.11
 O      -3.280252    -2.996202    -2.721526     279.99
 H      -2.379729    -3.036983    -2.608379      31.32
 C      -5.046355    -1.301751    -2.307139      88.32
 H      -5.145192    -1.620559    -1.194253      27.26
 O      -5.430159     0.092671    -2.271544     197.84
 H      -4.786722     0.803360    -1.726228      24.51
 C      -6.139154    -1.917863    -3.094095     119.79
 O      -6.008367    -3.358731    -3.431568     193.24
 H      -5.010149    -3.604153    -3.338270      30.43
 H      -6.244442    -1.302713    -4.012100      28.74
 H      -7.146291    -1.698654    -2.610549      27.18
55
name = lig-ACN-frame_233
 C       4.132079     2.831802    -0.244046      63.16
 H       3.770447     3.842088    -0.162024      25.21
 C       4.029383     0.559000     0.591447      60.91
 H       3.617390    -0.213417     1.248942      21.81
 C       5.204937     0.357264    -0.119882      -9.68
 O       6.150653    -0.889474    -0.062849     179.55
 C       5.605937    -1.851330     0.902735     112.83
 H       5.605215    -1.324313     1.850548      27.87
 H       6.458304    -2.622840     0.818187      24.37
 H       4.505557    -2.141696     0.665111      25.34
 C       5.894155     1.348199    -0.965377      10.85
 O       7.048221     1.166696    -1.691880     110.80
 H       7.657884     0.477882    -1.244378      23.89
 C       5.264178     2.628839    -1.013217      48.88
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 H       5.611148     3.491339    -1.560039      25.15
 C       3.501292     1.878331     0.545205      36.43
 C       2.304702     2.280160     1.311311     101.26
 H       2.407408     3.268230     1.718282      24.89
 O       2.129332     1.425939     2.554601     234.78
 H       1.823011     0.438390     2.192131      19.14
 C       0.952610     2.248771     0.462489      76.88
 H       0.945281     2.868345    -0.471372      21.57
 C      -0.314489     2.853070     1.235270      99.35
 O      -0.143955     3.957953     1.974080     236.11
 H       0.494241     4.856410     1.479513      23.45
 H      -0.527459     2.109495     2.047231      23.12
 H      -1.106897     3.030969     0.534203      24.71
 C      -2.108442    -1.229485    -0.644562      83.30
 H      -2.675082    -2.195879    -0.147776      20.26
 C      -2.017754     0.467441    -2.286171      97.81
 H      -2.251683     0.914985    -3.253548      11.48
 C      -0.887377     1.022819    -1.600874      38.43
 O      -0.200453     2.128756    -2.126571     202.37
 C      -0.916495     2.883430    -3.183677      92.34
 H      -0.175354     3.788487    -3.084319      22.92
 H      -1.188441     2.222164    -3.903437      31.76
 H      -2.089798     3.402039    -2.692885      26.64
 C      -0.347348     0.388978    -0.506597      27.73
 O       0.797911     0.850428     0.050405     223.02
 C      -1.001505    -0.662612     0.024666      54.69
 H      -0.676006    -1.169410     0.948187      21.03
 C      -2.582440    -0.761469    -1.867428      55.44
 C      -3.648847    -1.406357    -2.730957      61.40
 H      -3.516511    -1.168886    -3.749412      28.55
 O      -3.367940    -2.983471    -2.705045     173.88
 H      -2.349245    -3.249599    -2.625443      26.45
 C      -5.015358    -1.212247    -2.252161     100.48
 H      -4.986860    -1.805676    -1.245435      28.57
 O      -5.485316     0.145133    -2.236395     240.17
 H      -4.858315     0.623149    -1.700175      30.62
 C      -6.135675    -1.952438    -3.157012     112.34
 O      -6.010328    -3.362165    -3.406120     214.76
 H      -5.087841    -3.594922    -3.325409      33.21
 H      -6.204157    -1.371818    -4.096580      30.39
 H      -7.064088    -1.937799    -2.536285      27.66
55
name = lig-ACN-frame_234
 C       4.133033     2.849677    -0.288057      54.62
 H       3.741778     3.894023    -0.175384      25.39
 C       4.133416     0.577184     0.575556      51.81
 H       3.689447    -0.139359     1.274525      22.76
 C       5.371885     0.295419    -0.139400       9.66
 O       6.037461    -0.829040    -0.047522     184.15
 C       5.649124    -1.874670     0.855127     114.25
 H       5.397303    -1.547939     1.824813      29.10
 H       6.420172    -2.704778     1.035861      25.71
 H       4.734991    -2.500688     0.429287      26.88
 C       5.879486     1.400952    -0.964527      17.28
 O       7.068635     1.152028    -1.691407     108.10
 H       7.492060     0.407948    -1.324731      28.16
 C       5.297606     2.668753    -1.058379      87.84
 H       5.733664     3.480304    -1.638783      25.70
 C       3.503076     1.833831     0.477236      12.25
 C       2.249182     2.258599     1.348093      90.27
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 H       2.567410     3.344777     1.675075      23.94
 O       2.085658     1.449053     2.500289     287.69
 H       1.772429     0.565169     2.217603      24.50
 C       0.949227     2.331415     0.480203      87.69
 H       1.260702     2.929287    -0.368202      24.18
 C      -0.370845     2.737273     1.161185      93.61
 O      -0.179003     4.009290     2.073819     198.62
 H       0.453089     4.686840     1.400520      25.07
 H      -0.798426     1.962152     1.750727      26.35
 H      -1.117671     2.892799     0.358932      25.55
 C      -2.110217    -1.293877    -0.647428      67.45
 H      -2.544989    -2.382726    -0.131022      18.27
 C      -1.952519     0.488430    -2.336830      28.16
 H      -2.377065     0.886024    -3.216120      22.54
 C      -0.907785     1.053893    -1.673729      12.15
 O      -0.200909     2.143548    -2.120529     242.37
 C      -0.891793     2.896999    -3.110237      96.83
 H      -0.431644     3.799374    -3.682757      24.65
 H      -0.865654     2.417465    -4.077804      27.07
 H      -2.157877     3.116566    -2.732003      24.56
 C      -0.423635     0.469406    -0.422051       6.28
 O       0.842867     0.873353     0.122755     157.48
 C      -1.117287    -0.711116     0.137829      48.53
 H      -0.512475    -1.246312     0.982469      19.77
 C      -2.591970    -0.699063    -1.881350      43.30
 C      -3.601584    -1.437487    -2.757501      69.99
 H      -3.653208    -0.979002    -3.763186      31.09
 O      -3.510855    -2.848054    -2.678905     185.09
 H      -2.365122    -3.005283    -2.780988      25.95
 C      -5.153213    -1.253075    -2.190484      78.09
 H      -5.262549    -1.516870    -1.062394      28.52
 O      -5.526001     0.183106    -2.197508     229.96
 H      -5.053794     0.746202    -1.674176      31.33
 C      -6.144870    -1.951156    -3.138713     121.54
 O      -5.978835    -3.388240    -3.356957     205.65
 H      -5.022162    -3.504533    -3.328861      31.68
 H      -6.136581    -1.386763    -4.100389      30.02
 H      -7.146873    -1.712457    -2.741979      29.08
55
name = lig-ACN-frame_235
 C       4.099055     2.932248    -0.313325      51.60
 H       3.481827     3.887097    -0.502805      24.69
 C       4.235079     0.617212     0.554239      72.17
 H       3.885750    -0.247084     1.111070      22.73
 C       5.370540     0.441689    -0.130937      26.98
 O       6.037780    -0.857657    -0.064068     213.74
 C       5.638255    -1.943059     0.847980     109.29
 H       5.232389    -1.656170     1.716626      28.90
 H       6.687555    -2.377476     0.901261      24.59
 H       4.831720    -2.568216     0.250739      26.21
 C       5.948415     1.351242    -0.985863      24.36
 O       7.091348     1.133567    -1.680079     144.69
 H       7.568132     0.338186    -1.298017      25.07
 C       5.308957     2.622599    -1.049842      25.76
 H       5.901687     3.270710    -1.717379      23.02
 C       3.524063     1.850023     0.445867      -0.94
 C       2.246378     2.232551     1.342058      90.84
 H       2.355747     3.366296     1.803622      23.40
 O       2.039794     1.452683     2.501810     302.65
 H       1.772447     0.620401     2.230019      28.33
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 C       1.000611     2.328634     0.517718      94.09
 H       1.093575     2.907190    -0.346737      25.46
 C      -0.359104     2.788928     1.190780     101.94
 O      -0.221995     3.943442     2.058344     264.99
 H       0.061062     4.704846     1.515680      30.83
 H      -0.654832     2.050739     1.827184      27.13
 H      -1.091912     3.071912     0.357464      25.63
 C      -2.158249    -1.328600    -0.639702      53.37
 H      -2.680035    -2.490262    -0.559228      20.28
 C      -1.971627     0.450652    -2.383181      60.82
 H      -2.233769     0.909237    -3.311594      15.07
 C      -0.858431     1.055443    -1.627230       3.15
 O      -0.181200     2.204013    -2.104444     194.76
 C      -0.895684     2.926707    -3.157745      71.87
 H      -0.383737     3.881126    -2.797639      23.17
 H      -0.988313     2.174649    -4.076533      24.82
 H      -2.158681     3.121663    -2.745910      25.37
 C      -0.453646     0.483763    -0.358954      33.21
 O       0.769403     0.896207     0.151390     187.10
 C      -1.076038    -0.670686     0.091772      51.39
 H      -0.864913    -1.142458     1.162552      20.71
 C      -2.560429    -0.729833    -1.819906      34.87
 C      -3.730689    -1.343530    -2.645276      84.70
 H      -3.583315    -1.018665    -3.725343      28.61
 O      -3.537162    -2.779518    -2.680434     197.96
 H      -2.518846    -3.138215    -2.840171      26.49
 C      -5.194498    -1.169516    -2.148528      93.89
 H      -5.205752    -1.754401    -1.141313      28.99
 O      -5.614556     0.184521    -2.208843     232.83
 H      -4.914714     0.676906    -1.571346      26.38
 C      -6.195577    -1.911785    -3.120928     107.50
 O      -5.967776    -3.381804    -3.280173     170.06
 H      -4.935863    -3.532108    -3.285609      28.33
 H      -5.936809    -1.416526    -4.075493      29.02
 H      -7.253680    -1.877620    -2.932888      28.75
55
name = lig-ACN-frame_236
 C       4.117259     2.857607    -0.398195      62.66
 H       3.668094     3.907007    -0.567578      23.71
 C       4.160534     0.719289     0.599336      51.63
 H       3.627020    -0.001977     1.222846      22.58
 C       5.409254     0.347366    -0.098154       6.17
 O       6.080120    -0.839234    -0.105260     202.02
 C       5.659441    -1.953433     0.781834     120.97
 H       5.252736    -1.615404     1.613425      30.05
 H       6.488876    -2.627538     1.073874      26.24
 H       4.933099    -2.704230     0.307921      27.16
 C       5.989716     1.385123    -0.971704      15.07
 O       7.176286     1.103642    -1.699690      93.24
 H       7.713740     0.371216    -1.152937      22.49
 C       5.307272     2.616048    -1.058304      71.36
 H       5.526349     3.488073    -1.701321      26.62
 C       3.527879     1.986927     0.513356      34.18
 C       2.297959     2.249208     1.304917      82.28
 H       2.543083     3.396694     1.711328      22.76
 O       2.018768     1.411151     2.558855     238.67
 H       1.830981     0.413696     2.234746      22.27
 C       0.927054     2.281006     0.489108      93.61
 H       1.143277     2.806331    -0.366354      24.97
 C      -0.280466     2.827277     1.240906     111.29
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 O      -0.249296     3.952033     2.055158     310.30
 H       0.036963     4.608939     1.595698      35.34
 H      -0.614891     2.075603     1.840430      27.71
 H      -1.137727     2.832776     0.440896      25.74
 C      -2.123553    -1.273186    -0.632764      77.81
 H      -2.510425    -2.209038     0.062104      18.69
 C      -1.889341     0.427293    -2.277328      16.27
 H      -2.184953     0.711043    -3.293252      21.78
 C      -0.886729     1.029386    -1.635607      23.97
 O      -0.215605     2.169154    -2.056179     232.83
 C      -0.898092     3.006048    -3.075987      93.53
 H      -0.485066     3.981778    -3.433619      24.26
 H      -0.606068     2.691744    -4.225813      24.04
 H      -2.190794     3.052957    -2.888749      23.81
 C      -0.457293     0.466449    -0.450829      22.28
 O       0.677531     0.900770     0.195846     183.44
 C      -1.113866    -0.714539     0.057174      50.15
 H      -0.704667    -1.026211     1.100635      18.86
 C      -2.629194    -0.699364    -1.851622      79.28
 C      -3.763568    -1.251671    -2.586635      49.22
 H      -3.874152    -0.717308    -3.637278      29.18
 O      -3.519555    -2.821903    -2.678363     190.05
 H      -2.625121    -2.813415    -2.793026      32.39
 C      -5.240408    -1.161770    -2.138647      91.54
 H      -5.386722    -1.448157    -1.030316      29.00
 O      -5.699981     0.204930    -2.173438     192.74
 H      -5.072935     1.030596    -1.756293      24.42
 C      -6.172624    -1.942372    -3.170408     124.29
 O      -5.998794    -3.334865    -3.190139     200.38
 H      -4.970717    -3.431992    -3.141907      28.37
 H      -6.150729    -1.456337    -4.160408      30.95
 H      -7.109203    -1.673272    -2.714746      29.63
55
name = lig-ACN-frame_237
 C       4.092309     2.885056    -0.428849      43.28
 H       3.689115     3.938477    -0.465510      22.24
 C       4.174932     0.699107     0.641262      71.31
 H       3.778296    -0.031447     1.365362      23.11
 C       5.359391     0.392434    -0.094410       1.46
 O       6.130505    -0.868081    -0.111760     207.47
 C       5.659144    -1.921688     0.738053     125.20
 H       5.268570    -1.604418     1.630662      29.22
 H       6.520692    -2.522647     0.868840      27.37
 H       4.808850    -2.335334     0.145545      27.47
 C       6.021380     1.350766    -0.913595      -1.06
 O       7.219180     1.089630    -1.669600     106.87
 H       7.843792     0.520587    -1.149607      24.30
 C       5.351583     2.602740    -1.145736      25.00
 H       5.925994     3.241922    -1.866659      22.38
 C       3.586474     1.964355     0.542372      18.21
 C       2.198632     2.252189     1.389288      86.54
 H       2.159985     3.374228     1.860024      22.57
 O       2.068568     1.421461     2.529038     247.46
 H       1.910971     0.392934     2.211998      22.04
 C       0.986663     2.296777     0.469733      85.78
 H       1.085531     2.821929    -0.412448      24.10
 C      -0.328104     2.692349     1.268035      85.94
 O      -0.212526     4.079145     2.080932     212.27
 H       0.330277     4.685771     1.501282      28.63
 H      -0.479629     1.979269     1.998296      26.24
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 H      -1.182547     2.912519     0.502761      24.25
 C      -2.201904    -1.262595    -0.563473      55.98
 H      -2.932492    -2.069085    -0.180881      21.14
 C      -1.967065     0.388353    -2.380656      71.51
 H      -2.231522     0.875654    -3.335147      21.56
 C      -0.887535     1.060504    -1.663316      12.79
 O      -0.263992     2.217480    -2.066492     218.71
 C      -0.850727     3.060127    -3.081596      73.57
 H      -0.415677     3.934410    -2.667488      24.45
 H      -0.764935     2.294472    -4.043322      22.58
 H      -2.151987     3.130151    -2.854947      26.57
 C      -0.397743     0.428015    -0.477671      24.00
 O       0.643962     0.851241     0.264663     206.71
 C      -1.031635    -0.675514     0.071789      56.91
 H      -0.588428    -1.244960     0.883157      24.15
 C      -2.645323    -0.686047    -1.737774      47.63
 C      -3.791670    -1.330278    -2.615754      74.87
 H      -3.657820    -0.889321    -3.732717      29.35
 O      -3.483293    -2.739346    -2.693723     242.09
 H      -2.583157    -2.970226    -2.780206      32.83
 C      -5.274540    -1.119381    -2.117301      95.56
 H      -5.427165    -1.653022    -1.144494      30.10
 O      -5.810965     0.272828    -2.174822     222.61
 H      -5.074331     0.775268    -1.723497      29.21
 C      -6.197199    -1.861066    -3.083706     113.63
 O      -6.036802    -3.332098    -3.105316     189.78
 H      -5.130720    -3.554084    -3.106228      32.89
 H      -6.001953    -1.434011    -4.086393      29.73
 H      -7.270830    -1.766406    -2.919678      28.22
55
name = lig-ACN-frame_238
 C       4.177343     2.901114    -0.407228      56.90
 H       3.630900     3.819870    -0.621974      27.34
 C       4.282799     0.632832     0.673870      47.20
 H       3.956266    -0.180297     1.354954      20.95
 C       5.417162     0.372780    -0.104485      19.64
 O       6.123869    -0.775260    -0.085406     218.99
 C       5.606262    -1.903555     0.691745     131.34
 H       5.528332    -1.632246     1.693954      29.47
 H       6.331796    -2.652517     0.621159      28.04
 H       4.719934    -2.421768     0.382059      28.98
 C       6.027245     1.348022    -0.939101      23.58
 O       7.195557     1.097666    -1.572506     185.91
 H       7.733165     0.509028    -1.084756      26.92
 C       5.357735     2.533121    -1.159948      58.91
 H       5.783149     3.294031    -1.857398      18.90
 C       3.564402     1.964081     0.519267     -19.23
 C       2.236398     2.287534     1.390766      84.73
 H       2.353913     3.363879     1.809564      23.85
 O       2.117868     1.398908     2.503201     288.71
 H       1.885237     0.536370     2.191361      26.54
 C       0.900765     2.238416     0.559308      90.12
 H       1.130023     2.790093    -0.326202      25.41
 C      -0.308440     2.810155     1.381705     102.52
 O      -0.141930     4.062568     2.002125     221.25
 H       0.323849     4.840840     1.280473      23.96
 H      -0.517645     2.119442     2.197799      25.45
 H      -1.293840     2.677968     0.726610      25.24
 C      -2.281551    -1.195492    -0.472161      57.45
 H      -2.588647    -2.139186    -0.064277      25.43
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 C      -2.001473     0.431523    -2.387844      22.21
 H      -2.449135     0.733819    -3.322809      19.58
 C      -0.926131     1.004022    -1.710888       8.42
 O      -0.288478     2.228426    -2.031141     214.51
 C      -0.858461     3.066519    -3.047234     115.98
 H      -0.338265     3.968592    -3.168257      26.36
 H      -0.606837     3.038795    -4.210675      25.09
 H      -2.089661     3.345929    -2.839409      24.45
 C      -0.399882     0.401459    -0.504118       7.60
 O       0.750470     0.823915     0.297151     172.74
 C      -1.054278    -0.793223     0.052769      37.25
 H      -0.632711    -1.114388     0.929779      19.57
 C      -2.704885    -0.626670    -1.786957      42.84
 C      -3.728457    -1.309317    -2.604812      71.21
 H      -3.696164    -0.818284    -3.726439      28.02
 O      -3.490324    -2.744278    -2.708183     179.22
 H      -2.363790    -2.740989    -2.733290      24.69
 C      -5.318113    -1.088589    -2.118255      85.82
 H      -5.240705    -1.312564    -1.051531      28.86
 O      -5.811636     0.273017    -2.156569     261.48
 H      -5.368921     0.872131    -1.681476      32.10
 C      -6.271823    -1.871668    -3.069429     118.11
 O      -6.107840    -3.324524    -3.017038     208.73
 H      -5.142885    -3.379183    -3.109521      31.94
 H      -5.923507    -1.472796    -4.049259      29.63
 H      -7.302349    -1.530570    -2.880565      28.99
55
name = lig-ACN-frame_239
 C       4.178318     2.809810    -0.346190      69.37
 H       3.763757     3.746447    -0.579133      27.39
 C       4.278956     0.732583     0.669604      77.81
 H       3.781033     0.017504     1.344677      20.78
 C       5.436683     0.414042    -0.071867      16.12
 O       6.135031    -0.812172    -0.045812     212.51
 C       5.603632    -1.920690     0.686218     126.84
 H       5.677509    -1.795793     1.783057      27.72
 H       6.181797    -2.719832     0.394018      27.28
 H       4.601221    -1.910026     0.434046      28.72
 C       5.978597     1.361198    -0.967622      12.76
 O       7.237230     1.107153    -1.525734     141.37
 H       7.657726     0.314168    -1.045938      24.49
 C       5.316861     2.578766    -1.130815      53.99
 H       5.651275     3.332396    -1.856406      22.23
 C       3.608347     1.879445     0.488617      34.51
 C       2.353381     2.255749     1.305928      86.48
 H       2.526220     3.273902     1.681990      26.43
 O       2.169618     1.374451     2.520040     251.18
 H       1.887623     0.554737     2.173066      27.24
 C       0.900602     2.232632     0.668590      81.55
 H       0.791655     2.820365    -0.261616      23.49
 C      -0.299240     2.783562     1.478824      97.78
 O      -0.052379     4.112635     1.931142     205.16
 H       0.268347     4.833064     1.011577      23.12
 H      -0.451322     2.180468     2.426551      24.56
 H      -1.234419     2.841087     0.773601      24.76
 C      -2.307181    -1.168499    -0.534103      56.69
 H      -2.826770    -1.930623    -0.159179      27.30
 C      -2.028233     0.473222    -2.303515     106.83
 H      -2.180357     0.900537    -3.274671      16.80
 C      -0.870728     1.010743    -1.662981      10.87
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 O      -0.303290     2.196804    -2.034597     204.70
 C      -0.849357     3.190006    -3.092937      79.86
 H      -0.323725     4.000818    -2.783455      27.81
 H      -0.871801     2.363382    -3.837711      25.73
 H      -2.073666     3.323130    -2.829542      25.28
 C      -0.392125     0.349515    -0.471279      25.43
 O       0.762891     0.780749     0.212941     176.74
 C      -1.073984    -0.756518     0.031333      51.28
 H      -0.790690    -1.211965     0.887442      19.36
 C      -2.722040    -0.641990    -1.736398      27.39
 C      -3.835450    -1.211398    -2.611674      55.82
 H      -3.819733    -0.716368    -3.729443      27.23
 O      -3.485250    -2.759924    -2.710204     128.12
 H      -2.376992    -2.957036    -2.809698      23.78
 C      -5.253123    -1.071855    -2.065290     102.08
 H      -5.475749    -1.584670    -1.152251      31.64
 O      -5.794881     0.275648    -2.181019     237.62
 H      -5.171420     0.847099    -1.638652      29.49
 C      -6.286416    -1.877232    -3.061435      99.50
 O      -6.196707    -3.283266    -2.930551     155.99
 H      -5.193592    -3.611388    -3.004378      28.69
 H      -6.285542    -1.546886    -4.133176      29.35
 H      -7.336154    -1.689769    -2.715194      27.71
55
name = lig-ACN-frame_240
 C       4.101561     2.891879    -0.404582      68.61
 H       3.615108     3.799573    -0.268847      26.24
 C       4.278742     0.612165     0.694286      45.76
 H       3.979151    -0.134000     1.444609      20.59
 C       5.445704     0.410371    -0.031786       5.53
 O       6.194545    -0.824347    -0.013696     226.00
 C       5.541757    -1.932558     0.704039     126.80
 H       5.871019    -1.924547     1.785618      26.13
 H       5.859637    -2.820853     0.234287      27.44
 H       4.550752    -2.021020     0.665152      28.56
 C       6.023230     1.349470    -0.957821       3.03
 O       7.253287     1.135366    -1.529333     131.48
 H       7.725887     0.304219    -1.067390      21.48
 C       5.333624     2.608739    -1.116567      51.65
 H       5.827594     3.341336    -1.751693      25.14
 C       3.545026     1.911188     0.481248     -19.27
 C       2.317543     2.162012     1.341085     100.38
 H       2.413904     3.145909     1.701862      25.89
 O       2.254737     1.388005     2.501942     243.20
 H       1.936035     0.377147     2.333569      22.19
 C       0.969486     2.207154     0.608440      67.24
 H       1.100394     2.926783    -0.280882      22.22
 C      -0.247159     2.688269     1.545755      83.66
 O      -0.014699     4.161914     1.950916     175.68
 H       0.607046     4.767813     1.098631      21.72
 H      -0.482988     2.097268     2.558213      23.06
 H      -1.198636     2.529740     0.896650      23.99
 C      -2.326903    -1.228493    -0.588346      49.54
 H      -2.885894    -1.877026    -0.123312      22.59
 C      -1.995197     0.509963    -2.244025      16.50
 H      -2.401670     0.975217    -3.125191      24.42
 C      -0.889284     1.041276    -1.572819      19.59
 O      -0.262251     2.226943    -2.025103     217.20
 C      -0.881995     3.070139    -3.032853     122.46
 H      -0.165885     3.808895    -3.209729      27.09
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 H      -0.802341     2.994355    -4.122246      27.00
 H      -1.947119     3.545913    -2.757438      27.34
 C      -0.374427     0.387886    -0.464785      17.47
 O       0.779350     0.771931     0.161044     188.99
 C      -1.147112    -0.728540     0.082748      40.72
 H      -0.704235    -1.238765     0.915769      23.74
 C      -2.741547    -0.551532    -1.809241      58.06
 C      -3.841191    -1.267432    -2.580519      60.23
 H      -3.797774    -0.793701    -3.704579      27.65
 O      -3.550163    -2.690619    -2.724924     224.95
 H      -2.613907    -2.711073    -2.876097      31.50
 C      -5.349003    -1.149175    -2.151585     102.19
 H      -5.300414    -1.459612    -1.136622      29.66
 O      -5.725639     0.272709    -2.173622     209.12
 H      -4.979922     0.994055    -1.755670      23.42
 C      -6.316156    -1.848796    -2.976847     122.32
 O      -6.264836    -3.319566    -2.858782     173.68
 H      -5.271921    -3.511689    -2.970693      29.93
 H      -6.163774    -1.449860    -4.018184      29.65
 H      -7.308050    -1.527100    -2.554774      27.16
55
name = lig-ACN-frame_241
 C       4.079640     2.877373    -0.422323      53.94
 H       3.741925     3.829187    -0.745761      24.52
 C       4.265054     0.613939     0.647221      76.68
 H       3.894770    -0.054593     1.417959      22.20
 C       5.494799     0.331818    -0.048226      17.17
 O       6.183877    -0.824268     0.045135     194.66
 C       5.515041    -1.979636     0.716254     109.70
 H       5.958140    -2.064029     1.805067      24.27
 H       5.888573    -2.838377     0.167653      25.71
 H       4.568693    -1.800661     0.750804      28.37
 C       6.015214     1.395573    -0.867695       4.70
 O       7.228510     1.170671    -1.578091      85.50
 H       7.856688     0.591726    -1.057970      22.62
 C       5.335489     2.611301    -1.053557      45.20
 H       5.805141     3.394180    -1.630268      19.52
 C       3.565418     1.834053     0.463365      -5.57
 C       2.278935     2.177850     1.378520      90.08
 H       2.359662     3.121715     1.739438      28.00
 O       2.315353     1.325964     2.562761     224.95
 H       2.118512     0.329608     2.221787      22.44
 C       0.981704     2.135948     0.592310      88.89
 H       1.102448     2.828135    -0.358457      22.77
 C      -0.103467     2.731705     1.511629      99.72
 O      -0.041093     4.026978     2.010173     241.95
 H       0.418239     4.688322     1.237674      25.72
 H       0.091547     1.990831     2.468972      22.52
 H      -1.156527     2.629135     1.085692      25.19
 C      -2.293367    -1.199034    -0.577327      47.33
 H      -2.622999    -2.130667    -0.320388      22.87
 C      -2.048202     0.598046    -2.291633     141.97
 H      -2.387913     1.175874    -3.160996      22.83
 C      -0.941798     1.136289    -1.589666      18.83
 O      -0.210120     2.220311    -2.025969     231.30
 C      -0.835034     3.051112    -3.035659     117.67
 H      -0.279996     3.998118    -3.012220      23.88
 H      -1.108850     2.300832    -3.751531      27.11
 H      -1.847843     3.364008    -2.549743      31.05
 C      -0.456050     0.387650    -0.413285      20.36
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 O       0.832317     0.793906     0.157062     180.20
 C      -1.186931    -0.700281     0.079012      36.72
 H      -0.868811    -1.179523     1.075523      18.50
 C      -2.769289    -0.612873    -1.760967      66.35
 C      -3.841162    -1.257513    -2.676538      48.88
 H      -3.854943    -0.734267    -3.763021      31.21
 O      -3.602785    -2.652530    -2.737824     270.09
 H      -2.772202    -2.916334    -2.939391      32.53
 C      -5.272215    -1.078624    -2.054896      91.12
 H      -5.425972    -1.469406    -1.083358      30.47
 O      -5.683989     0.257171    -2.200905     248.54
 H      -4.897385     0.803041    -1.651130      25.35
 C      -6.421964    -1.895267    -2.940335     102.17
 O      -6.313970    -3.325897    -2.811130     213.79
 H      -5.424092    -3.513510    -2.932615      34.31
 H      -6.296202    -1.673940    -4.036995      30.40
 H      -7.508141    -1.582640    -2.766514      28.57
55
name = lig-ACN-frame_242
 C       4.103649     2.759921    -0.416354      72.64
 H       3.357790     3.553015    -0.531950      24.56
 C       4.263725     0.673583     0.585757      64.58
 H       3.863602    -0.070555     1.251329      21.58
 C       5.442645     0.374411    -0.052401      11.56
 O       6.184285    -0.883665     0.105827     229.83
 C       5.549191    -1.979853     0.718709     127.08
 H       5.849177    -2.140052     1.868602      25.14
 H       5.748349    -2.907787     0.119967      25.84
 H       4.553081    -2.015981     0.710166      27.98
 C       6.077451     1.374303    -0.816035       5.28
 O       7.178852     1.241875    -1.611201     188.12
 H       7.847320     0.770863    -1.150293      23.36
 C       5.351088     2.587208    -0.975439      63.62
 H       5.725858     3.277389    -1.718882      27.86
 C       3.550256     1.880234     0.446476      23.96
 C       2.427322     2.163044     1.363052      88.79
 H       2.546744     3.071497     1.750066      28.38
 O       2.315355     1.237870     2.583611     238.65
 H       2.138819     0.353700     2.329716      26.61
 C       1.050118     2.190172     0.568840      80.16
 H       1.124408     2.863332    -0.416058      22.51
 C      -0.082880     2.598125     1.495568      95.00
 O      -0.004843     3.972434     2.069141     275.84
 H       0.102235     4.602907     1.428701      33.17
 H      -0.124508     1.904225     2.514040      23.08
 H      -1.067487     2.352881     0.991486      25.35
 C      -2.292606    -1.216267    -0.622604      60.78
 H      -2.680083    -2.220836    -0.357065      23.39
 C      -2.163309     0.614324    -2.237908      47.89
 H      -2.546430     0.949971    -3.229132      11.27
 C      -0.983494     1.105677    -1.576165      27.93
 O      -0.138137     2.187394    -1.983646     236.01
 C      -0.871152     3.014088    -2.990242     127.84
 H      -0.140042     3.675511    -3.565311      26.00
 H      -0.976125     2.548662    -3.964467      30.16
 H      -1.857342     3.366346    -2.647869      31.30
 C      -0.482777     0.516767    -0.401483      38.84
 O       0.748587     0.737528     0.146781     178.27
 C      -1.148520    -0.630951     0.116796      57.90
 H      -0.742432    -1.191219     1.113617      18.01
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 C      -2.706540    -0.549809    -1.833887      31.08
 C      -3.850179    -1.196115    -2.661588      51.80
 H      -3.845035    -0.716376    -3.738416      26.69
 O      -3.663949    -2.733667    -2.774796     174.53
 H      -2.596260    -2.849026    -3.014695      25.37
 C      -5.318018    -1.107176    -2.077215      90.97
 H      -5.150147    -1.415757    -1.086417      31.36
 O      -5.665233     0.301359    -2.219848     256.19
 H      -5.257343     0.988589    -1.666928      29.27
 C      -6.416146    -1.915832    -2.939653     108.78
 O      -6.378016    -3.353945    -2.741091     183.81
 H      -5.399374    -3.565541    -2.873625      31.35
 H      -6.300813    -1.545174    -3.987874      29.76
 H      -7.407671    -1.655713    -2.460172      27.65
55
name = lig-ACN-frame_243
 C       4.059327     2.821702    -0.438191      37.46
 H       3.761419     3.889077    -0.665015      19.16
 C       4.254017     0.565936     0.623972      80.16
 H       3.833479    -0.195560     1.268462      22.34
 C       5.506721     0.326547    -0.026251      14.79
 O       6.162813    -0.834574     0.114854     207.71
 C       5.507632    -2.057350     0.731697     104.09
 H       5.902771    -2.041848     1.859206      24.23
 H       6.103750    -2.896413     0.235774      24.29
 H       4.477625    -1.987394     0.675582      26.76
 C       6.076271     1.383620    -0.823153      15.19
 O       7.217200     1.295725    -1.628015     154.00
 H       7.792329     0.525440    -1.318522      21.70
 C       5.363825     2.578249    -1.001310      25.06
 H       5.799946     3.271277    -1.735317      27.80
 C       3.610321     1.777877     0.497684      17.25
 C       2.408037     2.069684     1.410892     114.58
 H       2.558765     2.972665     1.821617      27.60
 O       2.320407     1.224544     2.501313     307.98
 H       2.037303     0.386013     2.209701      28.47
 C       1.125546     2.172298     0.640067      75.91
 H       1.223962     2.930165    -0.274531      22.18
 C      -0.143591     2.517994     1.524921      92.47
 O       0.042386     3.886110     2.101025     264.28
 H       0.110556     4.414376     1.350363      32.18
 H      -0.200019     1.699581     2.437103      23.11
 H      -1.029368     2.557132     0.883829      25.10
 C      -2.191653    -1.184115    -0.652244      65.41
 H      -2.766952    -2.092158    -0.157577      20.76
 C      -2.129586     0.674920    -2.225741      96.56
 H      -2.450421     1.262372    -3.109891      18.21
 C      -0.981455     1.139100    -1.575073       8.09
 O      -0.206101     2.171986    -2.034789     251.49
 C      -0.816445     2.948473    -3.074065     120.53
 H      -0.116176     3.893393    -3.003260      23.29
 H      -1.153389     2.319862    -3.821624      27.84
 H      -1.639161     3.460834    -2.644206      29.25
 C      -0.552381     0.488017    -0.378069      28.62
 O       0.717610     0.791243     0.165944     161.57
 C      -1.229664    -0.631167     0.074246      47.51
 H      -0.610998    -1.158268     0.977095      19.55
 C      -2.753749    -0.641145    -1.814094      54.94
 C      -3.854860    -1.299142    -2.642524      59.78
 H      -3.836583    -0.830586    -3.689392      27.35
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 O      -3.689060    -2.735177    -2.822965     182.36
 H      -2.563730    -2.970900    -2.949210      24.44
 C      -5.280226    -1.080345    -2.146951     106.07
 H      -5.494263    -1.349756    -1.151021      30.92
 O      -5.750305     0.342464    -2.257224     236.65
 H      -5.132187     0.722554    -1.742666      34.10
 C      -6.364645    -1.890788    -2.823770     109.72
 O      -6.397896    -3.366936    -2.692779     183.96
 H      -5.393121    -3.691713    -2.833845      30.19
 H      -6.423820    -1.682151    -3.924868      29.76
 H      -7.335228    -1.488950    -2.500924      29.05
55
name = lig-ACN-frame_244
 C       4.146604     2.801294    -0.373156      68.81
 H       3.530580     3.767572    -0.344093      25.45
 C       4.296735     0.498251     0.641303      41.62
 H       3.961697    -0.237789     1.391033      21.11
 C       5.520253     0.341684     0.001330      10.57
 O       6.199999    -0.898871     0.094836     229.64
 C       5.568732    -2.021460     0.739517     112.59
 H       5.576587    -1.999427     1.910698      24.66
 H       6.050632    -2.967500     0.301713      24.61
 H       4.526006    -2.242712     0.426556      26.05
 C       6.041648     1.373968    -0.878584       3.11
 O       7.274678     1.295808    -1.608481      99.74
 H       7.835217     0.459911    -1.228808      23.51
 C       5.312727     2.570809    -1.077407      64.63
 H       5.781188     3.385416    -1.658594      18.89
 C       3.630675     1.792409     0.467438      -2.87
 C       2.383648     2.074181     1.398965      95.06
 H       2.466942     3.017704     1.781273      26.14
 O       2.312536     1.142705     2.492946     280.05
 H       1.978948     0.169789     2.197755      19.67
 C       0.966982     2.094572     0.705683      92.97
 H       1.151754     2.876154    -0.165454      23.53
 C      -0.134108     2.579746     1.529012     110.87
 O       0.076308     3.769089     2.134499     224.79
 H       0.468400     4.569506     1.428458      25.84
 H      -0.356120     1.794893     2.406094      23.52
 H      -1.043395     2.547009     0.926930      25.49
 C      -2.291000    -1.259077    -0.664278     106.42
 H      -2.668563    -2.383956    -0.291790      20.10
 C      -2.141028     0.575954    -2.236938     -22.42
 H      -2.640172     1.128594    -3.019507      24.06
 C      -1.026261     1.128475    -1.546315      31.40
 O      -0.265113     2.158435    -2.071825     246.48
 C      -0.787046     3.008523    -3.113817     131.01
 H       0.020803     3.736258    -3.561374      24.75
 H      -0.783640     2.540653    -4.051447      30.06
 H      -1.751867     3.281003    -2.885622      33.68
 C      -0.478098     0.514612    -0.385687      36.62
 O       0.739364     0.832533     0.174659     224.67
 C      -1.155213    -0.638419     0.099960      68.63
 H      -0.964761    -1.242105     1.097468      19.03
 C      -2.735242    -0.587264    -1.822991      86.16
 C      -3.834874    -1.327197    -2.693201      57.68
 H      -3.785659    -0.838146    -3.698745      31.52
 O      -3.676177    -2.758540    -2.851761     260.91
 H      -2.699987    -3.044948    -2.795208      29.50
 C      -5.329639    -1.031442    -2.090597      88.04
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 H      -5.128886    -1.272338    -1.069194      29.72
 O      -5.786211     0.302836    -2.305640     238.02
 H      -5.260924     1.110829    -2.019669      28.63
 C      -6.401727    -1.921732    -2.868737     110.14
 O      -6.381847    -3.337170    -2.609713     204.84
 H      -5.475515    -3.601530    -2.798282      32.64
 H      -6.279689    -1.678041    -3.956368      30.38
 H      -7.370105    -1.679685    -2.453311      28.89
55
name = lig-ACN-frame_245
 C       4.161816     2.747707    -0.263584      48.48
 H       3.579968     3.712939    -0.448418      26.50
 C       4.327462     0.606836     0.639957      64.44
 H       3.920000    -0.166202     1.322535      19.54
 C       5.542542     0.319914    -0.053078      10.80
 O       6.281983    -0.934403     0.041185     214.14
 C       5.596504    -2.014894     0.711020     112.53
 H       5.433053    -1.748190     1.810723      26.11
 H       6.374915    -2.854055     0.718873      24.57
 H       4.588675    -2.127141     0.213145      25.49
 C       6.062824     1.330495    -0.964124       6.06
 O       7.255220     1.262819    -1.551280     161.47
 H       7.959432     0.727382    -1.016668      24.34
 C       5.319709     2.554475    -1.117319      38.61
 H       5.705343     3.321761    -1.827005      18.28
 C       3.558435     1.736159     0.533324      31.14
 C       2.349259     2.041252     1.366920     101.67
 H       2.557295     2.938920     1.886391      27.14
 O       2.305540     1.090474     2.523665     212.44
 H       2.088593     0.091898     2.107978      20.41
 C       0.987270     2.141331     0.634386      83.67
 H       0.903015     2.865318    -0.255546      23.79
 C      -0.261700     2.528311     1.570162      96.91
 O       0.144312     3.837222     2.238094     157.95
 H       0.690977     4.491556     1.420353      26.36
 H      -0.433090     1.825873     2.446013      25.03
 H      -1.157279     2.647898     0.962931      27.05
 C      -2.255825    -1.250239    -0.600582      54.11
 H      -2.684480    -2.397855    -0.391194      22.29
 C      -2.164202     0.546990    -2.253846      77.34
 H      -2.394061     0.932685    -3.227414      14.21
 C      -1.037926     1.097581    -1.577386      16.19
 O      -0.273168     2.203845    -2.074034     203.01
 C      -0.791795     2.997761    -3.288912     120.59
 H      -0.144168     3.942323    -3.009797      24.89
 H      -0.795004     2.388679    -4.076308      31.41
 H      -1.687971     3.443513    -3.181576      32.98
 C      -0.504642     0.419531    -0.407290      31.55
 O       0.761073     0.751334     0.146914     163.87
 C      -1.194335    -0.721759     0.065318      41.07
 H      -0.705790    -1.031935     1.006707      17.88
 C      -2.769441    -0.717593    -1.824610      54.77
 C      -3.850908    -1.210964    -2.738832      65.73
 H      -3.839661    -0.833943    -3.734350      29.27
 O      -3.654586    -2.791272    -2.846794     251.58
 H      -2.795131    -2.956931    -2.803770      31.63
 C      -5.294687    -1.059665    -2.088856      88.24
 H      -5.388918    -1.231722    -1.023756      30.28
 O      -5.840061     0.282177    -2.381971     188.84
 H      -5.042532     0.853110    -1.834459      26.93
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 C      -6.437324    -1.918715    -2.855201     111.07
 O      -6.330140    -3.329085    -2.530238     221.02
 H      -5.431352    -3.540050    -2.683401      33.00
 H      -6.281555    -1.707424    -3.947043      29.86
 H      -7.442802    -1.509651    -2.731540      29.08
55
name = lig-ACN-frame_246
 C       4.130036     2.770342    -0.334480      69.10
 H       3.732436     3.793780    -0.472067      25.22
 C       4.387916     0.531641     0.658860      30.19
 H       4.025667    -0.313265     1.266087      16.16
 C       5.546667     0.280456    -0.137751      22.23
 O       6.323512    -0.848521    -0.029716     212.63
 C       5.636623    -1.961019     0.715748     123.62
 H       5.210125    -1.609566     1.646544      26.67
 H       6.332488    -2.813813     0.837488      25.44
 H       4.821938    -2.546678     0.098563      24.99
 C       6.013017     1.311434    -0.934837      16.42
 O       7.303513     1.235497    -1.559227     201.69
 H       7.826550     0.558242    -1.124780      26.62
 C       5.279404     2.465450    -1.036691      70.33
 H       5.588263     3.212473    -1.782072      22.46
 C       3.616570     1.769305     0.528744     -12.35
 C       2.306609     1.977155     1.460072      95.46
 H       2.388975     3.018662     1.849827      24.82
 O       2.264574     1.105041     2.499411     277.78
 H       2.021079     0.161367     2.230240      22.12
 C       0.919892     2.107712     0.621812      71.60
 H       1.193693     2.801719    -0.203013      23.58
 C      -0.225633     2.599090     1.620110     107.07
 O       0.191465     3.862917     2.300806     244.08
 H       0.478849     4.420163     1.491254      29.53
 H      -0.354952     1.768436     2.308989      25.16
 H      -1.160887     2.855023     1.131430      25.78
 C      -2.302359    -1.329935    -0.630006      77.45
 H      -2.788977    -2.206037     0.045453      16.81
 C      -2.105763     0.489694    -2.276774      25.42
 H      -2.408390     0.891015    -3.232403      19.41
 C      -1.006387     1.073258    -1.656763      11.91
 O      -0.365860     2.233799    -2.088041     244.41
 C      -0.782251     2.956766    -3.312961     126.90
 H      -0.101352     3.841644    -3.463722      25.64
 H      -0.490024     2.549960    -4.165046      30.26
 H      -1.771317     3.019662    -3.216700      30.69
 C      -0.513260     0.392683    -0.500886      22.90
 O       0.720505     0.660913     0.084658     184.52
 C      -1.155823    -0.752898     0.066761      53.58
 H      -0.765954    -1.387074     0.764146      23.43
 C      -2.728562    -0.684427    -1.823939      55.12
 C      -3.898184    -1.333966    -2.669776      61.41
 H      -3.875022    -0.778258    -3.548411      30.63
 O      -3.671904    -2.718588    -2.847558     261.93
 H      -2.700762    -2.921132    -2.903001      29.24
 C      -5.391649    -1.072243    -2.209897     105.64
 H      -5.323926    -1.388757    -1.153592      30.10
 O      -5.803741     0.288789    -2.410304     230.04
 H      -5.356182     1.080463    -1.876654      25.23
 C      -6.364811    -1.933411    -2.862708     122.48
 O      -6.309375    -3.322741    -2.460310     183.94
 H      -5.289150    -3.527143    -2.515463      29.09
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 H      -6.262090    -1.923008    -3.955115      30.56
 H      -7.324551    -1.601273    -2.467170      28.87
55
name = lig-ACN-frame_247
 C       4.044326     2.736409    -0.370408      56.39
 H       3.447944     3.622733    -0.409395      25.26
 C       4.336575     0.509898     0.621517      81.47
 H       3.911080    -0.171847     1.357655      23.85
 C       5.487638     0.272740    -0.123843      15.75
 O       6.299849    -0.868938    -0.052951     246.23
 C       5.746072    -1.927152     0.675735     127.98
 H       5.221819    -1.665123     1.536521      28.76
 H       6.613408    -2.444801     1.013535      26.75
 H       4.968877    -2.449210    -0.087015      24.77
 C       6.091925     1.286503    -0.941415       2.64
 O       7.275136     1.230275    -1.584462     150.25
 H       7.772272     0.436133    -1.346256      26.86
 C       5.296219     2.506872    -1.081568      26.47
 H       5.825549     3.270242    -1.660134      18.54
 C       3.658728     1.746132     0.576104      16.62
 C       2.318699     2.002408     1.374422      87.36
 H       2.404098     3.008954     1.944554      22.24
 O       2.195703     1.075969     2.571585     272.74
 H       1.924354     0.283176     2.223640      27.90
 C       0.959092     1.984763     0.666364      94.48
 H       0.932326     2.655129    -0.181328      22.79
 C      -0.119458     2.669159     1.612527     114.37
 O       0.243894     3.843877     2.310848     309.05
 H       0.273420     4.553707     1.865689      35.72
 H      -0.315134     2.090100     2.468510      26.27
 H      -1.067532     2.669082     1.037662      26.58
 C      -2.327733    -1.305854    -0.616008      57.32
 H      -2.964337    -2.197367    -0.356480      20.30
 C      -2.081320     0.402231    -2.389703     108.55
 H      -2.627945     0.911036    -3.195940      26.47
 C      -0.978815     1.036287    -1.711569       7.83
 O      -0.410889     2.261345    -2.081056     227.00
 C      -0.797019     2.837360    -3.342982     137.04
 H      -0.476390     3.863991    -3.190665      26.87
 H      -0.496881     2.242674    -4.056219      31.44
 H      -1.768361     3.056121    -3.566032      31.07
 C      -0.485136     0.337802    -0.551859      15.01
 O       0.692790     0.715685     0.070143     217.57
 C      -1.155011    -0.818110    -0.045289      21.93
 H      -0.737258    -1.106850     0.780416      20.92
 C      -2.784882    -0.698862    -1.784831      56.16
 C      -3.870238    -1.273590    -2.656766      90.19
 H      -3.789529    -0.910581    -3.603108      35.57
 O      -3.716029    -2.721713    -2.857999     201.04
 H      -2.599286    -2.966833    -2.800060      24.23
 C      -5.322018    -1.041499    -2.164098      88.70
 H      -5.562565    -1.189427    -1.081116      28.83
 O      -5.776273     0.325861    -2.450240     252.26
 H      -5.232790     0.766821    -1.890110      33.90
 C      -6.407895    -2.030123    -2.942740     109.18
 O      -6.266133    -3.353177    -2.373223     163.62
 H      -5.271173    -3.669933    -2.463418      27.45
 H      -6.419565    -1.857822    -4.029331      29.74
 H      -7.454735    -1.708103    -2.721628      28.36
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name = lig-ACN-frame_248
 C       4.097142     2.650654    -0.400918      70.78
 H       3.543539     3.487002    -0.703811      26.61
 C       4.260722     0.510036     0.622131      52.17
 H       3.944778    -0.308978     1.260638      22.65
 C       5.500235     0.313975    -0.116585       8.07
 O       6.279212    -0.837578    -0.085033     246.05
 C       5.856362    -2.003950     0.683023     131.40
 H       5.305102    -1.690753     1.480274      29.88
 H       6.651696    -2.640545     0.914486      26.27
 H       5.182040    -2.839829     0.098156      24.96
 C       5.992931     1.383355    -0.931630      -1.38
 O       7.232249     1.219939    -1.641039     143.96
 H       7.849787     0.513887    -1.155352      20.19
 C       5.308429     2.565048    -1.095699      83.80
 H       5.616642     3.394701    -1.717220      26.47
 C       3.570016     1.720829     0.539966      24.17
 C       2.372200     1.939267     1.401671      92.41
 H       2.498851     3.086937     1.759553      21.75
 O       2.147790     1.099055     2.580617     255.98
 H       1.946800     0.171894     2.315024      23.62
 C       1.024681     2.094268     0.625694      78.49
 H       1.192758     2.807709    -0.132281      24.62
 C      -0.099377     2.560098     1.639238     103.21
 O       0.311930     3.885779     2.324104     221.31
 H       0.305469     4.494924     1.500783      28.26
 H      -0.339960     1.836006     2.311578      26.11
 H      -0.916642     2.924821     0.966500      24.77
 C      -2.367451    -1.295723    -0.627285      66.52
 H      -2.640149    -2.196398    -0.196917      23.89
 C      -2.082182     0.398567    -2.411264      42.90
 H      -2.378968     0.839278    -3.389898      17.75
 C      -1.014206     0.950964    -1.772333      16.70
 O      -0.469723     2.221934    -2.024179     227.43
 C      -0.852283     2.775793    -3.403579     130.62
 H      -0.298089     3.661772    -3.430864      26.82
 H      -0.345685     2.332324    -4.164745      29.75
 H      -1.879936     2.677254    -3.364876      27.85
 C      -0.483599     0.330539    -0.614692      18.91
 O       0.697963     0.710291     0.121519     170.12
 C      -1.118618    -0.821542    -0.081837      41.75
 H      -0.835868    -1.215936     0.789994      16.77
 C      -2.803692    -0.672611    -1.869901      42.26
 C      -3.907021    -1.225900    -2.708222      69.21
 H      -3.915460    -0.714501    -3.571315      31.09
 O      -3.743371    -2.769716    -2.854617     141.72
 H      -2.639690    -3.143662    -2.655498      20.53
 C      -5.410771    -1.046146    -2.197799      90.37
 H      -5.338487    -1.329417    -1.094232      28.98
 O      -5.718063     0.351273    -2.481952     274.77
 H      -5.251958     1.062664    -2.087392      29.34
 C      -6.391287    -2.050271    -2.904709     116.14
 O      -6.246755    -3.407838    -2.338261     189.14
 H      -5.309945    -3.493504    -2.550477      30.57
 H      -6.032109    -2.256071    -3.899591      30.05
 H      -7.444648    -1.705753    -2.773987      29.59
55
name = lig-ACN-frame_249
 C       4.022004     2.700070    -0.406404      58.98
 H       3.453140     3.595235    -0.465366      24.34
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 C       4.311952     0.438149     0.608500      68.42
 H       3.869382    -0.393716     1.147886      18.31
 C       5.474280     0.360344    -0.097332      13.16
 O       6.279306    -0.824777    -0.124855     185.17
 C       5.933816    -2.091321     0.706082     108.98
 H       5.538724    -1.936079     1.656490      28.97
 H       6.893354    -2.435021     0.822316      26.43
 H       5.157893    -2.682643    -0.037302      24.61
 C       6.038504     1.376444    -0.955419       6.70
 O       7.150754     1.212727    -1.659587     157.93
 H       7.827481     0.627217    -1.127397      21.86
 C       5.271035     2.579702    -1.087314      49.25
 H       5.538556     3.267141    -1.883388      28.35
 C       3.551030     1.633421     0.425880      -3.73
 C       2.318956     1.966755     1.438201      88.01
 H       2.607934     2.966490     2.091134      22.31
 O       2.152833     1.125935     2.548435     239.60
 H       1.932429     0.126939     2.142268      21.29
 C       1.045291     2.171967     0.623549      78.53
 H       1.160662     2.769249    -0.201730      23.26
 C      -0.073430     2.599137     1.580472     105.12
 O       0.342210     3.829415     2.275683     175.91
 H       0.777252     4.596875     1.471785      25.16
 H      -0.168967     1.890915     2.316117      26.07
 H      -1.146566     2.630423     1.147136      24.95
 C      -2.328797    -1.264202    -0.701171      57.94
 H      -2.890724    -1.966919    -0.288420      21.23
 C      -2.127232     0.391239    -2.454218      95.60
 H      -2.324005     0.655288    -3.510067      17.14
 C      -0.956992     0.959859    -1.715453      19.99
 O      -0.502926     2.180518    -2.082022     220.31
 C      -0.854210     2.728105    -3.368655     133.67
 H      -0.636932     3.689491    -3.397063      29.53
 H      -0.609744     2.015370    -4.155608      29.20
 H      -1.929333     2.912803    -3.602493      28.22
 C      -0.422487     0.337982    -0.545280      19.83
 O       0.693146     0.719679     0.134105     195.02
 C      -1.153346    -0.785976    -0.067520      52.49
 H      -0.656887    -1.408827     0.664170      23.85
 C      -2.811550    -0.709973    -1.919911      29.90
 C      -4.000978    -1.356086    -2.781063      53.57
 H      -3.940678    -1.054616    -3.737293      31.22
 O      -3.787192    -2.743891    -2.868657     219.87
 H      -2.678877    -2.839640    -2.720392      23.23
 C      -5.381766    -1.030262    -2.209479      93.41
 H      -5.510107    -1.150434    -1.066319      28.02
 O      -5.750411     0.346730    -2.547432     205.12
 H      -5.073226     0.765200    -1.804786      24.62
 C      -6.310710    -2.083658    -2.871226     122.08
 O      -6.248585    -3.414144    -2.311044     213.97
 H      -5.356755    -3.703818    -2.260614      31.20
 H      -6.166763    -1.948358    -3.942455      30.75
 H      -7.395590    -1.800146    -2.865390      27.91
55
name = lig-ACN-frame_250
 C       3.948106     2.696222    -0.378126      48.20
 H       3.407019     3.650765    -0.381540      25.64
 C       4.276623     0.447360     0.554069      63.87
 H       3.956435    -0.361650     1.219130      23.05
 C       5.549070     0.263976    -0.108940      17.51
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 O       6.286746    -0.860794    -0.107789     228.81
 C       6.053049    -2.014603     0.629140     120.62
 H       5.703472    -1.770501     1.626919      27.46
 H       6.861828    -2.695996     0.579204      26.07
 H       5.165117    -2.786722     0.162633      24.67
 C       5.954923     1.381625    -0.903371      -7.03
 O       7.161345     1.204821    -1.680790     153.01
 H       7.663270     0.473379    -1.362451      28.15
 C       5.182179     2.545331    -1.107992      60.61
 H       5.672448     3.307941    -1.719018      14.71
 C       3.501037     1.637385     0.459446      23.88
 C       2.380119     2.014763     1.350852      74.01
 H       2.647358     3.157411     1.743135      22.50
 O       2.174782     1.057788     2.518786     226.16
 H       1.751539     0.167931     2.102826      21.54
 C       0.960611     2.119717     0.592495      91.85
 H       1.042494     2.761000    -0.215989      24.85
 C      -0.067205     2.649696     1.566927     107.79
 O       0.344440     3.799047     2.201964     213.10
 H       0.829606     4.608051     1.499385      24.89
 H      -0.019991     1.970878     2.367037      25.31
 H      -1.105673     2.719908     1.038999      25.10
 C      -2.370923    -1.240578    -0.740889      58.67
 H      -2.798799    -2.079940    -0.333499      27.23
 C      -2.042584     0.369223    -2.442243      55.30
 H      -2.398804     0.949159    -3.279552      20.50
 C      -1.050538     0.949712    -1.716201      15.80
 O      -0.451704     2.202491    -2.129141     207.95
 C      -0.940230     2.719532    -3.395299     113.29
 H      -0.234103     3.432616    -3.465081      26.91
 H      -0.530742     2.118663    -4.273714      26.44
 H      -2.069398     2.826942    -3.226833      27.28
 C      -0.475349     0.374840    -0.500628      21.69
 O       0.755908     0.777976     0.156789     178.55
 C      -1.171067    -0.784373    -0.064984      35.62
 H      -0.842797    -1.323976     0.942707      15.46
 C      -2.831749    -0.727321    -2.003915      58.98
 C      -3.925234    -1.344689    -2.778705      77.43
 H      -4.007886    -0.841257    -3.660195      33.51
 O      -3.807258    -2.816379    -2.873822     210.07
 H      -2.857147    -3.068114    -2.813583      27.87
 C      -5.381536    -1.066674    -2.216726      88.96
 H      -5.364223    -1.198158    -1.067070      29.20
 O      -5.780627     0.291821    -2.586996     200.43
 H      -5.329051     1.184224    -2.091908      23.40
 C      -6.359732    -2.069948    -2.878635     118.95
 O      -6.276775    -3.412506    -2.283622     165.41
 H      -5.234967    -3.564800    -2.272719      26.45
 H      -6.178550    -2.227542    -3.939186      29.96
 H      -7.354084    -1.729725    -2.552419      29.42
55
name = lig-ACN-frame_251
 C       3.972346     2.652014    -0.389563      68.10
 H       3.387587     3.593555    -0.619602      24.74
 C       4.237485     0.429449     0.548401      70.60
 H       3.860718    -0.308184     1.266155      24.23
 C       5.447036     0.276431    -0.121051       2.36
 O       6.398385    -0.854393    -0.176769     219.21
 C       6.069629    -2.031612     0.631434     112.82
 H       6.088736    -1.771723     1.721301      27.57
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 H       7.007385    -2.638086     0.516162      24.62
 H       4.959861    -2.440136     0.273334      23.63
 C       5.954048     1.314151    -0.963311      10.50
 O       7.123374     1.240678    -1.653988     143.39
 H       7.550364     0.402505    -1.389010      26.62
 C       5.148157     2.474288    -1.086038      48.03
 H       5.433585     3.398624    -1.619055      19.20
 C       3.557404     1.667090     0.472190      31.83
 C       2.304527     1.935502     1.336252      94.91
 H       2.437339     2.984745     1.965730      21.23
 O       2.215718     1.060505     2.420425     298.23
 H       1.837947     0.279298     2.092286      26.92
 C       0.997954     2.112338     0.547937      88.45
 H       1.079773     2.777752    -0.276040      23.99
 C      -0.114984     2.571635     1.582568      97.66
 O       0.354319     3.908890     2.184401     230.92
 H       0.422834     4.467991     1.326076      27.72
 H      -0.550751     1.824730     2.279684      24.59
 H      -1.046663     2.884408     1.012993      25.03
 C      -2.373790    -1.267920    -0.705094      53.11
 H      -2.778918    -2.235220    -0.374100      26.26
 C      -2.062213     0.404219    -2.465581     109.50
 H      -2.434722     0.862525    -3.353090      20.03
 C      -0.985877     1.041987    -1.661406      18.86
 O      -0.400763     2.131006    -2.136105     197.95
 C      -0.908262     2.769046    -3.435714     113.43
 H      -0.558399     3.675354    -3.638316      27.30
 H      -1.133066     1.978603    -4.254270      23.78
 H      -2.020472     3.216310    -3.378014      26.57
 C      -0.549376     0.409666    -0.485218      36.66
 O       0.690483     0.736855     0.100088     190.20
 C      -1.257106    -0.736700    -0.060374      47.57
 H      -0.999600    -1.234104     1.057402      16.10
 C      -2.706824    -0.713594    -1.937515      48.14
 C      -3.913052    -1.297467    -2.795916      58.26
 H      -3.752551    -1.006815    -3.793259      30.90
 O      -3.803199    -2.887560    -2.904729     214.87
 H      -2.959129    -3.089143    -2.739841      29.79
 C      -5.338351    -1.080128    -2.243412      86.54
 H      -5.365100    -1.294858    -1.106883      28.71
 O      -5.846737     0.225912    -2.643556     249.39
 H      -5.285686     0.821080    -2.085858      29.83
 C      -6.464493    -2.076545    -2.815193     117.97
 O      -6.305280    -3.390485    -2.238101     165.80
 H      -5.297106    -3.608266    -2.430370      26.01
 H      -6.355542    -2.040083    -3.922069      29.74
 H      -7.476621    -1.659166    -2.772477      29.91
55
name = lig-ACN-frame_252
 C       3.994884     2.633403    -0.428941      55.44
 H       3.326771     3.555654    -0.552961      23.45
 C       4.240705     0.393486     0.606087      50.47
 H       3.832112    -0.440260     1.189149      20.64
 C       5.462791     0.223529    -0.209387       9.59
 O       6.404355    -0.782568    -0.219623     205.21
 C       6.106373    -1.995373     0.663481     102.61
 H       6.175572    -1.765424     1.800276      25.96
 H       6.673140    -2.924240     0.233941      24.42
 H       4.963090    -2.449425     0.499369      23.89
 C       5.885866     1.282618    -1.028260       6.35
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 O       7.116301     1.262213    -1.638732     183.08
 H       7.773779     0.515973    -1.270784      20.67
 C       5.206191     2.497076    -1.138593      55.68
 H       5.666833     3.064754    -1.989575      26.32
 C       3.515155     1.642580     0.502500      19.56
 C       2.298250     1.929476     1.327986      94.80
 H       2.464672     3.035806     1.789030      22.82
 O       2.209362     0.979290     2.401147     265.88
 H       1.992577     0.106458     2.047403      26.07
 C       0.948085     2.046649     0.614428      81.17
 H       1.089229     2.740205    -0.244127      22.39
 C      -0.175797     2.670824     1.503759      99.98
 O       0.273514     3.886130     2.177843     292.33
 H       0.545950     4.499069     1.613700      33.95
 H      -0.179041     2.046261     2.481889      23.13
 H      -1.086166     2.719745     0.837726      24.54
 C      -2.349892    -1.301390    -0.668760      80.89
 H      -2.973858    -2.203304    -0.235916      20.02
 C      -2.080712     0.468915    -2.383948      33.72
 H      -2.271813     0.714931    -3.413366      19.49
 C      -1.055955     1.039227    -1.744885       7.63
 O      -0.289508     2.208525    -2.245153     205.28
 C      -0.944481     2.816404    -3.391853      95.28
 H      -0.117451     3.317103    -3.709540      26.87
 H      -0.889447     2.003544    -4.308275      24.89
 H      -1.998739     3.108210    -2.917449      26.59
 C      -0.617722     0.423341    -0.499744      23.50
 O       0.601380     0.675736     0.035689     175.46
 C      -1.333519    -0.659036     0.070143      38.49
 H      -0.659117    -1.215544     0.993692      21.01
 C      -2.744066    -0.732526    -1.934967      43.83
 C      -3.857517    -1.437523    -2.817011      54.91
 H      -3.868833    -0.910070    -3.806572      28.52
 O      -3.781177    -2.848746    -2.928553     248.80
 H      -2.858966    -3.037624    -2.731246      30.89
 C      -5.404625    -1.117426    -2.306439      89.05
 H      -5.308986    -1.076832    -1.176070      28.06
 O      -5.872806     0.191045    -2.656678     247.59
 H      -5.481111     0.872307    -2.237263      32.16
 C      -6.460235    -2.066132    -2.793504     121.72
 O      -6.371991    -3.369465    -2.206805     209.61
 H      -5.503674    -3.662727    -2.376067      31.75
 H      -6.462980    -2.139290    -3.909071      29.45
 H      -7.374485    -1.752840    -2.323426      28.89
55
name = lig-ACN-frame_253
 C       3.999258     2.618659    -0.445088      51.88
 H       3.449844     3.598920    -0.533293      25.65
 C       4.316170     0.384397     0.562035      77.31
 H       4.041951    -0.404056     1.262102      20.97
 C       5.417368     0.210674    -0.223232      19.97
 O       6.337503    -0.853444    -0.167992     216.98
 C       6.085246    -1.920388     0.615131     111.83
 H       6.597435    -1.712540     1.686597      25.09
 H       6.826766    -2.789435     0.242784      23.26
 H       4.905506    -2.078101     0.697129      23.95
 C       5.892910     1.300546    -1.057360       3.78
 O       7.174423     1.258423    -1.666682     160.17
 H       7.758394     0.661858    -1.078497      25.66
 C       5.170454     2.484288    -1.239810      55.31
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 H       5.464961     3.387216    -1.857001      16.28
 C       3.566957     1.584342     0.402861      13.98
 C       2.303428     1.879678     1.341500      82.43
 H       2.478357     2.865720     1.927054      24.36
 O       2.181279     0.877754     2.460740     220.10
 H       1.876151    -0.015692     1.898968      22.04
 C       0.882088     2.012148     0.566453      90.10
 H       1.063814     2.683317    -0.340110      23.45
 C      -0.166095     2.677489     1.498925     102.96
 O       0.154579     3.878672     2.163851     317.56
 H       0.594388     4.371617     1.592374      34.57
 H      -0.564312     1.787048     2.216192      23.75
 H      -1.163534     2.877112     1.022656      25.70
 C      -2.400630    -1.237147    -0.631288      85.36
 H      -2.814936    -2.277418    -0.152033      19.53
 C      -2.202926     0.398307    -2.430155     115.60
 H      -2.546734     0.853126    -3.374923      21.81
 C      -1.026878     1.096376    -1.739736       6.10
 O      -0.237322     2.145833    -2.273048     242.34
 C      -0.846881     2.825487    -3.384109     130.95
 H      -0.455293     3.768287    -3.692712      27.28
 H      -1.250871     2.115175    -4.308519      25.47
 H      -1.883873     3.437492    -3.274416      29.34
 C      -0.691586     0.465287    -0.535714      28.95
 O       0.597034     0.706705     0.067843     186.45
 C      -1.377086    -0.616767     0.086596      38.57
 H      -0.983365    -1.134915     1.155565      19.23
 C      -2.843238    -0.777267    -1.903962      31.64
 C      -3.894040    -1.395595    -2.804610      45.60
 H      -3.733221    -0.964591    -3.864802      29.45
 O      -3.709429    -2.850649    -2.941363     219.52
 H      -2.668676    -3.160219    -2.890135      23.17
 C      -5.338933    -1.102440    -2.281300      83.66
 H      -5.396348    -1.369542    -1.187641      28.23
 O      -5.904632     0.203756    -2.723742     196.03
 H      -5.294052     0.841434    -2.155829      28.18
 C      -6.508222    -2.083272    -2.746680     113.11
 O      -6.433975    -3.417363    -2.165637     210.37
 H      -5.497827    -3.691526    -2.237677      29.17
 H      -6.704608    -2.107335    -3.858181      28.82
 H      -7.399748    -1.563276    -2.465217      29.80
55
name = lig-ACN-frame_254
 C       3.962351     2.588609    -0.483554      66.18
 H       3.377843     3.503148    -0.529654      26.14
 C       4.310013     0.402668     0.511458      57.15
 H       4.030769    -0.213839     1.362884      21.54
 C       5.513537     0.291259    -0.286949      15.14
 O       6.290641    -0.818594    -0.241003     199.99
 C       6.074767    -1.960844     0.722176      97.44
 H       6.522718    -1.765878     1.839429      24.19
 H       6.489186    -2.885896     0.119328      24.59
 H       4.993941    -2.352174     0.909141      24.57
 C       5.996239     1.329915    -1.120725      10.28
 O       7.214028     1.242682    -1.679076     198.61
 H       7.793195     0.619116    -1.274506      27.01
 C       5.097834     2.449361    -1.274254      49.32
 H       5.576671     3.335151    -1.760889      17.87
 C       3.514795     1.565709     0.398963      17.63
 C       2.285519     1.752241     1.374047      98.28
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 H       2.482713     2.696802     1.917920      24.51
 O       2.144396     0.823956     2.417837     277.50
 H       1.687511    -0.126910     2.190602      21.85
 C       0.986632     2.078504     0.555405      73.40
 H       1.094460     2.837846    -0.330043      22.47
 C      -0.279222     2.554768     1.466283      83.72
 O       0.079559     3.880362     2.188453     236.38
 H       0.441929     4.466749     1.466215      28.64
 H      -0.591584     1.855659     2.406967      22.93
 H      -0.984636     2.739761     0.646054      24.70
 C      -2.519508    -1.208341    -0.607531      72.65
 H      -2.929834    -2.271378    -0.210356      22.55
 C      -2.200360     0.423475    -2.425574       3.29
 H      -2.767512     0.825841    -3.301241      21.03
 C      -1.149122     1.010606    -1.786025      15.91
 O      -0.267378     2.020566    -2.275974     191.16
 C      -0.844419     2.924362    -3.445609      89.12
 H       0.049864     3.578346    -3.633990      24.94
 H      -0.781876     2.149807    -4.416476      24.67
 H      -1.827700     2.996989    -2.886267      26.26
 C      -0.634770     0.498976    -0.488216      34.77
 O       0.547114     0.741841     0.116882     173.86
 C      -1.426989    -0.549634    -0.002998      52.94
 H      -1.160659    -0.821890     1.117908      18.73
 C      -2.839807    -0.694858    -1.873618      56.62
 C      -3.921361    -1.363101    -2.785027      40.21
 H      -3.850268    -0.839109    -3.878166      28.42
 O      -3.675145    -2.878832    -2.948230     154.43
 H      -2.526816    -2.873775    -2.803731      21.21
 C      -5.411483    -1.160508    -2.282707      90.52
 H      -5.273813    -0.950781    -1.220949      28.40
 O      -5.845062     0.193035    -2.738180     164.46
 H      -5.316101     1.008398    -2.158658      23.85
 C      -6.542984    -2.102712    -2.727713     115.50
 O      -6.490674    -3.440014    -2.120616     180.19
 H      -5.456141    -3.700361    -2.191049      27.76
 H      -6.416781    -2.153582    -3.837503      29.22
 H      -7.500564    -1.781447    -2.362296      29.37
55
name = lig-ACN-frame_255
 C       3.858707     2.543889    -0.532548      48.49
 H       3.304479     3.417925    -0.732694      23.32
 C       4.328544     0.461037     0.461007      70.28
 H       4.141813    -0.456031     0.993168      21.41
 C       5.509153     0.324551    -0.237415      12.33
 O       6.299398    -0.887430    -0.284505     188.63
 C       6.026355    -1.999846     0.765480     100.09
 H       6.649666    -1.657565     1.786021      24.02
 H       6.629083    -2.903605     0.394397      23.74
 H       4.946868    -2.019357     0.873191      25.25
 C       5.969128     1.347659    -1.113351       9.93
 O       7.279605     1.275664    -1.761330     162.69
 H       7.741832     0.561523    -1.287903      25.31
 C       5.158076     2.451937    -1.261581      46.23
 H       5.363303     3.191243    -2.054559      27.11
 C       3.461722     1.550592     0.414994      26.27
 C       2.294563     1.770894     1.354012     105.38
 H       2.535109     2.666127     1.889879      24.72
 O       2.095356     0.753701     2.388838     304.42
 H       1.788188    -0.000065     1.878158      26.16
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 C       0.949243     2.064731     0.700210      81.50
 H       1.315898     2.789980    -0.166274      22.12
 C      -0.206300     2.627221     1.421936     103.40
 O      -0.046718     3.784622     2.159232     226.66
 H       0.420805     4.628227     1.522820      24.65
 H      -0.406111     1.733703     2.220838      22.98
 H      -1.140880     2.575218     0.869081      25.55
 C      -2.551972    -1.135756    -0.637166      62.45
 H      -3.185790    -1.942396    -0.107945      21.16
 C      -2.244230     0.473058    -2.429884      89.79
 H      -2.282747     0.911420    -3.460279      12.66
 C      -1.061833     0.991049    -1.776162      21.88
 O      -0.331780     1.941001    -2.344408     243.93
 C      -0.767583     2.813886    -3.388910     109.79
 H      -0.147074     3.795460    -3.183941      24.98
 H      -0.791212     2.380008    -4.538005      23.97
 H      -1.702557     3.445084    -3.503730      26.34
 C      -0.719846     0.468460    -0.567756      22.87
 O       0.531832     0.769316     0.120829     183.15
 C      -1.486228    -0.544590     0.077115      36.06
 H      -1.055016    -0.995864     0.969769      22.47
 C      -2.954869    -0.692443    -1.932637      48.48
 C      -3.948977    -1.445081    -2.756211      42.68
 H      -4.004563    -0.905781    -3.866392      27.22
 O      -3.657530    -2.799218    -2.933614     192.07
 H      -2.631288    -3.156918    -2.729735      23.47
 C      -5.463328    -1.094516    -2.212092      89.45
 H      -5.563754    -1.297115    -1.139898      29.88
 O      -5.790365     0.174632    -2.778087     223.78
 H      -5.329972     0.837218    -2.051859      25.96
 C      -6.525976    -2.155317    -2.700270     113.65
 O      -6.490324    -3.439325    -2.079924     226.20
 H      -5.595149    -3.837624    -2.143578      29.84
 H      -6.550537    -2.260481    -3.821573      29.56
 H      -7.514841    -1.685837    -2.560432      29.88
55
name = lig-ACN-frame_256
 C       3.867554     2.529314    -0.628243      74.11
 H       3.189641     3.291968    -0.850286      24.31
 C       4.326103     0.386227     0.490070      36.17
 H       3.798032    -0.344156     1.093391      19.08
 C       5.588414     0.245248    -0.244220      15.11
 O       6.279825    -0.974499    -0.266295     232.17
 C       6.025686    -1.888204     0.731136     115.40
 H       6.371804    -1.498379     1.874805      24.29
 H       6.460080    -2.853038     0.426621      25.56
 H       5.018570    -2.191661     0.913730      27.21
 C       6.052560     1.346079    -1.099685      -1.17
 O       7.203848     1.319510    -1.798424     129.65
 H       7.943905     0.727644    -1.343674      26.47
 C       5.081135     2.473076    -1.251878      50.89
 H       5.273920     3.203608    -2.034722      26.49
 C       3.496115     1.578305     0.337881       6.03
 C       2.262557     1.812263     1.446982      93.88
 H       2.483008     2.614511     2.035575      25.41
 O       2.086497     0.714367     2.332747     316.29
 H       1.857426    -0.082624     1.959023      27.19
 C       0.947247     2.051970     0.591238      75.60
 H       1.018335     2.800227    -0.334727      21.98
 C      -0.217833     2.550490     1.487097      96.68
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 O      -0.147833     3.818521     2.173192     196.13
 H       0.545159     4.538842     1.475105      23.53
 H      -0.545024     1.790542     2.326458      23.25
 H      -0.920068     2.674419     0.673593      24.88
 C      -2.635981    -1.057709    -0.650407      83.79
 H      -3.175977    -1.865602    -0.182251      22.53
 C      -2.240624     0.425928    -2.498606      28.19
 H      -2.539915     0.657014    -3.525929      19.64
 C      -1.145208     0.940359    -1.814958      10.73
 O      -0.310936     1.941745    -2.395608     216.78
 C      -0.711703     2.835523    -3.416332      94.47
 H       0.016891     3.758612    -3.325913      23.61
 H      -0.270234     2.338871    -4.451032      23.35
 H      -1.828086     2.805965    -3.218008      27.16
 C      -0.690593     0.431761    -0.449025      41.88
 O       0.508697     0.748796     0.069994     184.66
 C      -1.507342    -0.584823     0.101811      25.15
 H      -1.274661    -1.043051     0.958303      19.74
 C      -2.942953    -0.609921    -1.952349      46.67
 C      -4.053308    -1.397572    -2.727750      40.81
 H      -4.062262    -0.974247    -3.901553      25.60
 O      -3.668962    -2.833274    -2.900183     223.82
 H      -2.777710    -2.847185    -2.663822      28.65
 C      -5.464414    -1.206371    -2.197899     102.11
 H      -5.497446    -0.994512    -1.154307      30.60
 O      -5.769699     0.162265    -2.761981     230.18
 H      -5.336033     0.819513    -2.247459      29.87
 C      -6.531992    -2.145260    -2.754457     111.69
 O      -6.479365    -3.438193    -2.007093     231.91
 H      -5.610405    -3.718224    -2.167679      32.12
 H      -6.372278    -2.252214    -3.847210      29.71
 H      -7.551324    -1.780514    -2.458104      28.29
55
name = lig-ACN-frame_257
 C       3.834391     2.527624    -0.646166      44.02
 H       3.219691     3.370833    -0.887376      24.50
 C       4.330144     0.394896     0.474524      67.32
 H       4.226998    -0.327896     1.278366      23.01
 C       5.523881     0.223838    -0.251022      14.16
 O       6.277150    -0.945145    -0.314321     198.14
 C       5.975421    -1.908478     0.800351     107.41
 H       6.362201    -1.378210     1.866323      25.03
 H       6.663568    -2.697163     0.659389      26.15
 H       4.959758    -2.158177     0.746459      27.23
 C       5.947667     1.339217    -0.995855      13.59
 O       7.154532     1.363980    -1.822410      96.98
 H       7.881124     0.849182    -1.269288      21.68
 C       5.146583     2.394195    -1.329409      39.53
 H       5.611977     3.177922    -1.908669      18.76
 C       3.528411     1.538092     0.395576      25.01
 C       2.284118     1.760457     1.295981     104.32
 H       2.397789     2.585472     1.827264      26.46
 O       2.105716     0.720827     2.313952     291.29
 H       1.703986    -0.063793     1.802947      23.12
 C       0.924654     2.045336     0.562500      72.28
 H       1.131086     2.827165    -0.311302      21.97
 C      -0.326832     2.501551     1.483119      87.27
 O      -0.161484     3.878735     2.182939     203.28
 H       0.490756     4.518240     1.484308      24.38
 H      -0.512024     1.732697     2.312745      23.57
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 H      -1.160596     2.516231     0.841390      25.80
 C      -2.703495    -1.060259    -0.594901      48.81
 H      -3.207406    -1.891008    -0.312470      23.26
 C      -2.190169     0.371139    -2.610470      56.94
 H      -2.450876     0.865847    -3.529341      22.26
 C      -1.126607     0.958042    -1.820451       3.87
 O      -0.193148     1.879608    -2.294050     173.14
 C      -0.693870     2.790296    -3.502126     100.91
 H      -0.493586     3.916174    -3.165657      24.77
 H      -0.384695     2.415510    -4.582433      24.39
 H      -1.777754     3.006798    -3.680268      27.98
 C      -0.766937     0.448925    -0.530304      20.87
 O       0.567348     0.698722     0.036570     168.05
 C      -1.544381    -0.610626     0.071557      30.72
 H      -1.338865    -0.889503     0.966576      19.92
 C      -3.018336    -0.650991    -1.929879      46.64
 C      -4.032209    -1.386147    -2.746339      47.05
 H      -4.085034    -0.834180    -3.882078      26.93
 O      -3.698231    -2.855320    -2.825329     214.57
 H      -2.790944    -3.043635    -2.757691      28.19
 C      -5.474931    -1.152865    -2.219804      96.59
 H      -5.481567    -1.374030    -1.170478      29.25
 O      -5.817442     0.140269    -2.746161     283.26
 H      -5.342905     0.674051    -2.189686      32.97
 C      -6.540584    -2.182859    -2.703946     111.71
 O      -6.456810    -3.402766    -1.985192     210.66
 H      -5.482353    -3.773514    -1.978180      26.94
 H      -6.442220    -2.356223    -3.807792      29.42
 H      -7.585583    -1.717462    -2.643901      28.84
55
name = lig-ACN-frame_258
 C       3.905951     2.476130    -0.618739      75.30
 H       3.275745     3.377235    -0.721649      24.58
 C       4.338873     0.411068     0.565884      45.09
 H       3.992682    -0.307551     1.325713      18.50
 C       5.466859     0.231249    -0.291350      12.27
 O       6.265445    -0.918627    -0.294238     208.91
 C       5.988143    -1.907430     0.818339     105.36
 H       5.924741    -1.313317     1.878959      27.02
 H       6.710488    -2.690548     0.793403      26.72
 H       5.015454    -2.329517     0.779283      29.19
 C       5.957556     1.296848    -1.102276      14.65
 O       7.111324     1.359125    -1.741172     174.11
 H       7.789352     0.805518    -1.352532      24.45
 C       5.062102     2.402587    -1.280368      61.75
 H       5.386390     3.159009    -1.992319      22.21
 C       3.514063     1.549921     0.318530      27.52
 C       2.265085     1.747998     1.213892     107.76
 H       2.503366     2.575799     1.684850      26.88
 O       2.138183     0.771951     2.257930     266.12
 H       1.707746    -0.185321     1.918901      19.56
 C       0.853900     1.974514     0.596222      79.88
 H       0.972288     2.749427    -0.289456      21.67
 C      -0.263361     2.588453     1.473265     109.08
 O      -0.152961     3.814113     2.113838     311.16
 H       0.344180     4.431324     1.534091      29.94
 H      -0.439780     1.860511     2.288565      24.84
 H      -1.118630     2.592798     0.827608      25.90
 C      -2.742208    -1.129858    -0.613204      70.54
 H      -3.258447    -1.769585    -0.037558      18.51
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 C      -2.152145     0.338271    -2.522979      32.17
 H      -2.296045     0.519892    -3.574074      23.48
 C      -1.050093     0.938515    -1.865646       7.97
 O      -0.180596     1.921722    -2.336350     217.75
 C      -0.689400     2.720225    -3.491247     105.18
 H      -0.181515     3.741466    -3.226171      24.16
 H       0.014426     2.425043    -4.330255      24.23
 H      -1.741617     2.526314    -3.557311      27.83
 C      -0.764185     0.396920    -0.597756      26.70
 O       0.520517     0.664438    -0.040273     190.56
 C      -1.576053    -0.535374     0.037576      40.65
 H      -1.179840    -0.949903     0.858947      23.32
 C      -2.959308    -0.633447    -1.975967      43.59
 C      -3.984595    -1.455962    -2.793654      31.67
 H      -3.835921    -1.177609    -4.021398      25.17
 O      -3.766155    -2.844797    -2.735894     143.83
 H      -2.681208    -3.003556    -2.942348      22.36
 C      -5.492699    -1.170722    -2.264304      93.06
 H      -5.524559    -1.050732    -1.203285      27.54
 O      -5.909283     0.154542    -2.680915     263.95
 H      -5.497680     0.928044    -2.114970      25.03
 C      -6.519187    -2.196813    -2.740340     108.85
 O      -6.450160    -3.402111    -1.925466     227.47
 H      -5.433583    -3.613603    -1.958685      28.13
 H      -6.452978    -2.440497    -3.825420      28.86
 H      -7.551444    -1.799257    -2.437054      27.40
55
name = lig-ACN-frame_259
 C       3.845469     2.537603    -0.555452      44.39
 H       3.161870     3.431625    -0.765883      22.27
 C       4.319920     0.420883     0.573627      53.00
 H       3.910600    -0.409322     1.171212      15.86
 C       5.455412     0.212073    -0.261097      13.06
 O       6.246570    -0.940803    -0.203138     214.40
 C       5.974180    -1.858078     0.798171     121.40
 H       5.964049    -1.364399     1.875008      27.68
 H       6.855227    -2.488170     0.779213      25.92
 H       5.114188    -2.487222     0.538755      28.14
 C       5.839030     1.270663    -1.180204      10.44
 O       7.195152     1.315920    -1.712423     183.62
 H       7.655729     0.642704    -1.216061      26.62
 C       5.086382     2.434437    -1.309795      53.54
 H       5.300740     3.222606    -2.044073      22.53
 C       3.420805     1.471436     0.307447      11.91
 C       2.217320     1.790015     1.237172     108.41
 H       2.297536     2.653524     1.712446      26.72
 O       2.176900     0.799442     2.247481     276.94
 H       1.870674    -0.087083     1.777371      21.52
 C       0.865501     1.961221     0.487455      78.65
 H       0.970605     2.693029    -0.395053      20.56
 C      -0.279273     2.476277     1.457590     102.87
 O      -0.077143     3.836035     2.054384     330.53
 H       0.384291     4.346405     1.560630      35.40
 H      -0.539138     1.847746     2.277653      25.23
 H      -1.095971     2.548144     0.762197      25.11
 C      -2.677048    -1.075656    -0.632368      37.80
 H      -3.360442    -1.809431    -0.294356      20.06
 C      -2.106757     0.327242    -2.548699     131.19
 H      -2.279564     0.503664    -3.612182      18.73
 C      -1.007306     0.896670    -1.900013      14.06
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 O      -0.211233     1.932176    -2.366431     256.29
 C      -0.575314     2.641828    -3.494960     154.71
 H      -0.640977     3.776109    -3.373374      28.66
 H      -0.178863     2.300275    -4.447597      28.08
 H      -1.625430     2.618507    -3.669261      30.66
 C      -0.690471     0.377579    -0.624404      30.68
 O       0.471781     0.656225    -0.046705     211.55
 C      -1.604504    -0.546608     0.004558      44.36
 H      -1.351610    -0.946024     0.989457      20.25
 C      -2.918458    -0.744744    -1.954851      69.43
 C      -4.001961    -1.416238    -2.813816      19.51
 H      -3.998196    -0.987814    -3.999957      26.48
 O      -3.797343    -2.902957    -2.638054     148.61
 H      -2.693086    -3.126069    -2.840043      20.82
 C      -5.436090    -1.131175    -2.316861      83.36
 H      -5.311856    -1.362707    -1.267341      27.42
 O      -6.028419     0.192767    -2.673926     238.19
 H      -5.418689     0.787400    -1.927833      23.34
 C      -6.531304    -2.205477    -2.732380     101.66
 O      -6.418288    -3.405851    -1.875242     229.25
 H      -5.581265    -3.792650    -1.885476      31.27
 H      -6.440990    -2.396504    -3.835000      29.71
 H      -7.577137    -1.749519    -2.599951      28.32
55
name = lig-ACN-frame_260
 C       3.811423     2.552582    -0.581703      59.56
 H       3.149870     3.486927    -0.704205      22.90
 C       4.214891     0.363252     0.467024      48.06
 H       4.132896    -0.382585     1.264562      20.87
 C       5.430875     0.260863    -0.258035      14.68
 O       6.255171    -0.854819    -0.189692     220.54
 C       5.995350    -1.926456     0.841613     110.08
 H       5.726554    -1.478455     1.833569      26.36
 H       6.921216    -2.575928     0.944379      24.79
 H       5.038021    -2.490652     0.617570      25.80
 C       5.868927     1.261016    -1.163003      -0.33
 O       7.180494     1.232038    -1.696618     153.03
 H       7.873033     0.719200    -1.096572      28.08
 C       5.010214     2.427714    -1.316357      48.78
 H       5.563157     3.234972    -1.820861      22.17
 C       3.404113     1.570036     0.333270      20.50
 C       2.187384     1.812015     1.230857     103.78
 H       2.407555     2.674190     1.721993      23.70
 O       2.163940     0.785844     2.286798     312.98
 H       1.837388     0.000994     1.931468      25.28
 C       0.840768     1.983488     0.454212      86.89
 H       1.038378     2.706517    -0.372004      20.52
 C      -0.312594     2.436757     1.377375      99.47
 O      -0.003880     3.806275     2.001579     310.08
 H       0.544793     4.266288     1.427084      31.31
 H      -0.293194     1.719276     2.111450      24.84
 H      -1.342106     2.414418     0.982065      24.14
 C      -2.689021    -1.093657    -0.687239      65.50
 H      -3.151777    -1.935805    -0.078512      19.51
 C      -2.103805     0.249829    -2.682106      29.59
 H      -2.425268     0.802533    -3.574495      18.28
 C      -1.039508     0.842656    -1.924911       9.64
 O      -0.183665     1.893382    -2.316556     192.26
 C      -0.644846     2.653535    -3.663335     113.52
 H      -0.144666     3.610553    -3.350689      24.34
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 H      -0.016442     2.311133    -4.409207      27.09
 H      -1.656960     2.533804    -3.846758      29.66
 C      -0.730602     0.343592    -0.627083      36.23
 O       0.567462     0.639546     0.029319     185.02
 C      -1.513515    -0.575267     0.038164      38.61
 H      -1.283240    -0.713598     1.195637      15.58
 C      -2.880617    -0.707729    -2.079041      50.53
 C      -3.994040    -1.399737    -2.791769      58.44
 H      -3.754944    -1.213494    -4.005026      25.95
 O      -3.818885    -2.907214    -2.598056     203.00
 H      -2.876673    -3.110845    -2.590853      26.43
 C      -5.494251    -1.136561    -2.299901      87.30
 H      -5.539169    -1.105264    -1.214149      28.02
 O      -6.044826     0.172699    -2.627416     276.91
 H      -5.622962     1.008487    -2.157589      25.58
 C      -6.466488    -2.230001    -2.718706     109.06
 O      -6.442335    -3.364359    -1.856317     241.65
 H      -5.520024    -3.698638    -2.031726      28.68
 H      -6.411305    -2.629916    -3.758593      29.39
 H      -7.495617    -1.792759    -2.535685      28.07
55
name = lig-ACN-frame_261
 C       3.822666     2.542399    -0.644214      58.47
 H       3.336030     3.561616    -0.715164      23.10
 C       4.120028     0.396105     0.374458      61.64
 H       3.656110    -0.228259     1.144695      22.18
 C       5.372519     0.244246    -0.282859      22.35
 O       6.291730    -0.836299    -0.129249     204.01
 C       5.967575    -1.913326     0.869153     107.82
 H       5.856008    -1.524190     1.843428      27.53
 H       6.936296    -2.587490     0.772294      24.57
 H       5.102259    -2.575617     0.435307      25.25
 C       5.909926     1.324534    -1.069223      17.74
 O       7.096821     1.175082    -1.714277      96.69
 H       7.770877     0.823036    -0.962176      21.67
 C       5.058162     2.383310    -1.295091      52.91
 H       5.296397     3.280763    -1.878716      22.51
 C       3.431224     1.600070     0.328980      27.22
 C       2.216175     1.814138     1.290925      90.44
 H       2.294987     2.719359     1.848781      21.38
 O       2.100395     0.808080     2.320951     327.02
 H       1.711461     0.020108     1.959290      23.58
 C       0.830809     1.993070     0.472077      76.33
 H       0.903821     2.589772    -0.410873      20.11
 C      -0.262911     2.493752     1.404725     109.35
 O       0.006103     3.682217     1.938522     316.21
 H       0.601910     4.409956     1.435616      26.49
 H      -0.300835     1.892205     2.223149      24.29
 H      -1.216992     2.486529     0.792714      23.19
 C      -2.561908    -1.112747    -0.720797      60.03
 H      -3.406082    -1.868895    -0.379317      18.53
 C      -2.063796     0.291277    -2.736511      50.15
 H      -2.363523     0.529341    -3.786023      22.72
 C      -1.008649     0.821576    -1.955053      -2.38
 O      -0.256105     1.876130    -2.410843     211.19
 C      -0.554575     2.606996    -3.676276     118.70
 H      -0.258927     3.646400    -3.600647      26.13
 H      -0.160889     2.087160    -4.449880      27.25
 H      -1.611392     2.851028    -3.798368      26.77
 C      -0.618151     0.327684    -0.579893      23.86
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 O       0.557522     0.594006     0.005852     208.06
 C      -1.530204    -0.593264    -0.013077      35.09
 H      -1.240425    -1.158685     1.069647      18.69
 C      -2.888802    -0.717822    -2.026244      67.86
 C      -4.007918    -1.492772    -2.774931      41.24
 H      -4.080916    -1.216239    -3.964582      25.23
 O      -3.847846    -2.871647    -2.578804     284.43
 H      -2.985404    -3.031027    -2.448786      32.45
 C      -5.496109    -1.100700    -2.212834      82.52
 H      -5.328892    -1.240166    -1.128704      26.81
 O      -6.049511     0.159793    -2.653318     304.88
 H      -5.517818     0.681166    -2.155624      31.57
 C      -6.497542    -2.217266    -2.739676     100.59
 O      -6.448162    -3.338152    -1.825050     215.52
 H      -5.513286    -3.818029    -1.715598      25.83
 H      -6.192909    -2.378532    -3.810758      30.07
 H      -7.543566    -1.824982    -2.730924      27.99
55
name = lig-ACN-frame_262
 C       3.845296     2.590930    -0.624520      61.81
 H       3.218000     3.468165    -0.841535      23.11
 C       4.089343     0.376325     0.372815      41.22
 H       3.756248    -0.596069     0.734809      17.38
 C       5.358491     0.193686    -0.237203      21.02
 O       6.270816    -0.825319    -0.042794     249.63
 C       5.974788    -1.871719     0.803759     120.82
 H       5.805900    -1.572700     1.763200      31.09
 H       6.904355    -2.634036     0.848351      24.72
 H       4.931363    -2.419905     0.579725      26.55
 C       5.853777     1.283213    -0.983425      13.91
 O       7.071699     1.158289    -1.736755     198.39
 H       7.799709     0.665317    -1.268564      20.21
 C       5.109944     2.463260    -1.304834      49.56
 H       5.536888     2.978893    -2.167074      21.91
 C       3.363507     1.622662     0.295811      27.94
 C       2.203292     1.841595     1.287537     103.66
 H       2.407930     2.814163     1.799433      21.82
 O       2.027464     0.846691     2.339272     279.75
 H       1.674695    -0.046511     1.844726      16.97
 C       0.923205     1.905568     0.506851      89.06
 H       1.070294     2.614034    -0.241060      20.34
 C      -0.262578     2.378806     1.386194      91.33
 O       0.010977     3.767134     2.004027     227.64
 H       0.631141     4.261921     1.134640      23.67
 H      -0.608157     1.708085     2.076820      24.62
 H      -1.173274     2.433905     0.699521      22.09
 C      -2.578642    -1.144886    -0.794417     102.46
 H      -3.125632    -1.965054    -0.126996      16.35
 C      -2.068861     0.243404    -2.625194      27.79
 H      -2.024475     0.504866    -3.694168      14.27
 C      -0.973752     0.825075    -1.965760      21.29
 O      -0.253749     1.912306    -2.491777     250.36
 C      -0.533477     2.557889    -3.690564     120.22
 H       0.159468     3.339001    -3.632841      26.12
 H      -0.429460     1.978033    -4.550937      29.31
 H      -1.613364     2.797737    -3.722419      28.56
 C      -0.650400     0.307848    -0.711443      47.75
 O       0.580858     0.595845    -0.010356     204.54
 C      -1.459895    -0.644701    -0.059211      68.98
 H      -1.069787    -1.258962     1.007813      17.02
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 C      -2.893455    -0.716050    -2.092017      56.69
 C      -4.072089    -1.409409    -2.714610      42.45
 H      -4.001875    -1.105763    -3.869225      25.05
 O      -3.870074    -2.913230    -2.565517     149.33
 H      -2.782436    -3.114575    -2.488644      24.50
 C      -5.485028    -1.162326    -2.185060     101.28
 H      -5.651226    -1.156233    -1.088489      26.95
 O      -5.975953     0.153087    -2.652925     290.92
 H      -5.647726     0.950762    -2.243750      28.15
 C      -6.461723    -2.173040    -2.705391     109.86
 O      -6.502326    -3.331504    -1.804321     247.92
 H      -5.555777    -3.534088    -1.833398      30.79
 H      -6.215200    -2.627571    -3.698788      31.03
 H      -7.497912    -1.820020    -2.776588      28.91
55
name = lig-ACN-frame_263
 C       3.880263     2.650075    -0.584379      55.18
 H       3.226243     3.464301    -0.776757      22.59
 C       4.077791     0.300794     0.386848      60.37
 H       3.537389    -0.356046     1.069463      19.38
 C       5.367733     0.272357    -0.159278      31.78
 O       6.268200    -0.788776    -0.046826     217.22
 C       5.905308    -1.913243     0.876201     105.18
 H       5.840592    -1.592990     1.810406      27.47
 H       6.788363    -2.707615     0.695400      23.19
 H       4.920055    -2.459218     0.438225      23.63
 C       5.887258     1.274027    -1.061093      19.71
 O       7.040018     1.151292    -1.739492     186.68
 H       7.557709     0.600984    -1.189626      29.34
 C       5.102131     2.412999    -1.254710      57.10
 H       5.452404     3.187881    -1.940487      23.88
 C       3.410543     1.542447     0.261347      17.06
 C       2.201897     1.784237     1.258122      89.51
 H       2.332641     2.830084     1.800364      21.02
 O       2.011589     0.896912     2.345601     288.04
 H       1.738614    -0.107990     1.975736      17.59
 C       0.859316     1.927322     0.511389      90.78
 H       0.986358     2.560946    -0.278416      22.08
 C      -0.304933     2.405680     1.363081      93.30
 O      -0.034998     3.726337     2.042802     217.17
 H       0.620518     4.518307     1.420077      24.40
 H      -0.366373     1.780161     2.220481      22.04
 H      -1.201701     2.547539     0.667984      21.62
 C      -2.577603    -1.199606    -0.710998      59.37
 H      -3.184730    -2.100598    -0.361843      18.34
 C      -2.062810     0.243375    -2.685157      65.58
 H      -2.509024     0.644143    -3.602120      21.28
 C      -0.968435     0.871034    -1.977154      10.08
 O      -0.166452     1.861852    -2.420390     187.03
 C      -0.593735     2.544127    -3.825848     106.19
 H       0.106038     3.252834    -3.992181      26.93
 H      -0.446567     1.789607    -4.557338      26.68
 H      -1.490429     3.212995    -3.782034      25.79
 C      -0.584100     0.313809    -0.692388      48.59
 O       0.621681     0.576632    -0.073007     208.56
 C      -1.376133    -0.717315    -0.218281      14.84
 H      -0.992132    -0.956239     0.974276      13.55
 C      -2.891349    -0.739143    -2.007340      57.61
 C      -4.076943    -1.416623    -2.720434      63.97
 H      -4.215096    -1.237912    -3.824226      28.13
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 O      -3.886732    -2.927344    -2.576260     153.44
 H      -2.752802    -3.060452    -2.733637      22.19
 C      -5.505378    -1.087540    -2.159044      87.90
 H      -5.413718    -1.155910    -1.037318      27.29
 O      -5.911800     0.166169    -2.688388     291.21
 H      -5.387978     0.729078    -1.887898      22.71
 C      -6.495863    -2.224650    -2.704334     105.13
 O      -6.535707    -3.294973    -1.780247     264.30
 H      -5.739845    -3.778616    -1.744964      31.87
 H      -6.220546    -2.454237    -3.766903      32.12
 H      -7.426060    -1.655674    -2.654507      29.27
55
name = lig-ACN-frame_264
 C       3.872670     2.533761    -0.485587      58.61
 H       3.488344     3.502104    -0.477167      24.34
 C       4.110830     0.355579     0.430047      57.30
 H       3.993169    -0.368245     1.227983      24.43
 C       5.411078     0.272945    -0.152833      12.11
 O       6.273303    -0.827867    -0.017661     211.30
 C       5.852591    -1.920899     0.865777     112.39
 H       5.800109    -1.690665     1.849761      27.48
 H       6.699132    -2.717356     0.777379      23.62
 H       4.748277    -2.344240     0.611495      23.36
 C       5.798293     1.283104    -1.075107      14.57
 O       7.072700     1.116529    -1.747335     156.70
 H       7.793752     0.683838    -1.166768      29.65
 C       5.063839     2.454254    -1.237043      55.35
 H       5.478518     3.336205    -1.725264      23.38
 C       3.369599     1.535753     0.303517      38.49
 C       2.173317     1.781131     1.183436      91.89
 H       2.477884     2.842371     1.720557      20.45
 O       2.051431     0.895514     2.372510     296.46
 H       1.677998     0.019733     2.042312      19.39
 C       0.807267     1.987754     0.397373      84.18
 H       0.885825     2.653191    -0.379389      21.05
 C      -0.317453     2.506407     1.413933     101.44
 O      -0.101078     3.670593     2.076760     306.85
 H       0.536070     4.305030     1.515178      27.13
 H      -0.531858     1.679369     2.147471      21.29
 H      -1.373840     2.408003     0.919223      21.80
 C      -2.508297    -1.243123    -0.722505      52.83
 H      -3.046656    -1.994742    -0.184451      17.91
 C      -2.141972     0.282406    -2.664259     122.92
 H      -2.524892     0.746944    -3.571843      21.30
 C      -0.996600     0.842830    -2.002905      30.48
 O      -0.119583     1.924096    -2.507500     249.84
 C      -0.531332     2.501627    -3.836183     141.17
 H       0.144639     3.071871    -4.216425      26.33
 H      -0.985783     1.663118    -4.472768      26.60
 H      -1.549016     2.881226    -3.592690      29.36
 C      -0.556106     0.290375    -0.768224      62.42
 O       0.657719     0.593843    -0.122177     195.01
 C      -1.310796    -0.782018    -0.150451      54.19
 H      -0.937335    -1.383352     0.859178      13.18
 C      -2.885892    -0.735066    -1.983397      63.45
 C      -4.057992    -1.513958    -2.740463      33.22
 H      -3.929577    -1.137230    -3.745927      34.77
 O      -3.884076    -2.897627    -2.612858     262.47
 H      -2.991408    -3.141861    -2.901547      28.44
 C      -5.467956    -1.146702    -2.207108      90.66
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 H      -5.555901    -1.129556    -1.084152      25.42
 O      -5.833136     0.233067    -2.661429     269.75
 H      -5.476808     1.113547    -2.145440      23.08
 C      -6.532500    -2.125883    -2.648519     111.75
 O      -6.585376    -3.304418    -1.735936     204.17
 H      -5.675398    -3.794463    -1.913253      28.70
 H      -6.320122    -2.519284    -3.672363      31.98
 H      -7.586573    -1.902341    -2.728946      29.36
55
name = lig-ACN-frame_265
 C       3.843218     2.555834    -0.452094      41.38
 H       3.220704     3.431955    -0.418900      22.47
 C       4.248145     0.377432     0.561326      50.85
 H       3.806980    -0.418045     1.147868      14.55
 C       5.401958     0.217822    -0.217559      19.28
 O       6.267181    -0.869514     0.022256     215.52
 C       5.811422    -1.909543     0.867081     120.29
 H       5.773321    -1.557018     1.837159      29.95
 H       6.492358    -2.793469     0.730924      25.10
 H       4.728884    -2.286707     0.520181      25.63
 C       5.883351     1.243020    -1.093278      10.84
 O       7.063640     1.114308    -1.751300     145.92
 H       7.777288     0.940729    -0.977350      23.60
 C       5.072188     2.451291    -1.177403      48.85
 H       5.482700     3.258450    -1.808029      22.78
 C       3.338893     1.467637     0.376393      10.76
 C       2.101271     1.855871     1.219563      87.01
 H       2.251443     2.996172     1.739664      21.13
 O       2.079034     0.926454     2.327594     302.79
 H       1.784682     0.112335     2.045316      25.34
 C       0.821026     2.002569     0.383735      86.65
 H       0.972433     2.716831    -0.372446      20.83
 C      -0.397056     2.345794     1.376767      87.07
 O      -0.117155     3.731101     2.141490     277.93
 H       0.383656     4.218625     1.640626      34.34
 H      -0.392071     1.554593     2.224798      21.06
 H      -1.281692     2.608530     0.739578      22.25
 C      -2.413726    -1.269300    -0.762009      49.20
 H      -2.928804    -2.029095    -0.343669      18.12
 C      -2.209744     0.358592    -2.554504      53.17
 H      -2.445740     0.581508    -3.594398      13.28
 C      -0.945330     0.860790    -2.040567       3.62
 O      -0.138797     1.896115    -2.588734     249.29
 C      -0.605355     2.395577    -3.791408     122.44
 H       0.201283     2.857597    -4.169472      28.25
 H      -0.650117     1.551840    -4.646749      25.97
 H      -1.286220     3.240710    -3.741611      27.88
 C      -0.551423     0.198442    -0.793966      31.60
 O       0.633107     0.676315    -0.187677     207.72
 C      -1.238598    -0.788097    -0.100323      50.59
 H      -0.699485    -1.316812     0.713870      19.13
 C      -2.900884    -0.752243    -2.000535      31.72
 C      -3.992101    -1.451226    -2.753068      58.75
 H      -4.029854    -1.239902    -3.760275      25.96
 O      -3.873694    -2.955771    -2.664170     263.34
 H      -3.046751    -3.158218    -2.881403      31.84
 C      -5.461196    -1.071948    -2.221254      73.62
 H      -5.354432    -1.165860    -1.094380      26.40
 O      -5.777581     0.257871    -2.676825     310.75
 H      -5.341871     0.712650    -1.965576      26.73
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 C      -6.624633    -2.136619    -2.641496      98.50
 O      -6.597955    -3.283195    -1.717017     210.84
 H      -5.658476    -3.675013    -1.874885      28.11
 H      -6.432165    -2.507651    -3.666801      30.91
 H      -7.428613    -1.408135    -2.519526      28.90
55
name = lig-ACN-frame_266
 C       3.851039     2.537863    -0.472635      59.25
 H       3.236150     3.350952    -0.893611      22.09
 C       4.227069     0.383978     0.643406      50.34
 H       3.934796    -0.418427     1.314811      16.51
 C       5.399159     0.175793    -0.190553      21.52
 O       6.289593    -0.881597    -0.020338     177.79
 C       5.743812    -1.942835     0.893174     121.52
 H       5.727799    -1.686863     1.942529      29.83
 H       6.468461    -2.719422     0.803234      26.45
 H       4.651586    -2.251650     0.596277      24.90
 C       5.847651     1.248545    -1.027985      20.32
 O       7.108049     1.140494    -1.760200     175.92
 H       7.870795     0.874953    -1.174106      23.93
 C       5.082407     2.375305    -1.105950      54.69
 H       5.330376     3.180171    -1.816331      23.95
 C       3.450991     1.574371     0.405326      23.79
 C       2.142671     1.851130     1.264035      99.73
 H       2.297623     2.983128     1.844820      21.88
 O       2.038041     0.978655     2.327421     287.28
 H       1.864009     0.067084     1.947766      22.34
 C       0.773814     1.985566     0.474466      96.05
 H       0.853483     2.795681    -0.245199      20.70
 C      -0.365382     2.380888     1.342171      96.18
 O      -0.160637     3.654623     2.145749     286.33
 H       0.349077     4.278308     1.628429      31.53
 H      -0.583944     1.600313     2.214993      21.27
 H      -1.353469     2.218981     0.839594      22.77
 C      -2.373646    -1.354001    -0.761203      28.62
 H      -2.736489    -2.249496    -0.517322      19.28
 C      -2.176009     0.418135    -2.558254      43.01
 H      -2.630564     0.877064    -3.443085      14.26
 C      -1.013628     0.800073    -1.981901      19.59
 O      -0.210959     1.748493    -2.533986     217.96
 C      -0.566165     2.407189    -3.931926      97.72
 H       0.270490     2.919754    -4.186990      24.97
 H      -1.067666     1.526085    -4.653766      22.81
 H      -1.465552     2.956688    -3.799713      26.26
 C      -0.478336     0.313452    -0.797846      42.13
 O       0.665342     0.722886    -0.254515     238.58
 C      -1.212049    -0.801816    -0.210676      53.50
 H      -0.954731    -1.061666     0.739731      16.12
 C      -2.802460    -0.732701    -1.953683      63.56
 C      -4.034333    -1.473246    -2.802045      71.28
 H      -3.920135    -1.119023    -3.732277      27.45
 O      -3.873617    -2.970903    -2.712424     243.64
 H      -2.801042    -3.139309    -2.760855      23.11
 C      -5.421461    -1.112760    -2.249473      88.98
 H      -5.446082    -1.082326    -1.128539      27.02
 O      -5.719491     0.252492    -2.679702     322.77
 H      -5.559819     0.905365    -2.116755      33.33
 C      -6.594977    -2.047367    -2.593032     112.86
 O      -6.584100    -3.193065    -1.727775     242.29
 H      -5.761534    -3.603849    -1.751550      33.19
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 H      -6.771857    -2.256672    -3.670314      30.33
 H      -7.643859    -1.803258    -2.341037      27.96
55
name = lig-ACN-frame_267
 C       3.866326     2.525682    -0.559498      49.75
 H       3.185371     3.428822    -0.727658      22.85
 C       4.201940     0.445541     0.616519      65.27
 H       3.976738    -0.118642     1.520758      25.30
 C       5.425094     0.213994    -0.060994      21.52
 O       6.238719    -0.951748    -0.013083     216.78
 C       5.755253    -1.984189     0.881332     119.14
 H       5.656448    -1.492412     1.890604      25.81
 H       6.342375    -2.839607     0.820732      26.47
 H       4.725248    -2.303377     0.546437      25.92
 C       5.917857     1.189764    -0.950487      18.05
 O       7.092456     1.176285    -1.732202     182.57
 H       7.695981     0.722537    -1.192799      29.98
 C       5.131928     2.382072    -1.193714      37.69
 H       5.597050     3.087885    -1.903898      23.76
 C       3.461764     1.625621     0.515084      22.66
 C       2.210187     1.884525     1.266114      77.09
 H       2.443702     3.027988     1.826936      19.29
 O       1.978473     0.974614     2.421821     257.96
 H       1.707524    -0.049036     2.089730      16.41
 C       0.874455     2.034117     0.488993      80.19
 H       0.967996     2.846091    -0.266949      20.78
 C      -0.416530     2.373633     1.464767      98.75
 O      -0.221941     3.547036     2.096715     233.21
 H       0.353572     4.264219     1.406943      25.09
 H      -0.472927     1.490894     2.249273      20.17
 H      -1.257576     2.531615     0.799301      22.06
 C      -2.305964    -1.405151    -0.870202      97.60
 H      -2.656687    -2.250064    -0.332419      14.72
 C      -2.286684     0.322099    -2.552401      50.90
 H      -2.721168     1.009698    -3.291552      14.01
 C      -1.021878     0.858928    -1.992062      16.44
 O      -0.221667     1.765332    -2.623316     247.84
 C      -0.587166     2.304949    -3.892730     100.51
 H       0.287950     2.923941    -4.357555      24.90
 H      -0.609446     1.384103    -4.719471      25.57
 H      -1.374734     2.996417    -3.807641      27.91
 C      -0.572738     0.292348    -0.743414      68.50
 O       0.785573     0.765802    -0.258174     175.25
 C      -1.155261    -0.777191    -0.186955      -8.70
 H      -0.785925    -1.186918     0.624057      17.00
 C      -2.901660    -0.822539    -2.042439      22.17
 C      -3.960119    -1.505455    -2.776710      60.52
 H      -3.977527    -1.256304    -3.734728      33.02
 O      -3.857151    -2.915355    -2.764352     188.20
 H      -2.710421    -3.170177    -2.774716      24.32
 C      -5.413249    -1.077896    -2.213998      77.34
 H      -5.268955    -1.153280    -1.102220      26.39
 O      -5.696438     0.252449    -2.759016     261.92
 H      -5.430272     0.726718    -1.895793      22.77
 C      -6.643942    -1.955821    -2.558451     102.17
 O      -6.538920    -3.167505    -1.723930     216.01
 H      -5.615206    -3.489496    -1.981770      30.07
 H      -6.525817    -2.268109    -3.602740      31.02
 H      -7.396361    -1.184939    -2.315783      28.73
55
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name = lig-ACN-frame_268
 C       3.910131     2.543582    -0.580374      61.13
 H       3.389688     3.550725    -0.739504      23.41
 C       4.266742     0.475562     0.709491      48.86
 H       3.797754    -0.295790     1.340980      18.50
 C       5.492755     0.251302     0.007508      16.39
 O       6.167992    -0.997570    -0.001954     188.07
 C       5.723764    -2.031149     0.888280     122.20
 H       5.718810    -1.747702     2.021048      27.69
 H       6.516687    -2.714100     0.839187      26.29
 H       4.713442    -2.366684     0.639389      26.89
 C       5.926949     1.269067    -0.939705      30.05
 O       7.081766     1.141936    -1.657750      85.91
 H       7.883302     0.720851    -1.192833      24.94
 C       5.130973     2.334593    -1.254327      63.61
 H       5.471466     3.073013    -1.979036      24.12
 C       3.490245     1.661103     0.410870      13.36
 C       2.183999     1.914268     1.419086      87.41
 H       2.247381     3.035592     2.053088      21.51
 O       1.958480     1.016163     2.497700     257.58
 H       1.685521     0.047575     2.046684      18.50
 C       0.920499     2.047554     0.493217      77.35
 H       1.008731     2.952258    -0.195564      21.38
 C      -0.369288     2.209851     1.394407      86.77
 O      -0.243830     3.597896     2.144835     148.76
 H       0.347060     4.291775     1.393961      25.97
 H      -0.539963     1.462301     2.275254      21.47
 H      -1.267782     2.071877     0.835099      23.51
 C      -2.225005    -1.413667    -0.886764      48.73
 H      -2.773813    -2.368630    -0.571113      16.54
 C      -2.307175     0.344348    -2.534587      50.60
 H      -2.731414     0.541005    -3.527924      16.74
 C      -1.097483     0.860055    -2.000000       0.55
 O      -0.194406     1.812405    -2.636981     220.31
 C      -0.591742     2.231770    -3.945568     100.12
 H       0.316901     2.947494    -4.134097      22.99
 H      -0.748996     1.324577    -4.782750      24.35
 H      -1.539699     2.708076    -4.002775      27.35
 C      -0.463127     0.407812    -0.758384      22.90
 O       0.767173     0.758423    -0.271669     191.13
 C      -1.182917    -0.843971    -0.168494      48.29
 H      -0.686859    -1.426979     0.509412      19.61
 C      -2.838165    -0.880367    -2.028785      29.41
 C      -4.043346    -1.507695    -2.833585      78.58
 H      -3.990296    -1.085440    -3.741522      27.55
 O      -3.828114    -2.953839    -2.782387     266.39
 H      -2.786314    -3.148067    -2.968604      26.96
 C      -5.353937    -1.037140    -2.212740      99.10
 H      -5.336096    -0.887242    -1.132471      27.29
 O      -5.651797     0.253279    -2.778095     247.59
 H      -5.387721     1.195274    -2.262623      23.67
 C      -6.560760    -1.904905    -2.538286     107.85
 O      -6.516237    -3.120464    -1.743955     199.04
 H      -5.595539    -3.618725    -2.023417      27.25
 H      -6.745748    -2.087502    -3.608782      29.94
 H      -7.622976    -1.583245    -2.325283      27.93
55
name = lig-ACN-frame_269
 C       3.910810     2.606214    -0.530718      46.52
 H       3.279009     3.468526    -0.902006      22.65
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 C       4.305557     0.533996     0.748495      61.57
 H       3.939566    -0.351312     1.292584      20.23
 C       5.480123     0.274349     0.020740      18.15
 O       6.131173    -0.949348     0.007302     174.64
 C       5.712381    -2.102098     0.937015     106.83
 H       5.640779    -1.679762     2.059188      25.54
 H       6.390339    -2.927620     0.719138      25.62
 H       4.810413    -2.523907     0.655277      28.07
 C       5.937538     1.243679    -0.888519      16.74
 O       7.155199     1.071443    -1.634105     139.31
 H       7.827484     0.896808    -0.830651      23.85
 C       5.094205     2.340126    -1.288409      41.11
 H       5.401332     2.979449    -2.108729      22.92
 C       3.463123     1.644482     0.499818       8.92
 C       2.182098     1.934512     1.401825      82.26
 H       2.444272     3.081240     1.915022      22.52
 O       1.983899     1.047647     2.538602     293.88
 H       1.847787     0.106333     2.248591      23.76
 C       0.871085     1.996545     0.565612      87.32
 H       1.007972     2.838455    -0.238554      21.43
 C      -0.295008     2.238811     1.391735     107.68
 O      -0.293635     3.549204     2.120711     264.36
 H       0.258606     4.219165     1.596877      30.29
 H      -0.146983     1.459444     2.200173      21.32
 H      -1.181942     2.206292     0.847975      25.80
 C      -2.263427    -1.455442    -0.842221      59.39
 H      -2.366505    -2.598913    -0.483210      20.89
 C      -2.204391     0.353419    -2.568597      42.82
 H      -2.393446     0.757757    -3.548574      15.85
 C      -1.028993     0.910705    -1.958961       3.55
 O      -0.261440     1.798324    -2.573678     202.99
 C      -0.621823     2.198888    -4.055970      64.19
 H       0.073799     3.037700    -4.699428      22.09
 H      -0.548135     1.204208    -4.620848      25.61
 H      -1.611636     2.644472    -3.949452      25.32
 C      -0.557886     0.292747    -0.779534      34.16
 O       0.748675     0.771034    -0.279527     198.31
 C      -1.071100    -0.794709    -0.280273      57.89
 H      -0.675282    -1.159988     0.681462      17.05
 C      -2.773380    -0.819457    -2.030365      40.37
 C      -3.962340    -1.498069    -2.795034      59.47
 H      -4.017723    -1.286280    -3.796883      28.59
 O      -3.839914    -2.995830    -2.819063     271.75
 H      -3.004497    -3.087351    -3.113045      31.45
 C      -5.380650    -0.955754    -2.200525      81.17
 H      -5.209853    -0.966234    -1.130992      28.80
 O      -5.627634     0.304199    -2.885898     267.79
 H      -5.257921     0.889187    -2.070651      24.20
 C      -6.550473    -1.933051    -2.541778     111.52
 O      -6.466426    -3.126720    -1.774718     232.37
 H      -5.690352    -3.669563    -1.975789      31.28
 H      -6.488350    -2.089842    -3.614627      31.24
 H      -7.438610    -1.378276    -2.168914      28.94
55
name = lig-ACN-frame_270
 C       3.847953     2.548288    -0.455402      57.61
 H       3.102919     3.303999    -0.710515      23.86
 C       4.260052     0.537439     0.767202      61.87
 H       3.967323    -0.017489     1.669637      23.68
 C       5.424429     0.280368     0.011634       6.13
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 O       6.135291    -0.970691     0.072089     166.88
 C       5.699693    -2.066708     0.889498     111.94
 H       5.755832    -1.751404     2.092468      24.51
 H       6.542218    -2.826707     0.839957      23.91
 H       4.720742    -2.267974     0.694593      27.01
 C       5.966265     1.245175    -0.953785      16.13
 O       7.187041     0.994033    -1.554086      73.58
 H       8.004809     0.943674    -0.987335      25.92
 C       5.084102     2.316867    -1.214505      48.12
 H       5.369892     2.934163    -2.057422      22.91
 C       3.495312     1.720648     0.579220      32.11
 C       2.219018     1.873417     1.311643      89.53
 H       2.221993     3.046881     1.817715      22.05
 O       2.060352     1.094229     2.559903     276.59
 H       1.972706     0.228931     2.308064      27.59
 C       0.918438     1.996341     0.463593      71.13
 H       0.988124     2.954804    -0.247122      20.76
 C      -0.342131     2.276211     1.506543     109.63
 O      -0.328235     3.519640     2.101920     328.06
 H       0.220862     4.024199     1.706835      36.45
 H      -0.516585     1.533377     2.296622      24.18
 H      -1.187446     2.182654     0.875010      24.74
 C      -2.205841    -1.390705    -0.869252      49.77
 H      -2.794607    -2.406721    -0.489313      20.99
 C      -2.098455     0.302876    -2.591310      70.92
 H      -2.642093     0.758877    -3.390354      19.58
 C      -0.994887     0.902464    -2.001189       6.34
 O      -0.253299     1.945389    -2.652803     233.36
 C      -0.670480     2.114743    -4.010491      85.85
 H       0.245473     2.930195    -4.191512      21.86
 H      -0.640586     1.243069    -4.701055      26.67
 H      -1.722356     2.550092    -4.208228      24.13
 C      -0.464709     0.371624    -0.789712      39.98
 O       0.716329     0.742211    -0.251965     197.12
 C      -1.101827    -0.906718    -0.254670      49.27
 H      -0.556728    -1.299168     0.718663      14.91
 C      -2.758045    -0.840020    -2.021711      49.24
 C      -3.892654    -1.498773    -2.755896      67.27
 H      -3.756905    -1.006129    -3.707593      28.69
 O      -3.878750    -2.968219    -2.812920     269.70
 H      -3.022267    -3.270883    -3.148993      31.31
 C      -5.308040    -1.011373    -2.271076      94.48
 H      -5.381052    -0.761687    -1.255363      28.34
 O      -5.582854     0.356779    -2.914489     250.70
 H      -5.484073     1.037984    -2.334428      31.47
 C      -6.497152    -1.922244    -2.569223     114.78
 O      -6.430832    -3.188080    -1.780682     251.98
 H      -5.607107    -3.448182    -2.096355      32.88
 H      -6.539986    -2.242523    -3.602950      31.03
 H      -7.491951    -1.477160    -2.533647      29.97
55
name = lig-ACN-frame_271
 C       3.877582     2.510225    -0.506770      58.46
 H       3.409169     3.411405    -0.797119      24.45
 C       4.281708     0.515042     0.840308      63.41
 H       4.070129    -0.233025     1.606134      21.65
 C       5.408956     0.206366     0.009124      18.53
 O       6.185129    -0.911347     0.103908     193.51
 C       5.675734    -1.968707     0.909661     116.76
 H       5.666256    -1.702570     2.127878      24.98
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 H       6.242969    -2.937381     0.582563      24.08
 H       4.740687    -2.315707     0.657902      26.62
 C       5.883570     1.173044    -0.878546      20.64
 O       7.164218     0.950610    -1.551118     138.59
 H       7.734487     0.837770    -0.830451      27.18
 C       5.083468     2.327852    -1.146779      44.35
 H       5.310958     3.142870    -1.831232      24.44
 C       3.536272     1.670589     0.600523      21.49
 C       2.178563     1.932490     1.360246      92.11
 H       2.241951     3.104144     1.823245      21.58
 O       2.142990     1.131469     2.514833     266.32
 H       1.877886     0.176072     2.333144      23.19
 C       0.854544     1.959026     0.517950      85.60
 H       0.914197     2.817646    -0.316003      20.34
 C      -0.400424     2.170077     1.426760      93.73
 O      -0.343069     3.615330     2.162886     199.36
 H       0.360148     4.194019     1.630028      27.67
 H      -0.333039     1.450531     2.186756      24.16
 H      -1.327380     2.092402     0.897305      24.69
 C      -2.203897    -1.405700    -0.828972      69.35
 H      -2.866286    -2.217347    -0.250761      17.02
 C      -2.105177     0.267297    -2.626478      41.98
 H      -2.558273     0.619682    -3.541974      18.52
 C      -0.912833     0.890436    -2.046026      -1.47
 O      -0.295113     2.005371    -2.629705     227.08
 C      -0.638365     2.151410    -4.023007      86.38
 H       0.027966     2.905105    -4.776250      22.33
 H      -0.601923     1.199012    -4.450997      28.71
 H      -1.720581     2.634071    -3.962582      23.94
 C      -0.451561     0.286012    -0.792851      35.79
 O       0.775126     0.723040    -0.189850     203.50
 C      -1.041061    -0.803617    -0.224612      60.51
 H      -0.605399    -1.591368     0.568976      19.82
 C      -2.700697    -0.844566    -2.015628      28.83
 C      -3.897740    -1.437886    -2.805008      56.08
 H      -3.847253    -1.283883    -3.906714      27.50
 O      -3.916310    -2.902593    -2.779344     187.51
 H      -2.842292    -3.072888    -3.111502      24.89
 C      -5.277559    -0.940303    -2.321779      92.62
 H      -5.148405    -1.010304    -1.274649      28.67
 O      -5.530071     0.326094    -2.956409     285.18
 H      -5.474644     0.866479    -2.162246      28.80
 C      -6.449965    -2.019734    -2.696231     107.57
 O      -6.386974    -3.169916    -1.821295     202.89
 H      -5.516314    -3.744736    -1.834584      27.80
 H      -6.385331    -2.210732    -3.754781      30.88
 H      -7.364728    -1.609183    -2.359104      29.16
55
name = lig-ACN-frame_272
 C       3.902859     2.512161    -0.471030      51.34
 H       3.254928     3.322378    -0.619915      23.26
 C       4.309796     0.461537     0.879757      63.54
 H       3.832228    -0.247241     1.531931      21.13
 C       5.387706     0.217799     0.055753      13.42
 O       6.270758    -0.885375     0.140444     173.47
 C       5.624360    -1.976132     0.915739      99.50
 H       5.749821    -1.669969     2.132887      25.72
 H       6.341575    -2.909510     0.817784      23.82
 H       4.595151    -1.879725     0.682783      26.74
 C       5.863806     1.157680    -0.905620      26.18
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 O       7.030536     0.946547    -1.537161     160.86
 H       7.832370     0.690363    -1.007684      26.82
 C       5.177919     2.317026    -1.150871      55.67
 H       5.782466     2.955319    -1.810916      23.49
 C       3.429988     1.620110     0.527864      -3.27
 C       2.209079     2.024675     1.401481      86.82
 H       2.382683     3.128622     1.877183      23.37
 O       2.158458     1.122794     2.531792     214.70
 H       1.898062     0.154311     2.061717      20.61
 C       0.806447     1.973251     0.572897      76.04
 H       0.904113     2.851992    -0.223233      21.46
 C      -0.402638     2.248562     1.460284     108.25
 O      -0.360451     3.566471     2.141206     189.66
 H       0.381747     4.289226     1.557614      25.24
 H      -0.382575     1.552694     2.231835      25.22
 H      -1.355703     2.203178     0.913413      24.89
 C      -2.244132    -1.361938    -0.750305      58.46
 H      -2.474119    -2.360258    -0.283193      23.35
 C      -2.033480     0.281555    -2.641071      44.68
 H      -2.237781     0.622399    -3.677852      18.48
 C      -0.894527     0.845408    -2.037519       9.17
 O      -0.287068     2.001400    -2.529666     185.78
 C      -0.671001     2.222106    -4.080542      71.01
 H       0.239978     2.852120    -4.506856      23.11
 H      -0.724544     1.311994    -4.546940      28.72
 H      -1.783493     2.676162    -4.262361      23.24
 C      -0.361516     0.285212    -0.856597      16.98
 O       0.839257     0.641121    -0.157766     163.35
 C      -1.061453    -0.815245    -0.240230      42.12
 H      -0.474462    -0.936517     0.785731      16.19
 C      -2.721319    -0.846750    -2.058211      34.46
 C      -3.891880    -1.430956    -2.872703      58.32
 H      -3.686974    -0.950157    -3.931440      25.53
 O      -3.873240    -2.851780    -2.729372     199.98
 H      -2.859579    -3.305780    -2.956127      23.26
 C      -5.288411    -1.016777    -2.385706      99.13
 H      -5.394323    -0.829955    -1.354508      28.89
 O      -5.501124     0.309376    -2.936290     235.36
 H      -5.364727     1.158038    -2.242249      24.57
 C      -6.331841    -2.050287    -2.758356     119.56
 O      -6.367121    -3.173717    -1.853481     212.68
 H      -5.364255    -3.500785    -2.088883      25.73
 H      -6.332052    -2.433142    -3.776627      29.97
 H      -7.256636    -1.540408    -2.752254      30.43
55
name = lig-ACN-frame_273
 C       3.951410     2.539129    -0.451394      55.15
 H       3.429366     3.421924    -0.744943      23.30
 C       4.159640     0.481827     0.809034      53.06
 H       4.020602    -0.108443     1.694496      25.09
 C       5.446429     0.230801     0.122420       1.69
 O       6.299980    -0.922495     0.219045     184.95
 C       5.650447    -1.932033     0.957679     107.39
 H       5.643378    -1.673170     2.170529      24.23
 H       6.076038    -2.982076     0.672758      23.99
 H       4.606351    -2.242075     0.658942      24.98
 C       5.842652     1.148456    -0.853572      21.43
 O       7.008246     0.932953    -1.634671     146.64
 H       7.677059     0.554309    -0.902485      24.95
 C       5.143589     2.347966    -1.118989      49.33
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 H       5.393164     3.141628    -1.852392      24.20
 C       3.449746     1.592340     0.467622      45.82
 C       2.223166     1.957014     1.378909      97.51
 H       2.383297     3.010346     1.861494      23.71
 O       2.114016     1.116436     2.549120     247.69
 H       1.973060     0.104112     2.310187      20.69
 C       0.915762     2.024158     0.578124      63.59
 H       0.849631     2.796929    -0.299775      21.50
 C      -0.427839     2.291534     1.551939     105.67
 O      -0.349850     3.542947     2.103769     235.33
 H       0.301536     4.238331     1.493467      25.73
 H      -0.638810     1.574745     2.297075      25.26
 H      -1.274955     2.151653     0.830732      25.17
 C      -2.249967    -1.295699    -0.815724      40.19
 H      -2.818300    -2.124752    -0.504558      19.61
 C      -1.965574     0.215239    -2.613978      63.42
 H      -2.491709     0.596163    -3.559954      21.27
 C      -0.842879     0.865226    -2.010754      10.79
 O      -0.310791     1.993548    -2.601758     215.17
 C      -0.619898     2.279579    -3.980067     102.04
 H       0.214722     2.993763    -4.180485      24.62
 H      -0.526644     1.490546    -4.668310      27.03
 H      -1.560845     2.994190    -4.049329      23.97
 C      -0.276413     0.266373    -0.820016      23.06
 O       0.849141     0.642806    -0.129736     176.38
 C      -1.068501    -0.747462    -0.229292      56.68
 H      -0.913910    -1.229187     0.775348      19.99
 C      -2.699532    -0.808761    -2.006543      46.25
 C      -3.794314    -1.432573    -2.813172      61.41
 H      -3.814291    -1.247343    -3.996479      26.61
 O      -3.787613    -2.890268    -2.713689     264.35
 H      -2.859100    -3.079498    -2.968682      31.05
 C      -5.246615    -1.004463    -2.400208      86.19
 H      -5.207103    -1.169711    -1.336633      27.82
 O      -5.528573     0.333050    -2.969408     250.22
 H      -5.210987     0.876268    -2.092545      25.04
 C      -6.350303    -2.040673    -2.891507     109.72
 O      -6.326473    -3.162602    -1.896663     229.62
 H      -5.512490    -3.612641    -1.911747      30.60
 H      -5.941144    -2.404304    -3.819703      30.29
 H      -7.354170    -1.678225    -2.959874      29.03
55
name = lig-ACN-frame_274
 C       3.877158     2.607252    -0.438143      54.57
 H       3.327715     3.550572    -0.605567      22.51
 C       4.229110     0.422592     0.721736      59.17
 H       3.787516    -0.164710     1.516592      23.74
 C       5.458616     0.247115     0.139385      16.92
 O       6.241610    -0.878431     0.300158     168.04
 C       5.652618    -2.033606     1.015355      99.67
 H       5.566925    -1.800650     2.195343      25.91
 H       6.458800    -2.816998     0.916986      24.27
 H       4.570145    -1.997780     0.591782      25.25
 C       5.899362     1.192452    -0.871628      23.76
 O       7.018241     0.902834    -1.701096     131.44
 H       7.762215     0.529560    -1.228903      30.07
 C       5.111984     2.341682    -1.110342      47.98
 H       5.494657     2.971840    -1.947682      23.19
 C       3.443090     1.654484     0.513167      20.27
 C       2.229979     1.865108     1.361678     103.68
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 H       2.421201     2.900962     1.766621      23.70
 O       2.056285     1.108466     2.567567     319.32
 H       1.952776     0.224178     2.358769      28.60
 C       0.877241     1.950838     0.620536      90.40
 H       1.061727     2.845242    -0.087971      22.64
 C      -0.364420     2.183715     1.437570      94.26
 O      -0.328069     3.650669     2.124826     244.92
 H       0.207653     4.157770     1.562878      31.55
 H      -0.309826     1.487616     2.278038      24.15
 H      -1.306646     2.228752     0.827769      24.56
 C      -2.265908    -1.286018    -0.802214      60.38
 H      -2.744987    -1.859361    -0.156710      20.15
 C      -1.941065     0.256928    -2.632111      53.77
 H      -2.251010     0.843769    -3.580363      20.56
 C      -0.804828     0.841263    -2.011862       9.09
 O      -0.263071     1.958139    -2.593250     224.77
 C      -0.522404     2.459033    -3.920211     113.29
 H       0.158278     3.134152    -4.309213      26.11
 H      -0.628334     1.574888    -4.516914      26.93
 H      -1.626681     2.785101    -3.991198      25.29
 C      -0.337799     0.275258    -0.747654      16.63
 O       0.876163     0.720666    -0.089459     187.97
 C      -1.108451    -0.755050    -0.156022      52.57
 H      -0.625027    -1.236032     0.648816      21.80
 C      -2.668046    -0.754957    -2.075186      39.62
 C      -3.820175    -1.489582    -2.801121      46.55
 H      -3.467143    -1.131479    -3.907484      27.06
 O      -3.639958    -2.953931    -2.694247     243.16
 H      -2.865232    -3.135057    -3.047010      33.67
 C      -5.250143    -1.007393    -2.421733      95.91
 H      -5.418875    -0.819152    -1.366642      27.35
 O      -5.534648     0.330934    -2.913335     278.04
 H      -5.346711     1.008526    -2.352466      31.59
 C      -6.240801    -2.100581    -2.975079     113.89
 O      -6.357503    -3.116802    -1.964830     248.22
 H      -5.509893    -3.536390    -2.042718      31.72
 H      -6.074378    -2.456370    -3.988930      30.57
 H      -7.250550    -1.668485    -3.022609      29.18
55
name = lig-ACN-frame_275
 C       3.872057     2.600465    -0.405616      49.08
 H       3.177402     3.483795    -0.585576      23.09
 C       4.220822     0.485239     0.711750      60.68
 H       3.878251    -0.459465     1.105210      20.29
 C       5.471603     0.272465     0.056430      16.16
 O       6.236823    -0.851967     0.379250     188.78
 C       5.667672    -2.021842     1.061065     114.67
 H       5.445359    -1.724112     2.137873      27.67
 H       6.328948    -2.876436     0.931254      25.88
 H       4.722222    -2.545241     0.572926      26.56
 C       5.949317     1.205069    -0.876896      30.87
 O       6.997319     0.896588    -1.744870     176.78
 H       7.725610     0.744093    -1.149078      26.96
 C       5.119710     2.324309    -1.155304      41.25
 H       5.508926     3.029486    -1.916802      24.32
 C       3.481424     1.623433     0.543849      30.61
 C       2.181402     1.929068     1.466016      98.90
 H       2.257899     2.905397     1.910096      25.74
 O       2.037820     1.055871     2.605280     314.50
 H       1.901353     0.131993     2.360086      25.00
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 C       0.915239     1.972359     0.563482      85.05
 H       0.922539     2.787626    -0.220536      22.64
 C      -0.294035     2.285881     1.474152      98.20
 O      -0.311196     3.607185     2.076517     303.41
 H       0.288801     4.147174     1.766802      34.83
 H      -0.413899     1.563870     2.350448      23.40
 H      -1.264684     2.022831     0.875503      24.19
 C      -2.273888    -1.236017    -0.702353      48.29
 H      -2.768698    -2.072450    -0.511326      22.51
 C      -1.938690     0.340015    -2.672761      46.77
 H      -2.233560     0.592505    -3.749419      21.48
 C      -0.798891     0.837644    -2.008967       5.07
 O      -0.066199     1.987466    -2.465139     132.26
 C      -0.576504     2.506601    -3.925126     100.96
 H       0.186413     3.186529    -3.955640      27.33
 H      -0.354783     1.828268    -4.791271      26.30
 H      -1.529922     3.044332    -3.873045      26.62
 C      -0.388596     0.371747    -0.723115      23.88
 O       0.806517     0.688961    -0.144833     209.54
 C      -1.064675    -0.756597    -0.124218      39.54
 H      -0.765386    -1.057751     0.803549      20.57
 C      -2.667959    -0.798602    -2.041767      21.35
 C      -3.738530    -1.481220    -2.834097      66.24
 H      -3.976282    -1.277192    -3.998890      25.36
 O      -3.552500    -2.963032    -2.667880     233.70
 H      -2.619496    -3.112297    -3.037862      26.66
 C      -5.246487    -1.035890    -2.443255      81.75
 H      -5.368518    -1.291923    -1.365022      27.04
 O      -5.541757     0.325659    -2.942587     272.98
 H      -5.292097     0.776104    -2.139850      29.12
 C      -6.228061    -2.047116    -2.999093     106.42
 O      -6.381183    -3.120269    -2.050302     198.80
 H      -5.486662    -3.713397    -1.962516      25.87
 H      -5.829701    -2.504138    -3.909580      29.48
 H      -7.200225    -1.519325    -3.187197      27.88
55
name = lig-ACN-frame_276
 C       3.973388     2.514625    -0.391219      54.84
 H       3.455403     3.464427    -0.780803      23.09
 C       4.216741     0.455413     0.712524      41.02
 H       3.832198    -0.205212     1.488871      23.39
 C       5.444405     0.241982     0.055544      14.74
 O       6.283932    -0.847451     0.390179     180.88
 C       5.678895    -1.966027     1.070967     116.41
 H       5.269231    -1.741011     2.043907      27.64
 H       6.494453    -2.611321     1.169815      26.04
 H       4.741394    -2.202168     0.377032      25.28
 C       5.882668     1.222074    -0.930791      24.60
 O       7.023950     0.916789    -1.741863     117.24
 H       7.936581     0.901504    -1.207310      25.78
 C       5.091879     2.359876    -1.160137      61.27
 H       5.274443     3.129732    -1.900594      23.84
 C       3.436908     1.680384     0.620065      36.68
 C       2.211800     1.945085     1.478441     104.81
 H       2.357007     2.841524     1.966158      24.77
 O       2.033231     1.017185     2.629441     277.90
 H       2.005625    -0.008579     2.255411      19.63
 C       0.937946     2.046226     0.547799      75.87
 H       1.130682     2.785239    -0.225281      23.28
 C      -0.314978     2.299975     1.514484      95.88
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 O      -0.304565     3.604243     2.043824     276.68
 H       0.510457     4.091343     1.631503      26.81
 H      -0.222865     1.507030     2.356928      21.04
 H      -1.270512     2.328622     0.837319      22.90
 C      -2.284141    -1.228387    -0.776202      64.47
 H      -2.583766    -2.099338    -0.284280      20.51
 C      -1.939992     0.282938    -2.629666      47.29
 H      -2.225547     0.544956    -3.652441      21.04
 C      -0.813044     0.963586    -1.996436       3.31
 O       0.015856     1.978791    -2.490110     212.43
 C      -0.479998     2.568473    -3.746489     111.56
 H      -0.030881     3.598941    -3.974498      24.81
 H      -0.484971     1.818048    -4.612683      25.71
 H      -1.508643     2.685155    -3.601762      28.31
 C      -0.473514     0.342490    -0.737083      23.17
 O       0.787668     0.684004    -0.166419     173.24
 C      -1.136245    -0.678972    -0.105275      41.04
 H      -0.812317    -1.062885     0.813802      19.59
 C      -2.596320    -0.704458    -2.009291      24.53
 C      -3.732881    -1.497139    -2.849441      45.43
 H      -3.255541    -1.224842    -3.913247      25.96
 O      -3.524337    -2.907655    -2.658260     216.83
 H      -2.413805    -3.082028    -2.886642      21.96
 C      -5.167580    -1.108409    -2.431539      87.31
 H      -5.192674    -0.926452    -1.328018      25.29
 O      -5.503026     0.261183    -2.902794     217.57
 H      -5.325062     1.107348    -2.217847      24.53
 C      -6.226140    -2.049910    -3.070697     101.26
 O      -6.443560    -3.163606    -2.108486     223.93
 H      -5.537548    -3.633957    -2.195667      29.29
 H      -5.843814    -2.329308    -4.071404      28.96
 H      -7.293889    -1.669472    -3.226592      26.78
55
name = lig-ACN-frame_277
 C       3.902782     2.594940    -0.374952      49.00
 H       3.226826     3.515450    -0.388852      22.22
 C       4.193676     0.447515     0.820260      72.39
 H       4.072074    -0.110287     1.739034      24.81
 C       5.412989     0.254980     0.070020       5.53
 O       6.342617    -0.766187     0.344555     183.84
 C       5.667230    -1.890794     1.052746     115.44
 H       5.228604    -1.549234     1.892594      27.82
 H       6.328502    -2.655680     1.316256      26.73
 H       4.912146    -2.482145     0.384165      26.97
 C       5.883044     1.118530    -0.977717      16.45
 O       7.049386     0.967383    -1.706196     156.02
 H       7.807483     0.927818    -0.998438      28.30
 C       5.129840     2.316537    -1.160378      29.21
 H       5.536303     2.939138    -1.946753      22.50
 C       3.530117     1.636804     0.613469      25.01
 C       2.244806     1.890615     1.476875     101.37
 H       2.338166     2.783396     1.896988      25.14
 O       2.052218     1.034403     2.579934     299.24
 H       2.021112    -0.028935     2.315064      19.65
 C       0.909502     2.008509     0.609397      91.60
 H       0.995613     2.841565    -0.026676      23.63
 C      -0.310726     2.256279     1.394394      80.68
 O      -0.286094     3.681664     2.084351     170.54
 H       0.444132     4.442475     1.563670      23.47
 H      -0.363262     1.501754     2.307522      21.69
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 H      -1.343567     1.986030     0.903316      23.10
 C      -2.238512    -1.269091    -0.742984      48.59
 H      -3.001705    -1.996944    -0.349149      19.34
 C      -1.856345     0.393867    -2.640862      52.98
 H      -2.173518     0.763211    -3.562966      23.05
 C      -0.839273     0.993314    -1.942151      14.11
 O       0.052943     1.928009    -2.497576     218.34
 C      -0.504696     2.578076    -3.594069     116.04
 H       0.155929     3.543289    -3.868548      23.56
 H      -0.263480     1.948524    -4.570227      24.01
 H      -1.507100     2.784812    -3.505137      27.53
 C      -0.397574     0.427085    -0.730646      12.95
 O       0.809294     0.763986    -0.124000     199.42
 C      -1.253399    -0.595048    -0.104320      48.22
 H      -0.736821    -1.050710     0.769752      21.25
 C      -2.684392    -0.731396    -2.026241      25.85
 C      -3.590027    -1.442222    -2.833460      68.45
 H      -3.743742    -1.150820    -3.984716      24.71
 O      -3.530982    -2.874309    -2.644585     161.63
 H      -2.428137    -3.200764    -2.945619      22.99
 C      -5.105976    -1.054849    -2.456912      73.97
 H      -5.262095    -1.375195    -1.368347      26.72
 O      -5.453021     0.219772    -2.906273     242.50
 H      -5.129450     0.830044    -2.065919      24.36
 C      -6.221946    -2.099683    -3.044739      94.79
 O      -6.477027    -3.217318    -2.224932     259.63
 H      -5.761934    -3.755355    -2.143630      32.38
 H      -6.029175    -2.533574    -4.069499      27.96
 H      -7.086839    -1.349096    -3.075322      26.74
55
name = lig-ACN-frame_278
 C       3.945749     2.587421    -0.386394      54.63
 H       3.439561     3.546433    -0.660757      23.73
 C       4.344056     0.494272     0.890730      54.54
 H       3.940337    -0.270476     1.561026      17.90
 C       5.459616     0.234370     0.079770      25.16
 O       6.334255    -0.764410     0.328246     215.99
 C       5.713358    -1.854842     1.041485     131.97
 H       5.197627    -1.591481     1.848511      31.74
 H       6.541883    -2.492597     1.259564      26.85
 H       4.947461    -2.262920     0.312353      28.81
 C       5.778513     1.131289    -0.946886      20.26
 O       7.077988     0.997255    -1.627510     181.37
 H       7.779083     0.772390    -1.048983      28.63
 C       5.055664     2.294929    -1.131009      53.15
 H       5.461744     3.061527    -1.771389      25.18
 C       3.498665     1.627175     0.591383      21.14
 C       2.246379     1.916304     1.441576     113.80
 H       2.358588     2.774676     1.881625      27.52
 O       2.092230     1.028705     2.570301     307.10
 H       1.980229     0.106293     2.303178      25.65
 C       0.961407     2.021689     0.619405      81.63
 H       1.097791     2.749228    -0.106466      25.03
 C      -0.344536     2.370825     1.503479      89.80
 O      -0.322601     3.617149     2.084052     206.46
 H       0.372499     4.307610     1.378935      22.34
 H      -0.496498     1.631300     2.418287      21.75
 H      -1.154916     2.393183     0.656601      22.38
 C      -2.321478    -1.151300    -0.795072      65.56
 H      -2.739046    -2.148778    -0.290861      20.14
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 C      -1.938311     0.428924    -2.592016      60.71
 H      -2.161400     0.707781    -3.555256      22.03
 C      -0.758142     0.944174    -1.888453       8.90
 O       0.057663     1.879834    -2.399585     161.85
 C      -0.506437     2.637930    -3.660914      98.25
 H       0.239405     3.512954    -3.527425      24.14
 H      -0.553315     2.050581    -4.679726      24.34
 H      -1.432161     3.068429    -3.432867      27.57
 C      -0.411664     0.444981    -0.625908      34.18
 O       0.833557     0.788934    -0.097832     218.47
 C      -1.153019    -0.543012    -0.066390      41.49
 H      -1.008023    -0.836317     1.048354      18.97
 C      -2.518145    -0.649049    -2.059019      25.40
 C      -3.716463    -1.441957    -2.909376      77.17
 H      -3.388777    -1.228220    -4.037920      23.48
 O      -3.524444    -2.874801    -2.656255     211.68
 H      -2.542146    -3.132493    -3.054568      24.37
 C      -5.108385    -1.218351    -2.476829      97.11
 H      -5.143501    -1.103282    -1.347927      26.22
 O      -5.389230     0.245803    -2.871314     262.73
 H      -5.166320     0.841426    -2.210505      30.90
 C      -6.159008    -2.067749    -3.054249     101.90
 O      -6.537060    -3.284685    -2.276413     222.16
 H      -5.668282    -3.857951    -2.308209      28.52
 H      -5.929412    -2.228721    -4.160452      28.01
 H      -7.180037    -1.589099    -2.999745      26.19
55
name = lig-ACN-frame_279
 C       3.908881     2.526511    -0.380604      52.15
 H       3.257710     3.385363    -0.576276      24.14
 C       4.349951     0.593068     0.870706      59.48
 H       3.977377    -0.128669     1.629850      18.35
 C       5.480407     0.307937     0.104518      23.29
 O       6.362034    -0.811913     0.329257     222.76
 C       5.784750    -1.919150     1.030953     133.25
 H       5.464507    -1.657930     1.969114      30.93
 H       6.567833    -2.672985     1.197885      26.32
 H       4.996028    -2.455962     0.464665      28.89
 C       5.895414     1.182119    -0.921958      21.85
 O       7.023131     1.030883    -1.563142     130.21
 H       7.652172     0.718002    -0.881627      26.31
 C       5.060479     2.329984    -1.165966      49.88
 H       5.389552     3.103516    -1.868950      25.68
 C       3.490257     1.650334     0.608023      43.33
 C       2.281611     1.962387     1.477688     111.26
 H       2.457747     2.815015     1.875806      27.71
 O       2.132385     1.019048     2.583466     326.42
 H       1.973796     0.180639     2.263687      28.11
 C       0.963466     2.106566     0.655545      81.29
 H       1.061461     2.885925    -0.005058      24.46
 C      -0.334171     2.373494     1.462529      88.30
 O      -0.349279     3.650470     2.152111     209.70
 H       0.433431     4.434952     1.695062      23.03
 H      -0.599413     1.484685     2.191521      22.54
 H      -1.283325     2.259070     0.776302      23.09
 C      -2.225661    -1.002786    -0.741109      52.79
 H      -2.759896    -2.035678    -0.413991      21.15
 C      -1.901915     0.490513    -2.567422      66.42
 H      -2.073360     0.949116    -3.516190      21.91
 C      -0.768315     0.885841    -1.910393       7.13
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 O       0.041701     1.938999    -2.453328     217.80
 C      -0.419817     2.725836    -3.576260     116.71
 H       0.309911     3.431557    -4.093088      24.76
 H      -0.559491     1.931720    -4.438243      24.95
 H      -1.447216     3.014839    -3.392534      26.86
 C      -0.409048     0.426767    -0.566376      26.23
 O       0.854312     0.753896    -0.051040     178.79
 C      -1.211748    -0.592400     0.029224      42.17
 H      -0.982276    -0.973285     1.120481      18.54
 C      -2.643060    -0.716964    -2.115184      31.40
 C      -3.620924    -1.508036    -2.910035      70.63
 H      -3.667733    -1.180943    -4.068024      24.66
 O      -3.495694    -2.906513    -2.714973     286.45
 H      -2.616056    -3.116721    -2.907847      30.76
 C      -5.104761    -1.097225    -2.414186      72.67
 H      -5.113518    -1.377364    -1.298498      26.76
 O      -5.352129     0.235030    -2.864356     291.35
 H      -5.235799     0.730809    -2.081039      30.06
 C      -6.257248    -2.097345    -3.069280      89.87
 O      -6.500582    -3.317389    -2.351586     222.10
 H      -5.686678    -4.001464    -2.330298      27.05
 H      -5.874247    -2.449917    -4.103681      27.60
 H      -7.133155    -1.420872    -3.202758      27.51
55
name = lig-ACN-frame_280
 C       3.821172     2.559159    -0.469145      57.79
 H       3.175598     3.401148    -0.710689      22.04
 C       4.305075     0.542776     0.901051      63.88
 H       4.272477    -0.029494     1.851511      24.97
 C       5.516845     0.344648     0.163624       9.45
 O       6.377324    -0.809308     0.302197     148.50
 C       5.852013    -2.046678     1.070194     102.72
 H       5.614098    -1.751211     2.068717      26.29
 H       6.701203    -2.812375     0.968505      24.10
 H       4.950968    -2.328747     0.627959      29.11
 C       5.886607     1.311331    -0.815794      21.67
 O       7.094779     1.051756    -1.594188      51.19
 H       7.960337     0.745516    -1.034183      21.30
 C       5.071180     2.367718    -1.170921      54.02
 H       5.406861     2.946445    -2.051929      24.48
 C       3.523471     1.694565     0.633358      28.96
 C       2.285235     1.998060     1.577028     103.82
 H       2.407470     2.800722     2.085817      26.68
 O       2.162606     1.049568     2.600801     286.22
 H       2.037504     0.069815     2.240647      21.49
 C       0.949434     2.116934     0.661033      92.51
 H       1.081002     2.776189    -0.134082      24.99
 C      -0.337107     2.326926     1.413962      88.78
 O      -0.367063     3.688165     2.251820     207.20
 H       0.396056     4.297388     1.772130      25.39
 H      -0.295531     1.634093     2.307658      22.61
 H      -1.203885     2.292557     0.685577      24.48
 C      -2.335891    -1.142319    -0.777998      39.31
 H      -3.060929    -1.843689    -0.195892      19.32
 C      -1.904351     0.423103    -2.625503      48.38
 H      -2.345376     0.867815    -3.577484      21.23
 C      -0.757728     0.976340    -1.885281      -4.98
 O       0.080590     2.005180    -2.425168     179.66
 C      -0.421865     2.662421    -3.596491     118.01
 H       0.448986     3.308163    -3.723389      25.15
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 H      -0.638461     1.981361    -4.496485      24.35
 H      -1.165724     3.497746    -3.404654      26.30
 C      -0.329491     0.400910    -0.598918      13.59
 O       0.848325     0.777173     0.030238     194.61
 C      -1.203893    -0.503455     0.051621      38.73
 H      -0.845163    -1.160743     0.921565      20.89
 C      -2.609374    -0.621249    -2.042389      27.63
 C      -3.655393    -1.493439    -2.843595      55.13
 H      -3.535931    -1.224920    -3.998401      24.82
 O      -3.451006    -2.983427    -2.789479     263.88
 H      -2.541750    -3.102907    -2.778747      31.21
 C      -5.115013    -1.145435    -2.433632      87.39
 H      -5.310166    -1.106813    -1.314376      25.60
 O      -5.339854     0.242327    -2.819699     242.62
 H      -5.282279     1.004727    -2.042126      24.22
 C      -6.210692    -2.091487    -3.099298      96.83
 O      -6.473871    -3.319090    -2.379493     286.33
 H      -5.648466    -3.717852    -2.449174      32.34
 H      -5.911858    -2.297883    -4.204522      27.68
 H      -7.236647    -1.703462    -3.103944      26.77
55
name = lig-ACN-frame_281
 C       3.808288     2.558642    -0.521581      58.65
 H       3.168774     3.360497    -0.919014      23.26
 C       4.361878     0.559755     0.954539      49.66
 H       3.925752    -0.086074     1.734441      21.02
 C       5.547986     0.306158     0.235158      33.14
 O       6.344969    -0.812148     0.307970     200.07
 C       5.906445    -1.997815     1.036451     118.10
 H       5.960997    -1.900813     2.184731      26.55
 H       6.696858    -2.779517     0.778271      24.09
 H       4.995779    -2.311047     0.723853      30.60
 C       5.993170     1.314462    -0.771589      26.87
 O       7.088528     1.111417    -1.641976      10.30
 H       7.906580     1.079797    -0.948285      19.67
 C       5.038805     2.369540    -1.135937      36.75
 H       5.346662     3.075640    -1.935943      24.65
 C       3.519535     1.750878     0.654176      19.35
 C       2.279029     2.037546     1.557055      99.98
 H       2.356790     2.921334     1.955157      27.90
 O       2.160403     1.043345     2.664892     247.26
 H       2.101855     0.060561     2.180747      21.19
 C       1.000789     2.098598     0.662842      87.91
 H       1.176451     2.898537    -0.046525      24.96
 C      -0.310902     2.449159     1.569820     107.80
 O      -0.361813     3.612451     2.242273     314.61
 H       0.055295     4.260751     1.790340      33.51
 H      -0.543613     1.550751     2.170882      24.84
 H      -1.232333     2.417685     0.911763      25.71
 C      -2.329418    -1.127997    -0.651944      40.51
 H      -2.889627    -1.969080    -0.240558      21.49
 C      -1.816515     0.407473    -2.575839      62.60
 H      -2.122811     0.757360    -3.667776      21.66
 C      -0.767365     1.029617    -1.889160      21.88
 O       0.052309     1.992190    -2.332846     199.37
 C      -0.321689     2.712507    -3.651150     110.13
 H       0.501182     3.206029    -4.112135      26.27
 H      -0.695033     2.021641    -4.452096      25.10
 H      -1.361837     3.211076    -3.353504      25.46
 C      -0.378258     0.408742    -0.683427      22.12
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 O       0.843742     0.767231     0.086629     168.58
 C      -1.226414    -0.570857    -0.120439      44.55
 H      -0.950828    -0.729386     0.922267      20.55
 C      -2.625466    -0.700197    -1.965319      44.24
 C      -3.691726    -1.475058    -2.806733      45.67
 H      -3.545263    -1.078277    -3.890373      27.31
 O      -3.427206    -2.972848    -2.815316     198.00
 H      -2.368248    -3.082950    -3.033220      23.74
 C      -5.163738    -1.189295    -2.432789      89.35
 H      -5.229450    -1.420196    -1.329614      25.91
 O      -5.356520     0.272468    -2.840826     230.81
 H      -5.129708     0.692882    -1.835137      22.31
 C      -6.191522    -2.037829    -3.116688     103.59
 O      -6.380986    -3.305296    -2.397309     266.13
 H      -5.619570    -3.894016    -2.248937      29.14
 H      -5.904562    -2.230322    -4.220633      28.65
 H      -7.057263    -1.388997    -3.115521      28.23
55
name = lig-ACN-frame_282
 C       3.845075     2.496057    -0.429487      61.91
 H       3.088553     3.265750    -0.727828      24.86
 C       4.378616     0.702756     0.959933      62.94
 H       4.066640    -0.149286     1.538381      21.77
 C       5.565120     0.388459     0.212599      33.92
 O       6.345485    -0.790194     0.304324     191.68
 C       5.946578    -1.945487     1.004990     116.99
 H       6.124613    -1.717754     2.164765      25.70
 H       6.565329    -2.794058     0.607861      24.17
 H       4.952869    -2.147691     0.917244      29.44
 C       5.949613     1.274213    -0.771239      38.17
 O       7.042795     1.203580    -1.631987      68.19
 H       7.894858     0.972619    -1.185528      22.60
 C       5.115967     2.303395    -1.086290      52.54
 H       5.509821     3.012435    -1.818967      26.39
 C       3.537425     1.730846     0.649655      35.15
 C       2.289157     1.978584     1.526168     109.42
 H       2.429112     2.830088     2.035491      27.80
 O       2.148404     1.089481     2.666463     277.88
 H       1.918143     0.182127     2.385172      26.66
 C       0.949476     2.087982     0.772664      84.51
 H       0.984861     2.812413    -0.069496      24.57
 C      -0.316751     2.359258     1.536772     104.21
 O      -0.316477     3.672861     2.314456     282.28
 H       0.017662     4.309939     1.778217      33.25
 H      -0.414798     1.709111     2.360395      25.82
 H      -1.083141     2.321688     0.748053      25.43
 C      -2.335825    -1.119632    -0.654828      46.83
 H      -2.692782    -1.941292    -0.158412      22.14
 C      -1.870776     0.290485    -2.495548      50.61
 H      -1.990530     0.578504    -3.656735      20.47
 C      -0.768460     0.952810    -1.898261       9.39
 O       0.063912     2.096220    -2.389990     201.66
 C      -0.302809     2.646961    -3.619597     118.22
 H       0.493403     3.285685    -3.920639      27.02
 H      -0.408640     1.789518    -4.292795      26.48
 H      -1.173325     3.501337    -3.673408      25.60
 C      -0.374381     0.482593    -0.619921      31.11
 O       0.752375     0.734393     0.058108     191.66
 C      -1.115629    -0.600818    -0.050951      36.73
 H      -0.912453    -0.863034     0.939483      20.47
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 C      -2.635497    -0.749360    -2.008289      29.38
 C      -3.627691    -1.482104    -2.842470      75.10
 H      -3.653479    -1.112024    -3.916139      26.04
 O      -3.419480    -2.865505    -2.820785     196.95
 H      -2.331582    -3.130764    -3.176740      21.34
 C      -5.100487    -1.130046    -2.410409      90.66
 H      -5.373730    -1.220527    -1.338989      27.21
 O      -5.381235     0.203598    -2.797898     296.43
 H      -5.139629     0.934745    -2.176585      28.82
 C      -6.172648    -2.052062    -3.131431      97.69
 O      -6.344878    -3.260151    -2.404045     232.49
 H      -5.307500    -3.577263    -2.502376      26.59
 H      -5.879081    -2.344021    -4.210210      28.30
 H      -7.175761    -1.685978    -3.108357      28.09
55
name = lig-ACN-frame_283
 C       3.906874     2.553743    -0.395583      57.78
 H       3.347458     3.475392    -0.769312      21.97
 C       4.455553     0.601293     0.996572      69.14
 H       4.253105     0.089885     1.903344      23.90
 C       5.580083     0.393223     0.212886      26.53
 O       6.389458    -0.693080     0.246551     176.35
 C       5.911964    -1.906048     1.055314     104.79
 H       6.325448    -1.915366     2.204682      23.88
 H       6.411413    -2.744231     0.598866      24.97
 H       4.859809    -1.938475     1.039224      27.13
 C       5.918631     1.297718    -0.845269      37.61
 O       7.052239     1.251505    -1.630859     130.84
 H       7.665169     0.775603    -1.132701      29.11
 C       5.081245     2.376339    -1.067371      54.92
 H       5.293932     3.001612    -1.923982      25.05
 C       3.494973     1.656708     0.692821       7.25
 C       2.264171     1.948421     1.565678     105.34
 H       2.411414     2.923400     1.867148      26.07
 O       2.130080     1.100503     2.673421     310.83
 H       1.875680     0.287495     2.371235      30.23
 C       0.920055     2.038522     0.737131      85.32
 H       1.103492     2.911722    -0.003493      23.72
 C      -0.352806     2.336875     1.622997     105.62
 O      -0.269490     3.694898     2.310270     228.27
 H       0.351333     4.354861     1.710614      26.28
 H      -0.477069     1.574511     2.296340      27.22
 H      -1.265407     2.313148     1.064488      26.46
 C      -2.231546    -1.185164    -0.668627      56.34
 H      -2.879062    -1.829989    -0.237353      21.06
 C      -1.841618     0.305273    -2.593156      42.12
 H      -2.281604     0.617718    -3.654608      21.23
 C      -0.728395     0.943842    -1.868637       3.35
 O       0.003642     2.069274    -2.338159     183.75
 C      -0.260969     2.597522    -3.703500     104.11
 H       0.566180     3.274088    -3.852905      26.06
 H      -0.338790     2.025467    -4.599598      26.27
 H      -1.424109     3.037214    -3.537218      23.76
 C      -0.448400     0.434123    -0.554491      24.55
 O       0.790311     0.790733     0.093095     184.21
 C      -1.156149    -0.598536     0.060285      59.24
 H      -0.667966    -1.180543     0.760708      22.84
 C      -2.556889    -0.742742    -1.945250      35.19
 C      -3.637058    -1.417370    -2.890045      38.54
 H      -3.389621    -1.020306    -3.906735      28.55
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 O      -3.430990    -2.861002    -2.835781     206.27
 H      -2.308453    -2.980670    -2.878560      23.54
 C      -5.112025    -1.112189    -2.404158      90.57
 H      -4.994364    -1.250211    -1.324055      26.61
 O      -5.430354     0.219172    -2.825772     306.98
 H      -5.144692     0.671194    -2.125174      32.88
 C      -6.157270    -2.038024    -3.134200     103.59
 O      -6.251837    -3.269728    -2.388052     278.22
 H      -5.475483    -3.867276    -2.320085      29.41
 H      -5.772770    -2.133361    -4.184255      28.59
 H      -7.074679    -1.459275    -3.248125      27.83
55
name = lig-ACN-frame_284
 C       3.850092     2.600482    -0.289398      52.20
 H       3.087021     3.438527    -0.360889      24.76
 C       4.410552     0.564439     1.034803      58.76
 H       4.291397    -0.146052     1.827024      22.36
 C       5.584903     0.413825     0.150911       1.91
 O       6.470028    -0.735495     0.279740     168.34
 C       5.925440    -1.804230     1.048259     110.43
 H       6.362741    -1.700874     2.175115      24.15
 H       6.183529    -2.707308     0.553841      25.94
 H       4.807924    -1.819657     1.129462      25.23
 C       5.903115     1.356665    -0.891852      10.37
 O       7.066131     1.233331    -1.647638      64.11
 H       7.881384     0.944836    -1.094193      24.54
 C       5.014141     2.491785    -1.132966      43.29
 H       5.314729     3.225736    -1.874711      23.57
 C       3.550464     1.637023     0.685096      24.47
 C       2.231560     2.007617     1.551657      86.31
 H       2.358286     2.910921     2.132612      25.51
 O       2.102694     1.061842     2.729959     210.18
 H       1.978489     0.109010     2.290866      24.55
 C       0.910523     2.077094     0.737672      69.31
 H       0.923710     2.924245    -0.084838      23.37
 C      -0.366063     2.414876     1.737160     113.87
 O      -0.215882     3.650697     2.273140     213.87
 H       0.592264     4.243245     1.639754      24.21
 H      -0.394457     1.780548     2.527559      26.96
 H      -1.237206     2.352848     1.148829      27.09
 C      -2.218455    -1.254929    -0.658239      80.14
 H      -2.680599    -2.159578    -0.289364      22.20
 C      -1.736518     0.377440    -2.593232      65.92
 H      -1.989218     0.904979    -3.565379      21.66
 C      -0.806237     0.921029    -1.858387      21.43
 O      -0.028615     1.956977    -2.298539     189.77
 C      -0.283247     2.564849    -3.728355      94.48
 H       0.318194     3.529175    -3.827957      25.32
 H       0.000334     1.740219    -4.324246      26.06
 H      -1.418742     2.996683    -3.903779      24.96
 C      -0.418103     0.418428    -0.541892      33.38
 O       0.816228     0.781450     0.079904     169.89
 C      -1.177607    -0.667995     0.076289      30.75
 H      -0.882703    -0.933031     1.100543      19.52
 C      -2.510939    -0.684065    -2.006671      68.46
 C      -3.586120    -1.371046    -2.824776      61.34
 H      -3.591946    -1.029971    -3.857886      30.93
 O      -3.425234    -2.874870    -2.864583     252.52
 H      -2.541390    -3.088023    -2.644234      31.24
 C      -5.051806    -1.124166    -2.475978      97.91
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 H      -5.352846    -1.305821    -1.444591      27.52
 O      -5.474490     0.292796    -2.828878     248.33
 H      -5.365635     0.959645    -2.080368      26.16
 C      -6.035649    -2.053721    -3.083958     111.40
 O      -6.250867    -3.297909    -2.367700     266.48
 H      -5.416067    -3.637937    -2.513096      32.70
 H      -5.822147    -2.368918    -4.108137      29.97
 H      -7.055880    -1.660554    -2.972779      28.60
55
name = lig-ACN-frame_285
 C       3.832260     2.615176    -0.246804      43.42
 H       3.151906     3.483669    -0.429231      24.66
 C       4.427729     0.592773     0.893302      73.09
 H       4.014296    -0.171035     1.544906      22.90
 C       5.569077     0.404148     0.119697      13.13
 O       6.482455    -0.663106     0.283139     176.29
 C       5.945016    -1.776570     1.078769     105.98
 H       6.321471    -1.770327     2.200310      25.84
 H       6.325628    -2.717807     0.695740      26.05
 H       4.786984    -1.648233     1.089494      25.75
 C       5.857129     1.430427    -0.876444      15.49
 O       7.038906     1.223288    -1.685503      53.89
 H       7.849155     1.183648    -0.973385      22.90
 C       4.956143     2.507216    -1.091716      58.78
 H       5.278819     3.393064    -1.675025      25.63
 C       3.520995     1.693187     0.792408      22.12
 C       2.271764     1.951583     1.625918      91.41
 H       2.487381     2.990846     2.055158      24.16
 O       2.068600     1.033828     2.702239     237.25
 H       2.004754    -0.000070     2.341305      22.85
 C       0.850028     2.092315     0.831713      67.99
 H       0.874829     2.920180    -0.026247      22.72
 C      -0.296052     2.334717     1.709592     110.71
 O      -0.136831     3.761874     2.302865     179.22
 H       0.346304     4.511840     1.570220      25.03
 H      -0.287297     1.693279     2.521764      26.48
 H      -1.193823     2.240359     1.201510      27.33
 C      -2.200834    -1.221958    -0.771789      66.51
 H      -2.715967    -2.205305    -0.461443      21.78
 C      -1.847470     0.323832    -2.549687      60.31
 H      -2.025557     0.590523    -3.580438      19.78
 C      -0.709325     0.952595    -1.730377       8.32
 O      -0.002409     2.006202    -2.328041     223.83
 C      -0.283609     2.432286    -3.618767     107.34
 H       0.364629     3.416595    -3.577091      24.73
 H       0.090592     1.906358    -4.514490      26.69
 H      -1.435638     2.523003    -3.897011      24.26
 C      -0.376047     0.355451    -0.503306      32.88
 O       0.790942     0.758174     0.053255     191.82
 C      -1.145895    -0.650452     0.023242      54.96
 H      -1.115075    -0.908199     1.143280      20.50
 C      -2.494837    -0.742769    -2.012954      20.62
 C      -3.553331    -1.411129    -2.848455      58.75
 H      -3.353404    -1.026568    -3.833386      27.36
 O      -3.427434    -2.845414    -2.869374     304.86
 H      -2.564403    -3.014136    -2.837152      31.94
 C      -5.050169    -1.005336    -2.403326      68.45
 H      -5.022483    -1.034453    -1.313732      27.10
 O      -5.488359     0.294955    -2.851665     238.25
 H      -5.229359     0.817462    -1.894248      22.65
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 C      -6.081288    -2.135420    -3.125228      96.86
 O      -6.203170    -3.326451    -2.338970     247.87
 H      -5.371509    -3.959652    -2.233737      26.47
 H      -5.847052    -2.257860    -4.162172      29.17
 H      -7.000082    -1.493747    -3.199589      27.72
55
name = lig-ACN-frame_286
 C       3.804348     2.689807    -0.234021      62.21
 H       3.237650     3.584672    -0.447395      21.63
 C       4.321247     0.598045     0.818205      53.98
 H       4.190691    -0.166298     1.610805      23.32
 C       5.543033     0.469122     0.077128      19.73
 O       6.441613    -0.562125     0.292426     160.28
 C       5.985190    -1.766385     1.126896     101.28
 H       6.252592    -1.561111     2.200106      24.91
 H       6.556911    -2.569489     0.624636      25.08
 H       4.800244    -2.127795     0.988170      23.45
 C       5.892604     1.399931    -0.876367      25.61
 O       6.953635     1.282626    -1.681757     120.27
 H       7.781861     0.900500    -1.151198      25.56
 C       4.968861     2.497466    -0.966448      37.44
 H       5.145908     3.190536    -1.859564      23.47
 C       3.511341     1.753155     0.761300      29.83
 C       2.251878     1.913862     1.665194      95.95
 H       2.269713     2.915700     2.319174      23.34
 O       2.055801     0.961413     2.700497     287.63
 H       1.877724     0.135413     2.225504      26.98
 C       0.985845     2.009845     0.807886      81.52
 H       1.156055     2.957844     0.086450      22.94
 C      -0.256160     2.401885     1.778385     105.15
 O      -0.102212     3.798912     2.320756     267.61
 H       0.065111     4.312662     1.540899      31.02
 H      -0.295514     1.727644     2.637556      25.63
 H      -1.164915     2.349520     1.292314      27.18
 C      -2.165308    -1.269373    -0.729487      67.29
 H      -2.844934    -2.075503    -0.141337      20.01
 C      -1.792333     0.386481    -2.456578      72.86
 H      -2.028268     0.669920    -3.411355      22.72
 C      -0.767897     0.912258    -1.844795      18.03
 O       0.063496     1.988220    -2.213803     226.93
 C      -0.269665     2.408638    -3.615674     101.60
 H      -0.077972     3.528051    -3.870821      25.06
 H       0.104191     1.606417    -4.312533      26.27
 H      -1.420106     2.491616    -3.555443      24.94
 C      -0.360528     0.397861    -0.553796      20.10
 O       0.838519     0.789290     0.150150     190.16
 C      -1.204284    -0.667443     0.006927      55.92
 H      -0.728589    -1.305187     0.888434      20.33
 C      -2.521647    -0.807769    -2.054621      35.27
 C      -3.592269    -1.400229    -2.957851      66.39
 H      -3.543672    -1.066015    -3.954622      29.07
 O      -3.431160    -2.845501    -2.855609     213.16
 H      -2.424505    -3.060568    -3.102206      26.86
 C      -5.065798    -1.079437    -2.440966      92.32
 H      -5.133973    -1.229986    -1.374224      28.02
 O      -5.456687     0.265808    -2.828891     246.09
 H      -5.182636     1.121798    -2.242192      24.88
 C      -6.047019    -2.077175    -3.058353     110.84
 O      -6.207115    -3.341817    -2.309860     228.82
 H      -5.221810    -3.705731    -2.361319      28.13
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 H      -5.577973    -2.348800    -3.965642      30.72
 H      -7.142539    -1.941870    -3.147988      27.29
55
name = lig-ACN-frame_287
 C       3.823457     2.766265    -0.205636      56.62
 H       3.183162     3.596388    -0.332845      24.34
 C       4.248476     0.609430     0.853373      69.53
 H       3.990974    -0.087416     1.682419      23.62
 C       5.443910     0.467000     0.145877      19.50
 O       6.366000    -0.561494     0.340498     172.35
 C       6.089905    -1.706334     1.087016     115.01
 H       6.081455    -1.528413     2.152746      26.15
 H       6.954478    -2.468579     1.018319      24.76
 H       4.922878    -2.116740     0.832462      23.71
 C       5.800571     1.447993    -0.826828      27.79
 O       6.960886     1.350160    -1.726172     112.57
 H       7.567806     0.771008    -1.333111      26.96
 C       5.030107     2.550025    -1.013199      41.45
 H       5.308574     3.234737    -1.906628      24.64
 C       3.452008     1.755557     0.741550      13.32
 C       2.261518     1.922711     1.685358      82.18
 H       2.394812     2.999655     2.295049      22.86
 O       2.077940     0.820030     2.713572     243.09
 H       1.806697     0.042299     2.322147      28.19
 C       1.004826     2.076351     0.857029      73.83
 H       1.139513     2.807980    -0.069924      23.59
 C      -0.204390     2.502765     1.809362     115.21
 O      -0.092081     3.775513     2.327264     314.40
 H       0.226513     4.366618     1.788062      35.45
 H      -0.227137     1.852387     2.752875      24.87
 H      -1.058224     2.351506     1.235075      27.27
 C      -2.255428    -1.307475    -0.712463      78.37
 H      -2.749986    -2.352295    -0.290736      20.48
 C      -1.861531     0.338770    -2.570164      44.67
 H      -2.201376     0.851761    -3.387894      20.15
 C      -0.635728     0.945548    -1.745369       0.02
 O       0.115357     2.000139    -2.183072     203.20
 C      -0.341274     2.430699    -3.558770      96.74
 H       0.460860     3.225280    -3.768154      25.24
 H      -0.013264     1.555640    -4.313772      26.30
 H      -1.383537     2.572988    -3.747085      27.21
 C      -0.363149     0.399286    -0.480409      34.90
 O       0.817249     0.719296     0.186004     192.17
 C      -1.071734    -0.681151    -0.031049      44.55
 H      -0.642628    -1.084622     1.000339      19.73
 C      -2.536950    -0.751577    -2.028362      18.31
 C      -3.630467    -1.409462    -2.933003      77.18
 H      -3.546063    -1.037667    -3.880656      30.85
 O      -3.451061    -2.878875    -2.893465     174.97
 H      -2.285861    -3.107322    -2.890947      21.53
 C      -5.072535    -1.140050    -2.439625      91.00
 H      -5.119959    -1.207429    -1.361283      29.17
 O      -5.428108     0.223956    -2.839575     288.94
 H      -4.999557     0.594536    -2.106976      31.06
 C      -6.064087    -2.133849    -3.066864     118.09
 O      -6.153449    -3.322331    -2.270745     262.62
 H      -5.343262    -3.735002    -2.243081      31.79
 H      -5.865563    -2.337108    -4.088404      29.93
 H      -6.886747    -1.375849    -3.169447      27.63
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name = lig-ACN-frame_288
 C       3.881794     2.785157    -0.202337      61.86
 H       3.339232     3.677247    -0.350028      25.49
 C       4.215628     0.607267     0.955092      69.77
 H       3.804517    -0.205603     1.563781      23.27
 C       5.394469     0.457701     0.181658      12.75
 O       6.359690    -0.521897     0.312496     177.58
 C       6.127467    -1.692758     1.162926     108.12
 H       5.828798    -1.448211     2.118171      27.55
 H       7.120390    -2.282638     1.006489      24.77
 H       5.301705    -2.475070     0.550612      24.76
 C       5.797550     1.465970    -0.839716      18.65
 O       6.901540     1.384811    -1.695644     147.44
 H       7.631717     0.897385    -1.252140      24.98
 C       4.952268     2.663867    -1.042843      34.71
 H       5.354218     3.575174    -1.616916      24.82
 C       3.449065     1.779448     0.725806      28.63
 C       2.269290     1.855842     1.711840      83.25
 H       2.547169     2.813074     2.501687      22.41
 O       2.137436     0.790100     2.672810     243.88
 H       1.885958    -0.049874     2.098311      23.27
 C       0.922637     2.100744     0.905429      77.94
 H       1.032168     2.942169     0.109944      23.65
 C      -0.201128     2.451553     1.741781     103.32
 O      -0.072957     3.876605     2.388381     202.59
 H       0.565739     4.370083     1.727380      28.11
 H      -0.226727     1.637120     2.593072      24.30
 H      -1.157283     2.413167     1.297034      26.91
 C      -2.156894    -1.207549    -0.751039      66.24
 H      -2.595074    -2.284234    -0.477428      22.26
 C      -1.743879     0.377990    -2.479567      65.84
 H      -2.051592     0.668805    -3.471511      22.00
 C      -0.742243     0.915653    -1.766446      12.02
 O       0.061352     2.023713    -2.226526     232.35
 C      -0.231069     2.463776    -3.512179     120.09
 H       0.519179     3.207855    -3.852036      26.33
 H      -0.507235     1.609467    -4.309798      24.56
 H      -1.048945     3.130142    -3.358866      27.75
 C      -0.359568     0.356152    -0.454978      32.93
 O       0.803980     0.694198     0.276556     159.88
 C      -1.094658    -0.818238    -0.023997      46.55
 H      -1.005936    -1.223233     1.035628      19.47
 C      -2.572398    -0.712949    -1.952170      44.36
 C      -3.582940    -1.468754    -2.817851      82.73
 H      -3.455846    -1.103355    -3.747876      30.37
 O      -3.441737    -2.907926    -2.952291     218.63
 H      -2.396108    -3.117963    -2.557735      23.47
 C      -5.034978    -1.184251    -2.464838      95.92
 H      -5.170877    -1.375999    -1.400069      28.62
 O      -5.366863     0.170724    -2.810911     293.44
 H      -5.295145     0.841601    -2.213983      32.17
 C      -6.104578    -2.126707    -3.108609     110.42
 O      -6.165284    -3.294542    -2.225624     223.73
 H      -5.266550    -3.725684    -2.335472      29.60
 H      -5.966065    -2.337017    -4.140518      30.74
 H      -7.161939    -1.941475    -2.868255      27.70
55
name = lig-ACN-frame_289
 C       3.787783     2.806519    -0.132366      56.71
 H       3.204167     3.713994    -0.107122      23.56
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 C       4.272047     0.613498     0.894252      69.92
 H       4.071880    -0.161503     1.616994      23.11
 C       5.423074     0.542860     0.098651      11.89
 O       6.391437    -0.506691     0.277340     129.33
 C       6.145105    -1.694893     1.152411     109.90
 H       5.676759    -1.496997     2.059897      26.34
 H       7.147145    -2.090174     1.496344      26.43
 H       5.430097    -2.611587     0.632103      24.62
 C       5.717932     1.529639    -0.840989      31.74
 O       6.858494     1.375828    -1.626513      88.48
 H       7.700715     1.152614    -0.994602      24.66
 C       4.994411     2.641657    -0.959890      53.08
 H       5.305917     3.441955    -1.667350      23.31
 C       3.475321     1.767658     0.776993      12.56
 C       2.239041     1.887285     1.693514      87.43
 H       2.238104     2.971693     2.414308      21.75
 O       2.189968     0.798337     2.592255     223.49
 H       1.906034    -0.194244     2.168677      20.04
 C       0.970681     2.032666     0.881111      75.72
 H       1.183061     2.748158     0.032302      23.35
 C      -0.331010     2.509664     1.842532      91.25
 O      -0.049140     3.855399     2.401433     165.02
 H       0.585674     4.503137     1.632304      23.74
 H      -0.454213     1.829650     2.814038      23.73
 H      -1.213618     2.508757     1.181491      25.01
 C      -2.145359    -1.308570    -0.736765      77.58
 H      -2.853297    -2.043824    -0.245890      22.79
 C      -1.802979     0.357049    -2.451687      39.89
 H      -1.761806     0.744614    -3.516445      17.60
 C      -0.707749     0.941579    -1.664870      14.50
 O       0.030838     1.937499    -2.164050     212.44
 C      -0.203501     2.659385    -3.535550     101.70
 H       0.767082     2.825939    -3.890909      27.75
 H      -0.599507     1.818035    -4.291168      22.61
 H      -0.926382     3.408737    -3.566676      27.51
 C      -0.349095     0.289151    -0.458985      31.42
 O       0.743963     0.748662     0.352351     206.41
 C      -1.071266    -0.784068     0.064740      51.07
 H      -0.641802    -1.402319     0.840283      24.16
 C      -2.532440    -0.691456    -1.976018      37.40
 C      -3.529202    -1.465480    -2.852313      61.77
 H      -3.456373    -1.084039    -3.774881      29.58
 O      -3.375426    -2.950232    -2.941805     250.50
 H      -2.478279    -3.250294    -2.730103      30.79
 C      -5.094824    -1.187533    -2.420189      80.92
 H      -5.216589    -1.281881    -1.319685      28.16
 O      -5.325475     0.182309    -2.842678     231.87
 H      -5.213723     0.574851    -1.849564      24.09
 C      -6.181271    -2.139431    -3.038005     113.61
 O      -6.158691    -3.343293    -2.215385     179.60
 H      -5.170527    -3.773195    -2.348464      26.30
 H      -5.876782    -2.409798    -4.034601      30.18
 H      -7.055032    -1.493484    -3.192963      29.39
55
name = lig-ACN-frame_290
 C       3.769385     2.803528    -0.069381      62.22
 H       3.102614     3.687653    -0.228604      22.83
 C       4.322375     0.646692     0.816045      73.13
 H       4.131998    -0.032585     1.622701      24.53
 C       5.490439     0.457134     0.100757      19.59
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 O       6.419861    -0.529123     0.245279     191.45
 C       6.127066    -1.612857     1.142680     116.79
 H       5.428415    -1.335832     1.908752      24.65
 H       7.069665    -2.057465     1.438498      27.30
 H       5.610705    -2.472194     0.353829      24.46
 C       5.761698     1.520870    -0.835036      12.81
 O       6.899976     1.376743    -1.594419     136.33
 H       7.670623     1.162153    -0.962321      24.41
 C       4.878895     2.735128    -0.855701      46.60
 H       5.113839     3.377263    -1.668024      21.97
 C       3.469867     1.790918     0.832309      35.46
 C       2.229912     1.901784     1.660022      85.93
 H       2.383895     3.008085     2.341371      22.19
 O       2.215983     0.819087     2.611590     246.46
 H       1.876004     0.042969     2.001203      23.16
 C       0.834513     2.031902     0.927754      85.63
 H       0.850915     2.790242     0.135707      24.20
 C      -0.304586     2.599275     1.849469     104.97
 O      -0.027889     3.822847     2.402982     181.04
 H       0.184192     4.555732     1.509908      24.23
 H      -0.570342     1.852951     2.739626      24.37
 H      -1.307979     2.595540     1.272688      24.69
 C      -2.206469    -1.358910    -0.635494      63.69
 H      -2.714469    -2.220436    -0.268212      25.15
 C      -1.776267     0.371617    -2.430089      76.60
 H      -2.241933     0.794355    -3.406569      19.63
 C      -0.761630     0.900011    -1.659223      13.46
 O       0.078609     2.001120    -2.139645     196.83
 C      -0.158687     2.690228    -3.477085     125.80
 H       0.817053     2.996421    -3.610366      28.33
 H      -0.475245     1.991383    -4.288820      25.82
 H      -0.626439     3.622743    -3.346213      27.61
 C      -0.354861     0.339935    -0.397779      38.50
 O       0.699040     0.694363     0.374554     214.12
 C      -1.053831    -0.806287     0.048441      35.26
 H      -0.742776    -1.166557     0.987441      19.85
 C      -2.485446    -0.843404    -1.957413      51.18
 C      -3.609588    -1.489685    -2.909044      82.39
 H      -3.536276    -1.125527    -3.838920      30.45
 O      -3.307351    -2.956498    -2.906353     268.25
 H      -2.451584    -3.012279    -2.886803      30.22
 C      -5.053692    -1.179931    -2.406177      90.89
 H      -5.062393    -1.236218    -1.295143      29.20
 O      -5.306818     0.220838    -2.820357     245.15
 H      -4.950786     1.022170    -2.144415      24.71
 C      -6.100430    -2.136556    -2.993035     112.38
 O      -6.205505    -3.390439    -2.224959     235.78
 H      -5.267114    -3.681765    -2.269630      30.54
 H      -5.883250    -2.340024    -4.055222      30.13
 H      -7.131259    -1.814767    -2.878628      28.84
55
name = lig-ACN-frame_291
 C       3.761101     2.858168    -0.060663      47.38
 H       2.986823     3.683878    -0.216877      23.20
 C       4.285454     0.619234     0.906549      61.55
 H       3.854591    -0.205714     1.462694      23.49
 C       5.471289     0.526097     0.080084       6.40
 O       6.485850    -0.525702     0.201101     173.46
 C       6.076459    -1.600394     1.068412     114.78
 H       5.442973    -1.293345     1.973363      25.50
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 H       6.944181    -1.947427     1.556914      28.81
 H       5.489913    -2.564476     0.517476      25.66
 C       5.808976     1.563345    -0.787528      24.43
 O       6.976558     1.444961    -1.607820     198.28
 H       7.643567     0.968394    -1.191948      25.63
 C       4.941923     2.679769    -0.901499      50.84
 H       5.115460     3.532327    -1.447694      26.69
 C       3.455102     1.780369     0.773632       3.47
 C       2.201773     1.914251     1.707980      77.26
 H       2.388590     2.961414     2.480216      21.92
 O       2.177862     0.872071     2.666271     269.35
 H       1.947109     0.042812     2.366429      28.87
 C       0.801823     2.086140     0.945102      88.80
 H       0.907348     2.710618     0.102840      25.23
 C      -0.353906     2.494890     1.829698      92.90
 O       0.009642     3.897435     2.412048     206.06
 H       0.176747     4.543649     1.683808      29.59
 H      -0.404049     1.797528     2.768166      24.66
 H      -1.350792     2.591259     1.209249      24.67
 C      -2.181908    -1.378318    -0.647942      65.75
 H      -2.462774    -2.302371    -0.350718      24.04
 C      -1.848628     0.258014    -2.352940      68.21
 H      -2.217733     0.868837    -3.243745      20.64
 C      -0.721768     0.958377    -1.735457       4.89
 O       0.081866     2.035251    -2.080793     257.31
 C      -0.010185     2.716241    -3.303458     135.44
 H       0.852456     3.186801    -3.672424      28.51
 H      -0.376575     2.106164    -4.082736      29.08
 H      -0.897175     3.339585    -3.253357      27.93
 C      -0.491285     0.350201    -0.429946      27.77
 O       0.690189     0.672404     0.416520     155.72
 C      -1.154348    -0.840804     0.061477      45.50
 H      -1.032288    -1.122362     1.091786      21.78
 C      -2.491480    -0.908348    -1.949788      23.98
 C      -3.534435    -1.533310    -2.854006      92.03
 H      -3.505621    -1.131582    -3.776684      29.31
 O      -3.311727    -2.927961    -2.890857     295.66
 H      -2.398591    -3.106459    -2.702602      28.30
 C      -4.964801    -1.111362    -2.368285      80.14
 H      -5.060918    -1.243944    -1.252546      28.64
 O      -5.307213     0.237057    -2.816993     294.51
 H      -4.777203     0.729294    -2.206079      31.13
 C      -6.089030    -2.134530    -2.937586     105.43
 O      -6.189201    -3.424975    -2.248102     244.70
 H      -5.433681    -3.911997    -2.123154      32.49
 H      -5.963887    -2.266676    -4.047616      28.64
 H      -7.033293    -1.598372    -2.843947      28.44
55
name = lig-ACN-frame_292
 C       3.850223     2.783544    -0.143917      56.03
 H       3.346240     3.802144    -0.200931      23.35
 C       4.235151     0.609442     0.854739      66.83
 H       3.964981    -0.288949     1.435424      23.23
 C       5.457436     0.560279     0.139963      13.95
 O       6.428913    -0.477361     0.162911     177.35
 C       6.074728    -1.636199     1.069625     105.15
 H       5.400509    -1.155662     1.909463      24.21
 H       6.947313    -2.173096     1.365319      27.44
 H       5.382325    -2.393286     0.403662      25.85
 C       5.879041     1.624367    -0.788060      19.98
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 O       6.998887     1.556168    -1.611923      95.86
 H       7.600817     0.885561    -1.172709      22.53
 C       5.013721     2.717710    -0.941501      56.30
 H       5.471706     3.368666    -1.590905      26.06
 C       3.379317     1.756347     0.772668      21.94
 C       2.180159     1.914736     1.727434      80.59
 H       2.268217     3.094745     2.285943      21.53
 O       2.102064     0.921801     2.800693     264.40
 H       1.853593     0.136356     2.303299      26.55
 C       0.906165     2.017225     0.902474      87.11
 H       1.040604     2.740262     0.178096      24.24
 C      -0.328789     2.547595     1.879149      97.28
 O      -0.015309     3.870450     2.395145     283.19
 H       0.429406     4.263203     1.791451      35.73
 H      -0.461125     1.885604     2.783837      24.91
 H      -1.414600     2.415903     1.332820      23.76
 C      -2.169632    -1.548132    -0.740428      48.94
 H      -2.770373    -2.289331    -0.353183      20.29
 C      -1.835357     0.357921    -2.411266      40.57
 H      -2.068608     0.511604    -3.464124      19.35
 C      -0.751171     0.870138    -1.639618      -0.33
 O       0.102922     1.986203    -1.932851     193.26
 C      -0.041850     2.741275    -3.262168     105.97
 H       0.909528     3.315572    -3.060916      25.48
 H       0.102486     2.036262    -3.991328      27.89
 H      -0.839764     3.485804    -3.332989      26.78
 C      -0.452807     0.342851    -0.368449      28.52
 O       0.575832     0.707019     0.402675     233.90
 C      -1.239420    -0.693451     0.135423      47.66
 H      -0.731418    -1.218661     1.020037      22.08
 C      -2.454912    -0.833031    -1.897361      26.73
 C      -3.462316    -1.502755    -2.815209      68.57
 H      -3.285131    -1.104897    -3.739213      28.30
 O      -3.367560    -2.982187    -2.877063     219.27
 H      -2.354530    -3.295573    -2.598299      26.39
 C      -4.977981    -1.187106    -2.341511      86.40
 H      -4.971545    -1.081923    -1.225864      27.31
 O      -5.264214     0.195568    -2.799310     272.13
 H      -5.037220     0.831132    -2.182309      31.21
 C      -6.051326    -2.085779    -2.886272     107.36
 O      -6.194289    -3.422895    -2.249541     209.10
 H      -5.178500    -3.609793    -2.509755      28.13
 H      -5.840470    -2.297994    -3.986829      29.30
 H      -7.005827    -1.588808    -2.771214      29.32
55
name = lig-ACN-frame_293
 C       3.881309     2.756446    -0.178674      52.49
 H       3.285054     3.696970    -0.198669      23.68
 C       4.228279     0.603468     0.737071      61.09
 H       3.944549    -0.110214     1.541640      22.90
 C       5.502459     0.602662     0.116740      30.98
 O       6.336024    -0.494202     0.192330     226.51
 C       6.054465    -1.601060     0.998261     112.34
 H       5.752776    -1.506346     2.165984      23.34
 H       7.030506    -2.110142     1.051027      25.57
 H       5.243956    -2.297704     0.460306      24.65
 C       5.892079     1.595935    -0.775754      30.93
 O       7.008923     1.620535    -1.570044     212.54
 H       7.880149     1.087668    -1.206387      23.39
 C       5.090447     2.738049    -0.930530      57.79
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 H       5.083207     3.562982    -1.588509      23.70
 C       3.452613     1.767214     0.726636      20.88
 C       2.192829     1.897722     1.700075      77.27
 H       2.369959     3.028462     2.309302      22.33
 O       2.033221     1.017823     2.863830     236.57
 H       1.727324     0.004560     2.611393      22.12
 C       0.809115     2.039157     0.964974      97.63
 H       0.949650     2.663280     0.164157      24.80
 C      -0.218021     2.532019     1.875941     107.65
 O      -0.053435     3.844657     2.364348     269.42
 H       0.533911     4.420251     1.810403      29.57
 H      -0.297647     1.847544     2.708417      25.89
 H      -1.230023     2.630168     1.198145      24.02
 C      -2.101439    -1.397894    -0.651036      74.89
 H      -2.609223    -2.333107    -0.393342      21.14
 C      -1.733665     0.371478    -2.423737      37.19
 H      -1.783875     0.835974    -3.361296      16.48
 C      -0.791647     0.917151    -1.589481      24.68
 O       0.043240     1.936340    -1.856784     245.41
 C       0.041563     2.703878    -3.124679     123.87
 H       0.753658     3.630336    -3.029764      24.78
 H       0.223373     2.281097    -4.019703      29.33
 H      -1.061194     2.987517    -3.291537      27.32
 C      -0.541669     0.315330    -0.311205      45.58
 O       0.586389     0.730707     0.432717     203.88
 C      -1.279183    -0.817728     0.179335      27.65
 H      -1.056721    -1.159124     1.313031      18.03
 C      -2.439349    -0.815755    -1.944010      73.96
 C      -3.515266    -1.523024    -2.827589      47.21
 H      -3.550424    -1.204201    -3.835022      32.64
 O      -3.429998    -3.026715    -2.846216     169.64
 H      -2.259906    -3.220204    -2.793059      23.06
 C      -4.896948    -1.159983    -2.290364      89.05
 H      -4.954398    -1.427687    -1.197593      27.53
 O      -5.223344     0.148275    -2.804768     223.70
 H      -5.257548     0.756763    -1.901005      25.12
 C      -6.087443    -2.074670    -2.890867     100.12
 O      -6.106240    -3.361585    -2.271367     189.11
 H      -5.304218    -4.039160    -2.317378      27.26
 H      -5.934243    -2.074746    -4.035920      29.99
 H      -7.099205    -1.651451    -2.747030      28.93
55
name = lig-ACN-frame_294
 C       3.808350     2.853404    -0.133948      69.03
 H       3.104403     3.624540    -0.398617      23.18
 C       4.263711     0.607916     0.753626      72.21
 H       4.019224    -0.313857     1.310513      22.08
 C       5.482576     0.557721     0.055698      18.93
 O       6.334159    -0.482425     0.196969     190.25
 C       6.052579    -1.681888     0.969376     107.33
 H       5.990034    -1.285978     2.097710      24.67
 H       6.895813    -2.425316     0.740126      25.03
 H       5.074540    -2.238211     0.690140      25.83
 C       5.910452     1.666675    -0.803715      20.28
 O       7.098373     1.627084    -1.564176      95.35
 H       7.813507     1.233227    -0.942891      24.06
 C       5.008506     2.745674    -0.875226      49.67
 H       5.522961     3.449974    -1.571742      24.09
 C       3.461368     1.739941     0.705296      21.59
 C       2.223075     1.928480     1.663757      81.20
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 H       2.490619     3.054968     2.192276      21.99
 O       2.023054     1.107651     2.864264     229.26
 H       1.797034     0.126675     2.437674      22.07
 C       0.902116     2.086995     0.919581      85.34
 H       0.893173     2.809602     0.172750      23.17
 C      -0.302173     2.499970     1.868296      92.21
 O      -0.048281     3.903587     2.398025     180.29
 H       0.418534     4.455291     1.503911      25.02
 H      -0.385920     1.915947     2.714372      25.57
 H      -1.358460     2.274234     1.287487      22.56
 C      -2.256672    -1.286954    -0.734419      63.82
 H      -2.666296    -2.327695    -0.437434      22.42
 C      -1.712637     0.273654    -2.423585      38.38
 H      -2.039311     0.731118    -3.322269      18.94
 C      -0.804542     0.914997    -1.471712       1.71
 O       0.091261     1.970786    -1.821227     227.46
 C       0.006772     2.663298    -3.013935     103.87
 H       0.446881     3.732237    -2.751483      24.62
 H       0.602840     2.093856    -3.638888      26.94
 H      -1.082397     2.892720    -3.353497      24.87
 C      -0.568278     0.344084    -0.160155      35.37
 O       0.600936     0.681406     0.487153     201.90
 C      -1.157951    -0.820760     0.277580      34.16
 H      -1.230217    -1.249921     1.427046      19.56
 C      -2.410682    -0.858531    -2.054443      11.55
 C      -3.543903    -1.586216    -2.837014      83.29
 H      -3.458280    -1.189721    -3.853731      25.64
 O      -3.443208    -3.009048    -2.806618     198.09
 H      -2.321745    -3.344761    -2.896153      21.98
 C      -4.964042    -1.212033    -2.310378      92.64
 H      -4.965504    -1.069494    -1.208609      28.29
 O      -5.180678     0.164231    -2.734713     237.33
 H      -5.151657     0.882787    -1.918686      25.75
 C      -6.022854    -2.074349    -2.897230     110.36
 O      -6.076108    -3.367731    -2.261630     247.43
 H      -5.196034    -3.564258    -2.509237      31.53
 H      -6.046371    -2.200534    -4.045392      28.71
 H      -6.932063    -1.522689    -2.553360      28.29
55
name = lig-ACN-frame_295
 C       3.767334     2.855668    -0.122967      43.67
 H       3.161867     3.730654    -0.171691      23.49
 C       4.291702     0.613603     0.790392      54.25
 H       3.889316    -0.223692     1.353965      20.69
 C       5.463362     0.538455    -0.016115      15.78
 O       6.435097    -0.532202     0.121831     183.68
 C       6.017511    -1.704771     0.974290     101.86
 H       6.222800    -1.591815     2.139276      26.14
 H       6.707884    -2.588871     0.637512      25.50
 H       4.946617    -1.918307     0.812596      28.54
 C       5.888049     1.647587    -0.770236      23.64
 O       7.134263     1.636198    -1.510810     171.45
 H       7.788258     1.106435    -1.110064      23.15
 C       5.002052     2.788288    -0.877248      45.44
 H       5.172695     3.781437    -1.448947      25.23
 C       3.391016     1.765360     0.730257      10.94
 C       2.249767     2.043346     1.672312      87.11
 H       2.377024     3.203780     2.124165      22.68
 O       2.086444     1.158768     2.775510     277.56
 H       1.851133     0.285372     2.483164      26.46
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 C       0.888636     2.073243     0.920420      73.16
 H       1.066682     2.584657    -0.000032      20.78
 C      -0.323169     2.571367     1.916388      98.96
 O      -0.096557     3.877570     2.386583     191.62
 H       0.306751     4.603300     1.534858      23.84
 H      -0.317045     1.927138     2.712709      26.03
 H      -1.388723     2.640254     1.348608      22.51
 C      -2.255806    -1.354258    -0.641284      58.88
 H      -3.109119    -2.074432    -0.267686      20.63
 C      -1.680385     0.301434    -2.391742      80.73
 H      -1.655051     0.690499    -3.437889      18.46
 C      -0.799229     0.857189    -1.438962      16.01
 O       0.086022     1.934545    -1.643734     196.91
 C      -0.033352     2.676004    -3.013939     121.80
 H       0.309456     3.776529    -2.758276      25.27
 H       0.612455     2.389487    -3.828123      27.88
 H      -1.059729     2.597373    -3.588903      25.85
 C      -0.505040     0.358495    -0.113294      37.83
 O       0.671078     0.695960     0.575293     192.72
 C      -1.344504    -0.786539     0.161088      52.42
 H      -0.840339    -1.426990     1.050263      18.59
 C      -2.424651    -0.925458    -1.987868      57.95
 C      -3.497771    -1.551829    -2.861503      57.76
 H      -3.510000    -1.272863    -3.951990      27.79
 O      -3.425819    -3.038554    -2.783195     201.43
 H      -2.399849    -3.290401    -2.694594      25.77
 C      -4.923503    -1.140599    -2.324743      84.22
 H      -4.988486    -1.514315    -1.272532      28.28
 O      -5.161188     0.240487    -2.690450     307.53
 H      -4.778194     0.706616    -1.987133      30.80
 C      -6.115193    -2.051129    -2.856637     100.94
 O      -6.018302    -3.398987    -2.269240     220.37
 H      -5.177053    -3.832233    -2.223553      30.70
 H      -5.902709    -2.118037    -3.996138      29.05
 H      -7.182172    -1.658913    -2.773874      27.59
55
name = lig-ACN-frame_296
 C       3.826301     2.792259    -0.135531      62.69
 H       3.340989     3.733158    -0.048583      23.96
 C       4.228139     0.657068     0.787808      54.99
 H       4.105887    -0.011576     1.613496      23.10
 C       5.482423     0.509207     0.031184       5.07
 O       6.458622    -0.597942     0.069381     201.01
 C       5.988198    -1.660542     0.922954     114.62
 H       6.360044    -1.479294     2.004280      24.68
 H       6.378065    -2.642860     0.427128      25.07
 H       4.944054    -1.764375     0.918021      26.08
 C       5.872299     1.664985    -0.806590      11.11
 O       7.064981     1.659894    -1.437965     133.35
 H       7.574752     0.908484    -1.089786      25.72
 C       5.004164     2.801437    -0.856230      51.94
 H       5.344305     3.703265    -1.529215      20.91
 C       3.458191     1.809319     0.734343      34.73
 C       2.182739     2.113117     1.680393      82.17
 H       2.403315     3.177407     2.248659      22.43
 O       2.210258     1.181017     2.754703     285.98
 H       1.854330     0.410605     2.383992      27.41
 C       0.804193     2.110900     0.994342      94.68
 H       0.739776     2.821701     0.120717      20.21
 C      -0.261859     2.607065     1.839252     104.72
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 O      -0.139192     3.929846     2.429854     240.84
 H       0.410943     4.561226     1.723821      26.76
 H      -0.415334     1.998185     2.679586      26.15
 H      -1.274002     2.430211     1.204076      23.64
 C      -2.345485    -1.413797    -0.638663      94.21
 H      -2.851506    -2.307363    -0.074260      17.86
 C      -1.632256     0.228728    -2.282640      35.53
 H      -1.566287     0.477252    -3.395960      20.12
 C      -0.706715     0.873080    -1.432935      25.34
 O       0.029714     1.977230    -1.687021     227.03
 C      -0.040108     2.675753    -2.960256     106.49
 H      -0.091334     3.798086    -2.757631      25.76
 H       0.755818     2.260244    -3.629336      25.97
 H      -1.158961     2.432329    -3.195485      25.28
 C      -0.523156     0.238213    -0.198435      27.56
 O       0.651847     0.644629     0.637223     178.10
 C      -1.314406    -0.773589     0.237453      56.11
 H      -1.158029    -1.326572     1.238185      19.50
 C      -2.447803    -0.840362    -1.927347      72.16
 C      -3.489362    -1.562357    -2.857532      34.50
 H      -3.261173    -1.160566    -3.938830      26.82
 O      -3.372121    -3.049037    -2.768095     247.40
 H      -2.518116    -3.266043    -2.628185      31.92
 C      -4.937859    -1.126363    -2.325760      86.07
 H      -4.840180    -1.043595    -1.237287      26.81
 O      -5.145323     0.295993    -2.610463     308.02
 H      -4.634974     0.875043    -2.072901      28.63
 C      -6.073804    -2.093786    -2.906190     100.22
 O      -6.042250    -3.409366    -2.262573     214.00
 H      -4.965540    -3.495202    -2.323805      25.71
 H      -6.075874    -2.189886    -4.056910      28.20
 H      -7.082937    -1.688155    -2.545409      26.78
55
name = lig-ACN-frame_297
 C       3.878373     2.921803    -0.149143      50.26
 H       3.200008     3.749228    -0.380824      22.78
 C       4.308628     0.621653     0.832560      56.74
 H       4.013832    -0.091725     1.576338      21.87
 C       5.468383     0.561968     0.084715      26.90
 O       6.325644    -0.539963     0.004814     230.37
 C       5.960144    -1.665340     0.873458     117.89
 H       6.476238    -1.544976     1.870779      25.64
 H       6.329530    -2.655035     0.482178      25.58
 H       4.968425    -1.632109     1.046082      27.29
 C       5.816312     1.581136    -0.754947      21.86
 O       7.009922     1.651920    -1.432757     105.94
 H       7.769747     0.988353    -1.028042      23.62
 C       5.081210     2.760711    -0.890177      46.86
 H       5.574096     3.564247    -1.557424      23.58
 C       3.438830     1.846994     0.756554     -16.46
 C       2.263308     2.088044     1.662420      91.18
 H       2.345946     3.227235     2.049304      23.55
 O       2.312137     1.177291     2.795173     227.29
 H       1.900822     0.224953     2.532448      22.17
 C       0.871157     2.122727     0.989156      58.45
 H       1.014057     2.668667    -0.027099      19.98
 C      -0.391320     2.588313     1.897474      94.32
 O      -0.164781     4.003829     2.442839     269.31
 H       0.444352     4.485542     1.931393      31.68
 H      -0.546274     1.881413     2.748684      25.10
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 H      -1.318557     2.679723     1.208489      24.46
 C      -2.295955    -1.352641    -0.527138      55.92
 H      -2.820559    -2.341018    -0.542686      20.54
 C      -1.602190     0.162870    -2.313409      47.97
 H      -1.887701     0.603602    -3.326776      21.84
 C      -0.663910     0.808471    -1.445664       7.84
 O       0.043999     2.042899    -1.705882     232.48
 C      -0.180108     2.667259    -2.946107     130.57
 H       0.142319     3.720882    -2.755271      26.16
 H       0.696473     2.408485    -3.694413      26.31
 H      -1.017608     2.569247    -3.703336      25.71
 C      -0.412375     0.198483    -0.144417      13.87
 O       0.519142     0.626973     0.657245     172.40
 C      -1.323258    -0.905619     0.344107      42.08
 H      -1.333340    -0.926567     1.403446      20.11
 C      -2.495390    -0.882289    -1.829539      49.46
 C      -3.449048    -1.529727    -2.775764      66.35
 H      -3.389900    -1.198790    -3.936022      26.09
 O      -3.334942    -2.998574    -2.765481     258.74
 H      -2.467047    -3.177414    -2.843724      32.32
 C      -4.903481    -1.121150    -2.338917      89.04
 H      -5.064859    -1.489455    -1.316536      28.39
 O      -5.172823     0.312465    -2.622799     247.83
 H      -4.650131     0.785943    -1.756855      23.23
 C      -6.042239    -2.049351    -2.867484     102.71
 O      -6.014365    -3.375455    -2.272828     186.59
 H      -5.086497    -3.849900    -2.292450      26.98
 H      -6.032388    -2.160711    -4.004906      28.66
 H      -7.014307    -1.482681    -2.623609      27.98
55
name = lig-ACN-frame_298
 C       3.893774     2.948262    -0.151718      66.88
 H       3.247055     3.842862    -0.332765      23.13
 C       4.236414     0.745846     0.918050      72.32
 H       3.803008    -0.127319     1.402496      20.25
 C       5.419658     0.548239     0.120833      16.39
 O       6.186658    -0.547710    -0.035382     195.05
 C       5.953491    -1.670454     0.869344     128.23
 H       6.514331    -1.588111     1.788485      27.56
 H       6.302257    -2.444778     0.221968      27.35
 H       4.976495    -1.938328     1.048699      29.19
 C       5.868452     1.634560    -0.730793      22.57
 O       7.033947     1.584486    -1.494700     101.13
 H       7.816788     1.066849    -1.014096      22.06
 C       5.069891     2.758549    -0.888414      55.41
 H       5.352451     3.559160    -1.600877      25.36
 C       3.550636     1.898420     0.677040      24.88
 C       2.307240     1.998238     1.686721      89.09
 H       2.466105     3.039250     2.224621      24.22
 O       2.381355     1.183487     2.855659     204.71
 H       1.987821     0.200449     2.568976      21.92
 C       0.841830     2.020889     1.005273      75.94
 H       0.920507     2.664043     0.018420      20.11
 C      -0.388660     2.709894     1.902614      98.64
 O      -0.198605     3.977752     2.424857     325.34
 H       0.299805     4.414058     1.872484      34.99
 H      -0.545579     1.974835     2.787843      24.87
 H      -1.367463     2.633571     1.304379      24.46
 C      -2.265311    -1.417261    -0.445343      55.21
 H      -2.936459    -1.997308     0.152233      19.24
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 C      -1.625549     0.185107    -2.314136      42.77
 H      -1.833585     0.695278    -3.266514      17.87
 C      -0.651277     0.694621    -1.464157       3.94
 O      -0.033658     1.950824    -1.666777     165.69
 C      -0.176243     2.770631    -3.113237      86.51
 H      -0.153827     3.801770    -2.843282      26.28
 H       0.569201     2.266801    -3.907730      24.33
 H      -1.247083     2.562201    -3.244901      23.64
 C      -0.486473     0.160385    -0.146344      20.45
 O       0.519865     0.686506     0.794216     219.31
 C      -1.257411    -0.838216     0.388598      52.23
 H      -1.101405    -1.309145     1.246140      21.43
 C      -2.364768    -0.867894    -1.805344      46.68
 C      -3.480711    -1.490272    -2.703450      46.71
 H      -3.205655    -0.921748    -3.764065      26.50
 O      -3.311747    -2.936893    -2.773802     194.76
 H      -2.296875    -3.206134    -2.959249      24.10
 C      -4.906940    -1.167685    -2.286249      99.47
 H      -4.868691    -1.152156    -1.209751      27.77
 O      -5.173218     0.233686    -2.608979     259.49
 H      -5.088642     0.910453    -1.758476      24.56
 C      -6.003804    -1.994103    -2.916325     108.23
 O      -6.017894    -3.325964    -2.256848     249.35
 H      -5.210426    -3.645416    -2.527805      34.35
 H      -5.882835    -2.059433    -4.032910      30.10
 H      -7.047009    -1.660132    -2.653643      28.32
55
name = lig-ACN-frame_299
 C       3.880263     2.933408    -0.167170      54.76
 H       3.337393     3.927088    -0.138062      24.10
 C       4.246202     0.754593     0.816975      62.93
 H       3.891638     0.033435     1.584380      21.51
 C       5.390272     0.642204     0.087971      22.04
 O       6.079364    -0.624828    -0.038586     220.72
 C       5.967618    -1.754324     0.821079     132.02
 H       6.466605    -1.544738     1.730870      27.74
 H       6.434498    -2.562206     0.413340      28.08
 H       4.948415    -1.873347     1.077436      28.08
 C       5.934231     1.704647    -0.708329      15.61
 O       7.075765     1.504059    -1.554694      90.82
 H       7.618912     0.866212    -1.129237      23.96
 C       5.079974     2.850380    -0.916672      51.63
 H       5.405759     3.526369    -1.657904      23.07
 C       3.424734     1.951478     0.800435      11.74
 C       2.258206     2.070809     1.724198      92.65
 H       2.324020     3.162911     2.120284      23.22
 O       2.420135     1.140684     2.884088     251.13
 H       2.045490     0.262065     2.688232      25.93
 C       0.816798     2.069946     1.116006      77.09
 H       0.885350     2.605761     0.082459      20.37
 C      -0.310880     2.639571     1.857551      97.94
 O      -0.198046     4.016578     2.399980     286.08
 H       0.288735     4.681245     1.809517      28.78
 H      -0.569922     2.028113     2.841182      23.62
 H      -1.165614     2.568914     1.155052      24.34
 C      -2.231779    -1.389616    -0.424736      58.27
 H      -2.950972    -2.058761    -0.123686      22.41
 C      -1.646700     0.145149    -2.249218     120.11
 H      -1.773381     0.383747    -3.281141      21.56
 C      -0.622348     0.766240    -1.434383      17.30
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 O      -0.046955     1.938644    -1.775693     212.31
 C      -0.282696     2.695373    -3.047151     117.96
 H       0.191579     3.608030    -2.817528      26.92
 H       0.430342     2.293803    -4.003742      25.35
 H      -1.261343     2.700551    -3.467682      27.26
 C      -0.416561     0.275074    -0.063434      30.45
 O       0.497258     0.623008     0.860833     199.35
 C      -1.194992    -0.857144     0.386888      22.59
 H      -0.863715    -1.189433     1.221902      20.59
 C      -2.398564    -0.963467    -1.738616      31.25
 C      -3.408034    -1.452149    -2.664534      50.09
 H      -3.486363    -1.009263    -3.820941      25.26
 O      -3.312271    -2.895168    -2.817819     172.47
 H      -2.169114    -3.185258    -2.742604      20.68
 C      -4.910304    -1.094349    -2.137742      85.38
 H      -5.123824    -1.351112    -1.113068      29.32
 O      -5.182077     0.208118    -2.626199     286.78
 H      -5.225615     0.738526    -1.907421      31.99
 C      -6.004288    -2.017739    -2.899442     102.50
 O      -6.028982    -3.282713    -2.294119     222.25
 H      -5.125367    -3.721216    -2.348354      28.61
 H      -5.773918    -2.106011    -3.986289      29.99
 H      -6.920886    -1.403346    -2.844190      29.59
55
name = lig-ACN-frame_300
 C       3.853798     2.974620    -0.112846      51.41
 H       3.240219     3.884022    -0.368546      22.94
 C       4.185541     0.781134     0.779283      45.14
 H       4.113497    -0.088230     1.461905      21.49
 C       5.445169     0.623620     0.028543      20.67
 O       6.037707    -0.621496    -0.135878     179.90
 C       5.921038    -1.783456     0.889241     118.82
 H       6.405072    -1.600895     1.758273      27.42
 H       6.339471    -2.531979     0.341058      27.51
 H       4.905061    -2.181438     1.034088      25.71
 C       5.951397     1.696855    -0.789628      16.46
 O       7.044451     1.463080    -1.565848      98.51
 H       7.603910     0.756254    -1.227149      22.79
 C       5.119721     2.866747    -0.881788      51.00
 H       5.330441     3.697768    -1.456300      25.62
 C       3.421322     1.969939     0.784867      20.40
 C       2.207353     2.167687     1.870315      93.68
 H       2.234453     3.134300     2.415671      23.80
 O       2.408787     1.157094     2.876087     291.76
 H       1.984471     0.407545     2.595073      28.14
 C       0.910038     2.059058     1.114009      83.89
 H       1.038627     2.575998     0.115485      21.62
 C      -0.344372     2.647245     1.908809      94.55
 O      -0.200246     4.034283     2.373865     250.10
 H       0.525216     4.480590     1.605860      24.53
 H      -0.572940     1.880664     2.808035      23.69
 H      -1.185418     2.603369     1.252874      25.47
 C      -2.202255    -1.416054    -0.382600      65.99
 H      -2.464955    -2.362199    -0.100562      23.71
 C      -1.559946     0.095323    -2.156159      40.02
 H      -1.681018     0.419822    -3.155530      19.60
 C      -0.706599     0.833905    -1.350716      19.52
 O       0.014409     1.973454    -1.853600     231.46
 C      -0.320806     2.610717    -3.041234     104.80
 H       0.150305     3.563290    -2.958430      25.80
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 H       0.197303     1.889510    -3.936056      22.98
 H      -1.365246     2.765912    -3.144091      26.95
 C      -0.430652     0.297830    -0.070362      31.64
 O       0.554495     0.625894     0.923475     198.58
 C      -1.138833    -0.863402     0.348031      42.63
 H      -1.147382    -1.094267     1.304615      21.95
 C      -2.409010    -0.912718    -1.716197      34.90
 C      -3.510812    -1.503219    -2.599894      60.78
 H      -3.267124    -0.809856    -3.620391      24.14
 O      -3.330134    -2.913709    -2.860830     174.11
 H      -2.175978    -3.167797    -2.805807      20.91
 C      -4.935929    -1.144160    -2.159454     100.14
 H      -4.981989    -1.142219    -1.083338      28.96
 O      -5.207373     0.272505    -2.610688     257.48
 H      -4.956006     0.955954    -1.957609      28.22
 C      -5.911761    -1.962126    -2.869548     113.45
 O      -6.090479    -3.325577    -2.308140     204.78
 H      -5.063170    -3.593687    -2.087732      27.59
 H      -5.584758    -2.011873    -3.911777      30.52
 H      -6.930579    -1.667031    -2.821552      29.13
55
name = lig-ACN-frame_301
 C       3.913272     3.012351    -0.106539      61.82
 H       3.271099     3.891093    -0.272487      22.69
 C       4.242152     0.789318     0.785887      56.10
 H       3.646293     0.033248     1.291702      18.36
 C       5.336139     0.586370    -0.008469      24.64
 O       6.032524    -0.674481    -0.175369     221.10
 C       5.862940    -1.720253     0.837153     124.84
 H       6.279807    -1.479907     1.718996      29.46
 H       6.419620    -2.519313     0.427214      26.81
 H       4.767269    -1.910819     1.050146      26.95
 C       5.836236     1.646021    -0.824257      13.77
 O       7.022219     1.489084    -1.621959      92.21
 H       7.647598     0.818155    -1.058152      23.00
 C       5.101697     2.858174    -0.780383      59.48
 H       5.516634     3.604306    -1.394669      23.09
 C       3.490343     2.001213     0.788307       8.04
 C       2.331501     2.151053     1.879409      90.27
 H       2.460592     3.120508     2.286745      24.58
 O       2.350105     1.188136     2.916960     276.49
 H       1.946307     0.285422     2.578110      21.74
 C       0.845634     2.079404     1.137444      78.01
 H       0.950024     2.606687     0.189707      21.27
 C      -0.367865     2.681600     1.915527      98.85
 O      -0.200020     3.988385     2.346772     251.83
 H       0.605003     4.721384     1.814327      22.90
 H      -0.491217     2.118527     2.970753      22.58
 H      -1.255540     2.525554     1.382682      26.04
 C      -2.105072    -1.522638    -0.409657      50.91
 H      -2.690129    -2.273067     0.078914      21.87
 C      -1.564276     0.144835    -2.168666      41.11
 H      -1.710609     0.519752    -3.177984      19.16
 C      -0.673388     0.914583    -1.281187       6.52
 O       0.108407     1.912970    -1.716526     151.18
 C      -0.366914     2.555773    -3.172397      76.06
 H       0.111959     3.507987    -3.318735      24.93
 H      -0.249293     1.890337    -4.220480      23.06
 H      -1.431931     2.604520    -3.057440      26.31
 C      -0.399873     0.287655     0.020924      13.75
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 O       0.626804     0.688475     0.901986     230.49
 C      -1.157507    -0.808140     0.409248      54.51
 H      -0.769347    -1.277776     1.292970      20.51
 C      -2.425295    -0.936718    -1.636725      41.37
 C      -3.463259    -1.472272    -2.596591      55.53
 H      -3.483440    -1.021263    -3.762277      24.14
 O      -3.371049    -2.959109    -2.875485     177.98
 H      -2.348909    -3.145592    -3.078113      25.25
 C      -4.912880    -1.041549    -2.140314      87.37
 H      -5.084072    -1.156038    -1.060589      27.46
 O      -5.226555     0.316917    -2.582365     236.48
 H      -4.576933     0.866650    -1.858397      23.73
 C      -5.973817    -2.036033    -2.895173     107.19
 O      -6.106376    -3.351743    -2.295165     246.63
 H      -5.226978    -3.739997    -2.168459      29.94
 H      -5.676152    -2.096712    -3.933466      30.30
 H      -6.839070    -1.444381    -2.856912      29.86
55
name = lig-ACN-frame_302
 C       3.934898     3.062656    -0.035291      63.15
 H       3.532701     4.055044     0.038549      25.01
 C       4.193069     0.735633     0.824285      52.86
 H       3.904990    -0.103315     1.460154      19.90
 C       5.292102     0.471287    -0.092157      18.38
 O       6.015857    -0.674032    -0.210774     218.53
 C       5.798385    -1.617445     0.799485     127.16
 H       6.147494    -1.272895     1.667726      29.73
 H       6.213024    -2.636099     0.588965      25.74
 H       4.681835    -1.880174     0.883972      25.02
 C       5.796668     1.575447    -0.827097      27.68
 O       6.927283     1.544109    -1.617972     157.47
 H       7.689599     0.921652    -1.257865      22.08
 C       5.164335     2.855756    -0.818021      43.29
 H       5.551554     3.684762    -1.433410      21.60
 C       3.538193     2.013611     0.847178      29.09
 C       2.324608     2.137076     1.731055      99.01
 H       2.473009     3.014075     2.204583      24.53
 O       2.318968     1.211975     2.982437     190.65
 H       1.935219     0.218838     2.695721      19.49
 C       0.883866     2.196404     1.165103      78.88
 H       0.865459     2.761436     0.262561      20.29
 C      -0.338490     2.634954     1.977723      98.36
 O      -0.214168     4.060881     2.378529     252.90
 H       0.508008     4.541756     1.589628      23.65
 H      -0.460094     1.927181     2.907418      22.83
 H      -1.150929     2.531493     1.348596      25.07
 C      -2.039888    -1.505218    -0.376323      54.06
 H      -2.783458    -2.317087    -0.125212      21.26
 C      -1.657829     0.221462    -2.049168      46.58
 H      -1.824332     0.486922    -3.120982      16.70
 C      -0.637678     0.795507    -1.255480       4.32
 O       0.190374     1.955783    -1.766755     175.41
 C      -0.424120     2.426407    -3.137773      80.69
 H       0.297096     3.284673    -3.231426      24.88
 H      -0.059780     1.548576    -3.845317      24.00
 H      -1.534845     2.744550    -3.205169      24.92
 C      -0.392406     0.339449     0.059686      29.45
 O       0.679130     0.711769     0.829552     191.79
 C      -1.128875    -0.860646     0.513099      53.52
 H      -0.726167    -1.376268     1.472185      18.43
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 C      -2.306303    -0.941306    -1.693524      46.77
 C      -3.432538    -1.472814    -2.630637      49.67
 H      -3.159871    -0.815491    -3.663817      24.70
 O      -3.415089    -2.949927    -2.850145     245.71
 H      -2.582910    -3.187411    -3.013464      31.58
 C      -4.952773    -1.081986    -2.193011      84.48
 H      -5.072354    -1.268692    -1.108013      27.75
 O      -5.198779     0.309209    -2.530609     277.90
 H      -4.817883     1.116384    -1.944540      24.66
 C      -6.012202    -2.025553    -2.896381     112.89
 O      -6.133554    -3.337260    -2.254852     242.92
 H      -5.335741    -3.715935    -2.530489      32.19
 H      -5.791920    -2.201169    -3.920691      30.78
 H      -7.013845    -1.733780    -2.844247      30.16
55
name = lig-ACN-frame_303
 C       4.085658     3.035675     0.078271      58.81
 H       3.603961     3.987414     0.103244      23.58
 C       4.190791     0.659448     0.790445      57.20
 H       3.952745     0.027984     1.657804      20.03
 C       5.239906     0.506127    -0.125311      10.23
 O       6.016717    -0.680693    -0.297699     206.25
 C       5.686521    -1.624721     0.855041     103.52
 H       5.962476    -1.271521     1.784183      28.79
 H       6.404929    -2.453342     0.500176      24.87
 H       4.566832    -1.842988     0.897751      25.62
 C       5.761814     1.634795    -0.837541      22.28
 O       6.886962     1.563391    -1.639124     188.65
 H       7.389711     0.846268    -1.340130      25.94
 C       5.101815     2.831462    -0.808032      58.82
 H       5.586843     3.673554    -1.414771      24.58
 C       3.545612     1.929091     0.827526      10.56
 C       2.277358     2.180182     1.866497     100.33
 H       2.292348     3.113445     2.200122      26.68
 O       2.312052     1.293239     2.947487     306.45
 H       1.941249     0.410364     2.686394      24.15
 C       0.955450     2.169770     1.077488      84.45
 H       1.051189     2.825085     0.251636      23.52
 C      -0.261981     2.675540     2.049040     101.19
 O      -0.253540     4.063806     2.428056     302.57
 H       0.340941     4.637420     1.806933      28.46
 H      -0.400820     2.096772     3.019347      24.21
 H      -1.131753     2.441352     1.500856      26.10
 C      -2.042796    -1.438113    -0.357466      61.06
 H      -2.173865    -2.526790     0.033663      21.84
 C      -1.678877     0.286096    -1.988912      64.45
 H      -1.960227     0.856741    -2.914801      16.79
 C      -0.564910     0.812997    -1.285878       1.71
 O       0.081850     1.899020    -1.816127     239.15
 C      -0.265007     2.294545    -3.033401      98.38
 H       0.221348     3.191845    -3.542747      24.11
 H      -0.263755     1.456453    -3.885489      25.03
 H      -1.454646     2.517470    -2.990174      22.42
 C      -0.398915     0.256208     0.073463      24.31
 O       0.724496     0.778931     0.761353     221.93
 C      -1.052623    -0.879858     0.499163      53.75
 H      -1.150941    -1.193067     1.680794      20.44
 C      -2.284852    -0.985647    -1.649759      25.29
 C      -3.424244    -1.483250    -2.625294      70.32
 H      -3.280529    -1.019248    -3.771951      23.35
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 O      -3.442992    -2.896558    -2.813292     272.77
 H      -2.545731    -3.149337    -2.872589      29.88
 C      -4.917322    -1.139838    -2.241753      81.31
 H      -4.972773    -1.289726    -1.130533      28.13
 O      -5.202016     0.279112    -2.525853     296.88
 H      -5.107598     0.599857    -1.693818      31.23
 C      -6.071214    -1.995445    -2.896008     109.96
 O      -6.134346    -3.308036    -2.219488     183.05
 H      -5.271302    -3.894849    -2.439583      27.45
 H      -5.835126    -2.018719    -3.926601      30.71
 H      -6.936483    -1.395021    -2.754828      30.30
55
name = lig-ACN-frame_304
 C       4.064284     2.987347     0.218699      52.65
 H       3.529390     3.935646     0.303329      22.41
 C       4.173359     0.677635     0.758426      41.29
 H       3.776482    -0.255391     1.225159      16.95
 C       5.279988     0.534232    -0.132448       6.92
 O       5.936238    -0.696603    -0.263674     236.73
 C       5.671277    -1.644001     0.795216     105.17
 H       5.844826    -1.127090     1.725945      28.46
 H       6.258134    -2.661632     0.812556      24.48
 H       4.607853    -2.024158     0.715970      26.43
 C       5.757215     1.627794    -0.894055      18.04
 O       6.891668     1.532825    -1.678095     176.12
 H       7.360341     0.702416    -1.454713      25.75
 C       5.081881     2.896383    -0.779065      57.29
 H       5.424470     3.824643    -1.408095      24.44
 C       3.488364     1.934653     0.920754      31.21
 C       2.375566     2.261416     1.863001     103.54
 H       2.539502     3.140565     2.224614      28.59
 O       2.310298     1.342194     2.967587     311.45
 H       1.917755     0.586265     2.693990      28.29
 C       0.924019     2.189978     1.112519      82.32
 H       1.014729     2.706718     0.192258      23.58
 C      -0.182629     2.688862     2.019060     115.28
 O      -0.281466     4.084976     2.487974     345.58
 H       0.279821     4.571191     2.073880      36.16
 H       0.116569     2.096006     2.939108      23.85
 H      -1.141522     2.430246     1.722907      28.49
 C      -1.979917    -1.536204    -0.341759      48.85
 H      -2.627465    -2.514257    -0.095865      21.30
 C      -1.716364     0.239336    -2.000522      49.85
 H      -2.209245     0.732047    -2.851065      20.03
 C      -0.680014     0.751434    -1.246906      16.23
 O       0.108713     1.820170    -1.680297     177.21
 C      -0.255636     2.231157    -3.180936      75.02
 H       0.612115     3.033778    -3.172108      23.52
 H      -0.130063     1.360043    -3.884442      24.38
 H      -1.331459     2.810267    -3.220136      23.15
 C      -0.243154     0.309043    -0.027074      18.91
 O       0.769653     0.786798     0.728442     249.29
 C      -1.075728    -0.782225     0.467288      44.94
 H      -0.705036    -1.160735     1.651694      17.02
 C      -2.392734    -0.896617    -1.606029      35.19
 C      -3.439116    -1.469626    -2.624712      64.76
 H      -3.181997    -0.874290    -3.670238      26.26
 O      -3.411016    -2.931925    -2.761457     214.24
 H      -2.358164    -3.232092    -2.994324      24.64
 C      -4.872230    -1.139398    -2.218723      95.44
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 H      -5.033903    -1.423302    -1.130803      27.76
 O      -5.199705     0.213634    -2.509758     266.63
 H      -5.251683     0.928848    -1.870242      29.06
 C      -6.007312    -1.976564    -2.851062     112.26
 O      -6.176324    -3.254518    -2.218691     205.52
 H      -5.191304    -3.571641    -2.229496      28.44
 H      -6.115366    -2.171629    -3.892356      30.44
 H      -6.950554    -1.512874    -2.572262      30.25
55
name = lig-ACN-frame_305
 C       4.003307     3.048059     0.221134      59.69
 H       3.646578     4.088034     0.435683      24.01
 C       4.100291     0.679060     0.707157      61.38
 H       3.551613    -0.254439     0.999789      19.90
 C       5.274459     0.548469    -0.094873      17.52
 O       5.890036    -0.712881    -0.256020     204.22
 C       5.624080    -1.684210     0.768476     109.24
 H       5.620887    -1.290570     1.829431      26.73
 H       6.549885    -2.343404     0.562440      23.97
 H       4.621106    -2.158877     0.678281      26.40
 C       5.757772     1.652268    -0.914997      16.29
 O       6.901306     1.490956    -1.742788     153.91
 H       7.466417     0.645058    -1.372980      25.41
 C       5.084375     2.886126    -0.684904      54.30
 H       5.334849     3.835274    -1.288007      21.80
 C       3.597688     1.925069     0.959589      31.01
 C       2.340018     2.254859     1.825902      95.15
 H       2.470835     3.140927     2.154293      26.32
 O       2.322057     1.385577     3.047232     250.89
 H       1.977971     0.448399     2.762733      22.36
 C       0.999211     2.341881     1.074713      62.01
 H       0.941042     2.987025     0.191356      19.80
 C      -0.157711     2.634472     2.135425      99.83
 O      -0.264924     4.104047     2.506245     301.15
 H       0.390506     4.567529     2.056341      32.10
 H      -0.090944     2.053688     3.052562      24.34
 H      -1.065070     2.285470     1.650220      26.16
 C      -1.989480    -1.497115    -0.373841      55.08
 H      -2.562164    -2.293931     0.278535      21.56
 C      -1.807262     0.219621    -2.024277      63.09
 H      -1.899616     0.630607    -2.997580      19.29
 C      -0.723226     0.820229    -1.291630       1.20
 O       0.086069     1.813783    -1.745869     205.36
 C      -0.106216     2.237141    -3.144743      95.14
 H       0.779537     2.863747    -3.566416      23.98
 H      -0.111604     1.343282    -3.750265      25.60
 H      -1.178004     2.800104    -3.494546      23.27
 C      -0.297199     0.228728    -0.020339      14.79
 O       0.851056     0.765211     0.757967     166.95
 C      -1.047305    -0.789328     0.446545      57.39
 H      -0.548514    -1.437479     1.457932      17.64
 C      -2.482042    -0.942320    -1.534777      32.70
 C      -3.429952    -1.483103    -2.556618      66.47
 H      -3.221843    -1.050506    -3.642098      25.27
 O      -3.338726    -2.964306    -2.716151     166.85
 H      -2.187735    -3.174363    -3.036354      20.64
 C      -4.909629    -1.138181    -2.140213      83.07
 H      -4.903114    -1.211199    -0.997512      26.59
 O      -5.214923     0.228890    -2.554621     225.57
 H      -4.683034     0.762672    -1.726566      23.67
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 C      -6.050760    -1.965030    -2.810448     115.68
 O      -6.169507    -3.262837    -2.185735     255.80
 H      -5.379077    -3.667128    -2.047810      33.25
 H      -5.735949    -1.895760    -3.852545      29.96
 H      -6.952753    -1.328895    -2.637513      28.50
55
name = lig-ACN-frame_306
 C       4.090398     3.083900     0.192993      56.15
 H       3.615374     4.109802     0.318979      23.47
 C       4.065412     0.656719     0.637938      53.27
 H       3.621529    -0.156010     1.264030      22.31
 C       5.221325     0.532137    -0.120609      48.09
 O       5.855624    -0.663576    -0.279219     205.74
 C       5.615192    -1.763672     0.737775     102.44
 H       5.595710    -1.263015     1.829270      23.78
 H       6.454517    -2.488601     0.725226      24.56
 H       4.764721    -2.368718     0.456133      26.17
 C       5.762180     1.637160    -0.818536      16.66
 O       6.854752     1.465035    -1.764434     122.13
 H       7.471695     0.809436    -1.294232      26.34
 C       5.141689     2.893925    -0.687150      53.61
 H       5.630790     3.694035    -1.257355      23.29
 C       3.553702     2.011550     0.953709      15.53
 C       2.368212     2.223719     1.897281     108.46
 H       2.434858     3.113250     2.228151      25.98
 O       2.316605     1.452769     3.073439     263.33
 H       2.042864     0.405190     2.878262      20.72
 C       0.997103     2.248144     1.181747      60.33
 H       1.087303     2.936291     0.295417      20.36
 C      -0.159675     2.656055     2.186454     109.57
 O      -0.227020     4.048214     2.498848     270.15
 H       0.480796     4.636100     1.881065      26.09
 H      -0.088905     2.115871     3.069177      24.96
 H      -1.110921     2.465447     1.651517      24.53
 C      -2.106124    -1.421541    -0.242937      47.09
 H      -2.427316    -2.504508    -0.020840      20.96
 C      -1.786635     0.260760    -2.012921      54.73
 H      -2.021271     0.432941    -3.017491      20.27
 C      -0.714344     0.842829    -1.295727       2.43
 O       0.065002     1.888678    -1.847758     221.49
 C       0.046970     2.184081    -3.204887      97.65
 H       0.963476     2.882499    -3.362180      23.88
 H      -0.050495     1.397614    -3.874057      27.44
 H      -0.974514     2.927058    -3.175690      22.26
 C      -0.308090     0.348714     0.017364      15.09
 O       0.812182     0.781067     0.692571     210.33
 C      -0.953369    -0.946525     0.429012      35.24
 H      -0.813476    -1.424182     1.623465      18.91
 C      -2.428772    -0.914080    -1.570067      14.45
 C      -3.510084    -1.608076    -2.482711      67.55
 H      -3.392452    -1.020507    -3.498121      25.11
 O      -3.289279    -2.980232    -2.662805     205.87
 H      -2.089636    -3.110415    -2.852217      19.00
 C      -4.965978    -1.112764    -2.065154      93.14
 H      -5.184619    -1.154267    -0.941862      27.27
 O      -5.180622     0.259829    -2.561080     224.40
 H      -4.574718     1.037605    -2.083598      23.92
 C      -6.004087    -1.942119    -2.736989     111.61
 O      -6.210166    -3.290948    -2.159987     209.02
 H      -5.250892    -3.622410    -2.290894      29.55
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 H      -5.808075    -2.201248    -3.787814      29.16
 H      -7.064711    -1.538970    -2.797812      28.29
55
name = lig-ACN-frame_307
 C       4.148598     3.101757     0.201259      54.03
 H       3.701204     4.130400     0.197520      21.20
 C       4.010593     0.766518     0.715028      55.50
 H       3.713071    -0.132277     1.252469      18.52
 C       5.145779     0.494442    -0.145674      10.60
 O       5.875199    -0.732062    -0.283750     227.69
 C       5.624697    -1.778570     0.639954     115.32
 H       5.313502    -1.323339     1.759649      25.00
 H       6.500955    -2.361501     0.679847      27.09
 H       4.711780    -2.293202     0.400236      27.94
 C       5.808809     1.601139    -0.801734      32.18
 O       6.775833     1.444092    -1.701248     212.07
 H       7.449748     0.885696    -1.454308      24.13
 C       5.270748     2.908240    -0.729046      43.72
 H       5.619692     3.727497    -1.275837      26.08
 C       3.496714     2.012241     0.862029      41.04
 C       2.382608     2.273851     1.939111      97.76
 H       2.506216     3.176421     2.221591      27.72
 O       2.342482     1.442165     3.150449     273.24
 H       2.014131     0.553778     2.869618      25.21
 C       0.940326     2.087341     1.277333      80.99
 H       0.973065     2.812172     0.380041      21.40
 C      -0.185017     2.620078     2.140597     109.68
 O      -0.150874     4.046538     2.503164     206.36
 H       0.527173     4.646826     1.705175      23.93
 H      -0.117494     2.148660     3.045633      26.10
 H      -1.210015     2.225329     1.812570      24.92
 C      -2.112892    -1.426022    -0.246780      58.50
 H      -2.653704    -2.343012     0.009655      21.50
 C      -1.722041     0.251336    -2.026000      53.92
 H      -1.949360     0.812088    -2.908575      19.60
 C      -0.680590     0.858067    -1.286304       6.71
 O       0.100799     1.886346    -1.766915     149.38
 C       0.092713     2.251234    -3.342363      89.96
 H       1.109123     2.682605    -3.370990      25.39
 H       0.141096     1.403858    -3.918135      28.58
 H      -0.680263     3.038346    -3.935052      23.89
 C      -0.393168     0.337169     0.002768      44.89
 O       0.764244     0.837147     0.655381     231.11
 C      -0.955027    -0.854803     0.430719      42.45
 H      -0.394508    -1.267796     1.481781      18.76
 C      -2.417187    -0.894137    -1.513594      22.02
 C      -3.523177    -1.505764    -2.384273      65.89
 H      -3.479597    -1.162268    -3.463728      26.68
 O      -3.310218    -3.048636    -2.564207     147.57
 H      -2.210982    -3.113180    -2.991093      20.20
 C      -4.993782    -1.069405    -1.993096      84.17
 H      -5.170289    -1.095173    -0.863181      28.12
 O      -5.135182     0.248924    -2.589620     266.81
 H      -4.872914     0.840920    -1.905036      30.04
 C      -6.071082    -2.039280    -2.765400     101.73
 O      -6.201410    -3.297414    -2.117358     179.52
 H      -5.381913    -3.977852    -2.292026      26.71
 H      -5.699846    -1.993046    -3.828478      28.79
 H      -7.027957    -1.426059    -2.602444      28.05
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name = lig-ACN-frame_308
 C       4.166645     3.122568     0.140746      55.09
 H       3.830854     4.137574     0.295772      23.93
 C       4.071973     0.700341     0.747760      33.21
 H       3.428506     0.033462     1.246806      15.74
 C       5.157194     0.483610    -0.120695      22.99
 O       5.864891    -0.715826    -0.318704     221.57
 C       5.556701    -1.802681     0.589687     116.46
 H       5.457152    -1.407140     1.785463      26.24
 H       6.420126    -2.387101     0.626825      28.07
 H       4.810557    -2.463199     0.221635      28.93
 C       5.727356     1.590693    -0.802605      22.36
 O       6.833397     1.396057    -1.716656     185.74
 H       7.304184     0.592385    -1.321419      24.70
 C       5.257563     2.880132    -0.632396      56.60
 H       5.673849     3.578033    -1.255566      21.99
 C       3.500883     2.078641     0.849828      17.34
 C       2.285107     2.256348     1.907370      90.22
 H       2.244165     3.195557     2.257266      25.40
 O       2.424346     1.422629     3.192316     233.70
 H       2.062587     0.604162     3.074933      27.87
 C       0.908258     2.196316     1.198259      58.16
 H       0.897293     3.004585     0.365659      20.10
 C      -0.250784     2.532271     2.250016     100.73
 O      -0.082336     4.019428     2.472244     176.30
 H       0.556358     4.560417     1.642640      24.13
 H      -0.262970     2.068808     3.177237      25.35
 H      -1.191343     2.472761     1.581484      23.09
 C      -1.999966    -1.423858    -0.273537      62.02
 H      -2.478292    -2.090709     0.335193      24.22
 C      -1.697967     0.241736    -2.036973      61.01
 H      -2.074009     0.572959    -3.033576      20.26
 C      -0.673244     0.890161    -1.322775       7.36
 O       0.110486     1.951717    -1.803006     199.59
 C       0.236669     2.242839    -3.356861      88.85
 H       1.129249     2.795038    -3.545454      24.92
 H       0.106230     1.293058    -3.787748      25.60
 H      -0.806510     2.892295    -3.496302      22.19
 C      -0.355225     0.380598    -0.033048      17.07
 O       0.759660     0.764455     0.687910     178.76
 C      -1.075379    -0.745934     0.478069      51.40
 H      -0.582968    -1.370692     1.356695      18.55
 C      -2.447385    -0.833887    -1.487290      37.73
 C      -3.505770    -1.495806    -2.350091      68.38
 H      -3.306401    -1.029216    -3.330314      28.16
 O      -3.399088    -3.018494    -2.426015     197.25
 H      -2.422853    -3.134563    -2.819023      26.47
 C      -4.990515    -1.155133    -2.041648      98.82
 H      -5.192018    -1.073262    -0.939053      27.70
 O      -5.122149     0.230042    -2.568879     227.82
 H      -5.262797     0.915325    -1.948431      29.62
 C      -6.049980    -2.011898    -2.688426     107.12
 O      -6.209215    -3.339553    -2.082057     231.27
 H      -5.398797    -3.760366    -2.325206      32.06
 H      -5.877982    -2.176778    -3.822623      29.16
 H      -7.132258    -1.632552    -2.683146      28.54
55
name = lig-ACN-frame_309
 C       4.048276     3.143765     0.217411      47.07
 H       3.740619     4.147605     0.314656      23.75
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 C       4.038651     0.741207     0.735794      65.37
 H       3.749719    -0.154375     1.181674      20.91
 C       5.190539     0.498203    -0.066239      39.69
 O       5.814391    -0.699389    -0.341088     231.50
 C       5.549407    -1.872390     0.541505     109.48
 H       5.176967    -1.417219     1.657622      23.17
 H       6.407469    -2.507307     0.551118      25.95
 H       4.629517    -2.311512     0.209410      26.77
 C       5.759390     1.528476    -0.883435       9.63
 O       6.855151     1.330003    -1.671694     167.65
 H       7.394052     0.434127    -1.392715      26.80
 C       5.258711     2.866465    -0.644975      49.50
 H       5.778482     3.698512    -1.068081      21.72
 C       3.526104     2.031420     0.952690      30.46
 C       2.289931     2.225485     1.865026      98.67
 H       2.479202     3.193862     2.226640      23.51
 O       2.477660     1.459733     3.104810     255.46
 H       2.104630     0.498645     2.957049      22.84
 C       0.857835     2.151582     1.229422      75.29
 H       0.851846     2.770304     0.244528      19.08
 C      -0.250053     2.608446     2.187077     112.14
 O      -0.074686     3.948518     2.503298     288.54
 H       0.602531     4.351315     1.850023      27.15
 H      -0.114965     1.950512     3.042762      24.60
 H      -1.372577     2.297565     1.923133      23.88
 C      -2.034070    -1.376604    -0.231441      39.13
 H      -2.430132    -2.296185    -0.136710      22.22
 C      -1.748798     0.252417    -2.061227      60.19
 H      -1.883397     0.464227    -3.178430      18.25
 C      -0.636494     0.934412    -1.385225      11.34
 O       0.163917     2.028025    -1.872120     226.55
 C       0.230765     2.165186    -3.212469     123.83
 H       1.093864     2.788803    -3.354671      25.47
 H       0.332407     1.355558    -3.902416      27.54
 H      -0.701795     2.862418    -3.697349      24.89
 C      -0.295756     0.425791    -0.050207      31.88
 O       0.793434     0.765212     0.752224     219.70
 C      -1.044922    -0.650611     0.523645      43.18
 H      -0.932222    -0.845187     1.616882      19.37
 C      -2.439151    -0.851010    -1.488543      31.47
 C      -3.510278    -1.554459    -2.395702      81.34
 H      -3.383071    -1.309862    -3.445129      29.06
 O      -3.475212    -2.929177    -2.282798     306.11
 H      -2.690511    -3.180384    -2.496207      35.87
 C      -4.970344    -1.122367    -2.038311      87.09
 H      -5.105761    -1.308405    -0.946633      28.49
 O      -5.143802     0.191181    -2.576270     204.79
 H      -5.215145     0.869709    -1.698515      24.12
 C      -6.094504    -2.063297    -2.672076     106.49
 O      -6.196040    -3.370736    -2.054714     219.53
 H      -5.329032    -3.734263    -2.009546      29.99
 H      -5.844738    -2.177591    -3.808919      28.36
 H      -6.992577    -1.397547    -2.475172      28.52
55
name = lig-ACN-frame_310
 C       4.120818     3.013579     0.234130      44.12
 H       3.631521     3.959533     0.298462      22.86
 C       4.078358     0.710203     0.734252      50.47
 H       3.610595    -0.013442     1.350436      19.83
 C       5.191574     0.540727    -0.103490      34.87
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 O       5.783054    -0.769525    -0.317747     224.03
 C       5.452588    -1.857875     0.476614     120.79
 H       5.446530    -1.649830     1.687821      24.56
 H       6.347635    -2.544619     0.393713      25.91
 H       4.620113    -2.471529     0.110936      27.00
 C       5.763231     1.605229    -0.832165      15.85
 O       6.875611     1.285343    -1.656714     110.75
 H       7.422596     0.568997    -1.185079      24.97
 C       5.144147     2.847233    -0.629895      77.46
 H       5.476909     3.764883    -1.254183      24.87
 C       3.494177     1.992990     0.943500      41.29
 C       2.379403     2.278065     1.890427      99.34
 H       2.326469     3.347438     2.156221      25.00
 O       2.453211     1.467801     3.002572     257.86
 H       2.180713     0.429624     2.732478      20.80
 C       0.918048     2.098145     1.194479      83.49
 H       0.990758     2.870999     0.335163      22.08
 C      -0.195124     2.523311     2.164579     102.72
 O      -0.099346     3.964158     2.584517     278.28
 H       0.426931     4.445078     2.116742      35.33
 H      -0.056682     2.046770     3.143386      25.05
 H      -1.282096     2.359634     1.732424      24.64
 C      -2.100107    -1.292874    -0.229795      59.19
 H      -2.368048    -2.128753     0.325542      22.45
 C      -1.673896     0.333349    -2.058023      49.60
 H      -1.885310     0.705841    -3.098134      21.53
 C      -0.615612     0.910048    -1.350603      17.59
 O       0.137833     1.953692    -1.782602     193.99
 C       0.258254     2.219964    -3.304428      95.18
 H       1.120106     2.830420    -3.393473      25.61
 H       0.454127     1.183664    -3.592652      26.54
 H      -0.751642     2.699854    -3.850551      24.04
 C      -0.320856     0.407360    -0.068478      23.52
 O       0.789975     0.773010     0.786324     204.81
 C      -1.077093    -0.584563     0.516559      40.38
 H      -0.814133    -0.732210     1.503234      20.35
 C      -2.379693    -0.838635    -1.578418      48.90
 C      -3.509913    -1.496402    -2.425575      61.57
 H      -3.315702    -1.260562    -3.435634      27.65
 O      -3.513780    -3.003669    -2.121852     221.92
 H      -2.626953    -3.301891    -2.413043      28.47
 C      -4.951842    -1.149900    -2.031547      95.68
 H      -5.028770    -1.014902    -0.954606      27.85
 O      -5.207904     0.186424    -2.536415     225.75
 H      -4.779269     0.923510    -1.815920      24.24
 C      -6.069865    -2.077889    -2.643758     105.86
 O      -6.208935    -3.377828    -2.029228     204.72
 H      -5.195259    -3.661737    -1.793260      26.59
 H      -6.028417    -2.076998    -3.825983      27.69
 H      -7.104372    -1.707804    -2.470247      27.46
55
name = lig-ACN-frame_311
 C       4.092548     3.020729     0.223312      52.83
 H       3.695556     4.040657     0.328420      23.01
 C       4.095234     0.634594     0.797790      61.38
 H       3.720885    -0.308138     1.202946      18.20
 C       5.149285     0.440722    -0.102970      18.72
 O       5.766157    -0.721691    -0.339013     207.41
 C       5.393879    -1.948758     0.461151      99.36
 H       5.297188    -1.650082     1.596096      26.44
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 H       6.225750    -2.726833     0.200062      25.93
 H       4.355083    -2.251978     0.181056      27.14
 C       5.802662     1.577920    -0.765460      20.95
 O       6.846346     1.332050    -1.635922     200.15
 H       7.504786     0.840977    -1.206828      23.82
 C       5.159562     2.855045    -0.755483      46.35
 H       5.391694     3.733717    -1.528539      23.91
 C       3.541809     1.938539     0.884874      45.22
 C       2.348683     2.288934     1.818699      90.86
 H       2.564806     3.307219     2.340239      23.55
 O       2.402149     1.418726     3.027090     220.75
 H       2.073876     0.480272     2.781195      22.59
 C       1.053937     2.241507     1.178086      66.31
 H       0.900496     2.820176     0.233803      21.55
 C      -0.093555     2.520994     2.230814      99.60
 O      -0.147641     3.964272     2.665636     265.19
 H       0.254038     4.413946     1.953249      31.95
 H      -0.203223     1.711549     3.039385      24.04
 H      -1.018428     2.261412     1.605357      24.90
 C      -2.123172    -1.172083    -0.248601      59.73
 H      -2.978269    -1.765134     0.087531      23.17
 C      -1.641688     0.311654    -2.070708      49.52
 H      -1.966211     0.816511    -2.953786      21.60
 C      -0.603472     0.877924    -1.297515      12.16
 O       0.142485     1.984019    -1.770824     201.32
 C       0.294230     2.173515    -3.295281     100.48
 H       0.980875     3.039956    -3.501679      25.08
 H       0.450640     1.306296    -4.030371      25.63
 H      -0.774586     2.530019    -3.595583      24.78
 C      -0.285031     0.415334     0.017991      27.59
 O       0.771747     0.723193     0.735550     176.63
 C      -1.166218    -0.606753     0.506745      60.44
 H      -0.911255    -1.157483     1.249120      22.69
 C      -2.361471    -0.794503    -1.588380      52.67
 C      -3.467663    -1.568663    -2.363827      62.72
 H      -3.370579    -1.511912    -3.375591      29.35
 O      -3.475553    -3.036481    -2.008038     154.27
 H      -2.509722    -3.528211    -2.459748      25.09
 C      -4.967901    -1.103520    -2.013988      93.55
 H      -5.084541    -1.329188    -0.959556      28.79
 O      -5.290555     0.223057    -2.513250     268.21
 H      -4.757199     0.857857    -2.067621      30.45
 C      -6.085857    -2.056014    -2.585120     107.16
 O      -6.186371    -3.384398    -1.997755     200.69
 H      -5.218624    -3.766629    -2.000544      27.28
 H      -5.782899    -2.281249    -3.699552      27.10
 H      -6.974987    -1.439941    -2.470244      28.68
55
name = lig-ACN-frame_312
 C       4.105500     3.055005     0.075040      60.96
 H       3.633503     4.049281     0.279456      22.07
 C       4.071790     0.587006     0.796195      50.42
 H       3.515092    -0.190120     1.378887      19.25
 C       5.183129     0.451682    -0.067167      24.77
 O       5.797835    -0.821631    -0.360871     215.94
 C       5.314057    -1.924966     0.402292     108.83
 H       5.478990    -1.800725     1.492455      27.35
 H       5.944545    -2.913407     0.129137      25.47
 H       4.217430    -2.200987     0.136007      26.35
 C       5.740273     1.538252    -0.768320      30.73
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 O       6.840793     1.420113    -1.637244     110.06
 H       7.486199     0.729105    -1.306526      21.40
 C       5.155697     2.796343    -0.793545      50.66
 H       5.791372     3.561656    -1.413029      26.43
 C       3.595643     1.915476     0.906328      35.92
 C       2.478413     2.154844     1.854676      85.82
 H       2.634296     3.345276     2.097056      23.31
 O       2.342464     1.399878     3.056084     299.96
 H       2.007588     0.572295     2.879077      28.04
 C       0.988847     2.254467     1.179638      68.70
 H       1.071475     2.913735     0.328617      23.30
 C      -0.085229     2.582233     2.175325     106.09
 O      -0.169247     3.859209     2.715665     215.20
 H       0.196209     4.722107     2.067525      25.94
 H       0.283095     2.029644     3.170590      21.78
 H      -1.091943     2.314998     1.816501      25.08
 C      -2.316130    -1.117815    -0.290320      40.73
 H      -2.833105    -2.034634     0.218947      20.73
 C      -1.619080     0.296595    -2.104520      44.60
 H      -1.667093     0.588071    -3.105092      21.82
 C      -0.591097     0.908920    -1.311175      -4.75
 O       0.213904     2.005947    -1.840240     195.87
 C       0.186192     2.186198    -3.205314     103.60
 H       1.066095     2.935975    -3.259960      24.25
 H       0.589519     1.165091    -3.672278      25.25
 H      -0.763834     2.599387    -3.703996      25.53
 C      -0.350882     0.370437     0.039038       5.14
 O       0.884546     0.798398     0.759959     174.92
 C      -1.145261    -0.680320     0.583217      35.46
 H      -1.004834    -0.859785     1.520620      22.46
 C      -2.443718    -0.757800    -1.624030      27.43
 C      -3.487275    -1.642863    -2.323405      96.40
 H      -3.294667    -1.552870    -3.299260      29.28
 O      -3.399807    -3.030257    -1.914498     181.69
 H      -2.379523    -3.271872    -2.451309      23.29
 C      -4.968575    -1.138679    -1.956351      91.65
 H      -5.067777    -0.940537    -0.913746      28.28
 O      -5.337034     0.203346    -2.495242     249.14
 H      -5.121105     0.842879    -1.863602      30.83
 C      -6.029729    -2.051587    -2.606220     105.03
 O      -6.171519    -3.344882    -1.943720     243.80
 H      -5.423574    -3.797483    -2.171536      32.85
 H      -5.912273    -2.052101    -3.784283      27.90
 H      -7.033525    -1.672885    -2.500568      28.74
55
name = lig-ACN-frame_313
 C       4.051673     2.941084     0.046840      62.07
 H       3.623673     3.969594     0.003518      23.11
 C       4.121565     0.640338     0.723286      71.13
 H       3.728158    -0.147110     1.418584      22.71
 C       5.251891     0.341986    -0.068148      60.53
 O       5.830027    -0.878577    -0.375029     253.69
 C       5.236917    -1.963780     0.355716     111.56
 H       5.427372    -1.873437     1.402035      25.21
 H       5.771664    -2.900725    -0.161946      23.57
 H       4.063189    -1.967368     0.239957      22.22
 C       5.729783     1.463424    -0.862694      36.64
 O       6.864623     1.457858    -1.640645     155.37
 H       7.408135     0.570158    -1.302249      29.79
 C       5.161989     2.772509    -0.756590      55.71
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 H       5.592050     3.653632    -1.299131      20.47
 C       3.628008     1.966849     0.872079      39.14
 C       2.433315     2.204577     1.896329      75.90
 H       2.573554     3.283345     2.491455      20.78
 O       2.352555     1.405212     3.104654     287.78
 H       2.152131     0.498169     2.870886      25.65
 C       1.069381     2.181822     1.144926      84.93
 H       1.077230     2.854003     0.331744      22.42
 C      -0.109448     2.518698     2.189951      94.61
 O      -0.159735     3.894124     2.743520     161.87
 H       0.383047     4.608260     1.906340      22.63
 H       0.122521     1.746336     3.100997      21.96
 H      -1.063447     2.121815     1.903064      25.22
 C      -2.284114    -1.114621    -0.112097      44.96
 H      -2.914041    -2.073202     0.243443      20.96
 C      -1.585195     0.268022    -2.151559      72.61
 H      -1.511341     0.306018    -3.222558      20.29
 C      -0.599797     0.905401    -1.302086      10.95
 O       0.198839     1.918972    -1.725192     191.89
 C       0.180830     2.229792    -3.215079      99.65
 H       0.945282     3.028546    -3.674615      23.17
 H       0.308325     1.187289    -3.808991      24.15
 H      -0.820254     2.477718    -3.547670      26.28
 C      -0.300076     0.416216     0.008554      22.59
 O       0.842299     0.858220     0.716777     217.66
 C      -1.213911    -0.612491     0.536502      46.61
 H      -1.168407    -0.920906     1.499567      22.67
 C      -2.491972    -0.721490    -1.546468      35.43
 C      -3.555579    -1.550974    -2.349426      72.29
 H      -3.551763    -1.509503    -3.332189      31.34
 O      -3.289626    -3.014056    -1.872693     221.43
 H      -2.393435    -3.281376    -2.196583      29.09
 C      -4.998657    -1.138344    -1.937393      97.42
 H      -5.093085    -1.348246    -0.892845      28.86
 O      -5.305937     0.159738    -2.492916     210.83
 H      -5.375591     0.859856    -1.668438      25.23
 C      -6.060656    -2.062303    -2.571480     106.56
 O      -6.158657    -3.314964    -1.935967     231.34
 H      -5.336660    -3.907481    -2.031795      28.19
 H      -5.769836    -2.224614    -3.691665      28.15
 H      -6.982940    -1.507853    -2.463354      29.10
55
name = lig-ACN-frame_314
 C       3.988624     2.964863     0.043332      49.32
 H       3.459887     3.930835     0.053933      23.20
 C       4.222898     0.651125     0.750388      47.05
 H       3.933164    -0.214175     1.364280      17.88
 C       5.267846     0.390630    -0.208484      34.14
 O       5.842734    -0.902606    -0.373308     203.16
 C       5.176687    -2.045941     0.317578     116.29
 H       5.438352    -2.101294     1.296445      28.76
 H       5.428512    -3.096089    -0.152997      24.96
 H       3.998572    -1.905341     0.189129      22.50
 C       5.786504     1.461959    -0.916075      38.28
 O       6.929915     1.403807    -1.673109     150.12
 H       7.690769     0.715390    -1.382664      24.58
 C       5.161600     2.707625    -0.769366      62.63
 H       5.473817     3.444988    -1.463008      20.53
 C       3.519563     1.901766     0.948896      44.27
 C       2.392161     2.246358     1.910161      77.26
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 H       2.514338     3.507391     2.111122      21.85
 O       2.431793     1.421770     3.138352     228.83
 H       2.222574     0.406868     2.866274      19.95
 C       1.022547     2.220617     1.212784      71.66
 H       1.040101     2.879949     0.395242      22.57
 C      -0.097118     2.439992     2.219261     102.33
 O      -0.118962     3.895483     2.700074     182.97
 H       0.509699     4.456716     1.939798      25.30
 H      -0.116318     1.739925     3.210469      22.59
 H      -0.937417     2.391934     1.668460      26.52
 C      -2.256342    -1.067031    -0.177299      51.43
 H      -3.038300    -1.675436     0.465927      22.15
 C      -1.605435     0.132196    -2.057577      63.85
 H      -1.772991     0.375073    -3.141391      21.05
 C      -0.624783     0.826296    -1.341140       7.20
 O       0.234143     1.906194    -1.733044     185.81
 C       0.099291     2.198967    -3.199825     100.90
 H       0.950722     3.040761    -3.157045      22.51
 H       0.294145     1.315994    -4.010617      23.08
 H      -0.809150     2.667606    -3.275307      26.95
 C      -0.356563     0.450677    -0.006577      16.29
 O       0.782302     0.785881     0.641249     177.37
 C      -1.184577    -0.443381     0.606343      48.71
 H      -0.690699    -0.876963     1.469205      20.10
 C      -2.481139    -0.704604    -1.454027      45.76
 C      -3.513932    -1.496067    -2.266819      84.13
 H      -3.306764    -1.352318    -3.219465      30.50
 O      -3.247750    -2.927667    -1.898072     259.16
 H      -2.484338    -3.016423    -2.258596      33.97
 C      -5.022634    -1.206194    -1.924331     100.63
 H      -5.206857    -1.103506    -0.869099      27.75
 O      -5.257888     0.146435    -2.451227     214.72
 H      -4.977161     0.911639    -1.666149      23.16
 C      -6.074203    -2.076867    -2.581235     110.76
 O      -6.190721    -3.367123    -1.897711     217.34
 H      -5.136125    -3.596020    -1.910293      27.15
 H      -5.877217    -2.210468    -3.714199      28.08
 H      -7.069046    -1.620435    -2.560036      28.41
55
name = lig-ACN-frame_315
 C       4.001525     2.884778     0.059061      54.68
 H       3.552730     3.859785     0.029101      23.26
 C       4.258512     0.635510     0.824186      54.38
 H       3.942376    -0.141363     1.497302      19.70
 C       5.209130     0.374357    -0.215026      26.72
 O       5.824181    -0.943242    -0.357682     205.54
 C       5.114690    -2.062408     0.254124     115.16
 H       5.397326    -2.215636     1.204049      30.19
 H       5.485872    -2.852565    -0.461398      25.99
 H       3.919553    -1.978873     0.224996      24.68
 C       5.854541     1.509162    -0.917981       3.52
 O       7.022334     1.358279    -1.767148     187.57
 H       7.552751     0.811954    -1.179166      25.57
 C       5.060597     2.715581    -0.841866      48.02
 H       5.427703     3.505255    -1.382224      27.23
 C       3.561133     1.871162     0.868698      36.62
 C       2.408419     2.140839     1.891156      81.23
 H       2.619415     3.320971     2.376497      21.19
 O       2.524688     1.512897     3.133311     227.12
 H       2.122123     0.469740     2.998831      21.00
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 C       0.941816     2.120540     1.273521      85.56
 H       0.875982     2.904438     0.546225      23.46
 C      -0.184459     2.545641     2.204897     114.99
 O      -0.050766     3.830257     2.651440     298.38
 H       0.400434     4.446799     2.070256      30.27
 H      -0.059618     1.851063     3.208545      23.39
 H      -1.093699     2.233631     1.864768      27.02
 C      -2.253464    -0.979904     0.020974      50.72
 H      -2.884077    -1.785795     0.511384      22.34
 C      -1.597564     0.178506    -2.091301      81.85
 H      -1.838989     0.499815    -3.161157      19.60
 C      -0.573151     0.835585    -1.363725      21.28
 O       0.218385     1.789078    -1.850012     235.11
 C       0.051687     2.311467    -3.101461     122.50
 H       0.894782     3.045057    -3.495375      24.20
 H       0.217438     1.301986    -3.779735      23.75
 H      -0.824222     2.676821    -3.418019      28.62
 C      -0.404510     0.504186    -0.012865      32.95
 O       0.845062     0.804267     0.641542     207.95
 C      -1.193771    -0.453872     0.676404      25.31
 H      -1.042057    -0.685573     1.818532      20.18
 C      -2.498149    -0.733588    -1.376401      47.71
 C      -3.501934    -1.515738    -2.161371      94.47
 H      -3.440164    -1.255622    -3.116749      33.47
 O      -3.248303    -2.859178    -1.977322     286.69
 H      -2.414542    -3.121701    -2.439665      28.25
 C      -5.002297    -1.145369    -1.907054      93.24
 H      -5.183066    -1.301907    -0.834295      28.34
 O      -5.208034     0.179562    -2.419466     272.00
 H      -4.657814     0.770326    -1.867549      29.34
 C      -6.105365    -2.139119    -2.604432     104.75
 O      -6.181716    -3.404069    -1.885837     255.38
 H      -5.359517    -3.818321    -1.679179      31.14
 H      -5.849030    -2.264697    -3.697000      28.47
 H      -7.115924    -1.677735    -2.449085      27.53
55
name = lig-ACN-frame_316
 C       4.019761     2.856159    -0.014204      46.98
 H       3.501530     3.788709     0.076736      22.79
 C       4.246719     0.581912     0.823316      49.27
 H       4.019377    -0.191734     1.522238      18.51
 C       5.283990     0.351867    -0.123440      39.62
 O       5.755017    -0.883244    -0.348773     216.01
 C       5.098214    -2.076868     0.145207     118.60
 H       5.355103    -2.255576     1.122524      28.63
 H       5.332119    -2.982935    -0.410799      26.47
 H       3.934367    -1.899415     0.093491      24.06
 C       5.806855     1.457292    -0.940176      36.08
 O       6.986742     1.336672    -1.757600     146.79
 H       7.635831     0.723160    -1.456189      24.56
 C       5.122565     2.727717    -0.958374      45.36
 H       5.385955     3.613090    -1.416592      27.76
 C       3.584957     1.808352     0.864091      39.99
 C       2.433922     2.135206     1.854503      74.63
 H       2.543226     3.429879     1.936480      22.18
 O       2.603029     1.504345     3.174440     239.10
 H       2.244314     0.526241     3.156058      22.63
 C       0.985440     2.086528     1.234283      77.18
 H       1.072994     2.785061     0.421853      22.65
 C      -0.258211     2.446115     2.276855      98.28
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 O      -0.009802     3.897775     2.649471     288.75
 H       0.280856     4.313406     1.976815      35.49
 H      -0.170429     1.825409     3.285920      23.96
 H      -1.206827     2.418097     1.861941      26.09
 C      -2.361443    -0.990972     0.120029      46.42
 H      -2.880759    -1.821829     0.535949      21.69
 C      -1.684518     0.240184    -2.030203      63.27
 H      -1.741263     0.209919    -3.145151      20.79
 C      -0.618358     0.801558    -1.340484      -0.74
 O       0.294901     1.761681    -1.866557     153.45
 C       0.006243     2.349590    -3.255429     102.52
 H       0.787713     3.190964    -3.213848      24.82
 H       0.004504     1.630966    -4.249018      24.91
 H      -0.879448     2.764036    -3.091763      29.00
 C      -0.304052     0.474405     0.093414      25.03
 O       0.859879     0.841268     0.640219     224.70
 C      -1.195083    -0.385729     0.759894      38.08
 H      -1.076824    -0.478448     1.995062      20.05
 C      -2.422620    -0.662283    -1.282520      21.51
 C      -3.545286    -1.455085    -2.203815      73.70
 H      -3.365272    -1.237367    -3.161809      28.96
 O      -3.282942    -2.967663    -2.048241     228.33
 H      -2.271919    -2.964975    -2.543998      22.19
 C      -5.028292    -1.175106    -1.862596      94.58
 H      -5.321886    -1.118028    -0.792108      27.95
 O      -5.174853     0.213357    -2.399449     252.84
 H      -4.823178     0.796691    -1.818300      32.60
 C      -6.013723    -2.164623    -2.544936     110.93
 O      -6.202547    -3.428660    -1.880586     266.88
 H      -5.327817    -3.757667    -2.035871      31.84
 H      -5.825364    -2.364605    -3.614901      29.35
 H      -7.011899    -1.618103    -2.552833      28.16
55
name = lig-ACN-frame_317
 C       4.035139     2.817065    -0.107335      54.54
 H       3.543739     3.780634    -0.120227      24.20
 C       4.243691     0.537526     0.807772      53.19
 H       3.916307    -0.291432     1.429156      21.49
 C       5.319666     0.426542    -0.061076      20.43
 O       5.795005    -0.909066    -0.405266     239.79
 C       5.051123    -2.054640     0.085848     118.19
 H       5.263212    -2.292205     1.088603      26.67
 H       5.428045    -2.761270    -0.571042      26.50
 H       3.894626    -1.961776    -0.059183      24.16
 C       5.768155     1.427978    -0.965686      45.29
 O       6.871173     1.315308    -1.731582     176.75
 H       7.411532     0.553336    -1.274010      29.17
 C       5.158162     2.647968    -0.928030      68.13
 H       5.598517     3.221917    -1.712089      21.03
 C       3.587618     1.832849     0.843176      30.29
 C       2.474796     2.190977     1.854854      74.25
 H       2.657357     3.381658     2.330874      20.97
 O       2.652704     1.499233     3.171695     250.86
 H       2.441907     0.634911     2.977339      27.51
 C       1.013896     2.153467     1.279102      76.45
 H       0.825747     2.954352     0.570004      22.57
 C      -0.132663     2.485518     2.275075     104.60
 O      -0.023914     3.887496     2.697084     277.56
 H       0.343863     4.436544     1.979026      29.98
 H      -0.232240     1.830841     3.188693      24.66
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 H      -1.022297     2.275526     1.703846      25.63
 C      -2.311474    -0.932422     0.100179      55.02
 H      -2.994600    -1.456386     0.635486      24.12
 C      -1.701125     0.243335    -1.871472      37.41
 H      -1.777529     0.378030    -2.945686      20.28
 C      -0.540638     0.859621    -1.252632       6.48
 O       0.365423     1.697207    -1.943951     179.69
 C      -0.071594     2.415977    -3.255784     101.91
 H       0.714486     3.176460    -3.371519      24.80
 H      -0.002919     1.758868    -4.265376      23.80
 H      -0.997681     2.850966    -3.246330      27.74
 C      -0.349395     0.396211     0.036453      18.82
 O       0.903446     0.764429     0.641093     181.64
 C      -1.300074    -0.315467     0.827508      51.23
 H      -0.764291    -0.727380     1.914335      18.17
 C      -2.612669    -0.742297    -1.266186      33.59
 C      -3.488142    -1.509163    -2.133653      80.91
 H      -3.393006    -1.139819    -3.088658      27.95
 O      -3.336969    -2.984543    -2.136565     189.70
 H      -2.251273    -3.355525    -2.437565      22.39
 C      -4.987326    -1.161030    -1.828033      87.06
 H      -5.094056    -1.168498    -0.702248      27.15
 O      -5.198196     0.215471    -2.396626     194.78
 H      -5.270561     0.811875    -1.528084      25.62
 C      -5.987806    -2.113019    -2.540712     106.49
 O      -6.177063    -3.418509    -1.882844     206.31
 H      -5.417830    -4.155153    -2.049325      27.87
 H      -5.541531    -2.199345    -3.510470      30.25
 H      -7.049223    -1.683976    -2.600532      28.16
55
name = lig-ACN-frame_318
 C       3.990684     2.838779    -0.115998      57.58
 H       3.466114     3.800859    -0.266125      23.60
 C       4.214263     0.633833     0.802325      61.11
 H       3.771914    -0.185236     1.411503      17.57
 C       5.289424     0.289120    -0.090771      65.80
 O       5.855140    -0.899875    -0.431915     207.18
 C       5.048841    -2.041919    -0.013391     124.42
 H       5.128353    -2.207768     1.086723      26.60
 H       5.380014    -2.887408    -0.460307      27.64
 H       3.968864    -1.872536    -0.252932      24.98
 C       5.776181     1.351748    -0.861070      58.74
 O       6.826830     1.212725    -1.747506      71.76
 H       7.642299     0.576928    -1.392522      19.17
 C       5.109322     2.621604    -0.944825      55.41
 H       5.302962     3.526124    -1.597055      24.95
 C       3.603853     1.891383     0.804687      41.73
 C       2.539495     2.233306     1.914599      77.64
 H       2.778364     3.479893     2.140679      22.89
 O       2.670238     1.484861     3.091102     252.25
 H       2.415988     0.533291     2.946714      24.71
 C       1.090555     2.143739     1.303329      75.32
 H       1.171928     2.702703     0.373371      23.89
 C      -0.017668     2.540916     2.247676     115.34
 O      -0.058746     3.850627     2.768472     248.27
 H       0.416265     4.613651     2.068683      25.18
 H       0.147118     1.926621     3.111867      25.89
 H      -1.038492     2.318005     1.847148      25.56
 C      -2.417241    -0.929538     0.189078      40.99
 H      -2.999291    -1.572320     0.721995      22.85
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 C      -1.694225     0.237120    -1.836047      55.70
 H      -2.039242     0.581081    -2.768218      22.88
 C      -0.602758     0.855426    -1.291978      10.65
 O       0.357069     1.639924    -2.037221     215.53
 C      -0.099899     2.421183    -3.175206     120.36
 H       0.595039     3.184499    -3.392532      27.05
 H      -0.130843     1.572029    -3.943481      25.80
 H      -1.097660     2.752803    -3.032274      28.64
 C      -0.253477     0.481599     0.111560      27.19
 O       0.929777     0.741665     0.698441     202.95
 C      -1.260579    -0.303619     0.733642      42.78
 H      -1.190572    -0.758208     1.946130      18.60
 C      -2.525372    -0.682320    -1.216796      26.44
 C      -3.536057    -1.565322    -2.153703      68.83
 H      -3.293394    -1.267751    -3.139048      28.47
 O      -3.406912    -2.977015    -2.179616     216.50
 H      -2.271197    -3.015660    -2.532604      20.73
 C      -4.952699    -1.143885    -1.794391      94.80
 H      -5.243309    -1.215230    -0.697122      27.07
 O      -5.235624     0.167794    -2.343772     187.46
 H      -5.382693     0.989708    -1.593867      24.15
 C      -5.933416    -2.119509    -2.547366     104.64
 O      -6.168052    -3.374483    -1.897350     239.76
 H      -5.313961    -3.895912    -2.116473      29.49
 H      -5.704726    -2.269226    -3.570164      30.91
 H      -6.949109    -1.579344    -2.562918      28.79
55
name = lig-ACN-frame_319
 C       3.944764     2.922832    -0.130523      52.49
 H       3.353111     3.872199    -0.147751      22.75
 C       4.201265     0.613609     0.794118      53.34
 H       3.836236    -0.087999     1.592755      19.94
 C       5.207380     0.306009    -0.148400      33.79
 O       5.881962    -0.965710    -0.401315     212.60
 C       5.052563    -2.065717    -0.076983     127.55
 H       4.982307    -2.149918     1.050895      26.73
 H       5.442979    -2.904195    -0.512775      28.60
 H       4.046700    -1.889860    -0.487429      27.02
 C       5.810131     1.399516    -0.855656      12.33
 O       6.847994     1.093075    -1.787998     122.24
 H       7.523588     0.546039    -1.249207      23.59
 C       5.041252     2.608683    -0.947668      55.61
 H       5.635178     3.310133    -1.680026      24.39
 C       3.609275     1.929587     0.845580      26.59
 C       2.583505     2.218549     1.843155      83.75
 H       2.626619     3.403231     2.285158      21.79
 O       2.695906     1.451122     3.068196     214.60
 H       2.182675     0.493199     2.820606      20.32
 C       1.242379     2.162868     1.167621      72.56
 H       1.179977     2.922658     0.346417      22.14
 C       0.022609     2.483244     2.294159      86.92
 O      -0.046182     3.901778     2.844566     169.28
 H       0.354498     4.616608     1.927825      22.22
 H       0.183997     1.847930     3.091166      25.99
 H      -0.997921     2.247714     1.803482      23.07
 C      -2.417788    -0.885211     0.186611      57.01
 H      -2.935240    -1.680110     0.678439      22.57
 C      -1.757829     0.278783    -1.924450      55.86
 H      -1.878341     0.366211    -2.990064      21.11
 C      -0.528993     0.846425    -1.262589       2.36
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 O       0.320903     1.578893    -1.993504     203.52
 C      -0.179379     2.319444    -3.140762     120.33
 H       0.522098     3.071505    -3.151796      27.36
 H      -0.363691     2.002265    -4.171785      26.25
 H      -1.045964     2.908398    -2.787341      27.17
 C      -0.302271     0.532824     0.087971      17.74
 O       0.978827     0.780304     0.839830     179.53
 C      -1.204671    -0.353008     0.754835      24.11
 H      -0.854456    -0.224844     1.964022      18.44
 C      -2.526663    -0.755472    -1.214098      19.74
 C      -3.514761    -1.406367    -2.147681      77.85
 H      -3.453250    -0.995279    -3.172337      25.83
 O      -3.412978    -2.968378    -2.168316     213.11
 H      -2.491752    -3.280403    -2.603976      25.09
 C      -5.024938    -1.196259    -1.830163      93.16
 H      -5.148261    -1.242459    -0.693963      28.07
 O      -5.275684     0.162003    -2.295553     232.29
 H      -4.894968     0.710611    -1.536954      28.28
 C      -5.983360    -2.081818    -2.568513     122.06
 O      -6.138806    -3.348155    -1.912940     256.66
 H      -5.328445    -3.758432    -1.856318      33.10
 H      -5.643039    -2.157100    -3.560554      31.24
 H      -6.991990    -1.545783    -2.529257      28.48
55
name = lig-ACN-frame_320
 C       4.006831     2.893659    -0.137059      62.36
 H       3.531793     3.888038    -0.231029      24.15
 C       4.223889     0.599763     0.771538      62.16
 H       4.011555    -0.189816     1.516683      23.09
 C       5.227824     0.348909    -0.168125      25.69
 O       5.842508    -0.925076    -0.328898     190.97
 C       5.004238    -2.143857    -0.109754     119.13
 H       4.747859    -2.420916     1.001917      24.19
 H       5.686436    -2.887227    -0.412307      27.46
 H       4.117754    -2.149956    -0.647991      27.21
 C       5.746421     1.368793    -0.973848      29.78
 O       6.849987     1.040466    -1.759309     149.85
 H       7.428370     0.487640    -1.307137      26.97
 C       5.114103     2.646988    -0.990713      62.11
 H       5.352398     3.473330    -1.807289      19.10
 C       3.704252     1.919631     0.817146      28.24
 C       2.588737     2.234701     1.858175      75.81
 H       2.817379     3.399258     2.246192      21.74
 O       2.691664     1.392750     3.031078     228.86
 H       2.212954     0.403297     2.971148      19.73
 C       1.123133     2.228047     1.232671      79.31
 H       1.050270     2.826010     0.264174      21.62
 C       0.123908     2.544896     2.285897     101.88
 O       0.005775     3.871480     2.856890     200.42
 H       0.224626     4.653645     1.974405      23.43
 H       0.230548     1.935039     3.084087      26.71
 H      -0.920089     2.238525     1.782693      23.56
 C      -2.231041    -0.901013     0.135017      57.60
 H      -2.986737    -1.456554     0.779045      23.20
 C      -1.687027     0.229402    -1.879154      58.59
 H      -1.625246     0.246837    -2.985340      19.75
 C      -0.623688     0.747444    -1.284128      14.13
 O       0.343615     1.533592    -1.977603     211.16
 C      -0.237738     2.395434    -3.073061     112.15
 H       0.527525     3.014622    -3.461192      26.38
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 H      -0.380472     1.640962    -3.748546      27.13
 H      -1.290722     2.798167    -2.850570      26.50
 C      -0.288454     0.489958     0.112010      17.78
 O       0.914236     0.819187     0.836551     191.56
 C      -1.192585    -0.300759     0.830315      45.86
 H      -1.017539    -0.787726     1.933491      19.11
 C      -2.534862    -0.665137    -1.283132      46.19
 C      -3.560820    -1.470997    -2.154238      66.12
 H      -3.286036    -1.083390    -3.208715      26.01
 O      -3.401547    -2.874397    -2.146678     292.44
 H      -2.540357    -2.998284    -2.405079      31.60
 C      -5.036105    -1.149158    -1.823568      97.39
 H      -5.288260    -1.401049    -0.740058      27.00
 O      -5.322081     0.216858    -2.205866     265.63
 H      -4.815036     0.814422    -1.803514      32.59
 C      -6.057223    -2.064917    -2.605846     111.27
 O      -6.147501    -3.357521    -1.931675     231.64
 H      -5.154696    -3.564937    -1.796960      28.65
 H      -5.780979    -2.178445    -3.617632      30.27
 H      -7.114241    -1.689314    -2.625693      28.04
55
name = lig-ACN-frame_321
 C       4.161509     2.829775    -0.145394      49.95
 H       3.558933     3.735376    -0.162657      23.07
 C       4.268176     0.641144     0.772037      46.10
 H       3.854402    -0.125870     1.400068      20.85
 C       5.245202     0.323295    -0.167601      29.64
 O       5.765949    -0.921401    -0.224180     227.08
 C       5.022413    -2.197506    -0.141950     117.92
 H       4.627855    -2.246535     0.957799      24.40
 H       5.722335    -3.018621    -0.411507      26.76
 H       4.286999    -2.194334    -0.847127      27.57
 C       5.698845     1.326296    -1.100892      42.08
 O       6.868281     1.052029    -1.769503     158.13
 H       7.406607     0.378421    -1.279762      28.08
 C       5.180285     2.665746    -1.099189      51.90
 H       5.448944     3.513450    -1.840626      20.00
 C       3.665957     1.892552     0.822646      37.09
 C       2.595048     2.213135     1.845761      85.57
 H       2.788163     3.327078     2.286888      23.29
 O       2.672634     1.360467     3.004946     253.75
 H       2.378499     0.515534     2.640815      26.02
 C       1.131383     2.255584     1.285927      72.32
 H       1.102811     3.033123     0.428620      22.89
 C       0.039848     2.582452     2.330850     109.66
 O       0.095874     3.886707     2.839584     272.79
 H       0.275407     4.592739     2.132291      28.74
 H       0.312865     1.971044     3.121880      26.00
 H      -1.086904     2.361615     1.952353      23.63
 C      -2.238076    -0.962682     0.068074      52.29
 H      -2.965045    -1.716584     0.625721      21.73
 C      -1.619545     0.113733    -1.976490      43.58
 H      -1.915505     0.401242    -3.043772      19.98
 C      -0.487305     0.788854    -1.184403      -2.43
 O       0.344293     1.590062    -1.944756     200.44
 C      -0.252936     2.301424    -3.040729     114.22
 H       0.424731     3.121923    -3.329275      25.31
 H      -0.564041     1.799906    -3.870562      26.62
 H      -1.177612     2.930633    -2.626249      25.52
 C      -0.274345     0.448339     0.184494      23.40
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 O       0.847811     0.877438     0.766733     232.76
 C      -1.198725    -0.347305     0.831482      51.47
 H      -0.949837    -0.684659     1.894206      20.34
 C      -2.555603    -0.648273    -1.230552      43.84
 C      -3.612721    -1.428467    -2.170584      60.77
 H      -3.528151    -1.081672    -3.288022      25.97
 O      -3.350825    -2.854382    -2.091949     293.29
 H      -2.484017    -2.960475    -2.234139      33.26
 C      -5.100631    -1.098458    -1.839366      94.52
 H      -5.227427    -1.197361    -0.723556      26.83
 O      -5.397866     0.281412    -2.161391     247.19
 H      -4.916902     0.844231    -1.391554      24.36
 C      -6.098879    -2.066578    -2.629524     112.04
 O      -6.149273    -3.352619    -1.958780     214.04
 H      -5.169361    -3.802249    -1.977744      27.02
 H      -5.869401    -2.190399    -3.667725      29.98
 H      -7.057195    -1.555024    -2.516326      29.24
55
name = lig-ACN-frame_322
 C       4.178867     2.899503    -0.135609      54.45
 H       3.855027     3.913761    -0.136060      23.48
 C       4.236533     0.619069     0.798309      49.83
 H       3.973033    -0.152383     1.472432      20.81
 C       5.159991     0.337665    -0.197346      13.30
 O       5.834639    -1.006559    -0.163831     221.16
 C       5.012407    -2.157546    -0.167780     123.31
 H       4.383243    -2.437266     0.800595      25.10
 H       5.831023    -2.971088    -0.169340      26.99
 H       4.342871    -2.242651    -0.929524      27.85
 C       5.751183     1.275268    -1.118670      15.85
 O       6.926822     1.069107    -1.850524     124.41
 H       7.464054     0.294395    -1.315343      22.52
 C       5.168686     2.557585    -1.126385      49.92
 H       5.753274     3.251044    -1.747076      25.23
 C       3.670489     1.924444     0.760237      28.25
 C       2.562239     2.214366     1.840296      84.94
 H       2.761403     3.304521     2.268510      23.76
 O       2.652436     1.336883     2.971161     272.07
 H       2.362755     0.469995     2.871173      27.47
 C       1.116561     2.257762     1.263005      75.64
 H       1.062197     3.043472     0.420067      21.98
 C      -0.024080     2.543856     2.408966      87.40
 O       0.184250     4.001856     2.842140     270.59
 H       0.405594     4.454327     2.148822      34.36
 H      -0.067760     1.883554     3.285893      25.23
 H      -1.073619     2.341571     1.848290      23.05
 C      -2.361591    -1.049815     0.134471      38.04
 H      -2.865661    -2.030759     0.596727      20.07
 C      -1.527570     0.138418    -1.893453      42.96
 H      -1.624523     0.435344    -2.987437      19.33
 C      -0.513097     0.718866    -1.288725      17.71
 O       0.381197     1.651717    -1.865913     214.26
 C      -0.267218     2.322699    -3.012295     102.59
 H       0.588845     3.022781    -3.319070      25.03
 H      -0.432343     1.744419    -3.784607      27.58
 H      -1.273924     2.833917    -2.588820      24.54
 C      -0.339925     0.513727     0.097228      14.83
 O       0.937448     0.949073     0.773451     186.94
 C      -1.225269    -0.493627     0.782927      34.42
 H      -1.074957    -0.541455     1.808077      21.66
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 C      -2.528172    -0.703026    -1.344552      30.73
 C      -3.619177    -1.299461    -2.140797      72.38
 H      -3.402717    -0.911456    -3.243624      26.33
 O      -3.334453    -2.870090    -2.015184     177.13
 H      -2.394178    -2.992589    -2.423829      25.09
 C      -5.146596    -1.101249    -1.840115      96.03
 H      -5.381727    -1.379057    -0.787800      28.97
 O      -5.454486     0.333419    -2.148376     184.39
 H      -5.484929     0.906973    -1.160699      23.01
 C      -6.096470    -2.021491    -2.576129     117.16
 O      -6.164617    -3.349709    -1.991236     231.75
 H      -5.366927    -3.790626    -2.246534      33.30
 H      -5.812983    -2.015319    -3.622350      32.28
 H      -7.127903    -1.729366    -2.513086      31.35
55
name = lig-ACN-frame_323
 C       4.177143     2.932315    -0.188164      46.61
 H       3.887978     3.964563    -0.219278      23.37
 C       4.192829     0.645032     0.711925      39.39
 H       3.954556     0.025587     1.553841      21.60
 C       5.230532     0.172606    -0.238308      41.55
 O       5.901085    -0.969691    -0.119689     206.47
 C       4.998362    -2.197592    -0.173950     111.83
 H       4.296821    -2.081651     0.729221      23.96
 H       5.668816    -3.179481    -0.178251      26.64
 H       4.565213    -2.173307    -1.112768      28.03
 C       5.789478     1.185319    -1.047766      32.95
 O       6.938028     1.047674    -1.896043     122.97
 H       7.636946     0.425516    -1.494863      21.69
 C       5.179795     2.487025    -1.068001      50.65
 H       5.507871     3.286960    -1.660246      27.94
 C       3.646863     1.959334     0.767908      27.24
 C       2.549109     2.250797     1.824759      87.17
 H       2.767872     3.270693     2.276719      24.33
 O       2.654417     1.344557     2.984789     230.80
 H       2.066955     0.546990     2.689476      22.82
 C       1.019019     2.240466     1.349500      77.59
 H       0.857473     2.969361     0.503653      22.92
 C       0.033295     2.675004     2.371203     104.90
 O       0.207462     4.000248     2.832289     292.83
 H       0.444785     4.447608     2.079589      33.66
 H       0.130184     1.982430     3.276343      24.60
 H      -1.061369     2.708093     1.890460      23.14
 C      -2.335296    -1.074530     0.047506      42.52
 H      -3.130440    -1.724892     0.594005      19.84
 C      -1.635051     0.129393    -1.952212     107.88
 H      -1.704141     0.071488    -3.051136      19.64
 C      -0.432985     0.749219    -1.231401      -4.96
 O       0.373430     1.689500    -1.816536     205.13
 C      -0.177315     2.385510    -2.982180      97.61
 H       0.417558     3.316875    -3.436095      24.47
 H      -0.271065     1.687280    -3.649361      28.91
 H      -1.308881     2.750662    -2.949077      25.24
 C      -0.318170     0.479120     0.169538      34.35
 O       0.880336     0.869154     0.694952     235.33
 C      -1.223798    -0.486361     0.702009      38.60
 H      -1.048845    -0.872604     1.580315      22.93
 C      -2.477170    -0.746496    -1.238690      26.09
 C      -3.599698    -1.380753    -2.141425      50.14
 H      -3.509922    -1.136605    -3.338659      26.43
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 O      -3.390688    -2.781893    -1.994546     211.87
 H      -2.336423    -2.978089    -2.423908      21.52
 C      -5.123315    -1.031640    -1.737999      90.84
 H      -5.213211    -1.151970    -0.652846      28.42
 O      -5.518255     0.316337    -2.125574     224.06
 H      -5.423405     0.961408    -1.307758      26.40
 C      -6.126781    -1.995215    -2.585638     106.64
 O      -6.170855    -3.350858    -2.050265     240.84
 H      -5.301012    -3.712983    -2.165137      33.28
 H      -5.899802    -2.073976    -3.673077      30.47
 H      -7.052759    -1.478252    -2.495293      31.06
55
name = lig-ACN-frame_324
 C       4.139317     2.835782    -0.196323      54.76
 H       3.636012     3.791614    -0.394726      23.05
 C       4.194826     0.646389     0.620294      46.74
 H       3.768820    -0.110958     1.294649      21.01
 C       5.257185     0.238438    -0.175886      26.04
 O       5.965423    -1.093875    -0.068694     208.98
 C       5.029922    -2.141480    -0.206779     125.84
 H       4.152503    -2.141127     0.517711      23.67
 H       5.657928    -3.135267     0.064770      25.84
 H       4.501627    -2.203769    -1.153191      26.45
 C       5.827124     1.202758    -1.043698      29.35
 O       6.903256     1.003886    -1.893577     180.44
 H       7.534148     0.577875    -1.383540      30.11
 C       5.236995     2.488669    -1.019799      53.07
 H       5.629249     2.988281    -1.821800      22.71
 C       3.622206     1.944551     0.727011      28.71
 C       2.520566     2.269273     1.838800      87.42
 H       2.643499     3.309499     2.163631      24.60
 O       2.643859     1.393601     2.967208     241.11
 H       2.178131     0.391649     2.858233      19.69
 C       1.073685     2.217968     1.257603      75.73
 H       1.071228     2.879456     0.381752      22.64
 C      -0.012346     2.707363     2.369213      92.44
 O       0.251711     4.051417     2.820292     258.29
 H       0.443215     4.797622     2.131563      27.76
 H       0.070112     2.058893     3.357570      23.86
 H      -1.088888     2.417206     1.984639      23.99
 C      -2.260641    -1.024813     0.044048      57.27
 H      -2.973285    -1.610835     0.666768      21.98
 C      -1.570073     0.150959    -1.959841      44.23
 H      -1.712137     0.410356    -2.978079      20.35
 C      -0.610834     0.786659    -1.247693      16.20
 O       0.359652     1.777680    -1.772075     191.60
 C      -0.113655     2.366567    -3.041910     107.41
 H       0.643533     3.262934    -2.907679      23.09
 H      -0.000480     1.960756    -3.956345      27.93
 H      -1.156281     2.714482    -2.684666      25.21
 C      -0.328724     0.394999     0.085970      10.38
 O       0.833285     0.811617     0.762763     207.57
 C      -1.183727    -0.518031     0.803166      35.84
 H      -0.862480    -0.792787     1.667859      21.15
 C      -2.550892    -0.693350    -1.366527      63.37
 C      -3.614100    -1.383317    -2.105279      65.50
 H      -3.472153    -0.945658    -3.243396      24.55
 O      -3.486778    -2.811367    -2.006381     148.24
 H      -2.313526    -3.044844    -2.085011      22.71
 C      -5.077897    -1.042663    -1.736313     104.20
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 H      -5.242135    -1.219492    -0.676618      28.53
 O      -5.539321     0.302908    -2.090793     274.12
 H      -5.006719     0.878736    -1.657244      32.26
 C      -6.104002    -1.941766    -2.514330     111.28
 O      -6.192267    -3.330250    -2.116374     212.29
 H      -5.170450    -3.546825    -1.852246      28.44
 H      -5.752851    -1.784162    -3.571471      29.86
 H      -7.126029    -1.651760    -2.396757      29.06
55
name = lig-ACN-frame_325
 C       4.109954     2.812217    -0.267808      50.21
 H       3.636074     3.831848    -0.372114      22.18
 C       4.152887     0.532377     0.674106      50.23
 H       3.689854    -0.348678     1.192582      21.10
 C       5.368877     0.274759    -0.098964      11.26
 O       5.951859    -1.063529    -0.032365     196.07
 C       5.005902    -2.172813    -0.224264     111.19
 H       4.195875    -2.097748     0.521210      22.32
 H       5.649366    -3.158612    -0.047347      25.10
 H       4.783291    -2.244299    -1.308164      25.27
 C       5.843979     1.241171    -0.990990      42.31
 O       6.903580     0.950286    -1.866583     180.98
 H       7.637946     0.402056    -1.436515      28.55
 C       5.261003     2.517991    -1.074082      37.04
 H       5.541908     3.333465    -1.657985      21.06
 C       3.596090     1.841837     0.699709      22.26
 C       2.506180     2.197134     1.750625      98.61
 H       2.690271     3.167740     2.095346      25.05
 O       2.648441     1.446683     2.986856     244.90
 H       2.358081     0.487408     2.724918      23.78
 C       1.067679     2.199154     1.156564      86.08
 H       0.997743     2.814475     0.284196      22.60
 C       0.009826     2.664756     2.309179      81.69
 O       0.264288     4.113553     2.825483     175.70
 H       0.267588     4.512320     1.718619      24.09
 H       0.205958     1.944810     3.263687      22.08
 H      -1.061287     2.718940     1.920592      22.23
 C      -2.282387    -0.985858     0.066393      54.48
 H      -2.867523    -1.825554     0.341142      19.36
 C      -1.617761     0.231044    -2.041593      57.86
 H      -1.711053     0.542715    -3.043013      18.60
 C      -0.601665     0.884756    -1.227919      27.23
 O       0.259900     1.733278    -1.749612     214.83
 C      -0.007918     2.484891    -2.991910     114.28
 H       0.562059     3.491509    -3.155286      23.80
 H       0.225033     1.748151    -3.680464      27.07
 H      -1.057249     2.747407    -3.295381      27.93
 C      -0.309289     0.391919     0.116218      28.01
 O       0.816521     0.795789     0.885241     226.26
 C      -1.120111    -0.520259     0.762522      28.10
 H      -1.072101    -0.685347     1.758522      20.44
 C      -2.493109    -0.624399    -1.293334      56.26
 C      -3.663795    -1.300910    -2.145590      40.26
 H      -3.522727    -1.147057    -3.363969      25.86
 O      -3.559603    -2.903716    -2.019481     181.43
 H      -2.482751    -3.127984    -2.025518      23.24
 C      -5.117388    -1.077849    -1.691939     105.53
 H      -5.170448    -1.273237    -0.623843      28.47
 O      -5.498791     0.288539    -2.060552     266.01
 H      -4.810305     0.925852    -1.706641      28.22
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 C      -6.095226    -1.907309    -2.487178     117.13
 O      -6.164765    -3.299718    -2.150720     230.63
 H      -5.231527    -3.669173    -1.907184      28.46
 H      -5.978787    -1.834339    -3.620211      29.31
 H      -7.024744    -1.349692    -2.287137      29.28
55
name = lig-ACN-frame_326
 C       4.084804     2.727146    -0.254191      55.33
 H       3.698871     3.789719    -0.138862      23.55
 C       4.197743     0.468448     0.700190      52.66
 H       3.793838    -0.210666     1.499176      21.62
 C       5.321608     0.234337    -0.010756      18.33
 O       5.940247    -0.976741    -0.017207     206.48
 C       5.047347    -2.191929    -0.259418     112.03
 H       4.139270    -2.196696     0.322335      25.42
 H       5.684002    -3.085201    -0.052406      27.42
 H       4.534990    -2.139560    -1.308726      25.39
 C       5.900178     1.260700    -0.943060      12.36
 O       6.944326     0.906292    -1.841438      79.36
 H       7.593534     0.223735    -1.296293      22.82
 C       5.186223     2.544813    -1.086767      53.13
 H       5.709088     3.267418    -1.717423      25.03
 C       3.597174     1.736138     0.609642      37.10
 C       2.546421     2.197782     1.640160      89.21
 H       2.745912     3.169762     1.835246      26.60
 O       2.639214     1.473700     2.966823     257.83
 H       2.354848     0.619502     2.908147      29.75
 C       1.015878     2.193858     1.195985      91.83
 H       0.914094     2.711226     0.281350      23.72
 C       0.098327     2.745492     2.225271      96.60
 O       0.249107     4.021489     2.743409     209.73
 H       0.484949     4.922260     1.966661      23.96
 H       0.114362     1.961680     3.209173      23.05
 H      -0.938800     2.538533     1.847411      24.42
 C      -2.312469    -1.017532    -0.010746      52.39
 H      -2.854597    -1.711262     0.561688      20.18
 C      -1.702951     0.355347    -1.921991     102.77
 H      -1.817753     0.330850    -3.016691      18.60
 C      -0.589796     0.836763    -1.204623      19.05
 O       0.248887     1.863473    -1.741942     208.84
 C       0.083125     2.498890    -3.030253     115.07
 H       0.738381     3.376030    -2.782362      25.13
 H       0.590107     2.068495    -3.937491      27.19
 H      -0.967487     2.691876    -3.166504      27.24
 C      -0.296654     0.479313     0.180533      27.48
 O       0.785139     0.779775     0.948671     222.48
 C      -1.202324    -0.520806     0.692694      49.37
 H      -0.867403    -0.921174     1.674032      17.97
 C      -2.525709    -0.631282    -1.342882      64.07
 C      -3.608274    -1.421127    -2.100295      41.84
 H      -3.559778    -0.994037    -3.293532      24.74
 O      -3.577626    -2.874583    -2.023718     246.87
 H      -2.724620    -3.071998    -2.283468      30.12
 C      -5.067853    -1.041623    -1.692459     105.48
 H      -5.232157    -1.231551    -0.630006      30.08
 O      -5.438157     0.299614    -2.030866     239.62
 H      -4.978274     0.958758    -1.215298      23.77
 C      -6.168749    -1.904173    -2.507440     100.75
 O      -6.168875    -3.292422    -2.138021     241.40
 H      -5.285878    -3.456823    -2.319108      35.17
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 H      -5.919366    -1.696303    -3.621413      31.06
 H      -7.221041    -1.614935    -2.223649      29.17
55
name = lig-ACN-frame_327
 C       4.083732     2.687976    -0.241125      62.20
 H       3.513815     3.669447    -0.263571      21.17
 C       4.200460     0.485178     0.785994      39.15
 H       4.019020    -0.273014     1.573280      19.58
 C       5.325073     0.270844    -0.116022      23.97
 O       5.961164    -1.040684    -0.012206     220.35
 C       5.103294    -2.096069    -0.295807     127.56
 H       4.425743    -2.285819     0.505164      24.46
 H       5.775557    -2.941625    -0.330236      28.30
 H       4.757859    -2.095557    -1.445710      24.72
 C       5.854095     1.211371    -0.939246      21.98
 O       6.954400     0.892633    -1.741442     187.25
 H       7.562718     0.316443    -1.224053      19.84
 C       5.236578     2.408697    -1.052682      56.62
 H       5.465298     3.176893    -1.853066      25.11
 C       3.522135     1.713300     0.599639      35.45
 C       2.551127     2.208165     1.639334     107.58
 H       2.835669     3.141420     1.858641      27.72
 O       2.651155     1.534329     2.897464     237.04
 H       2.074430     0.732530     2.833821      25.09
 C       1.145323     2.200404     1.162095      87.20
 H       1.059294     2.764354     0.256877      23.42
 C       0.037676     2.691529     2.196484      89.51
 O       0.266618     4.033247     2.693058     224.19
 H       0.603933     4.603836     1.774346      26.21
 H       0.192106     2.042468     3.265842      22.31
 H      -0.953890     2.602918     1.729260      23.66
 C      -2.304400    -1.077929     0.002618      28.65
 H      -3.032082    -1.797307     0.379436      20.07
 C      -1.752211     0.363352    -1.819790      98.40
 H      -1.765813     0.891127    -2.834107      13.90
 C      -0.571886     0.914759    -1.209664      18.79
 O       0.292347     1.938266    -1.679490     242.05
 C       0.176265     2.549039    -3.044886     121.32
 H       0.560358     3.563846    -2.952905      26.56
 H       0.581113     1.932919    -3.903985      28.29
 H      -0.812498     2.767010    -3.307030      28.91
 C      -0.426213     0.459691     0.139015      38.23
 O       0.735671     0.776726     0.978754     198.88
 C      -1.242434    -0.500322     0.680424      25.70
 H      -0.928112    -1.084941     1.665489      18.39
 C      -2.617694    -0.700821    -1.354237      45.70
 C      -3.652792    -1.419636    -2.136779      49.38
 H      -3.421620    -1.158514    -3.358323      24.86
 O      -3.507686    -2.843235    -2.026679     247.46
 H      -2.707906    -3.066924    -2.405841      30.20
 C      -5.133077    -1.068677    -1.722250      97.75
 H      -5.191752    -1.314723    -0.637800      29.43
 O      -5.327545     0.378479    -1.973765     206.37
 H      -5.348806     0.962363    -1.075268      25.19
 C      -6.202205    -1.862573    -2.464444     107.95
 O      -6.164507    -3.298171    -2.153582     206.86
 H      -5.320587    -3.741461    -2.373506      33.07
 H      -6.129824    -1.750038    -3.625870      29.97
 H      -7.253955    -1.419331    -2.255711      29.89
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name = lig-ACN-frame_328
 C       4.056941     2.644124    -0.309259      49.41
 H       3.618657     3.602909    -0.646231      22.71
 C       4.260669     0.515450     0.767601      55.65
 H       3.882505    -0.195969     1.484523      20.66
 C       5.282154     0.125546    -0.065944      38.46
 O       6.039287    -0.992387    -0.005143     244.13
 C       5.189984    -2.164542    -0.361927     115.95
 H       4.431887    -2.289938     0.375019      25.61
 H       5.757021    -3.010322    -0.523144      28.95
 H       4.375162    -1.776711    -1.188601      23.37
 C       5.834940     1.094016    -0.992646      18.95
 O       7.006871     0.899431    -1.665670     164.78
 H       7.628128     0.420998    -1.173203      26.42
 C       5.184000     2.396474    -1.050850      50.21
 H       5.617081     3.152766    -1.811693      21.19
 C       3.572436     1.732607     0.684963      39.37
 C       2.543452     2.268052     1.694796      98.02
 H       2.669713     3.244363     1.888645      26.59
 O       2.674575     1.526653     2.900268     222.83
 H       1.998248     0.651167     2.861796      21.82
 C       1.053304     2.195207     1.132876      87.15
 H       1.055511     2.758491     0.186047      20.91
 C       0.047241     2.656015     2.174799      92.30
 O       0.305543     4.090819     2.604139     267.59
 H       0.423515     4.562042     1.802400      31.85
 H      -0.046462     1.772259     3.071165      23.42
 H      -0.941982     2.615107     1.766702      25.29
 C      -2.382537    -1.163493    -0.021774      45.16
 H      -2.726029    -2.143210     0.447752      17.65
 C      -1.748166     0.412397    -1.891715      77.44
 H      -2.432083     0.776186    -2.732806      20.07
 C      -0.667180     1.006195    -1.147040      22.25
 O       0.310143     1.966894    -1.646066     208.39
 C       0.171570     2.599072    -3.007556     117.18
 H       0.782337     3.425092    -3.051214      26.73
 H       0.775992     1.788203    -3.552142      25.51
 H      -0.792412     2.610863    -3.338946      28.76
 C      -0.377698     0.470998     0.161917      21.29
 O       0.672136     0.776710     0.921267     214.11
 C      -1.281590    -0.560296     0.710475      51.30
 H      -1.049801    -0.691287     1.934160      17.23
 C      -2.543825    -0.610657    -1.288093      73.73
 C      -3.730241    -1.349378    -2.243978      21.77
 H      -3.730807    -0.983059    -3.482116      26.40
 O      -3.424997    -2.885035    -2.043606     185.86
 H      -2.340515    -2.844530    -2.084979      23.09
 C      -5.129127    -1.036950    -1.738932     104.23
 H      -5.253203    -1.308723    -0.652253      29.11
 O      -5.259037     0.417240    -1.921672     300.05
 H      -4.983075     0.774904    -1.150743      31.40
 C      -6.229675    -1.870772    -2.477588      99.50
 O      -6.217615    -3.284960    -2.161611     206.93
 H      -5.136718    -3.405429    -2.253627      28.84
 H      -6.164253    -1.645377    -3.633129      29.99
 H      -7.224934    -1.524845    -1.977689      28.25
55
name = lig-ACN-frame_329
 C       3.997986     2.651534    -0.395143      54.95
 H       3.446047     3.569547    -0.313869      22.75
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 C       4.212070     0.484604     0.809767      39.68
 H       3.902566    -0.164263     1.595668      21.99
 C       5.320707     0.155772    -0.072176       2.70
 O       6.107022    -1.092113     0.014826     204.53
 C       5.202235    -2.204052    -0.378694     109.74
 H       4.756265    -2.652770     0.475213      24.73
 H       5.825084    -2.916553    -0.788357      29.02
 H       4.616739    -1.912896    -1.406166      23.87
 C       5.799308     1.085342    -0.979053      14.88
 O       7.081956     0.906085    -1.652691     164.66
 H       7.676799     0.387486    -0.961778      25.06
 C       5.181109     2.293791    -1.150463      49.50
 H       5.734345     3.075206    -1.752735      20.69
 C       3.677976     1.855901     0.702343       9.64
 C       2.470194     2.243995     1.671574      85.77
 H       2.643620     3.201952     1.992874      26.21
 O       2.672314     1.488920     2.994339     206.25
 H       2.292781     0.526322     2.836123      23.32
 C       0.993735     2.169031     1.145543      92.33
 H       0.828799     2.797099     0.203986      20.69
 C      -0.000592     2.778229     2.126976     104.44
 O       0.331081     4.057327     2.527890     305.76
 H       0.294224     4.597941     1.828842      34.84
 H       0.226411     2.314910     3.266079      22.55
 H      -0.989631     2.601257     1.764793      26.23
 C      -2.263686    -1.153231    -0.018231      69.07
 H      -2.944797    -2.058379     0.279965      19.27
 C      -1.830089     0.499264    -1.875297      42.94
 H      -1.809970     0.932206    -2.931173      14.58
 C      -0.739080     1.056991    -1.154835      29.36
 O       0.227854     1.992358    -1.585911     235.73
 C       0.208251     2.474690    -2.934352     136.82
 H       0.615396     3.399148    -2.810572      27.50
 H       0.522564     1.945142    -3.885986      27.25
 H      -0.744260     2.813764    -3.206560      29.99
 C      -0.495002     0.417958     0.122356      31.89
 O       0.717008     0.790784     0.876843     206.58
 C      -1.303262    -0.535167     0.715097      19.65
 H      -1.092435    -0.969892     1.888569      17.72
 C      -2.610285    -0.627431    -1.373849      56.57
 C      -3.610242    -1.359347    -2.162482      40.81
 H      -3.459125    -1.021343    -3.395678      25.21
 O      -3.373185    -2.791653    -2.113659     180.41
 H      -2.207079    -3.046346    -2.061640      21.76
 C      -5.095628    -1.026989    -1.733101      85.55
 H      -5.139603    -1.291007    -0.616254      27.63
 O      -5.260114     0.414120    -1.880165     255.65
 H      -4.538887     0.900117    -1.468437      29.34
 C      -6.302345    -1.803838    -2.450868     100.36
 O      -6.195342    -3.236051    -2.182093     220.75
 H      -5.282973    -3.609544    -2.030123      31.81
 H      -6.296343    -1.638799    -3.624314      28.12
 H      -7.395119    -1.459364    -2.170899      27.02
55
name = lig-ACN-frame_330
 C       4.035730     2.676152    -0.397001      49.63
 H       3.730042     3.635354    -0.739202      22.65
 C       4.264363     0.526471     0.801191      52.36
 H       3.996268    -0.173596     1.570665      22.84
 C       5.368698     0.130916    -0.000556      15.24
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 O       6.036505    -1.147595     0.039117     247.88
 C       5.327406    -2.293261    -0.418429     121.47
 H       4.761357    -2.731700     0.393963      26.18
 H       5.999213    -2.965927    -0.858913      28.89
 H       4.339616    -1.943340    -1.014224      24.13
 C       5.906056     1.091197    -0.989790      10.24
 O       7.070892     0.909174    -1.618831      67.43
 H       7.860741     0.381452    -1.102140      18.64
 C       5.113914     2.311427    -1.254640      43.42
 H       5.425624     3.003006    -2.062452      26.11
 C       3.600877     1.783705     0.711343      26.35
 C       2.508341     2.161349     1.737574      87.44
 H       2.584990     3.192209     1.939124      25.91
 O       2.619874     1.470706     3.001526     254.64
 H       2.406049     0.606503     2.887808      30.78
 C       1.024160     2.165856     1.138625      71.49
 H       1.187682     2.815062     0.194051      22.50
 C      -0.042204     2.760750     2.198294      95.05
 O       0.345486     4.177863     2.462245     220.35
 H       0.421244     4.690972     1.492822      25.98
 H      -0.035627     1.994103     3.141446      24.22
 H      -1.066526     2.781747     1.886392      25.53
 C      -2.286290    -1.079844    -0.167714      70.42
 H      -2.909475    -1.890135     0.366185      20.86
 C      -1.888461     0.544491    -1.878293      83.36
 H      -1.946809     0.625569    -2.966824      18.66
 C      -0.785082     0.985952    -1.099179      13.79
 O       0.114611     1.926984    -1.535858     224.46
 C       0.135677     2.512972    -2.885399     120.07
 H       0.917759     3.191386    -2.953037      27.54
 H       0.559267     1.596592    -3.442769      27.25
 H      -0.855899     2.732179    -3.187484      28.77
 C      -0.466327     0.514722     0.188641      30.47
 O       0.699054     0.749399     0.792883     205.71
 C      -1.270249    -0.524454     0.712997      54.34
 H      -0.791437    -1.128640     1.700342      19.33
 C      -2.524755    -0.560827    -1.345199      48.52
 C      -3.547273    -1.376084    -2.203682      27.76
 H      -3.419480    -0.906435    -3.401869      24.62
 O      -3.369505    -2.764178    -2.156303     168.11
 H      -2.240289    -2.866719    -2.575181      20.18
 C      -5.081717    -1.011914    -1.693956      91.57
 H      -5.171933    -1.358143    -0.596816      29.17
 O      -5.312273     0.393313    -1.884961     191.33
 H      -4.366005     0.885641    -1.539319      26.34
 C      -6.230981    -1.740489    -2.434734     102.03
 O      -6.204236    -3.186760    -2.184496     246.38
 H      -5.294635    -3.220527    -2.179007      35.38
 H      -6.153116    -1.523594    -3.588741      28.80
 H      -7.172540    -1.296575    -1.916588      27.57
55
name = lig-ACN-frame_331
 C       4.075807     2.614436    -0.368668      58.58
 H       3.395680     3.434059    -0.447462      24.41
 C       4.347785     0.537440     0.791346      45.42
 H       3.951225    -0.199163     1.501014      22.74
 C       5.412295     0.160998    -0.038731      29.67
 O       5.993189    -1.098653     0.103711     227.99
 C       5.322624    -2.380134    -0.402740     105.12
 H       5.080761    -3.030289     0.439703      26.30
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 H       6.083689    -2.918387    -0.978941      28.12
 H       4.568310    -2.141755    -1.253155      25.11
 C       5.893651     1.120480    -0.925081      11.26
 O       7.096118     0.919170    -1.666150     179.97
 H       7.652248     0.369944    -1.076084      22.45
 C       5.109292     2.226900    -1.254326      62.24
 H       5.298579     2.736453    -2.175636      25.04
 C       3.575285     1.728997     0.614446      12.27
 C       2.506740     2.145892     1.761121      94.27
 H       2.819909     3.132771     2.067298      24.85
 O       2.573764     1.443305     2.999198     236.18
 H       2.103854     0.575397     2.938067      26.20
 C       1.082765     2.135031     1.215784      83.18
 H       0.959920     2.792648     0.257710      21.55
 C       0.014234     2.764772     2.150777      95.86
 O       0.333639     4.254169     2.426446     143.09
 H       0.738214     4.645390     1.365652      23.90
 H       0.037711     2.383312     3.248121      24.41
 H      -0.955176     2.630421     1.648541      25.41
 C      -2.294824    -1.052503    -0.006168      54.86
 H      -2.711549    -2.053801     0.146123      23.43
 C      -1.828719     0.539743    -1.922629      39.49
 H      -2.121186     1.035463    -2.803759      20.00
 C      -0.829232     1.020801    -1.101492      13.87
 O       0.077230     1.967657    -1.488780     215.87
 C       0.065890     2.406192    -2.846308     120.14
 H       0.809590     3.185015    -2.853470      26.78
 H       0.171499     1.550281    -3.633871      26.70
 H      -0.786108     2.983949    -3.267961      26.70
 C      -0.527382     0.527424     0.216389      46.89
 O       0.776397     0.794771     0.772128     188.51
 C      -1.224108    -0.579725     0.651972      36.41
 H      -0.953179    -1.078199     1.688266      20.26
 C      -2.602027    -0.582739    -1.420705      34.76
 C      -3.641454    -1.224892    -2.265711      62.00
 H      -3.736941    -0.925234    -3.503794      25.81
 O      -3.359526    -2.801212    -2.220884     129.46
 H      -2.314706    -3.040780    -2.487150      22.78
 C      -4.979414    -1.017996    -1.702076     102.32
 H      -4.991697    -1.219986    -0.576013      29.05
 O      -5.347500     0.377692    -1.896615     203.38
 H      -4.747662     1.086690    -1.318209      26.62
 C      -6.140740    -1.685670    -2.398899     107.29
 O      -6.172487    -3.084278    -2.191752     210.68
 H      -5.371877    -3.656680    -2.407600      31.08
 H      -6.175677    -1.354781    -3.528793      28.86
 H      -7.153691    -1.324647    -2.024763      28.04
55
name = lig-ACN-frame_332
 C       3.960015     2.545873    -0.386104      57.36
 H       3.535868     3.507093    -0.675295      22.91
 C       4.292001     0.461835     0.802934      58.02
 H       4.058512    -0.293115     1.593733      22.89
 C       5.380736     0.152793    -0.046655      25.52
 O       6.003112    -1.119823     0.160135     237.77
 C       5.393593    -2.353844    -0.394183     113.31
 H       5.026927    -2.961948     0.473845      26.69
 H       6.279876    -2.847969    -0.910030      27.25
 H       4.449111    -2.247134    -0.960379      26.35
 C       5.939770     1.092652    -0.982328      17.39
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 O       7.075254     0.926328    -1.712956     144.63
 H       7.722627     0.430716    -1.288145      20.80
 C       5.112317     2.215995    -1.216769      46.13
 H       5.452005     2.911360    -1.968477      27.58
 C       3.645890     1.665714     0.691283      35.64
 C       2.569614     2.144532     1.696833      78.43
 H       2.771156     3.211983     1.964755      25.46
 O       2.555011     1.364619     3.004096     188.33
 H       1.904937     0.478519     2.828436      22.28
 C       1.105510     2.208868     1.228445      79.32
 H       1.197574     2.928677     0.303714      23.11
 C       0.109856     2.890551     2.149189     114.43
 O       0.304985     4.215779     2.341891     224.27
 H       0.677855     4.855402     1.425638      23.91
 H       0.051714     2.395831     3.170631      26.20
 H      -0.912217     2.696048     1.732074      26.63
 C      -2.379279    -1.121205    -0.121824      81.14
 H      -2.802850    -1.970733     0.297944      24.63
 C      -1.846591     0.491355    -1.887508      61.12
 H      -2.045173     1.052937    -2.762542      21.51
 C      -0.815429     1.087889    -1.059519      32.73
 O       0.063916     2.074639    -1.481320     226.34
 C       0.011615     2.388916    -2.891770      97.66
 H       0.964331     2.967294    -3.138137      25.41
 H       0.058855     1.473927    -3.646809      25.53
 H      -0.960896     2.886597    -2.902607      27.32
 C      -0.469944     0.497892     0.182345      43.47
 O       0.803201     0.825184     0.795438     188.15
 C      -1.211007    -0.615852     0.708233      41.64
 H      -0.890924    -1.073902     1.654100      18.53
 C      -2.603526    -0.577320    -1.388365      25.93
 C      -3.624144    -1.306376    -2.300884      32.77
 H      -3.429917    -0.736716    -3.438693      26.52
 O      -3.398837    -2.745337    -2.310052     243.73
 H      -2.461514    -2.725094    -2.269305      28.19
 C      -5.007801    -0.939917    -1.656428      92.85
 H      -4.935419    -1.320014    -0.581532      29.39
 O      -5.364608     0.451583    -1.890514     236.51
 H      -5.063066     0.904733    -1.173273      32.31
 C      -6.104440    -1.672780    -2.400917     102.91
 O      -6.173346    -3.088551    -2.189542     182.49
 H      -5.298488    -3.320913    -2.749895      29.91
 H      -5.972322    -1.436398    -3.529288      29.30
 H      -7.025218    -1.249973    -1.976818      29.35
55
name = lig-ACN-frame_333
 C       3.960568     2.451896    -0.451018      47.99
 H       3.399174     3.417918    -0.524815      22.26
 C       4.264626     0.364902     0.800662      26.88
 H       4.021023    -0.343131     1.643026      20.69
 C       5.370280     0.043321    -0.045887      10.38
 O       6.059161    -1.125036     0.193738     263.19
 C       5.467584    -2.291538    -0.315839     117.68
 H       5.110383    -2.966959     0.545787      24.94
 H       6.115914    -3.004657    -0.991287      26.41
 H       4.729399    -1.984656    -0.991298      26.54
 C       5.857432     1.028017    -0.997711       7.76
 O       7.070995     0.921799    -1.789991     163.72
 H       7.769546     0.473411    -1.173594      25.19
 C       5.116273     2.267375    -1.160747      50.85
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 H       5.494549     3.104187    -1.766682      21.51
 C       3.624940     1.678076     0.753934       5.01
 C       2.584904     2.090071     1.794883     100.88
 H       2.933155     3.107523     2.177388      26.11
 O       2.568085     1.334565     2.937178     252.92
 H       2.109256     0.362657     2.732016      22.28
 C       1.189571     2.290819     1.085799      69.28
 H       1.189002     2.810326     0.070980      21.15
 C       0.096928     2.845575     2.141851     100.80
 O       0.319733     4.332904     2.308362     237.81
 H       0.299947     4.636727     1.329706      28.22
 H       0.272365     2.371297     3.092831      26.81
 H      -0.949948     2.661827     1.748176      25.48
 C      -2.263137    -1.161507    -0.101416      56.06
 H      -2.982648    -1.763078     0.209777      22.86
 C      -1.828503     0.550435    -1.789001      53.96
 H      -2.022611     0.577200    -2.852360      19.61
 C      -0.777749     1.066726    -1.038965      10.27
 O       0.068488     2.132785    -1.499174     196.81
 C      -0.071807     2.437054    -2.952529      93.15
 H       0.879259     3.017666    -3.346625      24.85
 H      -0.201454     1.322701    -3.308751      25.06
 H      -0.851654     3.045772    -3.489860      26.05
 C      -0.374352     0.424668     0.206421      20.24
 O       0.743338     0.846387     0.843813     196.24
 C      -1.280652    -0.593067     0.646135      63.63
 H      -0.994363    -1.124195     1.454955      26.08
 C      -2.552232    -0.616039    -1.363309      49.06
 C      -3.560429    -1.248736    -2.225560      46.34
 H      -3.629964    -0.830489    -3.452207      25.13
 O      -3.431728    -2.671635    -2.405915     249.61
 H      -2.607997    -2.956997    -2.390767      33.39
 C      -5.044606    -0.915830    -1.702844      90.97
 H      -5.192995    -1.057123    -0.595736      27.78
 O      -5.342927     0.531649    -1.840394     207.84
 H      -4.814951     1.050591    -1.218188      29.36
 C      -6.190547    -1.654793    -2.417507     108.15
 O      -6.145387    -3.131786    -2.220653     224.47
 H      -5.345908    -3.521045    -2.501272      33.03
 H      -6.092357    -1.424893    -3.537964      28.81
 H      -7.165388    -1.318745    -2.168359      29.51
55
name = lig-ACN-frame_334
 C       3.942232     2.446025    -0.323071      47.34
 H       3.319841     3.375695    -0.498708      21.54
 C       4.285410     0.363135     0.801266      59.58
 H       3.979835    -0.364283     1.573347      22.22
 C       5.350509     0.055533    -0.069448      13.11
 O       6.206649    -1.100526     0.230302     226.29
 C       5.463495    -2.320654    -0.291909     105.02
 H       5.006158    -2.925935     0.590627      25.74
 H       6.415963    -2.836053    -0.776371      26.00
 H       4.688178    -2.101672    -0.922079      27.18
 C       5.820990     1.002602    -1.039323      24.20
 O       6.981593     0.894040    -1.783150     124.82
 H       7.795488     0.435125    -1.217905      23.94
 C       5.159043     2.212202    -1.117815      36.57
 H       5.571204     2.896709    -1.928605      20.22
 C       3.627207     1.547020     0.661009      36.95
 C       2.587539     2.129956     1.744309      72.14
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 H       2.891065     3.172793     2.184998      24.82
 O       2.573210     1.252277     2.939889     236.74
 H       2.205837     0.376573     2.785525      26.95
 C       1.136000     2.253782     1.095841      95.34
 H       1.234055     2.862337     0.185357      24.59
 C       0.172840     2.882585     2.042854     112.52
 O       0.291797     4.368468     2.285787     288.32
 H       0.333875     4.856866     1.596188      35.13
 H       0.370928     2.517822     2.973220      28.47
 H      -0.895926     2.526713     1.842105      26.49
 C      -2.250867    -1.174501    -0.066237      57.56
 H      -2.582985    -2.040928     0.335507      27.16
 C      -1.795472     0.514118    -1.790760      73.38
 H      -1.912827     1.193456    -2.664626      18.57
 C      -0.697540     1.076237    -1.080802      14.66
 O       0.008174     2.189154    -1.565733     216.15
 C      -0.117094     2.398663    -3.034643      87.22
 H       0.975473     2.890418    -3.137069      24.10
 H      -0.123703     1.555375    -3.878277      25.80
 H      -1.012581     3.101177    -2.959480      24.13
 C      -0.391492     0.479225     0.148994      24.11
 O       0.739523     0.836384     0.941749     177.69
 C      -1.152465    -0.610999     0.726821      29.07
 H      -1.021880    -0.860576     1.653837      20.79
 C      -2.478170    -0.614931    -1.361922      46.69
 C      -3.655570    -1.135522    -2.217258      40.72
 H      -3.467373    -0.391317    -3.265467      25.28
 O      -3.472993    -2.672399    -2.473589     162.61
 H      -2.442784    -2.638405    -2.636773      23.20
 C      -5.083897    -0.856113    -1.686809      92.18
 H      -5.068630    -1.313174    -0.663058      30.00
 O      -5.296099     0.580287    -1.817852     179.92
 H      -4.362069     1.064030    -1.442451      25.64
 C      -6.239193    -1.717462    -2.505778     112.14
 O      -6.158241    -3.136893    -2.242052     216.92
 H      -5.200268    -3.188311    -2.197093      30.20
 H      -6.269649    -1.461210    -3.601442      28.83
 H      -7.106051    -1.447710    -1.992118      29.53
55
name = lig-ACN-frame_335
 C       4.056434     2.502589    -0.321365      52.05
 H       3.586184     3.513770    -0.500811      25.46
 C       4.318056     0.298722     0.794409      31.14
 H       4.165954    -0.423190     1.593909      21.85
 C       5.460113     0.037781    -0.020055      23.19
 O       6.221158    -1.067888     0.193513     261.33
 C       5.564836    -2.335045    -0.228802     103.22
 H       5.072865    -2.792163     0.723527      24.71
 H       6.250901    -3.204534    -0.709099      25.69
 H       4.866202    -2.122942    -0.958116      28.23
 C       5.824176     0.983604    -0.995283      15.98
 O       6.920619     0.830555    -1.779186     120.78
 H       7.570012     0.213971    -1.265381      22.82
 C       5.062974     2.189666    -1.126968      64.01
 H       5.343040     2.980950    -1.911864      24.94
 C       3.529925     1.532913     0.668449       0.98
 C       2.563728     1.999185     1.666517      71.25
 H       2.949946     3.124847     1.895721      22.22
 O       2.586788     1.247818     2.931193     245.93
 H       2.021206     0.518850     2.786498      28.03
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 C       1.173713     2.197262     1.143408      90.32
 H       1.185588     2.573251     0.153710      25.26
 C       0.181513     2.992978     2.081950     116.84
 O       0.242091     4.352895     2.287479     305.15
 H       0.635773     4.669124     1.460310      30.12
 H       0.269388     2.551848     2.974371      28.45
 H      -0.857117     2.814300     1.619271      25.43
 C      -2.112256    -1.163012    -0.013239      54.95
 H      -2.589539    -2.100718     0.198163      24.91
 C      -1.745915     0.516637    -1.836736     113.05
 H      -2.428189     0.922665    -2.605638      23.10
 C      -0.670246     1.047521    -1.115884      16.01
 O      -0.028141     2.128737    -1.661618     207.44
 C      -0.096380     2.492438    -3.049975      95.72
 H       0.770574     3.234632    -3.474750      24.41
 H      -0.324458     1.474052    -3.610093      25.80
 H      -1.007658     3.157513    -3.494600      24.36
 C      -0.347564     0.524986     0.230226      30.48
 O       0.723039     0.841366     1.000978     206.33
 C      -1.070995    -0.563471     0.718740      15.50
 H      -0.735926    -0.921577     1.606856      21.63
 C      -2.510350    -0.618035    -1.318843      62.73
 C      -3.670760    -1.125825    -2.260705      45.23
 H      -3.704363    -0.678349    -3.476699      27.47
 O      -3.487277    -2.531560    -2.531802     149.74
 H      -2.399251    -2.909650    -2.763841      23.04
 C      -5.109944    -0.888236    -1.746182      98.66
 H      -5.282640    -1.075593    -0.673443      28.85
 O      -5.273646     0.571404    -1.796567     185.95
 H      -4.392500     1.113146    -1.401515      27.82
 C      -6.247183    -1.665583    -2.472695     117.68
 O      -6.125009    -3.113586    -2.251426     185.99
 H      -5.129386    -3.493565    -2.215544      26.79
 H      -6.238416    -1.491036    -3.562722      29.08
 H      -7.167313    -1.296580    -2.122111      29.79
55
name = lig-ACN-frame_336
 C       4.018845     2.486967    -0.246213      51.61
 H       3.556715     3.479824    -0.135693      24.76
 C       4.305375     0.301864     0.788808      68.63
 H       3.920132    -0.333968     1.574373      22.97
 C       5.445734     0.086973     0.057736       3.86
 O       6.285453    -1.126500     0.121877     254.21
 C       5.624029    -2.338191    -0.141163     112.80
 H       5.028182    -2.736552     0.784626      25.05
 H       6.572368    -3.018657    -0.366331      25.53
 H       4.966887    -2.264910    -0.987671      27.65
 C       5.827136     1.011377    -0.967604      25.42
 O       6.927268     0.738624    -1.810324     160.41
 H       7.476734     0.137265    -1.385033      25.24
 C       5.076989     2.168408    -1.229921      48.53
 H       5.520721     2.885444    -1.995651      26.72
 C       3.650512     1.502610     0.618733      36.70
 C       2.582021     1.961263     1.705625      86.72
 H       2.970605     3.023750     2.119416      23.41
 O       2.593184     1.296346     2.896691     238.90
 H       2.045711     0.407745     2.977739      23.96
 C       1.179024     2.212056     1.143767      84.35
 H       1.243308     2.769652     0.276373      26.63
 C       0.074836     2.901721     2.129064      96.74
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 O       0.280899     4.439889     2.274821     177.50
 H       0.734026     4.951850     1.348522      24.36
 H      -0.048918     2.536241     3.018883      29.26
 H      -0.894992     2.667067     1.579346      25.86
 C      -2.050844    -1.168749    -0.110474      63.97
 H      -2.585937    -1.970509     0.505978      22.70
 C      -1.841532     0.447228    -1.812362      60.45
 H      -1.777009     0.891741    -2.809039      21.46
 C      -0.709612     1.014837    -1.147217       6.17
 O       0.046111     2.162487    -1.696180     188.52
 C      -0.166121     2.530435    -3.144497      83.03
 H       0.913062     3.040903    -3.211708      24.42
 H       0.034103     1.613533    -3.856125      26.13
 H      -1.234173     3.128148    -3.229741      24.04
 C      -0.342700     0.567052     0.164292      22.07
 O       0.701737     0.845781     1.055413     182.83
 C      -1.061088    -0.569777     0.665754      52.08
 H      -0.651150    -1.210228     1.465745      23.23
 C      -2.536937    -0.598891    -1.285028      48.22
 C      -3.606590    -1.157960    -2.246684      43.49
 H      -3.452252    -0.273298    -3.176574      26.90
 O      -3.491380    -2.514521    -2.593217     172.43
 H      -2.324072    -2.625928    -2.587650      23.90
 C      -5.079034    -0.875264    -1.708173      97.61
 H      -5.045028    -1.321048    -0.700131      30.12
 O      -5.309534     0.557109    -1.828168     220.30
 H      -4.797325     0.891566    -1.110306      31.60
 C      -6.172003    -1.614693    -2.480185     112.04
 O      -6.127383    -3.074914    -2.224142     185.09
 H      -5.175223    -3.201298    -2.587820      28.76
 H      -6.104929    -1.362883    -3.522501      30.07
 H      -7.151205    -1.359519    -2.053833      29.12
55
name = lig-ACN-frame_337
 C       4.079525     2.463916    -0.342329      56.13
 H       3.556476     3.399489    -0.478359      24.96
 C       4.284234     0.256553     0.840600      31.87
 H       3.956683    -0.573130     1.498929      20.59
 C       5.495183     0.043306     0.011931       4.15
 O       6.330359    -1.052136     0.082594     239.01
 C       5.677691    -2.403424    -0.058985     108.98
 H       5.021612    -2.667756     0.843898      24.31
 H       6.515242    -3.205248    -0.117049      26.44
 H       5.101373    -2.556997    -1.011059      27.00
 C       5.866170     0.991675    -1.006951      21.48
 O       6.902496     0.660618    -1.834852      92.18
 H       7.605726     0.226469    -1.298468      25.71
 C       5.110310     2.190452    -1.199328      59.35
 H       5.348622     2.860295    -2.038027      22.89
 C       3.647847     1.554365     0.726641      16.96
 C       2.645417     2.090135     1.725487      54.52
 H       3.012585     3.219652     1.970649      23.58
 O       2.613207     1.266963     3.001785     177.04
 H       2.096053     0.367543     2.593086      22.13
 C       1.108267     2.263563     1.246686      87.15
 H       1.109586     2.703985     0.317108      27.33
 C       0.051636     2.962372     2.082171     116.39
 O       0.309691     4.404394     2.281848     179.81
 H       0.512938     4.793045     1.159961      24.19
 H       0.138543     2.596162     2.967238      29.58
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 H      -0.977337     2.853602     1.681263      27.04
 C      -2.152631    -1.208089    -0.108928      60.24
 H      -2.622693    -2.258113     0.245454      25.12
 C      -1.738835     0.508719    -1.840978      55.92
 H      -2.040564     0.576756    -2.871660      20.17
 C      -0.675350     1.143939    -1.145046      12.90
 O       0.073623     2.106469    -1.707643     216.44
 C      -0.116618     2.505182    -3.134758      99.58
 H       0.407160     3.518293    -3.374594      25.54
 H      -0.222029     1.774213    -4.001807      26.99
 H      -1.264014     3.060279    -3.208990      25.27
 C      -0.362975     0.503659     0.124672      40.21
 O       0.660319     0.879961     0.987150     196.44
 C      -1.012132    -0.635545     0.536315      45.08
 H      -0.710081    -0.893317     1.662884      18.69
 C      -2.528336    -0.622269    -1.317790      47.67
 C      -3.628629    -1.049326    -2.204145      54.62
 H      -3.562592    -0.614141    -3.382037      25.63
 O      -3.413024    -2.572984    -2.665521     155.91
 H      -2.451386    -2.866413    -2.628583      26.49
 C      -4.980822    -0.883188    -1.657925     102.69
 H      -5.120886    -1.113241    -0.604943      29.82
 O      -5.368438     0.522811    -1.813401     210.56
 H      -5.055441     1.114529    -1.198250      31.97
 C      -6.120546    -1.605039    -2.465684     113.23
 O      -6.103407    -3.000668    -2.245822     218.89
 H      -5.375392    -3.417219    -2.580863      32.93
 H      -6.131050    -1.372319    -3.494953      30.09
 H      -7.037731    -1.108918    -1.992856      28.42
55
name = lig-ACN-frame_338
 C       4.054820     2.411814    -0.348476      47.64
 H       3.447951     3.232337    -0.657261      23.71
 C       4.353935     0.309559     0.807383      35.93
 H       4.136959    -0.407331     1.655340      20.39
 C       5.408866     0.043476    -0.049355      10.26
 O       6.329034    -1.081205     0.063464     238.56
 C       5.760568    -2.425914     0.038085     117.23
 H       4.973544    -2.455331     0.847287      23.47
 H       6.590966    -3.110067     0.219210      26.35
 H       5.265145    -2.529285    -1.008898      25.72
 C       5.872759     0.940462    -1.023351      22.62
 O       6.916000     0.613284    -1.890173     155.87
 H       7.743110     0.231762    -1.307037      22.10
 C       5.203282     2.146357    -1.177714      56.57
 H       5.391606     2.781124    -2.001070      20.05
 C       3.680517     1.608497     0.754233       4.63
 C       2.559169     2.144162     1.852714      63.69
 H       2.908899     3.240939     2.372288      22.91
 O       2.631406     1.310248     3.004550     219.70
 H       2.114206     0.381694     2.942084      23.14
 C       1.097874     2.284641     1.161298      86.27
 H       1.226913     2.865286     0.296021      26.50
 C       0.073814     3.021318     2.153354     120.07
 O       0.328333     4.364943     2.273403     224.55
 H       0.576492     4.896160     1.311517      25.36
 H       0.033618     2.642189     3.059650      29.51
 H      -0.913309     2.790819     1.723644      27.22
 C      -2.183798    -1.221465    -0.122610      56.41
 H      -2.744785    -2.286246     0.090580      23.73
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 C      -1.695122     0.499817    -1.901335      49.83
 H      -2.008372     1.112340    -2.709560      21.09
 C      -0.699156     1.121520    -1.177080      21.33
 O       0.188409     2.105298    -1.765226     217.88
 C      -0.214162     2.569842    -3.069482      97.00
 H       0.577242     3.294899    -3.291127      25.80
 H       0.190754     1.676673    -3.613407      26.14
 H      -1.456767     2.731534    -3.202157      23.98
 C      -0.349136     0.524952     0.061508      30.80
 O       0.665291     0.911198     0.934299     186.79
 C      -1.076674    -0.722950     0.503919      40.21
 H      -0.728297    -1.175917     1.626200      19.16
 C      -2.406568    -0.563014    -1.390026      55.23
 C      -3.543504    -1.176059    -2.314014      50.19
 H      -3.714001    -0.339231    -3.235939      27.49
 O      -3.361017    -2.582599    -2.689716     253.28
 H      -2.514698    -2.643812    -2.646463      32.85
 C      -5.027954    -0.855963    -1.612464      90.41
 H      -4.993236    -1.189942    -0.582656      29.46
 O      -5.446628     0.540658    -1.803799     197.38
 H      -4.574073     0.985407    -1.341833      26.43
 C      -6.055578    -1.561852    -2.411533     113.72
 O      -6.138604    -3.009277    -2.257694     214.07
 H      -5.162582    -3.192147    -2.469433      29.16
 H      -5.904833    -1.247772    -3.395140      29.59
 H      -7.130400    -1.294143    -2.107225      27.22
55
name = lig-ACN-frame_339
 C       4.027944     2.421640    -0.358249      54.10
 H       3.508935     3.365915    -0.465637      24.05
 C       4.391708     0.457310     0.878532      39.39
 H       4.190703    -0.199219     1.799367      20.40
 C       5.417779    -0.032929    -0.102808      35.34
 O       6.277163    -1.094277     0.080216     257.32
 C       5.793278    -2.389949     0.125313     137.23
 H       4.980191    -2.663698     0.806386      27.37
 H       6.636992    -2.965225     0.390300      28.56
 H       5.514596    -2.943986    -0.887437      27.98
 C       5.897057     0.891501    -1.079390      17.21
 O       6.957929     0.598757    -1.937267      76.10
 H       7.604954    -0.068912    -1.391871      20.20
 C       5.180463     2.117456    -1.180991      49.06
 H       5.602867     2.774965    -1.876011      25.08
 C       3.681267     1.631020     0.757959      27.06
 C       2.529198     2.068611     1.818645      70.89
 H       2.763354     3.297595     2.077992      23.58
 O       2.594330     1.347485     3.039200     255.71
 H       2.097454     0.577380     2.897330      29.05
 C       1.145035     2.292718     1.182064      87.43
 H       1.203704     2.865691     0.259887      24.25
 C       0.075495     2.906153     2.135098     107.27
 O       0.360693     4.468006     2.307990     219.36
 H       0.768271     4.720036     1.462245      30.43
 H       0.188384     2.498020     3.064351      28.25
 H      -0.913465     2.815900     1.773112      27.24
 C      -2.105088    -1.161356    -0.310956      56.44
 H      -2.739407    -1.996475     0.268064      22.45
 C      -1.731248     0.556017    -1.977065      67.82
 H      -2.047102     0.907820    -2.954372      21.36
 C      -0.567244     1.057372    -1.203210      -1.72
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 O       0.220519     2.107097    -1.686404     210.05
 C      -0.177617     2.518059    -3.060487     107.13
 H       0.161611     3.521839    -3.135254      27.54
 H      -0.097136     1.941886    -3.975629      27.88
 H      -1.363432     2.953995    -3.153616      24.55
 C      -0.368111     0.450121     0.102220      30.04
 O       0.698729     0.920774     0.884501     202.35
 C      -1.066671    -0.632288     0.563590      52.50
 H      -0.562036    -1.436101     1.394167      20.52
 C      -2.463156    -0.653324    -1.537757      39.42
 C      -3.555351    -1.134406    -2.340846      56.36
 H      -3.370717    -0.689438    -3.478196      25.02
 O      -3.313983    -2.537423    -2.677788     225.26
 H      -2.430250    -2.750902    -2.803320      29.68
 C      -4.989494    -0.871285    -1.621551      91.18
 H      -4.963287    -1.098744    -0.566031      29.56
 O      -5.405516     0.546115    -1.741673     162.74
 H      -4.646337     1.356440    -1.530244      24.93
 C      -6.138675    -1.592829    -2.422110     118.61
 O      -6.116879    -3.035832    -2.273872     180.42
 H      -5.139556    -3.459293    -2.307358      28.00
 H      -5.958416    -1.370901    -3.419360      29.88
 H      -7.094304    -1.095513    -2.082166      28.61
55
name = lig-ACN-frame_340
 C       4.082066     2.495959    -0.380618      46.53
 H       3.739677     3.529247    -0.623460      23.08
 C       4.485996     0.438606     0.937486      42.90
 H       4.294073    -0.297947     1.789433      19.50
 C       5.395019     0.053368    -0.061433      35.03
 O       6.240303    -1.082949     0.131720     240.80
 C       5.820921    -2.543977     0.202383     108.67
 H       4.911277    -2.488261     0.749869      26.85
 H       6.569765    -2.998289     0.713385      27.80
 H       5.662116    -2.785680    -0.950642      25.35
 C       5.826942     0.871258    -1.134303       6.86
 O       6.962324     0.602502    -1.941837     173.74
 H       7.501763    -0.056218    -1.498023      24.88
 C       5.125998     2.113427    -1.208742      52.57
 H       5.392892     2.912949    -1.860334      25.98
 C       3.647489     1.636187     0.720535       9.11
 C       2.614780     2.097685     1.685117      58.98
 H       3.053224     3.224003     2.109762      22.11
 O       2.506803     1.370955     3.049841     198.95
 H       2.155223     0.515019     2.919159      28.08
 C       1.123128     2.221575     1.183319      89.53
 H       1.202488     2.820957     0.236264      23.47
 C       0.153409     2.985859     2.138761     119.61
 O       0.372478     4.411600     2.332641     300.38
 H       0.744418     4.766875     1.660638      36.42
 H       0.226525     2.526006     3.106967      27.21
 H      -0.806117     2.751570     1.781892      28.14
 C      -2.023234    -1.148880    -0.325341      67.38
 H      -2.614703    -2.094764    -0.102797      23.13
 C      -1.680525     0.532544    -2.010466      79.41
 H      -1.760426     0.837188    -3.056686      20.60
 C      -0.603069     0.947378    -1.261377      26.37
 O       0.195064     2.048244    -1.660948     224.84
 C      -0.168066     2.646233    -3.023724     106.41
 H       0.450654     3.431657    -3.208127      27.10
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 H       0.156015     1.858286    -3.678159      29.08
 H      -1.341952     2.628231    -2.840322      23.04
 C      -0.287512     0.539113     0.071323      54.06
 O       0.769728     0.860030     0.866419     208.89
 C      -1.082749    -0.611160     0.475490      44.37
 H      -0.861765    -1.006846     1.634295      18.16
 C      -2.390238    -0.529198    -1.589313      49.60
 C      -3.595505    -1.095498    -2.436022      36.49
 H      -3.923027    -0.363655    -3.386254      26.33
 O      -3.345498    -2.569841    -2.649830     192.58
 H      -2.268706    -2.543120    -2.621816      24.12
 C      -4.936457    -0.858192    -1.744263      95.44
 H      -4.883655    -1.291362    -0.750303      29.48
 O      -5.347250     0.534094    -1.719324     233.77
 H      -4.603493     0.977797    -1.120200      27.18
 C      -6.124149    -1.639005    -2.444765     113.49
 O      -6.122604    -3.078915    -2.253580     231.95
 H      -5.188272    -3.222606    -2.389443      31.56
 H      -6.278120    -1.352297    -3.457086      30.48
 H      -7.054292    -1.400475    -1.935562      28.35
55
name = lig-ACN-frame_341
 C       4.115427     2.485975    -0.333083      54.07
 H       3.421575     3.384565    -0.384856      23.82
 C       4.426168     0.451269     0.904313      50.12
 H       4.241906    -0.160111     1.810856      20.93
 C       5.468314     0.048842    -0.019105       4.18
 O       6.267329    -1.113182     0.205080     236.70
 C       5.783767    -2.490505     0.234676     119.24
 H       4.839096    -2.799801     0.588324      27.90
 H       6.552131    -2.945588     0.739578      26.93
 H       5.881896    -3.148868    -0.803949      26.10
 C       5.761312     0.906375    -1.148465      21.90
 O       6.870441     0.622278    -1.921039     183.26
 H       7.474379     0.192094    -1.360995      27.34
 C       5.130754     2.149570    -1.323714      46.11
 H       5.512837     2.667419    -2.228600      20.92
 C       3.749314     1.598488     0.665013      28.62
 C       2.613071     2.111120     1.761833      61.40
 H       2.917255     3.323411     2.115831      22.01
 O       2.478050     1.429622     2.963667     222.24
 H       2.102495     0.439215     2.749479      22.29
 C       1.224759     2.255452     1.098700      77.04
 H       1.095080     2.802738     0.096420      21.93
 C       0.195504     2.961374     2.158119     108.06
 O       0.406075     4.356965     2.366837     243.12
 H       0.630424     4.688943     1.441515      29.96
 H       0.211356     2.547671     3.194994      25.77
 H      -0.769448     2.876201     1.774451      26.91
 C      -2.088576    -1.176294    -0.405497      75.11
 H      -2.417075    -2.127217    -0.053648      20.75
 C      -1.563644     0.505560    -2.133051     104.51
 H      -1.776441     1.083307    -3.072815      27.68
 C      -0.533505     1.058474    -1.267222      16.95
 O       0.214121     2.048197    -1.694298     229.80
 C      -0.128728     2.645964    -2.909129     127.47
 H       0.441954     3.520074    -2.811779      27.20
 H       0.085702     2.028117    -3.749467      28.00
 H      -1.042512     3.144871    -3.345198      27.49
 C      -0.305513     0.485157     0.011553      27.67
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 O       0.833102     0.810625     0.878436     190.74
 C      -1.044275    -0.544110     0.451147      41.90
 H      -1.037561    -0.858593     1.568139      18.95
 C      -2.448841    -0.546189    -1.603514      60.72
 C      -3.560051    -1.057281    -2.483094      59.52
 H      -3.267311    -0.699556    -3.597955      30.70
 O      -3.401540    -2.509692    -2.639373     147.77
 H      -2.297347    -2.926409    -2.615003      24.08
 C      -4.995097    -0.948761    -1.819533      93.95
 H      -4.869735    -1.352178    -0.815782      28.55
 O      -5.252121     0.492487    -1.702944     265.95
 H      -4.920902     0.872780    -0.974424      31.30
 C      -6.174449    -1.655932    -2.420588     126.18
 O      -6.070851    -3.119645    -2.246240     194.18
 H      -5.280270    -3.491128    -2.550752      31.90
 H      -6.264390    -1.395609    -3.451325      30.78
 H      -6.954500    -1.275605    -1.812732      30.18
55
name = lig-ACN-frame_342
 C       4.119196     2.486648    -0.423009      36.98
 H       3.569455     3.461529    -0.671066      23.45
 C       4.429789     0.352343     0.857934      25.39
 H       4.164381    -0.271694     1.691084      23.71
 C       5.464088    -0.002686     0.006380      21.96
 O       6.285495    -1.097040     0.262788     262.88
 C       5.803713    -2.468738     0.231099     107.56
 H       4.810987    -2.364366     0.574160      26.00
 H       6.338334    -2.994843     0.991160      24.04
 H       5.945191    -2.741278    -0.951516      24.13
 C       5.773489     0.907300    -1.048449      23.61
 O       6.802788     0.626193    -1.928530     117.14
 H       7.616769     0.173997    -1.441382      21.99
 C       5.061139     2.138301    -1.341087      56.17
 H       5.238466     2.843743    -2.222555      24.47
 C       3.760184     1.686907     0.780221      -1.63
 C       2.645728     2.165052     1.678605      55.15
 H       2.982515     3.366449     2.076621      21.37
 O       2.507947     1.416543     2.914591     219.46
 H       1.949622     0.472118     2.690798      19.69
 C       1.225715     2.265395     1.111544      77.10
 H       1.394978     2.844384     0.130173      21.73
 C       0.188509     2.828375     2.085163      98.01
 O       0.482800     4.361080     2.385258     130.49
 H       0.685219     4.859492     1.323704      24.21
 H       0.411822     2.180443     3.035227      23.88
 H      -0.780050     2.637230     1.747383      26.80
 C      -2.104482    -1.126112    -0.384380      62.94
 H      -2.751910    -1.825462    -0.067392      22.78
 C      -1.550347     0.461018    -2.098783      27.46
 H      -1.931127     0.929858    -3.041426      21.11
 C      -0.564232     1.021438    -1.291936      16.16
 O       0.286266     2.128181    -1.693483     237.47
 C       0.014689     2.816282    -2.985526     107.80
 H       0.656616     3.693171    -3.103014      26.21
 H       0.255232     2.242146    -3.846685      28.59
 H      -0.965495     2.909856    -2.715753      27.29
 C      -0.216763     0.478407     0.010591      13.46
 O       0.822824     0.831674     0.833314     202.10
 C      -1.150194    -0.607488     0.427624      57.52
 H      -0.726874    -1.192548     1.235333      21.28
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 C      -2.378087    -0.530546    -1.674941      53.69
 C      -3.481142    -1.146581    -2.535824      53.30
 H      -3.644691    -0.481648    -3.565005      26.87
 O      -3.453874    -2.547240    -2.646317     162.49
 H      -2.270622    -2.710114    -2.818777      22.72
 C      -4.888044    -0.924862    -1.818154      87.59
 H      -4.782404    -1.436521    -0.844697      28.75
 O      -5.258954     0.436094    -1.738189     274.99
 H      -4.600430     0.817652    -1.123863      28.21
 C      -6.207155    -1.718869    -2.425083     104.30
 O      -6.073127    -3.149741    -2.234682     161.98
 H      -5.117781    -3.189000    -2.708782      27.42
 H      -6.409161    -1.493825    -3.477709      30.34
 H      -7.114964    -1.494869    -1.978784      30.64
55
name = lig-ACN-frame_343
 C       4.013043     2.486691    -0.388905      60.88
 H       3.571518     3.487613    -0.574112      23.21
 C       4.331783     0.414433     0.908950      54.91
 H       4.041871    -0.309580     1.605815      20.94
 C       5.418245     0.034850     0.003029      16.73
 O       6.367727    -1.025604     0.314092     245.22
 C       5.753468    -2.357399     0.199017     110.97
 H       4.691746    -2.484274     0.350036      27.56
 H       6.346703    -3.112597     0.813634      25.38
 H       5.861234    -2.945369    -0.891404      25.79
 C       5.838561     0.907515    -1.037723      11.45
 O       6.824091     0.614031    -1.962804     124.38
 H       7.470306    -0.083958    -1.464023      20.42
 C       5.026952     1.996621    -1.266125      46.60
 H       5.395366     2.589532    -2.193246      24.17
 C       3.809380     1.691000     0.714914      40.50
 C       2.668893     2.151806     1.677652      57.51
 H       2.919805     3.366270     2.118983      22.72
 O       2.592282     1.383707     2.908803     213.14
 H       2.147558     0.499747     2.693485      23.99
 C       1.215930     2.242349     1.012838      81.79
 H       1.048352     2.843220     0.061951      21.24
 C       0.245434     2.857905     2.028265     100.45
 O       0.506548     4.209887     2.379138     126.23
 H       0.953541     4.793595     1.406376      25.09
 H       0.268453     2.429147     3.165547      23.85
 H      -0.766090     2.787585     1.674000      25.94
 C      -2.217701    -1.059680    -0.385198      53.56
 H      -2.768366    -1.798949    -0.003961      23.89
 C      -1.558480     0.550432    -2.115094      99.17
 H      -1.485866     0.902961    -3.157992      20.33
 C      -0.460084     1.063949    -1.316312       3.15
 O       0.390522     2.135980    -1.676057     215.36
 C       0.046059     2.920245    -2.972542     108.89
 H       0.378546     3.986629    -2.690735      25.94
 H       0.369125     2.318315    -3.804838      27.90
 H      -0.880097     3.105278    -3.356601      29.61
 C      -0.275623     0.444511    -0.035093      17.39
 O       0.814564     0.865523     0.774922     220.97
 C      -1.025381    -0.651275     0.436024      23.98
 H      -0.862428    -1.180380     1.273414      20.65
 C      -2.343043    -0.630121    -1.693286      37.65
 C      -3.579669    -1.136702    -2.526390      65.89
 H      -3.559251    -0.656135    -3.663408      26.17
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 O      -3.401457    -2.645819    -2.718084     174.14
 H      -2.375790    -2.925948    -2.915212      23.15
 C      -4.908621    -0.975730    -1.801034      97.43
 H      -4.780160    -1.284883    -0.741065      29.71
 O      -5.274816     0.425283    -1.773516     238.64
 H      -4.501756     1.149723    -1.435511      25.44
 C      -6.151270    -1.743223    -2.430873     120.10
 O      -6.053717    -3.177473    -2.258683     188.30
 H      -5.118121    -3.592450    -2.433882      27.92
 H      -6.217474    -1.449338    -3.483957      30.21
 H      -6.898395    -1.381320    -1.791588      29.85
55
name = lig-ACN-frame_344
 C       4.051606     2.441944    -0.409812      51.37
 H       3.437672     3.293681    -0.593408      24.80
 C       4.373230     0.448656     0.880206      40.11
 H       4.099288    -0.047261     1.768785      22.29
 C       5.479814     0.067860     0.087997      12.75
 O       6.323709    -0.978655     0.337963     256.43
 C       5.732152    -2.319502     0.121359      88.76
 H       4.702590    -2.242128     0.525437      25.29
 H       6.345565    -2.932955     0.908146      22.37
 H       5.935316    -2.472169    -1.054499      23.64
 C       5.804659     0.834965    -1.043535      17.86
 O       6.885863     0.573372    -1.946473     183.63
 H       7.402229    -0.140904    -1.602755      28.47
 C       5.040266     2.020096    -1.291958      58.27
 H       5.259169     2.628309    -2.237939      24.00
 C       3.641129     1.656820     0.733654       8.22
 C       2.626398     2.089790     1.685806      62.49
 H       2.899903     3.335476     2.050024      21.32
 O       2.684298     1.362258     2.901158     272.71
 H       2.367771     0.531709     2.787835      29.43
 C       1.211202     2.208119     0.995423      83.40
 H       1.379277     2.797825     0.067262      23.40
 C       0.192750     2.848564     2.018567     106.20
 O       0.574110     4.177977     2.368683     195.15
 H       1.057282     4.586345     1.444479      26.16
 H       0.161021     1.985449     2.904907      23.62
 H      -0.767507     2.832226     1.510659      25.83
 C      -2.151574    -1.043265    -0.320490      73.57
 H      -2.718275    -1.848420     0.032127      23.69
 C      -1.492682     0.543992    -2.166739      36.19
 H      -1.708308     0.865704    -3.177673      20.49
 C      -0.466976     1.070268    -1.357252      10.24
 O       0.377575     2.126800    -1.745113     248.59
 C       0.094261     2.943925    -2.901774     129.11
 H       0.487516     3.993913    -2.564987      25.22
 H       0.883295     2.846926    -3.602198      27.30
 H      -0.859054     2.871808    -3.061564      31.20
 C      -0.245833     0.479153    -0.062038      46.06
 O       0.820461     0.828281     0.727607     207.01
 C      -1.025129    -0.654645     0.359405      42.46
 H      -0.886140    -0.795812     1.295683      21.35
 C      -2.386120    -0.513931    -1.719494      44.71
 C      -3.523039    -1.240713    -2.508306      56.98
 H      -3.628725    -0.669659    -3.595251      25.34
 O      -3.359670    -2.703676    -2.802057     223.22
 H      -2.406421    -2.749867    -2.716529      26.77
 C      -4.922719    -0.976846    -1.763686      95.81
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 H      -4.857278    -1.387356    -0.709350      29.06
 O      -5.336505     0.437070    -1.862197     233.14
 H      -4.512296     0.893371    -1.227458      24.16
 C      -6.023679    -1.754286    -2.388013     121.85
 O      -6.062793    -3.221985    -2.272882     239.96
 H      -5.164935    -3.370105    -2.308576      33.69
 H      -6.157162    -1.464236    -3.458724      30.22
 H      -7.007024    -1.483726    -2.037848      29.15
55
name = lig-ACN-frame_345
 C       4.026689     2.395097    -0.456463      54.23
 H       3.540039     3.254310    -0.796359      23.20
 C       4.442308     0.458455     0.954663      38.72
 H       4.454315    -0.216327     1.804355      20.63
 C       5.517234     0.164605     0.098813      -5.22
 O       6.293881    -0.980494     0.403250     256.03
 C       5.741644    -2.234093     0.095325      99.14
 H       4.620621    -2.370627     0.335158      26.42
 H       6.323762    -3.171730     0.501099      22.86
 H       5.661488    -2.581428    -1.061713      24.75
 C       5.796049     0.859494    -1.127397      21.58
 O       6.892785     0.526686    -1.881031     201.32
 H       7.468746    -0.017089    -1.352233      29.89
 C       5.089280     2.052756    -1.349823      48.99
 H       5.266034     2.712823    -2.220896      22.34
 C       3.637383     1.579857     0.616369      15.56
 C       2.558072     2.052749     1.696470      64.34
 H       2.910888     3.279094     2.035960      21.36
 O       2.736348     1.335775     2.947678     236.36
 H       2.298954     0.432978     2.824532      24.06
 C       1.211289     2.147680     1.084423     101.14
 H       1.295357     2.740641     0.183136      22.85
 C       0.118001     2.736518     1.882336      88.37
 O       0.654891     4.195903     2.384143     186.80
 H       0.931492     4.608797     1.593342      31.97
 H       0.043921     2.284241     3.041434      23.33
 H      -0.925680     2.849327     1.472374      24.67
 C      -2.073618    -1.043055    -0.447321      57.96
 H      -2.776807    -1.793971     0.002734      21.19
 C      -1.541335     0.447207    -2.234573      59.12
 H      -1.757740     0.968267    -3.137450      23.05
 C      -0.523767     1.053657    -1.439862      10.29
 O       0.371019     2.049325    -1.753413     273.66
 C       0.171653     3.008547    -2.802405     133.88
 H      -0.026017     4.043096    -2.477160      26.25
 H       0.481655     2.546387    -3.711831      26.08
 H      -0.726290     2.838331    -3.277229      28.71
 C      -0.197432     0.512294    -0.156447      18.22
 O       0.861339     0.778956     0.709125     229.94
 C      -1.030898    -0.497803     0.380709      42.83
 H      -0.753648    -1.041464     1.160831      21.63
 C      -2.393455    -0.485269    -1.611503      61.79
 C      -3.490738    -1.222906    -2.469870      53.27
 H      -3.662642    -0.653419    -3.545078      26.14
 O      -3.294905    -2.664782    -2.831292     272.02
 H      -2.469713    -2.868508    -2.721075      33.90
 C      -4.865074    -0.998383    -1.741713      88.61
 H      -4.772989    -1.101316    -0.612405      27.37
 O      -5.328314     0.395008    -1.912219     221.79
 H      -5.045789     1.005012    -1.178765      27.60
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 C      -6.104989    -1.810644    -2.459238     108.81
 O      -6.021814    -3.231698    -2.256128     205.04
 H      -5.135997    -3.580198    -2.460226      30.55
 H      -5.871949    -1.584028    -3.522748      30.44
 H      -7.029415    -1.398484    -2.015768      29.28
55
name = lig-ACN-frame_346
 C       3.955158     2.351255    -0.571529      49.83
 H       3.385645     3.247356    -0.554212      23.72
 C       4.534372     0.503781     0.968722      52.80
 H       4.206177    -0.066348     1.872064      16.82
 C       5.520311     0.158429     0.048799      23.41
 O       6.323213    -0.959996     0.462483     203.95
 C       5.661191    -2.273089    -0.011166      97.26
 H       4.674433    -2.399927     0.603606      23.18
 H       6.468153    -2.935490     0.478070      24.46
 H       5.709648    -2.147507    -1.147767      25.11
 C       5.837253     0.922266    -1.090776      13.39
 O       6.930946     0.474877    -1.850610     135.92
 H       7.566099    -0.025020    -1.148680      22.38
 C       5.097447     2.068833    -1.402527      64.63
 H       5.517523     2.668729    -2.185187      24.11
 C       3.683643     1.541494     0.630213      -8.94
 C       2.672450     2.003979     1.704233      59.36
 H       2.890474     3.270432     2.051766      22.76
 O       2.724038     1.312411     2.977292     203.67
 H       2.253759     0.298661     2.875295      20.14
 C       1.167509     2.072019     1.059832      85.21
 H       1.263108     2.685557     0.194106      23.55
 C       0.101381     2.875893     1.979840      99.67
 O       0.642694     4.103283     2.346365     272.18
 H       0.846107     4.558410     1.650273      35.86
 H      -0.290893     2.203853     2.968972      24.02
 H      -0.770670     2.945167     1.195606      24.23
 C      -2.038566    -1.047016    -0.389095     112.45
 H      -2.502157    -2.050706     0.077766      21.49
 C      -1.600909     0.505882    -2.265190      46.40
 H      -1.825548     0.762374    -3.282717      18.38
 C      -0.505270     1.010717    -1.464191      22.32
 O       0.412646     2.023405    -1.761525     252.58
 C       0.036339     2.965352    -2.858132     143.50
 H       0.514967     3.837506    -2.418506      25.95
 H       0.852888     2.979428    -3.423422      27.89
 H      -0.993338     3.031625    -3.045710      30.04
 C      -0.235342     0.471798    -0.154290      48.45
 O       0.916572     0.731774     0.649026     206.45
 C      -1.036413    -0.474018     0.376377      13.29
 H      -0.671593    -0.916735     1.274582      18.64
 C      -2.388728    -0.582479    -1.738302      95.50
 C      -3.538548    -1.125702    -2.451808      31.43
 H      -3.514238    -0.518591    -3.508350      29.03
 O      -3.268510    -2.571486    -2.800269     239.92
 H      -2.393492    -2.634567    -2.904697      27.29
 C      -4.936407    -1.018789    -1.774431      98.56
 H      -4.876526    -1.465815    -0.710576      29.10
 O      -5.307406     0.367347    -1.973780     267.07
 H      -4.994282     0.787513    -1.243768      32.24
 C      -6.005206    -1.836204    -2.486179     108.39
 O      -6.003983    -3.265496    -2.217363     173.86
 H      -5.046677    -3.475331    -2.686386      26.99
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 H      -6.171971    -1.590447    -3.576007      31.11
 H      -7.040112    -1.527542    -2.131396      29.86
55
name = lig-ACN-frame_347
 C       3.917011     2.305231    -0.575868      51.19
 H       3.333205     3.129016    -1.036715      23.97
 C       4.549727     0.528687     0.928590      43.81
 H       4.552368    -0.056528     1.909687      20.75
 C       5.550509     0.090108     0.105634      19.76
 O       6.317677    -0.981893     0.434421     273.36
 C       5.722862    -2.211896    -0.034625     110.51
 H       4.667359    -2.365576     0.477078      25.11
 H       6.312094    -3.156575     0.015154      24.37
 H       5.356513    -2.234910    -1.106007      28.82
 C       5.925742     0.896482    -1.017255       3.05
 O       6.985438     0.470444    -1.830393     114.89
 H       7.669329    -0.167796    -1.346991      20.93
 C       5.064437     2.055025    -1.403750      46.04
 H       5.229447     2.759453    -2.178767      25.78
 C       3.727259     1.658821     0.642467      19.68
 C       2.646746     1.981257     1.678328      57.80
 H       3.070583     3.187083     2.058082      22.07
 O       2.700026     1.300926     2.966745     195.60
 H       2.278162     0.266908     2.784110      19.84
 C       1.259163     2.088024     1.083935      89.31
 H       1.337114     2.712232     0.231010      23.87
 C       0.091020     2.824264     1.924053      93.02
 O       0.628963     4.106199     2.379367     195.01
 H       0.998101     4.477373     1.445094      28.09
 H      -0.291347     2.268341     2.961660      23.47
 H      -0.925657     3.104121     1.355871      23.00
 C      -2.099413    -1.106934    -0.387353      64.27
 H      -2.709544    -2.154672    -0.128176      20.99
 C      -1.600131     0.528647    -2.198232      87.13
 H      -1.753063     0.984161    -3.181699      18.51
 C      -0.465267     0.986482    -1.463653       8.42
 O       0.389168     1.989609    -1.853068     277.78
 C       0.064476     2.988248    -2.822511     134.87
 H       0.156656     3.969353    -2.417002      28.41
 H       0.214751     2.679788    -3.768679      29.00
 H      -1.016847     2.928770    -3.188922      25.79
 C      -0.229475     0.483698    -0.135078      53.77
 O       0.923648     0.702169     0.560235     214.38
 C      -1.050053    -0.611996     0.392020      30.96
 H      -0.992853    -0.800637     1.526105      20.00
 C      -2.289254    -0.577191    -1.682818      37.02
 C      -3.565691    -1.144218    -2.543092      46.67
 H      -3.865270    -0.435213    -3.544980      24.54
 O      -3.298829    -2.468310    -2.771941     257.81
 H      -2.303644    -2.616563    -2.858061      24.11
 C      -4.952544    -1.046701    -1.888487      95.17
 H      -4.982038    -1.255707    -0.752236      29.76
 O      -5.313664     0.363486    -1.966255     258.75
 H      -4.609403     0.941065    -1.418257      26.22
 C      -6.051311    -1.880731    -2.525481     114.33
 O      -5.930011    -3.289625    -2.219323     205.08
 H      -5.089931    -3.737561    -2.474677      30.02
 H      -5.948122    -1.719920    -3.638778      30.73
 H      -6.986755    -1.506438    -1.975314      28.69
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name = lig-ACN-frame_348
 C       3.953443     2.314924    -0.602041      49.26
 H       3.070347     2.955677    -0.962806      21.39
 C       4.534799     0.561918     0.978016      42.39
 H       4.329231     0.016481     1.948689      20.73
 C       5.613570     0.170457     0.092048       6.26
 O       6.379855    -1.080575     0.392678     241.24
 C       5.674134    -2.227537    -0.105958     118.12
 H       4.859382    -2.547367     0.669663      24.65
 H       6.486524    -2.942703    -0.010377      24.95
 H       5.393316    -1.983090    -1.127780      27.88
 C       5.965405     0.895076    -1.041410      23.42
 O       7.032834     0.528248    -1.836455     165.04
 H       7.490123    -0.090360    -1.307490      25.86
 C       5.099874     1.896365    -1.331843      62.99
 H       5.273645     2.246871    -2.335008      23.45
 C       3.740005     1.655042     0.683804       3.88
 C       2.621467     2.044076     1.729561      58.64
 H       2.656110     3.311719     2.158468      21.45
 O       2.679334     1.277091     2.909476     250.12
 H       2.304142     0.305874     2.790083      20.92
 C       1.222587     2.119590     1.012222      97.24
 H       1.388198     2.765564     0.171414      24.06
 C       0.142746     2.714406     1.868036      81.09
 O       0.625410     4.144620     2.403149      69.56
 H       1.191518     4.786363     1.566822      23.47
 H       0.035385     2.110529     2.872262      23.85
 H      -0.852500     2.624612     1.165058      22.61
 C      -2.119779    -1.174283    -0.468292      62.24
 H      -2.972207    -1.885524     0.076072      20.26
 C      -1.558429     0.511287    -2.127300      29.39
 H      -1.946911     1.038581    -3.027370      23.73
 C      -0.451576     0.995057    -1.391699       6.68
 O       0.433873     1.962895    -1.926765     241.04
 C      -0.075280     2.973223    -2.908506     101.81
 H       0.455276     3.867404    -2.679790      27.00
 H       0.422965     2.816602    -3.759797      26.95
 H      -1.178733     3.112613    -2.616646      25.99
 C      -0.258682     0.359073    -0.108186      19.26
 O       0.969825     0.756747     0.558669     207.53
 C      -1.090867    -0.640030     0.377192      49.41
 H      -0.858715    -1.202765     1.451842      17.52
 C      -2.434750    -0.526119    -1.678666      69.13
 C      -3.490852    -1.063566    -2.550731      48.66
 H      -3.300883    -0.576769    -3.662946      27.26
 O      -3.316637    -2.536849    -2.814190     152.28
 H      -2.202155    -2.751557    -2.675140      24.16
 C      -4.908629    -0.968567    -1.893131      83.86
 H      -4.715761    -1.406737    -0.835370      26.98
 O      -5.356590     0.392369    -1.960230     222.02
 H      -4.511273     1.034252    -1.498041      21.07
 C      -6.062672    -1.942611    -2.580473     103.19
 O      -5.894374    -3.337220    -2.203498     248.43
 H      -4.998178    -3.336799    -2.382883      33.30
 H      -6.166722    -1.796472    -3.712655      30.00
 H      -7.151571    -1.656620    -2.315174      28.04
55
name = lig-ACN-frame_349
 C       3.995304     2.242574    -0.530539      47.51
 H       3.440345     3.161328    -0.997704      22.93
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 C       4.622008     0.550693     1.011991      39.36
 H       4.348836    -0.131725     1.825430      20.83
 C       5.676430     0.112878     0.237912      12.29
 O       6.387644    -1.029027     0.345731     268.76
 C       5.679591    -2.301367    -0.158953     100.71
 H       4.833725    -2.615017     0.535431      26.28
 H       6.348049    -3.091077    -0.311188      25.77
 H       5.154380    -2.181771    -1.084169      30.36
 C       5.984329     0.831588    -0.979003      -5.45
 O       7.077428     0.591121    -1.842312     162.27
 H       7.693956    -0.057403    -1.498004      24.40
 C       5.054840     1.885475    -1.449470      38.48
 H       5.153093     2.306548    -2.469356      23.12
 C       3.728627     1.687367     0.712469       6.20
 C       2.611265     2.105436     1.671906      53.23
 H       2.976705     3.284896     2.166623      21.70
 O       2.646297     1.272830     2.883903     236.32
 H       2.260415     0.453767     2.676219      26.46
 C       1.261615     2.141861     0.897729      88.76
 H       1.286124     2.738184    -0.021890      22.46
 C       0.255074     2.750316     1.905338      99.41
 O       0.541458     4.061303     2.374327     147.15
 H       0.860472     4.592165     1.366561      24.96
 H       0.155782     2.070007     2.782867      24.87
 H      -0.896554     2.953898     1.498718      22.50
 C      -2.155584    -1.127962    -0.415614      80.85
 H      -2.787302    -2.069050    -0.014555      21.84
 C      -1.620794     0.524632    -2.110733      13.46
 H      -1.704243     0.931591    -3.150976      17.51
 C      -0.479154     0.987867    -1.362718      32.05
 O       0.468127     1.903401    -1.927078     225.11
 C      -0.129206     2.932281    -2.924685     116.75
 H       0.463248     3.781691    -2.629242      25.63
 H      -0.219438     2.586847    -3.860056      28.92
 H      -1.310561     3.260681    -3.073557      26.54
 C      -0.145486     0.369333    -0.118380      37.01
 O       0.960792     0.743652     0.606072     229.68
 C      -1.096227    -0.694257     0.314516      63.50
 H      -0.628121    -1.411589     1.262606      18.35
 C      -2.456543    -0.487924    -1.652233      45.83
 C      -3.480233    -1.108631    -2.620130      25.77
 H      -3.556743    -0.421711    -3.624957      25.81
 O      -3.303717    -2.602448    -2.844295     157.57
 H      -2.126352    -2.917957    -2.847672      20.52
 C      -4.932613    -0.952560    -1.993777      84.02
 H      -4.931760    -1.291898    -0.894085      26.70
 O      -5.407973     0.426215    -1.965074     240.77
 H      -4.892625     0.973332    -1.142648      20.28
 C      -6.035841    -1.920941    -2.609002     108.00
 O      -5.830024    -3.319941    -2.203389     198.51
 H      -4.866327    -3.640508    -2.237126      28.17
 H      -5.899651    -1.889278    -3.726699      30.20
 H      -7.009646    -1.583490    -2.139068      29.12
55
name = lig-ACN-frame_350
 C       4.068138     2.265905    -0.561691      48.04
 H       3.427317     3.204127    -0.709359      23.12
 C       4.620982     0.510440     1.104163      51.41
 H       4.468021    -0.060308     1.984507      21.25
 C       5.702932     0.153500     0.172252     -13.19
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 O       6.391881    -1.139062     0.328073     253.96
 C       5.667290    -2.304918    -0.186505     116.06
 H       5.047335    -2.614622     0.654439      26.18
 H       6.424646    -3.003679    -0.323241      25.69
 H       5.186240    -2.014453    -1.050587      30.08
 C       5.965366     0.882250    -1.026815      16.86
 O       7.080984     0.640366    -1.820283     130.66
 H       7.713584    -0.049355    -1.279164      21.79
 C       5.044807     1.794129    -1.433295      62.63
 H       5.241711     2.474003    -2.304736      24.22
 C       3.883532     1.605431     0.701943      30.58
 C       2.707696     2.059068     1.578465      63.07
 H       2.810438     3.336848     1.961840      22.64
 O       2.586243     1.360236     2.828133     254.46
 H       2.282806     0.497488     2.694327      27.91
 C       1.297556     2.172071     0.906250      75.21
 H       1.351223     2.697989    -0.083583      22.73
 C       0.197556     2.722275     1.923447     102.26
 O       0.519891     4.057166     2.334929     226.04
 H       0.611387     4.706887     1.573944      28.73
 H       0.318652     2.154696     2.812417      25.65
 H      -0.905595     2.436817     1.402714      22.82
 C      -2.189226    -1.062727    -0.380705      51.88
 H      -2.565923    -2.123134    -0.231998      20.63
 C      -1.635469     0.567185    -2.121233      54.67
 H      -1.727624     0.873164    -3.182393      17.22
 C      -0.487149     0.974141    -1.404417      13.11
 O       0.368899     1.877606    -1.955152     248.66
 C      -0.127632     2.828924    -2.939359      81.69
 H       0.421239     3.771858    -3.168195      24.67
 H       0.006976     2.382873    -3.829880      26.56
 H      -1.110550     2.957106    -2.265017      22.27
 C      -0.184739     0.380711    -0.151505      34.16
 O       0.956599     0.691010     0.680368     198.56
 C      -0.892802    -0.700183     0.275788      34.89
 H      -0.683635    -1.291190     1.403345      17.72
 C      -2.439890    -0.531000    -1.680770       8.24
 C      -3.572090    -1.178420    -2.613272      70.13
 H      -3.510189    -0.756727    -3.743902      27.06
 O      -3.275223    -2.585630    -2.870371     164.65
 H      -2.104207    -2.535551    -3.097339      20.62
 C      -4.963186    -0.991556    -2.002353      95.16
 H      -4.831296    -1.318514    -0.934483      29.43
 O      -5.441250     0.443881    -2.006998     274.63
 H      -5.134594     0.720655    -1.176559      30.54
 C      -5.930474    -1.916616    -2.642693     119.50
 O      -5.799610    -3.272259    -2.180590     198.56
 H      -4.762197    -3.432891    -2.484520      26.39
 H      -6.081980    -1.784798    -3.747140      31.55
 H      -6.956227    -1.629015    -2.323557      30.68
55
name = lig-ACN-frame_351
 C       4.097496     2.268713    -0.500869      55.62
 H       3.391979     3.047008    -0.851979      22.87
 C       4.760443     0.435698     1.042857      77.17
 H       4.553950    -0.013513     1.964675      23.16
 C       5.677693     0.033263     0.126158      18.40
 O       6.411788    -1.139402     0.336871     296.10
 C       5.665096    -2.288015    -0.173193     118.11
 H       4.979811    -2.746695     0.470862      29.02
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 H       6.370459    -3.010616    -0.458565      26.49
 H       5.118178    -2.077120    -1.013820      31.95
 C       5.965833     0.834446    -1.036209      -0.03
 O       7.093567     0.655363    -1.788197     123.81
 H       7.728875    -0.076082    -1.297769      20.77
 C       5.076858     1.899650    -1.436084      40.19
 H       5.390422     2.323883    -2.438176      21.99
 C       3.908868     1.581694     0.700558      15.96
 C       2.727597     2.059156     1.536915      73.21
 H       3.074201     3.290456     1.840374      21.50
 O       2.566888     1.459101     2.804520     237.89
 H       2.221428     0.472688     2.642758      24.41
 C       1.290119     2.054285     0.947912      97.36
 H       1.257814     2.704563     0.017320      23.00
 C       0.236085     2.603253     1.878610      93.05
 O       0.468251     4.123173     2.316588     237.41
 H       0.596282     4.537080     1.596428      34.84
 H       0.214782     2.108496     2.762686      27.06
 H      -0.908339     2.540970     1.392520      23.42
 C      -2.019513    -1.103755    -0.435366      79.61
 H      -2.677767    -1.759334     0.093979      23.11
 C      -1.673249     0.498112    -2.189526      62.20
 H      -2.029318     1.061573    -3.052878      18.72
 C      -0.511842     0.950056    -1.442290      22.15
 O       0.418186     1.898698    -1.942544     246.36
 C      -0.198076     2.706711    -2.961154     121.87
 H       0.662198     3.444710    -2.863410      23.51
 H      -0.480102     2.275164    -3.838190      27.42
 H      -1.219530     3.321166    -3.035364      25.40
 C      -0.149404     0.403755    -0.142331      47.85
 O       0.929641     0.708128     0.679435     214.73
 C      -0.946583    -0.727603     0.250877      49.52
 H      -0.497278    -1.157082     1.350046      15.17
 C      -2.453174    -0.557571    -1.713167      57.24
 C      -3.504069    -1.124185    -2.578254      26.83
 H      -3.555177    -0.371863    -3.533038      27.92
 O      -3.242224    -2.554987    -2.880654     189.03
 H      -2.186918    -2.801529    -2.979458      23.15
 C      -4.952015    -0.980842    -1.942608      90.46
 H      -4.986178    -1.346131    -0.894616      27.43
 O      -5.437152     0.365052    -2.063424     305.47
 H      -4.984645     0.963356    -1.588100      32.45
 C      -6.039015    -1.909137    -2.687586     112.44
 O      -5.734745    -3.238793    -2.194611     231.09
 H      -4.905575    -3.578934    -2.532463      30.68
 H      -5.796736    -1.906735    -3.758047      31.84
 H      -7.048865    -1.624718    -2.390714      31.04
55
name = lig-ACN-frame_352
 C       4.105719     2.257280    -0.534894      44.77
 H       3.415389     3.035582    -0.767687      23.43
 C       4.717047     0.472217     0.992750      40.40
 H       4.669159    -0.229578     1.788402      18.67
 C       5.689950    -0.019596     0.048177      -4.20
 O       6.436273    -1.161031     0.346128     285.49
 C       5.666038    -2.346202    -0.202114     108.59
 H       5.099322    -2.571628     0.585683      28.30
 H       6.358948    -3.136888    -0.448403      25.58
 H       5.128579    -2.009792    -0.995823      30.40
 C       5.964555     0.787488    -1.048717      21.37
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 O       7.137764     0.626970    -1.788772     210.39
 H       7.699123    -0.083573    -1.425060      23.47
 C       5.206848     1.953452    -1.373310      69.24
 H       5.184877     2.519292    -2.324774      22.91
 C       3.886643     1.544266     0.691682      13.46
 C       2.701612     2.062205     1.571646      55.60
 H       2.801344     3.341795     1.791288      23.34
 O       2.616131     1.484006     2.872422     196.95
 H       2.218355     0.430633     2.786541      20.15
 C       1.303645     2.061361     0.884817      82.54
 H       1.273567     2.615045    -0.100404      21.17
 C       0.254812     2.697755     1.946879     105.29
 O       0.392480     4.034201     2.260003     255.33
 H       0.870817     4.543750     1.517075      28.12
 H       0.125194     2.100034     2.751178      26.93
 H      -0.776871     2.662535     1.251316      22.53
 C      -2.020240    -1.256757    -0.508212      45.15
 H      -2.695320    -1.851949    -0.065099      19.60
 C      -1.603959     0.497908    -2.182649      35.86
 H      -1.928859     1.020045    -3.058276      20.52
 C      -0.496625     0.916225    -1.447167      13.51
 O       0.343435     1.896016    -1.912725     239.65
 C      -0.178833     2.732402    -3.108672      81.29
 H       0.456478     3.544847    -3.663431      24.10
 H      -0.250702     2.001813    -3.836150      26.64
 H      -1.016621     3.147064    -2.482908      24.97
 C      -0.156275     0.351260    -0.215727      26.88
 O       0.914881     0.678514     0.616964     241.30
 C      -0.926531    -0.657693     0.305851      59.92
 H      -0.808307    -1.314210     1.273414      19.09
 C      -2.337462    -0.576381    -1.658077      66.51
 C      -3.516496    -1.099451    -2.518278      35.36
 H      -3.577730    -0.550408    -3.591350      25.92
 O      -3.216152    -2.503706    -2.906469     259.55
 H      -2.344668    -2.631131    -2.732689      33.02
 C      -5.004395    -1.013832    -1.931719     103.50
 H      -4.985900    -1.237815    -0.861839      27.06
 O      -5.452453     0.328180    -2.142465     269.39
 H      -4.601706     0.863944    -1.770821      25.64
 C      -5.975306    -1.910498    -2.680801     118.11
 O      -5.757049    -3.268642    -2.210324     254.03
 H      -4.900557    -3.347374    -2.543794      32.43
 H      -5.916372    -1.764401    -3.769323      32.17
 H      -7.003915    -1.675558    -2.481733      30.39
55
name = lig-ACN-frame_353
 C       4.114176     2.255991    -0.534936      62.42
 H       3.627619     3.131980    -0.817702      23.53
 C       4.627282     0.398699     0.940741      49.34
 H       4.348922    -0.028519     1.906316      20.35
 C       5.660734     0.066231     0.052909      -1.52
 O       6.431270    -1.225073     0.299918     249.12
 C       5.678915    -2.375826    -0.160903     114.99
 H       5.018316    -2.778750     0.451479      30.66
 H       6.443672    -3.166233    -0.350387      25.32
 H       5.183717    -2.217694    -1.054463      29.84
 C       6.060042     0.840729    -1.121297       9.92
 O       7.186712     0.566889    -1.849033     148.43
 H       7.710062    -0.046577    -1.379087      27.44
 C       5.248635     1.940367    -1.298684      52.53
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 H       5.715784     2.581415    -2.046642      23.39
 C       3.815221     1.573553     0.668444      -2.58
 C       2.666061     2.021277     1.592602      64.66
 H       2.939007     3.251720     1.919333      22.18
 O       2.691369     1.458639     2.957652     212.18
 H       2.324043     0.461805     2.860397      23.35
 C       1.278478     2.104402     0.895375      83.19
 H       1.427263     2.744591    -0.000928      23.61
 C       0.178026     2.648972     1.811435     103.52
 O       0.376234     4.053898     2.244310     165.04
 H       1.082169     4.659100     1.503151      23.38
 H       0.323908     2.203402     2.734038      25.93
 H      -0.938349     2.370903     1.403851      23.66
 C      -2.017339    -1.313806    -0.445570      56.71
 H      -2.298233    -2.244959    -0.342430      22.67
 C      -1.569555     0.476001    -2.150723      70.57
 H      -1.782987     0.778898    -3.163358      17.60
 C      -0.418535     0.949662    -1.480631       9.96
 O       0.365305     2.017830    -1.970028     245.04
 C      -0.180358     2.651453    -3.163694     106.67
 H       0.639959     3.457464    -3.286491      24.63
 H      -0.597011     2.114912    -4.047513      25.62
 H      -1.187688     3.210963    -3.091742      25.91
 C      -0.176676     0.282936    -0.198094      49.24
 O       0.961792     0.662182     0.551544     188.28
 C      -1.014525    -0.776757     0.322094      13.09
 H      -0.636620    -0.929558     1.310346      18.08
 C      -2.358402    -0.630135    -1.718234      65.93
 C      -3.543464    -1.144620    -2.506869      48.74
 H      -3.569783    -0.393314    -3.461694      26.75
 O      -3.206455    -2.474655    -2.917970     283.65
 H      -2.344468    -2.616999    -2.828206      30.51
 C      -4.969982    -1.013994    -1.940156      98.94
 H      -5.029432    -1.303382    -0.889477      30.12
 O      -5.459345     0.357463    -2.235604     225.47
 H      -4.932157     1.110855    -1.499754      21.30
 C      -5.946544    -1.943032    -2.644302     122.65
 O      -5.776104    -3.310106    -2.283215     230.94
 H      -4.788787    -3.607370    -2.220918      28.62
 H      -5.831751    -1.849119    -3.716350      32.10
 H      -6.895504    -1.612771    -2.302597      31.26
55
name = lig-ACN-frame_354
 C       4.158832     2.326369    -0.518213      45.49
 H       3.637561     3.223400    -0.725778      26.35
 C       4.517332     0.395825     0.869451      34.62
 H       4.402250    -0.401685     1.651430      18.79
 C       5.688465    -0.026702     0.088677       6.97
 O       6.331509    -1.167490     0.248415     276.88
 C       5.700236    -2.452549    -0.149331     105.60
 H       5.020795    -2.648513     0.533286      29.31
 H       6.539760    -3.195341    -0.155342      23.75
 H       5.291560    -2.321918    -1.125399      29.26
 C       6.115553     0.791265    -0.982760      10.54
 O       7.206830     0.517267    -1.927262     139.70
 H       7.860282    -0.044125    -1.421130      22.76
 C       5.315110     2.017339    -1.330304      48.19
 H       5.570736     2.801381    -2.021949      24.76
 C       3.751983     1.529046     0.613538      12.10
 C       2.678362     2.021273     1.664680      58.54
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 H       2.953745     3.225108     1.871905      22.45
 O       2.743797     1.386183     2.952956     259.20
 H       2.399296     0.530673     2.895466      27.19
 C       1.259174     2.049872     0.899889      86.89
 H       1.346251     2.655658    -0.002129      24.09
 C       0.140597     2.587578     1.781943      92.72
 O       0.354852     4.090088     2.207854     143.43
 H       0.849320     4.631364     1.243670      22.90
 H       0.063204     1.925813     2.658992      25.17
 H      -0.915917     2.614767     1.319491      23.06
 C      -2.020418    -1.346795    -0.490603      59.48
 H      -2.477550    -2.201835    -0.153940      17.96
 C      -1.571916     0.388529    -2.160817      54.73
 H      -1.874126     0.900053    -3.082142      18.78
 C      -0.449839     0.905318    -1.464138       5.72
 O       0.349724     2.064364    -2.011820     233.40
 C      -0.200264     2.669607    -3.246655      96.11
 H       0.635146     3.385217    -3.647185      25.18
 H       0.035089     1.869329    -3.947058      26.13
 H      -1.074682     3.260002    -2.995364      26.93
 C      -0.150216     0.356408    -0.187732      53.57
 O       1.015613     0.676326     0.505602     215.84
 C      -0.933632    -0.777394     0.325677      31.09
 H      -0.778817    -1.341577     1.117726      19.05
 C      -2.353759    -0.668283    -1.641929      44.13
 C      -3.466160    -1.103703    -2.576253      27.36
 H      -3.595649    -0.471473    -3.578355      26.59
 O      -3.232424    -2.539945    -2.942778     186.25
 H      -2.183976    -2.628281    -3.167419      26.13
 C      -4.928766    -0.969031    -1.932735      94.25
 H      -4.925909    -1.004277    -0.846054      25.44
 O      -5.439759     0.377585    -2.282344     203.23
 H      -5.404415     0.851477    -1.330693      23.08
 C      -5.944172    -1.971912    -2.643546     111.84
 O      -5.791880    -3.396661    -2.324054     224.22
 H      -4.732036    -3.463115    -2.328385      28.07
 H      -5.876914    -1.798548    -3.709657      32.22
 H      -6.952228    -1.764134    -2.357481      30.60
55
name = lig-ACN-frame_355
 C       4.236329     2.378049    -0.470267      59.15
 H       3.672819     3.280472    -0.726200      23.63
 C       4.495870     0.288008     0.791553      55.05
 H       4.002441    -0.347507     1.572014      18.60
 C       5.596292     0.020021    -0.009501      21.56
 O       6.322658    -1.225520     0.264833     278.15
 C       5.705588    -2.465404    -0.119565     116.09
 H       4.929652    -2.757654     0.466468      30.88
 H       6.480710    -3.252966     0.065062      24.93
 H       5.347101    -2.575865    -1.150950      27.94
 C       6.137891     0.894135    -1.021249       3.99
 O       7.116514     0.497679    -1.897335     101.81
 H       7.893231    -0.101186    -1.453669      19.61
 C       5.367603     2.031181    -1.237834      64.40
 H       5.602274     2.427255    -2.208590      22.60
 C       3.782470     1.514695     0.575867      -7.95
 C       2.680983     2.014099     1.601283      69.30
 H       2.789899     3.180285     1.992710      22.55
 O       2.764096     1.304728     2.891638     231.68
 H       2.411967     0.426805     2.806652      26.61
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 C       1.310028     2.019623     0.943198      82.01
 H       1.391894     2.670263     0.079557      23.52
 C       0.086788     2.688931     1.811176     105.11
 O       0.314792     3.980123     2.154820     249.18
 H       0.664870     4.555603     1.321059      26.38
 H      -0.269090     2.230715     2.807847      24.19
 H      -0.709328     2.551922     1.030646      23.31
 C      -1.947742    -1.299037    -0.447571      55.71
 H      -2.691814    -1.916302     0.068497      20.56
 C      -1.558502     0.384832    -2.169492      70.50
 H      -1.990496     0.891417    -3.061339      22.10
 C      -0.475064     0.968128    -1.478329      12.64
 O       0.262334     1.992527    -1.954724     238.28
 C      -0.091055     2.642089    -3.333840     107.42
 H       0.401059     3.605364    -3.494881      24.19
 H      -0.453333     1.979973    -4.195842      24.37
 H      -1.156490     2.842968    -3.298033      26.71
 C      -0.140803     0.349906    -0.186908      38.07
 O       1.063093     0.662355     0.497689     215.84
 C      -0.833404    -0.780587     0.233520      28.97
 H      -0.419410    -1.173817     0.983943      20.46
 C      -2.345189    -0.666843    -1.692299      78.27
 C      -3.465917    -1.154808    -2.618498      30.74
 H      -3.241680    -0.555195    -3.559470      31.20
 O      -3.271937    -2.588598    -2.972976     145.17
 H      -2.105122    -2.769515    -3.230714      22.43
 C      -4.912878    -0.962795    -2.024178      98.00
 H      -4.786248    -1.217803    -0.965583      26.60
 O      -5.435176     0.369494    -2.291778     301.98
 H      -5.244214     0.899736    -1.605219      31.47
 C      -5.956100    -1.997463    -2.624613     115.99
 O      -5.746397    -3.417226    -2.361933     239.13
 H      -4.915119    -3.659031    -2.705649      33.82
 H      -5.898597    -1.831550    -3.691048      32.89
 H      -6.953842    -1.685635    -2.292766      31.33
55
name = lig-ACN-frame_356
 C       4.307025     2.412745    -0.421392      57.17
 H       3.760013     3.385899    -0.647487      23.62
 C       4.412019     0.281511     0.688250      30.24
 H       4.218458    -0.499989     1.450656      21.03
 C       5.570980    -0.081874    -0.059765       4.20
 O       6.322838    -1.231504     0.255226     273.29
 C       5.684150    -2.532609    -0.059428     111.48
 H       4.780107    -2.631755     0.425910      28.11
 H       6.452576    -3.273091     0.176329      24.88
 H       5.567720    -2.461892    -1.177286      26.60
 C       6.077764     0.834623    -0.998848       8.11
 O       7.057067     0.495358    -1.867971      69.84
 H       7.651600    -0.133986    -1.230295      19.26
 C       5.381147     2.118032    -1.250958      57.66
 H       5.661073     2.798268    -2.073717      24.41
 C       3.844471     1.570167     0.610373      29.18
 C       2.732506     1.948785     1.572599      70.85
 H       3.131100     3.075113     1.785372      21.81
 O       2.773745     1.239624     2.793984     255.29
 H       2.229983     0.314480     2.683223      19.50
 C       1.276236     2.039204     1.012406      94.20
 H       1.395581     2.692711     0.166471      24.98
 C       0.038909     2.604544     1.698571     102.85
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 O       0.292542     4.012339     2.144321     296.98
 H       0.749369     4.462955     1.546278      33.78
 H      -0.110133     1.923754     2.674718      23.45
 H      -0.886336     2.559234     1.129464      24.96
 C      -1.962543    -1.192506    -0.439006      61.68
 H      -2.407042    -2.191397     0.004921      21.37
 C      -1.599473     0.444669    -2.198516      63.48
 H      -1.711166     0.806082    -3.249503      17.97
 C      -0.540882     0.969833    -1.472352       9.93
 O       0.241599     2.021178    -2.007461     239.70
 C      -0.183555     2.536446    -3.310097     114.50
 H       0.603004     3.275486    -3.238764      26.19
 H       0.458104     2.008923    -4.035805      25.82
 H      -1.076002     3.043472    -3.246451      28.22
 C      -0.046606     0.373681    -0.295045      24.50
 O       1.074095     0.644485     0.498639     212.39
 C      -0.725852    -0.805614     0.205015      39.24
 H      -0.462371    -1.145255     1.093843      18.60
 C      -2.303749    -0.704018    -1.723629      38.73
 C      -3.432124    -1.235889    -2.652906      75.29
 H      -3.563218    -0.611857    -3.583776      27.25
 O      -3.293510    -2.623909    -3.009356     186.28
 H      -2.136312    -2.852489    -2.856440      20.60
 C      -4.876449    -1.059190    -2.112934      88.67
 H      -4.961276    -1.175952    -1.014666      28.70
 O      -5.434683     0.335514    -2.294235     278.29
 H      -4.681986     0.770598    -1.865851      30.52
 C      -5.941814    -1.994401    -2.688011     112.87
 O      -5.685953    -3.373239    -2.392553     212.48
 H      -4.955897    -3.587599    -3.002686      30.96
 H      -6.173210    -1.867301    -3.727625      31.18
 H      -6.863775    -1.804624    -2.057482      29.61
55
name = lig-ACN-frame_357
 C       4.325575     2.506352    -0.370643      32.15
 H       3.882453     3.578841    -0.349754      23.45
 C       4.400987     0.248278     0.662191      53.61
 H       3.950431    -0.332794     1.449683      21.51
 C       5.528523    -0.133001    -0.070474       6.93
 O       6.317612    -1.234392     0.248243     276.60
 C       5.691850    -2.534353    -0.049455     102.04
 H       4.724044    -2.595594     0.442176      27.70
 H       6.239902    -3.333932     0.403351      24.80
 H       5.484126    -2.798178    -1.157911      25.91
 C       5.953170     0.795384    -1.065170      16.58
 O       7.092799     0.472754    -1.836865     168.20
 H       7.729355    -0.162792    -1.526414      23.89
 C       5.388851     2.129563    -1.246152      47.00
 H       5.949213     2.918414    -1.809490      24.58
 C       3.862534     1.537170     0.574661      18.57
 C       2.757741     1.988864     1.611464      70.89
 H       2.865905     3.076224     2.097419      22.51
 O       2.783225     1.169928     2.758350     246.73
 H       2.294951     0.164611     2.599593      18.35
 C       1.293326     2.058505     0.820915      78.82
 H       1.365220     2.661834    -0.070099      22.73
 C       0.067624     2.545537     1.704153      91.69
 O       0.242649     4.009068     2.147359     285.49
 H       0.900312     4.338613     1.666448      32.87
 H      -0.157285     1.876695     2.700907      22.74
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 H      -0.738443     2.451694     1.051634      25.81
 C      -1.907378    -1.204527    -0.497833      73.02
 H      -2.447015    -2.265678    -0.168751      22.03
 C      -1.635600     0.435657    -2.242769      92.82
 H      -1.863060     0.775017    -3.272007      12.72
 C      -0.499281     0.986026    -1.510758      42.65
 O       0.193818     2.028617    -1.990312     260.58
 C      -0.045701     2.587269    -3.279365     136.59
 H       0.336185     3.528822    -3.481215      26.91
 H      -0.102781     1.772366    -4.100815      27.79
 H      -1.067783     2.592038    -3.576016      29.65
 C      -0.008645     0.280630    -0.306215      33.24
 O       1.086651     0.691665     0.484952     231.83
 C      -0.757544    -0.751052     0.166025      40.75
 H      -0.477663    -1.343895     1.014641      19.53
 C      -2.313231    -0.684886    -1.750612      67.69
 C      -3.446189    -1.257856    -2.688941      41.44
 H      -3.239261    -0.719605    -3.609950      29.83
 O      -3.223643    -2.687763    -3.040798     265.33
 H      -2.273239    -2.945309    -2.834939      26.19
 C      -4.920283    -1.089063    -2.096046      88.02
 H      -4.762042    -1.444336    -1.035826      27.59
 O      -5.348959     0.239247    -2.338025     253.07
 H      -4.787916     1.072406    -1.796545      23.15
 C      -5.994820    -1.996211    -2.722575     110.56
 O      -5.643140    -3.363431    -2.453063     183.81
 H      -4.661903    -3.573520    -2.877944      24.26
 H      -6.132287    -1.732590    -3.768978      31.27
 H      -6.987377    -1.707996    -2.195529      29.74
55
name = lig-ACN-frame_358
 C       4.390923     2.517128    -0.332417      62.20
 H       4.073208     3.620456    -0.360219      21.95
 C       4.359006     0.251503     0.715571      39.53
 H       4.028795    -0.471711     1.418780      19.86
 C       5.465112    -0.094637    -0.123374       3.93
 O       6.301370    -1.277825     0.195604     227.80
 C       5.652958    -2.548392     0.021471     102.41
 H       4.597919    -2.555374     0.409836      26.03
 H       6.340243    -3.210110     0.490150      25.62
 H       5.683287    -2.760815    -1.133234      24.93
 C       5.961605     0.764384    -1.170240       8.68
 O       7.116227     0.494004    -1.856697     212.74
 H       7.504267    -0.030546    -1.187247      24.12
 C       5.419721     2.067801    -1.152607      51.13
 H       5.987612     2.675699    -1.917696      21.07
 C       3.791617     1.598511     0.568223       8.00
 C       2.688469     2.015367     1.544524      74.89
 H       3.015174     3.064038     1.896528      23.38
 O       2.758997     1.122784     2.774985     211.73
 H       2.319915     0.180662     2.597539      20.17
 C       1.373634     2.090918     0.774130      82.15
 H       1.468501     2.751565    -0.087840      22.44
 C       0.165927     2.617505     1.671381      99.86
 O       0.176888     3.901167     2.136449     257.57
 H       0.904743     4.569123     1.659652      25.65
 H       0.138517     1.891248     2.670725      22.09
 H      -0.727980     2.483466     1.192803      24.92
 C      -1.901066    -1.331904    -0.628838      57.50
 H      -2.584316    -2.180817    -0.006108      20.81
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 C      -1.585331     0.421490    -2.253286      38.82
 H      -2.032751     1.016379    -3.042494      20.30
 C      -0.479147     0.903555    -1.578132       9.49
 O       0.244815     2.114362    -1.916202     227.90
 C      -0.098658     2.571175    -3.404879      92.90
 H       0.451363     3.474796    -3.421013      26.42
 H       0.535763     1.934501    -4.116229      24.92
 H      -1.053464     2.921441    -3.272751      25.88
 C      -0.045032     0.327565    -0.347596      10.28
 O       1.096201     0.676024     0.407681     194.84
 C      -0.846468    -0.801626     0.159371      46.04
 H      -0.288613    -1.275827     1.081916      18.04
 C      -2.371487    -0.667194    -1.801334      64.19
 C      -3.407346    -1.297530    -2.710837      59.47
 H      -3.556046    -0.750978    -3.588852      29.79
 O      -3.109258    -2.743638    -3.044947     264.24
 H      -2.261504    -2.844356    -3.061431      33.17
 C      -4.879440    -1.126021    -2.088262      97.50
 H      -4.956356    -1.218851    -0.959382      25.81
 O      -5.272868     0.221910    -2.389201     231.57
 H      -5.128493     0.669491    -1.345635      20.32
 C      -5.987912    -1.999517    -2.736215     109.36
 O      -5.652407    -3.390139    -2.544648     240.66
 H      -4.638998    -3.321607    -2.477444      28.51
 H      -5.896500    -1.841232    -3.827077      31.18
 H      -7.090122    -1.875076    -2.386783      28.48
55
name = lig-ACN-frame_359
 C       4.442492     2.454225    -0.299920      44.28
 H       4.056987     3.479803    -0.509984      24.75
 C       4.377880     0.326910     0.658625      51.92
 H       4.098307    -0.313026     1.465258      20.17
 C       5.441210    -0.132042    -0.152277      19.88
 O       6.217716    -1.202565     0.129826     250.99
 C       5.651726    -2.579230     0.059541      95.16
 H       4.564417    -2.627437     0.509292      24.17
 H       6.186914    -3.312736     0.640426      25.24
 H       5.525972    -2.932033    -1.046469      24.88
 C       5.959466     0.732667    -1.101412      21.82
 O       7.134192     0.486512    -1.859427     190.84
 H       7.972402    -0.034417    -1.492507      23.83
 C       5.487460     2.059785    -1.189217      44.57
 H       5.756244     2.874108    -1.889804      22.92
 C       3.820593     1.560779     0.606110      24.07
 C       2.697966     1.945258     1.545133      90.25
 H       2.842732     2.993794     1.957160      23.36
 O       2.695971     1.208359     2.732603     313.68
 H       2.221212     0.435810     2.668551      27.10
 C       1.357179     2.108016     0.805330      77.78
 H       1.577848     2.694366    -0.106875      23.16
 C       0.218231     2.525143     1.612805     100.96
 O       0.160767     3.939394     2.164415     187.42
 H       0.788586     4.605945     1.359569      23.51
 H       0.334736     1.819526     2.601937      21.59
 H      -0.599889     2.258954     1.112554      25.98
 C      -1.919713    -1.378905    -0.651399      60.82
 H      -2.519512    -2.432377    -0.356435      18.70
 C      -1.599759     0.457126    -2.284535      53.08
 H      -1.909232     0.984242    -3.180107      10.34
 C      -0.398959     0.945761    -1.580461       9.58
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 O       0.241286     2.131915    -1.974598     241.40
 C      -0.067583     2.657207    -3.324662     121.48
 H       0.637463     3.482060    -3.376702      25.42
 H       0.138039     1.816879    -4.088220      28.67
 H      -0.945706     2.779324    -3.862531      27.88
 C      -0.133737     0.304283    -0.346427      65.27
 O       1.074907     0.663790     0.291231     195.01
 C      -0.832403    -0.820613     0.063824      33.45
 H      -0.796414    -1.330148     1.185988      17.19
 C      -2.304928    -0.742104    -1.844680      22.88
 C      -3.455240    -1.355257    -2.719201      74.35
 H      -3.465475    -0.853186    -3.604710      26.33
 O      -3.002254    -2.732791    -3.021959     258.99
 H      -2.081173    -2.663738    -3.097335      27.68
 C      -4.882587    -1.181571    -2.095379      89.88
 H      -4.822140    -1.431284    -0.990791      27.89
 O      -5.218133     0.275882    -2.373948     252.78
 H      -5.095229     0.837077    -1.561839      25.61
 C      -5.874699    -2.055065    -2.824282     121.18
 O      -5.678327    -3.455729    -2.604669     261.89
 H      -4.810933    -3.667063    -2.506238      34.54
 H      -5.995067    -1.692824    -3.882617      30.73
 H      -6.872285    -1.714412    -2.327869      28.42
55
name = lig-ACN-frame_360
 C       4.433281     2.467161    -0.373880      65.84
 H       3.953735     3.419518    -0.379759      25.19
 C       4.407576     0.230317     0.686575      59.39
 H       4.003340    -0.422589     1.470491      20.72
 C       5.439710    -0.116951    -0.186538      16.18
 O       6.177497    -1.285873     0.100086     245.05
 C       5.592312    -2.568432     0.103058     104.92
 H       4.525014    -2.544241     0.667816      24.63
 H       6.410153    -3.067699     0.668431      24.25
 H       5.541229    -3.028824    -0.930259      25.21
 C       6.114120     0.822855    -1.087561      23.61
 O       7.141213     0.464378    -1.901784     118.56
 H       7.827605    -0.052571    -1.222515      19.39
 C       5.471953     2.071742    -1.210249      60.35
 H       6.055599     2.643968    -1.917430      26.79
 C       3.915511     1.561074     0.605318      16.75
 C       2.723149     2.015326     1.521058      88.07
 H       2.927563     3.028836     1.809926      25.70
 O       2.605024     1.271314     2.784262     260.35
 H       2.253629     0.383165     2.605524      25.96
 C       1.394550     1.992416     0.702458      73.85
 H       1.383773     2.804129    -0.083758      22.16
 C       0.147314     2.489078     1.692776      89.57
 O       0.173638     3.917647     2.119833     203.74
 H       0.742143     4.539162     1.308355      25.24
 H      -0.031243     1.908429     2.714717      23.44
 H      -0.696804     2.393178     1.171107      25.55
 C      -1.907757    -1.364416    -0.712922      77.04
 H      -2.244678    -2.461561    -0.401888      20.09
 C      -1.591321     0.440974    -2.308097      13.42
 H      -1.858101     0.767170    -3.307596      17.60
 C      -0.553922     0.993580    -1.633551      23.15
 O       0.182527     2.097569    -2.018188     275.88
 C       0.004480     2.664293    -3.323220     102.38
 H       0.535651     3.680596    -3.562206      24.38
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 H       0.386334     1.930774    -4.066377      27.55
 H      -0.939328     3.052577    -3.087548      27.29
 C      -0.115317     0.314576    -0.385532      48.69
 O       1.067731     0.674693     0.250507     208.37
 C      -0.873709    -0.859584     0.046199      66.90
 H      -0.391686    -1.265958     1.160473      15.56
 C      -2.240921    -0.722042    -1.940689      42.52
 C      -3.342229    -1.326790    -2.746697      65.93
 H      -3.443598    -0.834178    -3.620467      29.46
 O      -2.976103    -2.724546    -2.985640     224.90
 H      -1.907781    -2.916207    -2.873971      23.83
 C      -4.769302    -1.152517    -2.147273      87.22
 H      -4.872928    -1.457150    -1.065818      28.56
 O      -5.190654     0.241606    -2.335828     333.42
 H      -4.656305     0.620106    -1.740801      32.68
 C      -5.848741    -2.058754    -2.874302      96.35
 O      -5.719988    -3.537354    -2.668274     189.93
 H      -4.779800    -3.697833    -3.045072      30.63
 H      -5.752108    -1.952936    -4.010822      29.81
 H      -6.910727    -1.900490    -2.486052      28.18
55
name = lig-ACN-frame_361
 C       4.401768     2.476466    -0.423789      39.69
 H       4.082292     3.454410    -0.573363      21.95
 C       4.433039     0.213756     0.678615      44.73
 H       4.080053    -0.652534     1.301310      19.51
 C       5.542122    -0.115761    -0.160543      21.33
 O       6.214388    -1.324431     0.026605     227.52
 C       5.554002    -2.612195     0.183959     106.94
 H       4.487244    -2.646276     0.822520      23.59
 H       6.165829    -3.402086     0.712930      25.29
 H       5.274271    -3.008218    -0.809383      26.39
 C       6.099310     0.831010    -1.045386      40.82
 O       7.187427     0.434115    -1.907869     172.25
 H       7.844799    -0.148061    -1.457871      13.53
 C       5.530497     2.122343    -1.254329      57.35
 H       5.824718     2.835233    -1.969296      24.63
 C       3.919519     1.551647     0.622414      15.96
 C       2.738092     2.048964     1.430231      82.52
 H       2.871913     2.994793     1.749656      27.83
 O       2.540361     1.326369     2.835926     175.22
 H       2.253890     0.281025     2.599610      20.11
 C       1.261256     2.008507     0.780534      76.33
 H       1.365297     2.599487    -0.195988      19.93
 C       0.070447     2.524154     1.685594     109.45
 O       0.211681     3.857403     2.057028     306.67
 H       0.918706     4.307204     1.506947      28.35
 H       0.137860     1.829975     2.604397      22.82
 H      -0.781657     2.323408     1.172895      26.01
 C      -1.817366    -1.356887    -0.740913      61.77
 H      -2.471329    -2.201287    -0.441537      18.04
 C      -1.612289     0.458835    -2.481872      78.82
 H      -1.900523     0.978828    -3.426515      20.32
 C      -0.614064     1.018377    -1.579113      11.12
 O       0.230405     2.058477    -1.976343     200.73
 C      -0.052030     2.719846    -3.329303      94.63
 H       0.931890     3.313639    -3.104347      21.79
 H      -0.040447     2.131630    -4.252004      25.52
 H      -0.981964     3.098668    -3.689407      25.31
 C      -0.152489     0.355559    -0.470115      25.23
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 O       1.092280     0.630238     0.231557     188.89
 C      -0.775265    -0.757802     0.040387      35.49
 H      -0.267333    -1.584009     0.846685      18.93
 C      -2.250036    -0.746177    -1.908919      34.43
 C      -3.232822    -1.323809    -2.857346      63.94
 H      -3.204052    -0.861439    -3.744620      30.26
 O      -3.018332    -2.765236    -2.962267     195.16
 H      -1.821272    -2.885278    -2.869524      22.76
 C      -4.728327    -1.210366    -2.209852      84.76
 H      -4.593267    -1.424907    -1.121382      26.65
 O      -5.140218     0.150449    -2.317060     298.56
 H      -4.837789     0.845224    -1.634970      25.70
 C      -5.817561    -2.125955    -2.956803     103.08
 O      -5.704121    -3.535532    -2.743496     183.13
 H      -4.849329    -3.879814    -3.312936      28.68
 H      -5.725220    -1.777582    -4.070235      30.22
 H      -6.818428    -1.696526    -2.700694      29.59
55
name = lig-ACN-frame_362
 C       4.427812     2.413997    -0.407067      62.33
 H       3.864702     3.284694    -0.528759      23.37
 C       4.472795     0.290036     0.617309      60.45
 H       3.936494    -0.304798     1.419001      21.39
 C       5.625612    -0.126094    -0.078199       9.11
 O       6.300181    -1.377383    -0.048401     200.20
 C       5.452838    -2.662121     0.218319      92.91
 H       4.657189    -2.274217     1.102111      21.09
 H       6.346243    -3.272755     0.595740      24.12
 H       5.038167    -3.028691    -0.691372      26.56
 C       6.146439     0.787976    -1.116090      19.48
 O       7.189641     0.448639    -1.890687     186.47
 H       7.808873    -0.070947    -1.401691      25.97
 C       5.526414     2.085105    -1.220853      58.77
 H       5.811107     2.632223    -2.081990      21.10
 C       3.863727     1.546703     0.521574      21.31
 C       2.579469     1.971831     1.539318      98.86
 H       2.888675     2.887905     1.764954      26.11
 O       2.540268     1.405115     2.772617     270.74
 H       2.212369     0.399023     2.760017      23.03
 C       1.237605     2.032688     0.752890      91.58
 H       1.220005     2.872546    -0.045226      20.32
 C       0.069454     2.413694     1.631337     104.22
 O       0.255486     3.879856     2.020260     302.68
 H       0.956134     4.231783     1.705916      35.43
 H       0.024494     1.882044     2.593941      23.93
 H      -0.855318     2.303679     1.162706      25.19
 C      -1.809694    -1.301145    -0.743434     111.37
 H      -2.170509    -2.162967    -0.315472      21.15
 C      -1.586909     0.477490    -2.423197     -28.78
 H      -2.003688     0.919515    -3.376950      17.08
 C      -0.592771     1.049193    -1.678515      25.31
 O       0.202828     2.074135    -2.029582     260.33
 C      -0.020922     2.745526    -3.303463     105.58
 H       0.629935     3.601396    -3.738604      23.77
 H       0.110324     1.886557    -3.874875      28.38
 H      -0.917469     3.311177    -3.078282      26.92
 C      -0.104295     0.355858    -0.392049      66.65
 O       1.073271     0.631226     0.218577     197.47
 C      -0.722040    -0.821590    -0.041841      47.35
 H      -0.266566    -1.232474     1.015089      15.26
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 C      -2.207321    -0.660351    -2.009544      40.77
 C      -3.283517    -1.422019    -2.896002      73.56
 H      -3.250903    -1.002518    -3.789156      31.03
 O      -3.042340    -2.836919    -2.967398     161.49
 H      -1.837504    -3.016530    -3.178782      20.28
 C      -4.648572    -1.298830    -2.292541     102.56
 H      -4.626176    -1.848331    -1.331439      28.59
 O      -5.133699     0.105430    -2.358678     246.87
 H      -5.044994     0.430721    -1.255666      20.94
 C      -5.713778    -2.071971    -3.045200     104.92
 O      -5.688216    -3.510610    -2.843690     216.57
 H      -4.826878    -3.790547    -3.093528      34.85
 H      -5.740338    -1.897853    -4.203260      30.48
 H      -6.672613    -1.893783    -2.558880      29.75
55
name = lig-ACN-frame_363
 C       4.374813     2.437918    -0.433195      46.59
 H       4.019687     3.419878    -0.731209      24.15
 C       4.501889     0.260021     0.675676      44.43
 H       4.220644    -0.529109     1.417087      21.42
 C       5.669948    -0.121587    -0.111539      16.64
 O       6.306104    -1.446857    -0.102167     215.85
 C       5.480985    -2.540111     0.256794     110.05
 H       4.776090    -2.491247     1.335110      22.45
 H       6.096136    -3.472562     0.485965      25.20
 H       4.776233    -2.844724    -0.487656      27.02
 C       6.132924     0.749152    -1.054840      21.45
 O       7.217601     0.472712    -1.923769     137.64
 H       8.027832     0.027530    -1.356436      18.23
 C       5.495171     1.975348    -1.219786      53.29
 H       5.990036     2.663417    -1.910385      25.36
 C       3.742867     1.515715     0.498919      -9.80
 C       2.609322     2.017797     1.439821      92.70
 H       2.695296     3.015353     1.614619      26.94
 O       2.545655     1.361260     2.798208     268.67
 H       2.153125     0.550595     2.746798      29.32
 C       1.260218     1.990243     0.714514      86.90
 H       1.455459     2.677791    -0.194651      20.94
 C       0.081613     2.458483     1.661425     110.18
 O       0.228312     3.846105     2.005971     310.96
 H       0.955885     4.158918     1.478770      30.15
 H      -0.009885     1.786051     2.466800      25.79
 H      -0.798072     2.395404     1.029129      24.51
 C      -1.852339    -1.309213    -0.809313      39.90
 H      -2.264943    -2.190756    -0.717491      18.82
 C      -1.600414     0.540091    -2.386633      72.54
 H      -1.821836     1.056881    -3.368924      14.83
 C      -0.434802     1.007623    -1.643373       2.61
 O       0.306074     2.200244    -2.033611     242.41
 C      -0.103814     2.715835    -3.322284     110.94
 H       0.776285     3.417262    -3.350242      23.86
 H      -0.332708     2.270779    -4.229359      28.98
 H      -1.133279     3.127195    -3.341185      26.23
 C      -0.089439     0.382986    -0.508881      33.12
 O       1.088377     0.729747     0.222659     208.58
 C      -0.716828    -0.836871    -0.058766      37.87
 H      -0.530465    -1.362723     0.934401      17.91
 C      -2.233125    -0.789902    -2.019809      24.14
 C      -3.223860    -1.451395    -2.903513      86.44
 H      -3.316219    -1.049677    -3.793310      27.02
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 O      -3.022826    -2.942554    -3.005996     182.11
 H      -1.826741    -3.112865    -3.091537      20.31
 C      -4.684016    -1.346810    -2.359022      94.56
 H      -4.722734    -1.581705    -1.306720      28.93
 O      -5.116084     0.017866    -2.343733     280.13
 H      -4.904731     0.475104    -1.366021      23.49
 C      -5.734642    -2.086359    -3.146101     109.91
 O      -5.632195    -3.515358    -2.959169     254.29
 H      -4.715776    -3.652609    -2.784156      33.04
 H      -5.693961    -1.696950    -4.266166      29.97
 H      -6.636506    -1.612307    -2.811734      29.94
55
name = lig-ACN-frame_364
 C       4.305020     2.351342    -0.497612      61.10
 H       3.938784     3.415961    -0.520621      24.25
 C       4.513525     0.192109     0.719593      74.43
 H       4.084479    -0.452592     1.488919      23.08
 C       5.595227    -0.223488    -0.111931      16.20
 O       6.270985    -1.402879    -0.109660     197.83
 C       5.455958    -2.525653     0.316316     105.45
 H       5.181575    -2.255066     1.539070      22.35
 H       6.098709    -3.409439     0.115650      25.77
 H       4.570689    -2.480110    -0.285844      26.87
 C       6.182099     0.753054    -1.069774      33.48
 O       7.218229     0.502480    -1.935538      72.24
 H       8.186671     0.114587    -1.550301      11.87
 C       5.457400     1.972489    -1.214897      50.45
 H       5.888989     2.734243    -1.943843      26.37
 C       3.846452     1.477080     0.499274      12.27
 C       2.686151     1.993488     1.405722      73.97
 H       3.155194     3.006975     1.826145      23.58
 O       2.571762     1.312613     2.770308     229.68
 H       2.184743     0.448844     2.541476      26.74
 C       1.282544     2.075449     0.723037      85.66
 H       1.240622     2.841156    -0.112586      20.49
 C       0.100255     2.501745     1.564688     109.01
 O       0.198948     3.834022     2.032113     245.41
 H       0.785094     4.579179     1.386124      26.24
 H       0.075530     1.984940     2.433285      26.28
 H      -0.846654     2.255438     1.046475      24.65
 C      -1.827101    -1.437590    -0.857957      79.97
 H      -2.191764    -2.227827    -0.381589      18.49
 C      -1.545544     0.506747    -2.378114      25.10
 H      -1.947936     0.991936    -3.282559      19.53
 C      -0.417006     1.043088    -1.727359       9.23
 O       0.324902     2.150734    -2.045192     229.52
 C      -0.183902     2.817527    -3.399679      92.65
 H       0.477009     3.625318    -3.719586      25.68
 H       0.009837     1.975270    -3.903482      29.03
 H      -1.111967     3.409084    -3.204972      26.68
 C      -0.009807     0.273093    -0.479899      25.51
 O       1.083277     0.661323     0.201606     194.31
 C      -0.812566    -0.795543    -0.085744      56.75
 H      -0.340781    -1.324449     0.687267      21.61
 C      -2.164716    -0.687802    -2.050533      24.90
 C      -3.219632    -1.524200    -2.961225      56.58
 H      -3.074017    -1.140338    -3.840561      27.99
 O      -2.952671    -2.986201    -3.045781     221.91
 H      -1.859326    -3.139009    -2.854749      24.95
 C      -4.724128    -1.336843    -2.300470      89.51
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 H      -4.676330    -1.945160    -1.411217      28.21
 O      -5.119618     0.021608    -2.341032     325.05
 H      -4.597867     0.574113    -1.826711      29.36
 C      -5.786830    -2.101515    -3.258900     101.09
 O      -5.608385    -3.519831    -3.082009     209.37
 H      -4.578219    -3.687460    -2.795955      28.13
 H      -5.490657    -1.899927    -4.370466      29.45
 H      -6.821179    -1.999461    -3.066599      28.75
55
name = lig-ACN-frame_365
 C       4.314606     2.231254    -0.511000      58.90
 H       3.630432     3.150051    -0.663523      21.90
 C       4.484504     0.140351     0.695255      67.02
 H       4.094010    -0.466815     1.476750      21.90
 C       5.569943    -0.146207    -0.177712       9.28
 O       6.252618    -1.391158    -0.095065     206.85
 C       5.431971    -2.506445     0.381640     102.84
 H       5.562922    -2.773863     1.631639      23.04
 H       5.856231    -3.406313    -0.043788      26.35
 H       4.348407    -2.512846     0.179764      25.89
 C       6.107447     0.776861    -1.064484      38.89
 O       7.203108     0.537165    -1.952126     149.76
 H       7.858977     0.072171    -1.285377      19.83
 C       5.471768     2.004704    -1.265101      55.36
 H       5.841124     2.609699    -2.185243      18.93
 C       3.924731     1.406979     0.546229      22.22
 C       2.772454     1.928577     1.504096      80.44
 H       3.004981     3.122598     1.768025      22.93
 O       2.604757     1.246765     2.645988     250.54
 H       2.200641     0.219307     2.590407      20.37
 C       1.362100     2.116069     0.670491      70.57
 H       1.537067     2.696754    -0.242075      20.63
 C       0.113212     2.480504     1.560577      95.58
 O       0.152266     3.912140     2.076015     184.33
 H       0.741240     4.562942     1.230139      23.01
 H       0.063839     1.864719     2.334156      25.89
 H      -0.782300     2.386024     0.860331      22.23
 C      -1.744196    -1.411933    -0.853199      37.91
 H      -2.310434    -2.313011    -0.696751      16.49
 C      -1.512024     0.464179    -2.471544     117.42
 H      -1.925703     1.002407    -3.296485      19.64
 C      -0.441985     0.985083    -1.696628      19.23
 O       0.285160     2.158803    -2.135036     242.60
 C      -0.158442     2.812812    -3.383054     117.06
 H       0.557797     3.512320    -3.688067      25.12
 H      -0.398636     2.305013    -4.279151      27.28
 H      -1.229116     3.008915    -3.198849      26.09
 C      -0.029704     0.310789    -0.584674      13.61
 O       1.143618     0.601532     0.239990     142.87
 C      -0.760526    -0.844751    -0.064921       3.24
 H      -0.548857    -1.216521     0.821607      19.40
 C      -2.199162    -0.817489    -2.050303     113.31
 C      -3.235569    -1.511410    -2.960980      51.20
 H      -3.400790    -1.148316    -3.848701      35.09
 O      -2.876726    -2.954524    -3.041780     265.73
 H      -1.843331    -3.057641    -3.017799      28.72
 C      -4.741142    -1.403779    -2.429793      98.52
 H      -4.869253    -1.635201    -1.402764      26.29
 O      -5.131596     0.054189    -2.345044     292.62
 H      -4.477213     0.473464    -1.775428      27.09
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 C      -5.728595    -2.147531    -3.338909     107.16
 O      -5.594399    -3.585984    -3.182534     220.99
 H      -4.535298    -3.753876    -3.293677      27.42
 H      -5.580483    -1.717319    -4.414857      30.53
 H      -6.702629    -1.791314    -3.107502      29.92
55
name = lig-ACN-frame_366
 C       4.292229     2.243449    -0.506108      47.75
 H       3.694328     3.140213    -0.917192      21.84
 C       4.491767     0.119063     0.672351      48.05
 H       4.392746    -0.670062     1.359889      19.26
 C       5.592792    -0.160189    -0.171972      -1.23
 O       6.191471    -1.420364    -0.084858     190.70
 C       5.471738    -2.566984     0.453491     104.11
 H       5.881340    -2.732372     1.633241      22.71
 H       5.576839    -3.360103    -0.246973      26.29
 H       4.399765    -2.215612     0.494407      23.59
 C       6.085821     0.803623    -1.169606      20.20
 O       7.158480     0.545282    -1.896773     124.59
 H       7.894583     0.042402    -1.645794      14.45
 C       5.419543     2.005986    -1.351694      50.06
 H       5.712486     2.768188    -2.180557      20.97
 C       3.868083     1.407850     0.580816      25.28
 C       2.758865     1.928816     1.401879      72.67
 H       3.062661     3.058983     1.925371      22.97
 O       2.634209     1.094701     2.668859     203.29
 H       2.133639     0.225261     2.292728      23.38
 C       1.482665     1.965528     0.661454     102.13
 H       1.576981     2.600989    -0.186213      24.52
 C       0.196612     2.573295     1.519660      95.22
 O       0.109541     3.907660     2.079693     248.08
 H       0.873587     4.460715     1.445825      24.78
 H       0.023147     1.919781     2.279574      26.68
 H      -0.731133     2.441443     0.806413      23.57
 C      -1.767203    -1.398992    -0.892933      68.46
 H      -2.068571    -2.429128    -0.413242      18.22
 C      -1.568697     0.328350    -2.525425      16.16
 H      -1.774578     0.759015    -3.468627      16.28
 C      -0.470892     0.959757    -1.795262       9.44
 O       0.237553     2.074363    -2.222757     239.82
 C      -0.239291     2.776128    -3.394771     131.06
 H       0.468283     3.535746    -3.309246      27.08
 H      -0.016579     2.160777    -4.204895      29.63
 H      -0.969186     3.528171    -3.238899      28.21
 C       0.022433     0.309690    -0.482837      32.60
 O       1.147668     0.646943     0.240427     214.19
 C      -0.642669    -0.850758    -0.070662      47.92
 H      -0.477500    -1.163831     0.842483      19.58
 C      -2.148777    -0.807172    -2.116709      25.35
 C      -3.274829    -1.497190    -2.932285      83.62
 H      -3.101556    -1.015185    -3.782810      29.31
 O      -2.852353    -2.891374    -3.045242     303.69
 H      -1.986708    -2.940732    -3.252482      31.09
 C      -4.714325    -1.368467    -2.455710     103.41
 H      -4.809079    -2.007494    -1.580426      28.51
 O      -5.119196     0.016803    -2.430436     286.85
 H      -4.833550     0.496143    -1.442053      21.88
 C      -5.678041    -2.157156    -3.404822     104.47
 O      -5.571629    -3.628846    -3.313783     248.56
 H      -4.740047    -3.851058    -3.614833      36.55
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 H      -5.576298    -1.907316    -4.501983      30.70
 H      -6.679111    -2.002595    -3.022217      29.68
55
name = lig-ACN-frame_367
 C       4.240625     2.316621    -0.536821      64.05
 H       3.729168     3.300976    -0.377172      24.37
 C       4.546175     0.191425     0.665009      84.21
 H       4.054890    -0.208175     1.532295      23.16
 C       5.578496    -0.192457    -0.186344      19.46
 O       6.211788    -1.450783    -0.130046     198.88
 C       5.485829    -2.551934     0.502390     104.98
 H       6.134152    -2.990696     1.454304      23.73
 H       5.533779    -3.395240    -0.164162      26.09
 H       4.395726    -2.429144     0.876638      24.51
 C       6.049110     0.739100    -1.151337      33.82
 O       7.195635     0.543574    -1.986737     134.06
 H       7.777863     0.075051    -1.361727      21.41
 C       5.291981     1.957256    -1.365785      55.54
 H       5.724894     2.689980    -2.115566      25.61
 C       3.893792     1.423865     0.457854       0.78
 C       2.751026     1.802815     1.498110      68.63
 H       3.008270     3.028104     1.888822      22.47
 O       2.655210     0.989558     2.642903     279.89
 H       2.176630     0.200342     2.550359      27.25
 C       1.398037     2.036641     0.669362      88.09
 H       1.612787     2.630898    -0.161209      23.54
 C       0.256249     2.557966     1.452067      97.07
 O       0.158080     3.902549     2.033251     319.12
 H       0.761045     4.523142     1.887546      33.13
 H       0.068858     1.940841     2.288970      25.04
 H      -0.639611     2.468958     0.669239      21.99
 C      -1.669196    -1.402366    -0.810704      97.77
 H      -2.340923    -2.392090    -0.432754      21.81
 C      -1.467681     0.338068    -2.564695     111.66
 H      -1.773736     0.677441    -3.536959      18.60
 C      -0.462166     0.832172    -1.784408      15.26
 O       0.173830     1.948236    -2.232288     237.16
 C      -0.178421     2.872364    -3.417544     128.18
 H       0.553797     3.544304    -3.701928      24.64
 H      -0.340068     2.278731    -4.321564      25.40
 H      -1.222411     2.884152    -3.392144      25.64
 C      -0.032499     0.342304    -0.556482      35.29
 O       1.150103     0.658621     0.227045     195.73
 C      -0.658546    -0.847885    -0.136014      25.07
 H      -0.190805    -1.424270     0.572915      21.57
 C      -2.170654    -0.853774    -2.023795     120.34
 C      -3.132836    -1.449029    -2.990562      60.19
 H      -3.263608    -1.045349    -3.909628      34.04
 O      -2.918262    -2.872896    -3.087441     318.25
 H      -2.072761    -2.976917    -3.014767      36.35
 C      -4.666792    -1.410871    -2.465041      89.26
 H      -4.732276    -1.724898    -1.404463      25.97
 O      -5.126034    -0.039040    -2.493781     245.20
 H      -5.234377     0.341804    -1.481343      22.66
 C      -5.690001    -2.211403    -3.467091     102.42
 O      -5.547943    -3.643433    -3.450450     252.46
 H      -4.590710    -3.791249    -3.580056      32.52
 H      -5.561472    -1.707454    -4.461612      32.56
 H      -6.745668    -1.967159    -3.225776      30.38
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name = lig-ACN-frame_368
 C       4.207965     2.407051    -0.537343      57.12
 H       3.957149     3.433613    -0.760745      23.07
 C       4.537899     0.271072     0.679363      69.82
 H       4.387335    -0.499234     1.442557      23.48
 C       5.570819    -0.235872    -0.217237       4.89
 O       6.224243    -1.477105    -0.169853     173.50
 C       5.573733    -2.599152     0.540046     109.59
 H       6.262226    -2.869376     1.446362      24.91
 H       5.349158    -3.386384    -0.210304      26.04
 H       4.577297    -2.111425     0.900910      23.80
 C       5.986934     0.718358    -1.206283      23.23
 O       7.158928     0.526089    -2.018169     134.27
 H       8.091903     0.128914    -1.699702      15.65
 C       5.288766     1.906649    -1.391381      37.16
 H       5.715566     2.528839    -2.182516      24.72
 C       3.818003     1.457797     0.495057      20.55
 C       2.748232     1.765668     1.470279      75.30
 H       3.126447     2.847249     2.124539      21.44
 O       2.683807     0.917284     2.652212     236.78
 H       2.155901     0.166409     2.431621      27.89
 C       1.460425     2.098520     0.667612      73.83
 H       1.662796     2.753288    -0.120253      24.32
 C       0.145629     2.549734     1.458963      96.86
 O       0.229980     3.908337     2.006783     308.96
 H       0.890713     4.205666     1.485632      31.90
 H       0.030408     1.736276     2.189310      25.37
 H      -0.811945     2.470436     0.743042      24.02
 C      -1.762224    -1.450363    -0.831083     120.95
 H      -2.216732    -2.575406    -0.379023      17.08
 C      -1.455623     0.213124    -2.532344      17.26
 H      -1.734855     0.728737    -3.465431      19.55
 C      -0.416576     0.892749    -1.848110      18.59
 O       0.284961     2.025336    -2.277475     243.30
 C      -0.255743     2.711404    -3.453681     131.47
 H       0.310890     3.595062    -3.206742      26.45
 H       0.010701     2.237103    -4.397087      28.99
 H      -1.056111     3.315880    -3.200138      28.98
 C      -0.019754     0.304423    -0.564983      38.43
 O       1.083258     0.666979     0.144691     179.88
 C      -0.604634    -0.901260    -0.108839      50.40
 H      -0.114083    -1.346316     0.811266      18.27
 C      -2.143720    -0.822051    -2.029091      36.48
 C      -3.190766    -1.473990    -2.990307      72.68
 H      -2.966893    -0.939106    -3.846754      32.31
 O      -2.939247    -2.925438    -3.151266     280.10
 H      -2.001276    -3.285145    -3.006763      28.38
 C      -4.677682    -1.446472    -2.498758     102.55
 H      -4.652132    -1.903466    -1.468490      27.64
 O      -5.163210    -0.060840    -2.559828     315.63
 H      -5.128176     0.291502    -1.747753      30.21
 C      -5.637703    -2.196040    -3.460224     102.70
 O      -5.506429    -3.647083    -3.602907     240.25
 H      -4.448456    -3.760731    -3.321221      27.57
 H      -5.419577    -1.778405    -4.435183      31.88
 H      -6.685097    -1.942230    -3.109368      28.46
55
name = lig-ACN-frame_369
 C       4.292825     2.315227    -0.569529      67.74
 H       3.635841     3.110167    -0.752819      24.99
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 C       4.565407     0.214685     0.628854      71.56
 H       4.205370    -0.279373     1.546602      23.76
 C       5.551130    -0.203186    -0.261852      21.11
 O       6.234934    -1.470212    -0.204581     218.36
 C       5.644008    -2.549480     0.550264     115.10
 H       6.322534    -2.951238     1.346057      26.35
 H       5.481446    -3.470386    -0.113137      25.34
 H       4.660184    -2.282874     1.078316      24.41
 C       6.027007     0.668609    -1.272615      12.88
 O       7.071620     0.518727    -2.077334      93.94
 H       7.669644    -0.018618    -1.385639      18.49
 C       5.319695     1.935359    -1.407450      63.04
 H       5.576559     2.564674    -2.222489      24.28
 C       3.872678     1.495255     0.509142     -34.10
 C       2.707985     1.874305     1.516344      63.79
 H       2.950456     3.094054     1.959763      21.96
 O       2.690708     0.906113     2.617533     216.39
 H       2.207895    -0.030070     2.375913      22.30
 C       1.355084     2.009734     0.680233      85.92
 H       1.590409     2.726536    -0.067332      24.20
 C       0.088224     2.532803     1.470569      92.99
 O       0.344040     3.859552     1.960015     265.66
 H       0.694994     4.623901     1.331797      27.10
 H      -0.221459     2.031069     2.458243      23.39
 H      -0.787262     2.484085     0.668430      22.63
 C      -1.735347    -1.473547    -0.794521      60.34
 H      -2.259436    -2.589378    -0.427130      19.73
 C      -1.407555     0.293549    -2.553702     146.92
 H      -1.789141     0.575899    -3.569101      20.56
 C      -0.352551     0.908376    -1.818701       0.56
 O       0.366166     2.031487    -2.296084     240.46
 C      -0.234641     2.751329    -3.400559     121.87
 H       0.389155     3.565474    -3.792929      24.15
 H      -0.197717     2.066780    -4.337400      24.74
 H      -1.308701     2.674517    -3.453656      26.01
 C      -0.005113     0.253298    -0.613451      32.72
 O       1.129787     0.752869     0.101126     197.36
 C      -0.660988    -0.942383    -0.142618      33.31
 H      -0.523427    -1.313310     0.994682      17.00
 C      -2.184037    -0.952077    -2.029191      78.49
 C      -3.197124    -1.564449    -2.955987      65.69
 H      -3.278327    -1.144059    -3.935343      29.70
 O      -2.946533    -3.008519    -3.207042     181.81
 H      -1.787316    -2.870726    -3.350088      23.02
 C      -4.683118    -1.444353    -2.544950     103.89
 H      -4.873954    -1.914545    -1.531946      25.93
 O      -5.199740    -0.088162    -2.600407     300.77
 H      -4.742101     0.480058    -1.945864      27.93
 C      -5.593517    -2.193410    -3.501387     106.29
 O      -5.434143    -3.622252    -3.706860     259.57
 H      -4.516912    -3.996213    -3.373584      30.66
 H      -5.631519    -1.631128    -4.410097      31.78
 H      -6.669181    -2.108364    -3.087343      27.98
55
name = lig-ACN-frame_370
 C       4.256776     2.244478    -0.577386      53.43
 H       3.774739     3.142658    -0.784754      22.95
 C       4.525278     0.201297     0.641312      49.39
 H       4.274924    -0.492234     1.442422      19.41
 C       5.548734    -0.210063    -0.283071       9.46
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 O       6.235321    -1.413744    -0.247645     186.87
 C       5.726509    -2.530362     0.573524     114.13
 H       6.490225    -2.705805     1.272736      27.66
 H       5.551463    -3.402248    -0.195715      25.03
 H       4.774505    -2.254406     1.052194      24.61
 C       5.945065     0.743612    -1.280099      16.94
 O       7.084378     0.431334    -2.137208     199.49
 H       7.766028    -0.170830    -1.917803      24.90
 C       5.360486     1.973433    -1.473975      44.52
 H       5.706563     2.568519    -2.286979      20.11
 C       3.977260     1.462587     0.537461      42.46
 C       2.677360     1.877022     1.486756      71.62
 H       2.752618     3.019874     2.142681      22.57
 O       2.697960     1.010735     2.571155     203.05
 H       1.995574     0.171523     2.334675      20.97
 C       1.249094     1.980579     0.735919      91.75
 H       1.328397     2.733769    -0.029206      23.67
 C       0.093461     2.572556     1.466795      98.70
 O       0.419681     3.857505     1.969093     199.29
 H       0.686139     4.396859     0.940413      23.19
 H      -0.195462     1.827546     2.354182      23.70
 H      -0.861754     2.603916     0.780561      23.00
 C      -1.735400    -1.514072    -0.867444      62.55
 H      -2.375213    -2.411198    -0.285184      15.56
 C      -1.482340     0.230216    -2.529549      36.64
 H      -1.645703     0.666406    -3.550886      16.48
 C      -0.372889     0.840291    -1.856732      12.24
 O       0.416594     1.998513    -2.237357     212.31
 C      -0.246002     2.673260    -3.498515      93.09
 H       0.076697     3.787241    -3.603040      25.19
 H       0.005572     1.946624    -4.344984      26.62
 H      -1.213079     2.952271    -3.140227      28.41
 C       0.055234     0.265732    -0.603965      28.60
 O       1.194588     0.673666     0.056432     202.84
 C      -0.707029    -0.837529    -0.117759      67.73
 H      -0.240878    -1.307173     0.952025      18.98
 C      -2.073471    -0.904638    -2.103873      34.30
 C      -3.205069    -1.639878    -3.002806      43.33
 H      -3.077132    -1.037460    -3.909351      26.59
 O      -2.875260    -3.039131    -3.222311     167.98
 H      -1.798059    -3.389381    -3.671218      23.59
 C      -4.722639    -1.490464    -2.508556      94.34
 H      -4.836458    -1.755392    -1.414684      25.02
 O      -5.205639    -0.104887    -2.618243     228.77
 H      -4.404060     0.579207    -2.201548      22.08
 C      -5.667444    -2.231118    -3.585461     103.44
 O      -5.383780    -3.617073    -3.801771     301.94
 H      -4.468745    -3.608934    -3.679467      34.82
 H      -5.606141    -1.690924    -4.494425      31.67
 H      -6.734105    -2.106310    -3.132954      27.47
55
name = lig-ACN-frame_371
 C       4.264636     2.345901    -0.630840      48.98
 H       3.827101     3.322107    -0.622189      25.07
 C       4.548036     0.149680     0.673600      85.84
 H       4.252547    -0.562444     1.414522      23.41
 C       5.527088    -0.157469    -0.286702       5.84
 O       6.243174    -1.373175    -0.298107     224.23
 C       5.844221    -2.471132     0.552811     125.63
 H       6.487012    -2.698825     1.302317      28.85
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 H       5.741873    -3.471523    -0.075076      25.12
 H       4.910818    -2.224218     0.969417      26.47
 C       6.072228     0.695622    -1.336325      22.19
 O       7.038644     0.364804    -2.198392     134.66
 H       7.561911    -0.206773    -1.644512      23.41
 C       5.329495     1.961573    -1.491542      55.50
 H       5.641563     2.731315    -2.202475      25.26
 C       3.846459     1.480936     0.542194     -36.83
 C       2.700543     1.885447     1.384792      70.45
 H       3.112126     3.119438     1.640694      21.17
 O       2.635579     1.064813     2.610418     206.52
 H       2.070324     0.251477     2.430980      24.53
 C       1.390779     1.985618     0.625404      63.02
 H       1.588018     2.642204    -0.238513      22.28
 C       0.029255     2.519738     1.534819      76.25
 O       0.442792     3.862335     1.985648     193.39
 H       1.189852     4.495109     1.276262      21.81
 H      -0.229558     1.883792     2.570892      21.62
 H      -0.852218     2.579179     0.817780      22.63
 C      -1.681688    -1.408261    -0.875366      54.96
 H      -2.215235    -2.400257    -0.509069      19.18
 C      -1.432044     0.263114    -2.593794     163.15
 H      -1.903198     0.703299    -3.510410      21.36
 C      -0.340589     0.823156    -1.846225       5.69
 O       0.338300     1.937035    -2.275701     219.64
 C      -0.233699     2.614773    -3.421586     117.54
 H       0.689148     3.306161    -3.455246      22.96
 H      -0.183635     2.183951    -4.536938      24.67
 H      -1.277105     2.780883    -3.503091      25.66
 C       0.014545     0.246896    -0.616879      34.67
 O       1.225461     0.555480     0.058136     156.68
 C      -0.712066    -0.788672    -0.103505      29.22
 H      -0.312464    -1.355761     0.929152      17.45
 C      -2.113344    -1.003790    -2.145898      95.41
 C      -3.121547    -1.599118    -3.060127      51.11
 H      -3.137696    -1.210702    -4.122952      31.62
 O      -2.841736    -3.084342    -3.215371     179.09
 H      -1.682218    -3.055282    -3.409449      21.92
 C      -4.729921    -1.529546    -2.565555      88.28
 H      -4.784948    -2.129506    -1.603303      25.60
 O      -5.145712    -0.136948    -2.653605     249.02
 H      -4.439711     0.479253    -2.188787      26.49
 C      -5.736307    -2.236216    -3.581802     103.73
 O      -5.341729    -3.618234    -3.884345     266.48
 H      -4.432785    -3.661387    -4.147603      36.58
 H      -5.583179    -1.612862    -4.431112      32.27
 H      -6.877649    -2.250250    -3.422601      28.04
55
name = lig-ACN-frame_372
 C       4.316891     2.326275    -0.522434      76.54
 H       3.875711     3.313991    -0.737212      23.66
 C       4.524908     0.279074     0.598907      83.66
 H       4.176326    -0.254406     1.459640      26.80
 C       5.595698    -0.135877    -0.301767      10.23
 O       6.284626    -1.362068    -0.353755     188.09
 C       5.930168    -2.430325     0.550579     122.84
 H       6.602902    -2.443670     1.276995      28.48
 H       6.016158    -3.385514    -0.112794      25.27
 H       4.950432    -2.421224     0.949798      27.35
 C       5.968327     0.757454    -1.321222      21.53
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 O       7.026042     0.280548    -2.216240     122.28
 H       7.825307    -0.244278    -1.740648      19.84
 C       5.299319     1.967523    -1.450618      56.35
 H       5.700323     2.569037    -2.311928      23.58
 C       3.856873     1.419715     0.326560      31.78
 C       2.754536     1.875393     1.364484      66.99
 H       2.826242     3.058847     1.921625      21.87
 O       2.554233     1.158448     2.627118     233.89
 H       2.218661     0.364217     2.385433      31.25
 C       1.385791     1.897560     0.545307      87.03
 H       1.377670     2.624437    -0.331264      22.84
 C       0.242636     2.537785     1.452295      90.99
 O       0.413510     3.839866     2.049090     269.41
 H       1.145947     4.302137     1.436731      26.73
 H       0.008736     1.808304     2.465506      22.82
 H      -0.702239     2.501546     0.852145      24.50
 C      -1.750497    -1.432275    -0.884434      90.25
 H      -2.020139    -2.430876    -0.517054      20.54
 C      -1.426270     0.217001    -2.630500      -7.28
 H      -1.670877     0.761268    -3.549224      14.55
 C      -0.431463     0.754023    -1.874425      33.78
 O       0.259164     1.873224    -2.326484     260.77
 C      -0.127679     2.633230    -3.458428     110.18
 H       0.261958     3.686902    -3.755373      24.05
 H      -0.067097     1.735121    -4.175701      25.19
 H      -1.073458     3.055694    -3.157375      28.39
 C       0.056015     0.253991    -0.593882      56.61
 O       1.225163     0.547517     0.095174     219.45
 C      -0.726871    -0.858626    -0.098545      72.87
 H      -0.571874    -1.262216     0.998975      16.83
 C      -2.086825    -0.880353    -2.181498      64.63
 C      -3.177061    -1.701016    -3.117836      23.95
 H      -3.084019    -1.060784    -4.101475      27.67
 O      -2.770568    -3.055916    -3.195382     263.32
 H      -1.760260    -3.197973    -3.052083      26.87
 C      -4.666549    -1.574888    -2.698162     104.10
 H      -4.801094    -1.849466    -1.609665      27.22
 O      -5.067341    -0.185595    -2.655240     324.26
 H      -4.735155     0.168690    -1.926533      30.99
 C      -5.647222    -2.250746    -3.670440     112.34
 O      -5.364303    -3.616824    -3.965360     237.86
 H      -4.312877    -3.586445    -4.228477      31.87
 H      -5.886166    -1.657661    -4.540872      31.00
 H      -6.565285    -2.285607    -3.017008      28.13
55
name = lig-ACN-frame_373
 C       4.345493     2.432470    -0.622754      36.56
 H       3.769088     3.417584    -0.649089      23.25
 C       4.562346     0.216625     0.524602      68.97
 H       4.418372    -0.487881     1.365793      20.94
 C       5.632436    -0.159021    -0.279276      22.19
 O       6.301052    -1.334280    -0.377606     226.77
 C       6.031350    -2.429007     0.561268     123.59
 H       6.546212    -2.346586     1.421872      27.03
 H       6.341181    -3.380686     0.047376      25.64
 H       4.981633    -2.385538     0.761639      25.27
 C       6.002954     0.693414    -1.356857       7.36
 O       6.953087     0.294393    -2.200703     108.85
 H       7.729931    -0.102363    -1.585722      20.96
 C       5.403400     2.007008    -1.501478      52.06
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 H       5.591985     2.775013    -2.328625      20.61
 C       3.830973     1.458533     0.420968     -20.11
 C       2.687345     1.881746     1.316178      76.39
 H       3.148427     3.080817     1.522193      21.24
 O       2.520044     1.214594     2.579048     221.06
 H       2.094834     0.288379     2.467518      24.53
 C       1.430590     1.976306     0.550329      85.09
 H       1.685939     2.531256    -0.426354      21.23
 C       0.347022     2.476836     1.387603      94.75
 O       0.440237     3.795856     2.077183     300.87
 H       0.666936     4.445721     1.518433      32.74
 H       0.219408     1.548206     2.247007      21.47
 H      -0.548942     2.518365     0.776259      24.21
 C      -1.817705    -1.485743    -0.932284      47.00
 H      -2.447608    -2.239286    -0.627913      18.13
 C      -1.477784     0.201531    -2.682796      86.92
 H      -1.653983     0.496762    -3.725520      17.37
 C      -0.379298     0.785893    -1.840591       7.74
 O       0.363211     1.905421    -2.266458     147.08
 C      -0.195104     2.630060    -3.550938      96.61
 H       0.839981     3.126476    -3.507981      21.84
 H      -0.325347     2.328622    -4.671068      25.00
 H      -1.203076     3.005895    -3.470069      26.41
 C      -0.027242     0.145573    -0.603444      18.62
 O       1.159915     0.570424     0.127246     177.46
 C      -0.754886    -0.898488    -0.126668      15.14
 H      -0.466961    -1.295556     0.817833      20.86
 C      -2.205890    -0.949517    -2.168793      62.15
 C      -3.063908    -1.642988    -3.116598      45.11
 H      -2.961611    -1.317167    -4.253774      27.28
 O      -2.722939    -3.076520    -3.168689     268.66
 H      -1.839128    -3.022186    -3.312321      32.36
 C      -4.568564    -1.586294    -2.756705     100.63
 H      -4.653887    -2.308094    -1.881524      26.85
 O      -4.993852    -0.198889    -2.672623     239.89
 H      -4.998668     0.145409    -1.695246      22.36
 C      -5.637047    -2.272288    -3.677761     105.83
 O      -5.359786    -3.637967    -4.081857     259.08
 H      -4.339563    -3.820411    -4.030726      33.23
 H      -5.853578    -1.662754    -4.563288      31.14
 H      -6.585339    -2.294881    -3.090591      29.70
55
name = lig-ACN-frame_374
 C       4.341378     2.344579    -0.635851      65.82
 H       4.038514     3.429492    -0.754690      22.36
 C       4.539508     0.165893     0.572050      56.27
 H       4.044866    -0.535834     1.332918      20.95
 C       5.603707    -0.111142    -0.351180       1.64
 O       6.363664    -1.384512    -0.358022     204.65
 C       6.089635    -2.399698     0.590476     126.42
 H       6.465456    -2.196324     1.535116      27.27
 H       6.511493    -3.279758     0.201839      27.69
 H       5.025926    -2.726556     0.686422      26.46
 C       5.995570     0.786095    -1.370084      18.90
 O       6.978797     0.320831    -2.246969     155.35
 H       7.630516    -0.226817    -1.811179      24.01
 C       5.414010     2.057333    -1.495693      50.85
 H       6.004763     2.581345    -2.316586      20.23
 C       4.013833     1.509389     0.419861      22.32
 C       2.783883     1.914881     1.283571      76.96
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 H       2.772836     3.136651     1.763726      22.00
 O       2.532630     1.233559     2.538643     187.13
 H       1.973987     0.321929     2.208959      21.89
 C       1.490367     2.046528     0.423016      58.25
 H       1.597773     2.800000    -0.468551      21.27
 C       0.217969     2.495695     1.362618      90.06
 O       0.488933     3.702146     2.091922     285.40
 H       0.483879     4.371613     1.435884      31.09
 H       0.056800     1.740931     2.349487      22.31
 H      -0.687058     2.436750     0.785957      24.29
 C      -1.918252    -1.507572    -0.898853      66.24
 H      -2.378113    -2.220562    -0.459422      19.55
 C      -1.410115     0.198006    -2.598342      -8.10
 H      -1.654779     0.574661    -3.597409      18.02
 C      -0.412604     0.777847    -1.904649      26.78
 O       0.368825     1.896836    -2.320083     261.59
 C      -0.121655     2.660319    -3.569070     103.24
 H       0.449894     3.616633    -3.890631      24.45
 H      -0.199198     1.714322    -4.187566      25.96
 H      -0.987876     3.229660    -3.171359      27.42
 C      -0.046104     0.197023    -0.650513      56.01
 O       1.033935     0.548785     0.138524     168.90
 C      -0.856344    -1.033821    -0.176468      27.46
 H      -0.600461    -1.533930     0.629691      17.32
 C      -2.151937    -0.897711    -2.174225      66.13
 C      -3.050316    -1.667620    -3.215506      24.38
 H      -2.824718    -1.057965    -4.243837      28.02
 O      -2.664402    -3.097715    -3.159079     217.12
 H      -1.819037    -3.385100    -3.455752      31.15
 C      -4.545547    -1.641730    -2.775914      98.58
 H      -4.520119    -1.952977    -1.696850      27.00
 O      -4.937269    -0.226235    -2.663598     228.52
 H      -4.882696     0.207495    -1.611039      21.20
 C      -5.627613    -2.290749    -3.723281     108.32
 O      -5.337411    -3.668088    -4.181873     287.06
 H      -4.522856    -3.800760    -3.818909      39.40
 H      -5.624221    -1.585313    -4.580261      31.41
 H      -6.621310    -2.274732    -3.283717      29.35
55
name = lig-ACN-frame_375
 C       4.439578     2.361256    -0.611236      49.02
 H       3.815591     3.281485    -0.584802      23.84
 C       4.565196     0.233919     0.543688      72.30
 H       4.082394    -0.508202     1.301597      20.75
 C       5.571233    -0.222055    -0.354560      16.76
 O       6.363472    -1.328439    -0.372981     195.05
 C       6.097566    -2.410189     0.668945     114.11
 H       6.259181    -1.969644     1.643590      26.55
 H       6.827141    -3.088446     0.476735      27.73
 H       5.019683    -2.706161     0.559189      26.28
 C       6.058309     0.754354    -1.351146      34.50
 O       7.021327     0.383984    -2.297080     183.49
 H       7.550297    -0.296555    -1.901679      23.12
 C       5.479289     2.021199    -1.530738      50.68
 H       5.675300     2.908117    -2.172934      22.57
 C       4.051533     1.497132     0.458587      31.64
 C       2.819235     2.001541     1.265894      55.51
 H       3.179301     3.204133     1.648693      22.58
 O       2.569486     1.185566     2.447089     220.22
 H       2.012129     0.365824     2.203165      23.14
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 C       1.301427     1.978149     0.439139      70.88
 H       1.378035     2.445037    -0.608397      19.17
 C       0.178797     2.497867     1.320812      97.64
 O       0.496243     3.652537     2.092276     224.12
 H       0.785578     4.566583     1.437350      24.89
 H      -0.002033     1.496308     1.987869      21.84
 H      -0.705062     2.723080     0.765480      23.81
 C      -1.998302    -1.495960    -0.902569      27.58
 H      -2.401220    -2.331617    -0.790475      19.76
 C      -1.442661     0.197228    -2.660729      47.22
 H      -1.769286     0.726711    -3.583210      15.33
 C      -0.342990     0.835260    -1.868556      -4.70
 O       0.410341     1.932500    -2.380465     234.50
 C      -0.120038     2.610121    -3.476562     116.70
 H       0.749193     3.227623    -3.909112      25.07
 H      -0.458082     2.103670    -4.486716      26.24
 H      -1.149419     2.975855    -3.308433      26.33
 C      -0.109468     0.148088    -0.620330      33.67
 O       0.991589     0.585971     0.133642     202.96
 C      -0.799769    -0.970587    -0.204901      46.87
 H      -0.506618    -1.333792     0.667576      20.29
 C      -2.157902    -0.947792    -2.228157      27.85
 C      -3.035296    -1.710637    -3.211247      70.63
 H      -3.053219    -1.359025    -4.396530      26.00
 O      -2.691635    -3.093513    -3.184560     216.23
 H      -1.532665    -3.076020    -3.404816      20.94
 C      -4.546288    -1.631879    -2.733127      93.93
 H      -4.693093    -2.267077    -1.802411      28.91
 O      -4.915139    -0.240853    -2.678188     297.43
 H      -4.411022     0.074448    -1.868486      26.75
 C      -5.553513    -2.294716    -3.780291     107.53
 O      -5.318582    -3.644702    -4.222030     269.82
 H      -4.432579    -3.935357    -3.918178      35.28
 H      -5.654210    -1.658293    -4.707823      30.21
 H      -6.511443    -2.256543    -3.299954      29.26
55
name = lig-ACN-frame_376
 C       4.516106     2.423933    -0.529320      62.24
 H       4.101805     3.358458    -0.851342      22.69
 C       4.614436     0.189124     0.524045      51.80
 H       4.412580    -0.506694     1.417969      21.19
 C       5.612011    -0.138877    -0.413971      14.10
 O       6.326618    -1.390077    -0.329981     252.34
 C       6.089769    -2.282064     0.712690     117.35
 H       5.942170    -1.837354     1.736095      25.71
 H       6.892795    -3.023262     0.785501      26.25
 H       5.187771    -2.967857     0.482118      26.34
 C       6.093418     0.717420    -1.409326       8.00
 O       7.065248     0.427741    -2.287689     129.51
 H       7.755407    -0.290037    -1.888107      19.23
 C       5.468741     2.003335    -1.464871      63.34
 H       5.874567     2.455381    -2.369852      22.56
 C       3.928394     1.542862     0.407926      -2.47
 C       2.703801     1.928284     1.202270      75.01
 H       2.835544     3.178407     1.588435      22.29
 O       2.634523     1.150855     2.379686     265.89
 H       2.202037     0.422249     2.102447      30.63
 C       1.279227     1.927275     0.434083      87.64
 H       1.410465     2.637526    -0.437054      22.64
 C       0.111644     2.525797     1.282706     100.60
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 O       0.505332     3.651448     2.134431     194.67
 H       1.211899     4.271982     1.379483      23.93
 H      -0.346894     1.863387     2.107480      24.11
 H      -0.668246     2.732317     0.561378      24.69
 C      -1.858540    -1.446922    -1.010208      40.20
 H      -2.279425    -2.212375    -0.592076      17.86
 C      -1.453200     0.259097    -2.698146      53.48
 H      -1.658263     0.580354    -3.740742      16.40
 C      -0.430577     0.782040    -1.923578      24.93
 O       0.422761     1.832592    -2.337703     231.32
 C      -0.184117     2.614054    -3.554622     114.12
 H       0.571024     3.446974    -3.566886      25.18
 H      -0.184055     1.901020    -4.389976      26.43
 H      -0.913766     3.368141    -3.198270      26.49
 C      -0.072447     0.252620    -0.658540      66.08
 O       1.024852     0.545102     0.177293     211.89
 C      -0.874920    -0.925300    -0.179238      63.80
 H      -0.618452    -1.378724     0.774711      15.31
 C      -2.145155    -0.931154    -2.273659      58.83
 C      -3.125611    -1.734678    -3.152134      14.91
 H      -2.950207    -1.158263    -4.258526      22.43
 O      -2.694310    -3.121530    -3.222591     125.66
 H      -1.456250    -3.129357    -3.202764      19.08
 C      -4.543148    -1.673579    -2.815691     109.97
 H      -4.660463    -2.169497    -1.805467      27.83
 O      -4.907972    -0.268004    -2.652924     305.49
 H      -4.292837     0.267017    -2.325174      33.09
 C      -5.520602    -2.249628    -3.811410     109.65
 O      -5.289319    -3.633578    -4.212960     219.40
 H      -4.185420    -3.747228    -4.189639      31.78
 H      -5.580359    -1.493294    -4.673677      29.94
 H      -6.478570    -2.272477    -3.378872      28.91
55
name = lig-ACN-frame_377
 C       4.505380     2.475202    -0.562123      50.82
 H       4.228635     3.485652    -0.463981      22.47
 C       4.579091     0.306554     0.475939      63.19
 H       4.268918    -0.366672     1.297115      20.47
 C       5.674171    -0.155624    -0.351954      20.15
 O       6.297961    -1.389082    -0.342986     189.75
 C       6.025105    -2.264819     0.832014     102.88
 H       5.643651    -1.589102     1.707645      22.73
 H       7.089412    -2.575318     1.098059      23.77
 H       5.256338    -3.056911     0.549620      24.62
 C       6.053608     0.726323    -1.414673      11.46
 O       7.145787     0.427234    -2.298989     133.24
 H       7.874900    -0.056825    -1.659308      23.46
 C       5.534829     1.975256    -1.464591      50.18
 H       5.844439     2.745549    -2.122814      22.97
 C       3.924847     1.498572     0.293765      11.85
 C       2.614536     1.855981     1.169472      75.83
 H       2.690377     3.090602     1.633573      20.74
 O       2.668874     1.085339     2.382351     225.67
 H       2.243950     0.165808     2.355181      22.31
 C       1.342527     1.922653     0.471921      81.25
 H       1.460173     2.437913    -0.481649      20.68
 C       0.049582     2.588353     1.330309      99.67
 O       0.521101     3.666640     2.122948     251.39
 H       1.091187     4.418983     1.569209      25.60
 H      -0.372671     1.755853     1.897852      24.43
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 H      -0.699885     2.990701     0.616813      23.28
 C      -1.731305    -1.460848    -1.023313      75.02
 H      -2.367060    -2.244925    -0.749399      19.66
 C      -1.497956     0.224252    -2.759274      27.75
 H      -1.584135     0.628216    -3.770431      17.96
 C      -0.438952     0.764785    -1.930979       7.23
 O       0.343862     1.777619    -2.384721     236.58
 C      -0.088548     2.688929    -3.489255     119.01
 H       0.586687     3.360567    -3.998208      25.54
 H      -0.369666     2.110640    -4.357384      27.40
 H      -1.156005     2.746007    -3.274105      27.69
 C      -0.107781     0.198057    -0.616183      35.11
 O       1.029557     0.498966     0.129400     205.95
 C      -0.852220    -0.772125    -0.185104      49.35
 H      -0.704425    -1.278122     0.855425      18.40
 C      -2.149240    -0.885157    -2.291459      60.55
 C      -3.022396    -1.705038    -3.214189      33.68
 H      -3.047193    -1.239791    -4.391789      26.97
 O      -2.685479    -3.134507    -3.253868     130.89
 H      -1.441612    -3.260057    -3.370119      22.57
 C      -4.588695    -1.647782    -2.744085      91.82
 H      -4.706966    -2.204779    -1.764254      27.24
 O      -4.959911    -0.274895    -2.683092     239.89
 H      -4.085001     0.179540    -2.254213      23.54
 C      -5.568778    -2.235463    -3.853301     101.34
 O      -5.235047    -3.587528    -4.182746     216.67
 H      -4.237986    -3.564083    -4.464981      32.93
 H      -5.451659    -1.581223    -4.794278      29.96
 H      -6.571057    -2.168871    -3.510455      29.03
55
name = lig-ACN-frame_378
 C       4.477875     2.465297    -0.646995      56.97
 H       4.210392     3.489655    -0.600517      23.93
 C       4.553706     0.279729     0.427485      55.51
 H       3.954863    -0.354021     1.030551      21.12
 C       5.644289    -0.116925    -0.350198      18.42
 O       6.243336    -1.407866    -0.305334     250.63
 C       6.012871    -2.198968     0.942752      94.50
 H       5.333016    -1.598855     1.754084      22.31
 H       6.994156    -2.673218     1.432079      23.55
 H       5.472147    -3.157728     0.616092      24.73
 C       6.137360     0.725276    -1.407851      12.10
 O       7.165901     0.423814    -2.238744     115.99
 H       7.919240    -0.093122    -1.809714      25.85
 C       5.544138     2.150945    -1.465596      63.05
 H       6.146214     2.811540    -2.006031      25.56
 C       3.867651     1.546367     0.258627      19.57
 C       2.761968     1.810837     1.234061      62.08
 H       3.133602     2.999149     1.624903      21.23
 O       2.675892     0.999457     2.452022     198.42
 H       2.005667     0.167287     2.104650      19.46
 C       1.218311     1.885636     0.441753      89.22
 H       1.413840     2.484118    -0.409408      23.35
 C       0.151271     2.589481     1.271231     106.77
 O       0.526720     3.717698     2.162531     304.90
 H       0.612974     4.396571     1.583301      32.03
 H      -0.284236     1.940323     1.969015      26.48
 H      -0.699441     2.914167     0.600111      23.59
 C      -1.838729    -1.475270    -1.044894      65.66
 H      -2.111433    -2.529323    -0.693313      16.91
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 C      -1.441966     0.237189    -2.753971      22.22
 H      -1.787641     0.660260    -3.678251      19.05
 C      -0.435284     0.787679    -1.966103      11.00
 O       0.385815     1.836304    -2.459170     259.52
 C      -0.169758     2.588539    -3.488265     139.26
 H       0.513136     3.394222    -3.202255      23.81
 H      -0.075726     2.133155    -4.403651      27.78
 H      -0.933082     3.357290    -3.303567      26.49
 C      -0.096066     0.274426    -0.705242      47.11
 O       1.033566     0.525595     0.067695     224.27
 C      -0.919450    -0.868720    -0.124620      58.52
 H      -0.535346    -1.114351     1.016345      13.62
 C      -2.103212    -0.968714    -2.306435      42.25
 C      -3.036302    -1.744654    -3.247566      23.25
 H      -2.954971    -1.231294    -4.406716      24.06
 O      -2.656846    -3.128866    -3.298554     156.17
 H      -1.457071    -3.015337    -3.486355      20.70
 C      -4.617164    -1.625183    -2.786598      94.62
 H      -4.708283    -2.189744    -1.818167      27.69
 O      -4.967104    -0.236109    -2.712524     248.09
 H      -4.609221     0.396174    -1.823135      20.22
 C      -5.541700    -2.205451    -3.847985     110.30
 O      -5.215278    -3.563265    -4.159861     269.46
 H      -4.341327    -3.589127    -4.356422      39.50
 H      -5.474019    -1.473207    -4.737878      30.35
 H      -6.599218    -2.257510    -3.609550      28.60
55
name = lig-ACN-frame_379
 C       4.429406     2.514195    -0.705130      58.39
 H       3.901846     3.442688    -0.928885      22.60
 C       4.437980     0.217309     0.330967      61.51
 H       4.182000    -0.546886     0.966292      20.66
 C       5.599896    -0.081121    -0.439501      16.16
 O       6.185586    -1.429047    -0.200352     217.32
 C       5.987500    -2.167698     0.989321      96.21
 H       5.242889    -1.647295     1.851662      22.90
 H       7.085368    -2.170248     1.509200      23.81
 H       5.547568    -3.182741     0.698393      24.39
 C       6.166438     0.902772    -1.304332      20.74
 O       7.189994     0.438911    -2.190499     168.90
 H       7.597631    -0.252469    -1.721370      18.14
 C       5.660867     2.116669    -1.438981      35.31
 H       6.066449     2.784448    -2.153259      21.03
 C       3.924223     1.494703     0.259562      12.65
 C       2.741643     1.865310     1.274987      70.46
 H       2.772325     3.003129     1.871670      21.13
 O       2.679480     0.954872     2.435427     227.18
 H       2.044637     0.078878     2.310172      18.11
 C       1.418770     1.991427     0.472431      79.95
 H       1.510813     2.584423    -0.383406      22.31
 C       0.163882     2.548502     1.331495     102.75
 O       0.520941     3.732854     2.154037     301.74
 H       0.744786     4.490051     1.643054      31.53
 H      -0.177671     1.840036     1.949834      26.28
 H      -0.650933     2.790895     0.565545      22.43
 C      -1.882707    -1.522769    -0.949338      75.94
 H      -2.406903    -2.594052    -0.676291      22.06
 C      -1.459907     0.185097    -2.721410      68.14
 H      -1.735250     0.667195    -3.632827      14.69
 C      -0.401484     0.796939    -1.995097      11.49
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 O       0.392643     1.810812    -2.425376     254.20
 C      -0.135284     2.764246    -3.532859     105.91
 H       0.504891     3.551303    -3.816631      25.22
 H      -0.110009     2.232381    -4.453899      28.88
 H      -1.292871     2.676781    -3.359880      25.20
 C      -0.200357     0.175296    -0.698061      68.83
 O       1.011215     0.589099     0.017110     204.51
 C      -0.923396    -0.852598    -0.244757      27.71
 H      -0.736411    -1.507565     0.767109      16.50
 C      -2.069083    -1.019543    -2.323669      27.69
 C      -3.102631    -1.714060    -3.230398      64.80
 H      -3.048625    -1.153627    -4.360093      25.06
 O      -2.616582    -3.127434    -3.369069     238.27
 H      -1.547738    -3.220025    -3.366325      23.68
 C      -4.544313    -1.571209    -2.834110      95.98
 H      -4.710601    -2.025970    -1.832484      30.19
 O      -4.980462    -0.147067    -2.722590     233.94
 H      -4.951940    -0.050102    -1.743255      26.97
 C      -5.528835    -2.175373    -3.859402     109.19
 O      -5.221820    -3.567825    -4.154770     229.90
 H      -4.238380    -3.664441    -4.010511      32.87
 H      -5.507133    -1.536965    -4.796343      30.75
 H      -6.509888    -2.092056    -3.342306      28.95
55
name = lig-ACN-frame_380
 C       4.440781     2.409035    -0.687964      65.26
 H       3.901127     3.390564    -0.828053      24.11
 C       4.391049     0.212679     0.233094      62.48
 H       3.903348    -0.319162     0.983777      22.32
 C       5.545864    -0.166868    -0.397163      22.26
 O       6.133708    -1.334461    -0.229104     228.69
 C       5.991916    -2.122198     1.069855      84.05
 H       5.103512    -1.628566     1.804260      22.72
 H       7.075823    -2.179954     1.636224      24.15
 H       5.833303    -3.229539     0.826444      24.55
 C       6.256116     0.819693    -1.235789      27.53
 O       7.190786     0.489992    -2.119626     154.07
 H       7.867438    -0.158960    -1.814475      18.23
 C       5.592101     2.214215    -1.403510      55.29
 H       5.882738     2.850492    -2.243387      21.85
 C       3.909331     1.584819     0.279244      29.54
 C       2.695659     1.833008     1.278812      82.44
 H       3.035673     2.997930     1.697060      21.72
 O       2.702886     0.994350     2.390372     280.67
 H       2.248471     0.177541     2.163245      25.50
 C       1.420910     2.063539     0.509633      75.27
 H       1.764195     2.658127    -0.275989      22.14
 C       0.249491     2.537990     1.379036     114.38
 O       0.486179     3.701358     2.150431     285.88
 H       1.041701     4.277546     1.436132      26.58
 H       0.035853     1.805970     1.994299      27.67
 H      -0.658154     2.738874     0.718363      23.30
 C      -1.929371    -1.551081    -1.061470      64.89
 H      -2.674205    -2.367986    -0.444487      17.28
 C      -1.471512     0.126543    -2.749622      12.38
 H      -1.671396     0.369039    -3.779637      16.37
 C      -0.455292     0.727506    -1.976992       7.32
 O       0.419568     1.888834    -2.417972     207.86
 C      -0.179940     2.731565    -3.599017      94.47
 H       0.186895     3.771120    -3.457100      24.77
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 H      -0.001221     2.116937    -4.486548      25.78
 H      -1.273564     3.032861    -3.339818      25.93
 C      -0.097578     0.273314    -0.681832      38.56
 O       1.001696     0.637099     0.000052     196.31
 C      -0.892196    -0.945220    -0.219798      84.54
 H      -0.444642    -1.235255     0.840539      15.08
 C      -2.164100    -1.001296    -2.275202      36.92
 C      -3.005471    -1.637016    -3.270782      36.37
 H      -2.902167    -1.154104    -4.404997      25.73
 O      -2.653836    -3.125135    -3.428197     226.71
 H      -1.747970    -3.054283    -3.454249      31.19
 C      -4.564848    -1.511511    -2.827272      97.29
 H      -4.664149    -2.088964    -1.889529      28.79
 O      -4.965287    -0.125447    -2.725755     292.51
 H      -4.705484     0.355795    -2.013764      28.14
 C      -5.512766    -2.183294    -3.832785     112.13
 O      -5.256789    -3.558676    -4.128583     217.77
 H      -4.234026    -3.785613    -3.807915      29.88
 H      -5.562296    -1.567719    -4.761397      30.54
 H      -6.601945    -2.164481    -3.488808      27.74
55
name = lig-ACN-frame_381
 C       4.410997     2.488421    -0.621107      68.19
 H       4.136852     3.599954    -0.641221      22.53
 C       4.312821     0.249002     0.312520      54.89
 H       3.801709    -0.611694     0.708849      19.83
 C       5.537472    -0.060365    -0.359796       4.41
 O       6.151844    -1.421779    -0.228300     216.01
 C       6.040663    -2.045126     1.059498      90.76
 H       5.052612    -1.674104     1.744873      22.63
 H       7.019627    -1.842965     1.748495      24.01
 H       5.819313    -3.125860     0.774070      25.00
 C       6.132883     0.859406    -1.209674      33.40
 O       7.263637     0.546382    -2.104395      69.24
 H       7.981240     0.098197    -1.465503      17.61
 C       5.564217     2.037684    -1.380307      42.10
 H       6.117988     2.771487    -2.027939      25.23
 C       3.830985     1.535757     0.271197      29.76
 C       2.807691     1.902254     1.202532      73.64
 H       3.005809     3.025585     1.742522      21.42
 O       2.718134     1.039998     2.383394     251.04
 H       2.251899     0.261790     2.265015      25.21
 C       1.322399     2.025521     0.466305      90.51
 H       1.209213     2.723315    -0.325416      21.99
 C       0.245086     2.472621     1.421835      98.26
 O       0.498850     3.715576     2.143784     235.85
 H       1.012531     4.650000     1.664652      24.46
 H       0.102422     1.797159     2.127666      26.66
 H      -0.717881     2.492756     0.820632      23.66
 C      -1.833401    -1.462922    -0.932005     102.72
 H      -2.526511    -2.490247    -0.600734      23.44
 C      -1.367349     0.142347    -2.794291      45.58
 H      -1.468263     0.520537    -3.826084      21.79
 C      -0.402279     0.831347    -1.996876       8.68
 O       0.294908     1.911681    -2.440040     238.28
 C      -0.236421     2.661551    -3.515656     120.74
 H       0.517055     3.468295    -3.440827      24.31
 H       0.141151     2.402855    -4.577751      26.44
 H      -1.343415     2.791178    -3.641529      27.98
 C      -0.133687     0.219200    -0.720246      41.75
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 O       1.073567     0.706507     0.045904     205.62
 C      -0.788340    -0.907165    -0.217000     -14.39
 H      -0.706480    -1.378707     0.772818      17.18
 C      -2.208381    -0.933334    -2.291242      92.19
 C      -3.097608    -1.668959    -3.358742      52.71
 H      -2.912221    -1.054585    -4.371214      30.67
 O      -2.723180    -3.049921    -3.460310     235.60
 H      -1.768547    -3.304905    -3.623196      29.60
 C      -4.544801    -1.505404    -2.836434      98.33
 H      -4.544707    -1.882482    -1.801752      27.44
 O      -4.956745    -0.113480    -2.755523     260.48
 H      -4.101148     0.271550    -2.379813      22.49
 C      -5.559446    -2.165324    -3.829648     101.98
 O      -5.293723    -3.576595    -4.063351     218.26
 H      -4.257485    -3.647954    -3.995859      28.92
 H      -5.402590    -1.574404    -4.739065      30.02
 H      -6.637588    -2.068966    -3.421568      26.63
55
name = lig-ACN-frame_382
 C       4.473374     2.541467    -0.548409      50.69
 H       4.185827     3.639252    -0.475183      22.45
 C       4.358200     0.148121     0.330286      42.40
 H       3.751491    -0.609848     0.903977      19.70
 C       5.572291    -0.159873    -0.295894      22.15
 O       6.126425    -1.395955    -0.252869     252.27
 C       6.060684    -2.006584     1.050780      98.81
 H       5.077108    -1.626846     1.656070      22.39
 H       7.010492    -1.677484     1.682919      24.38
 H       6.169773    -3.131149     1.068334      24.69
 C       6.130886     0.763127    -1.304936       5.52
 O       7.280370     0.623681    -1.986288     150.46
 H       7.992315    -0.055220    -1.562724      24.73
 C       5.487597     2.092649    -1.379253      64.87
 H       6.111723     2.863929    -1.937404      24.83
 C       3.797839     1.558703     0.196540       2.78
 C       2.637412     2.023677     1.185774      72.71
 H       2.940621     3.157172     1.546693      22.80
 O       2.741646     1.141548     2.386028     210.94
 H       2.115849     0.318479     2.186338      21.07
 C       1.305268     2.047232     0.465665      82.54
 H       1.506784     2.655426    -0.411222      21.80
 C       0.160359     2.457759     1.545221     104.26
 O       0.494328     3.733588     2.182465     248.97
 H       0.625627     4.214987     1.147361      24.47
 H       0.144877     1.731046     2.282495      25.35
 H      -0.835566     2.551404     1.057738      22.75
 C      -1.838562    -1.349285    -1.024935      89.34
 H      -2.151025    -2.439170    -0.505970      17.81
 C      -1.322836     0.167740    -2.802483      15.28
 H      -1.539315     0.555647    -3.818715      18.02
 C      -0.417693     0.769348    -1.968778      23.46
 O       0.209693     1.913929    -2.394362     256.55
 C      -0.208547     2.689003    -3.566877     105.36
 H      -0.096680     3.794218    -3.503357      23.63
 H      -0.027012     1.918804    -4.394492      25.08
 H      -1.287966     2.733168    -3.465123      29.43
 C      -0.005852     0.280668    -0.681645      28.04
 O       1.071195     0.628425     0.024040     223.23
 C      -0.729960    -0.825171    -0.208126      80.87
 H      -0.323653    -1.214757     0.653640      15.70
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 C      -2.054779    -0.899867    -2.313572      97.92
 C      -3.105317    -1.583696    -3.293132      39.46
 H      -3.177741    -1.149202    -4.354615      29.54
 O      -2.818785    -3.040467    -3.498134     189.62
 H      -1.737375    -2.777095    -3.604127      23.64
 C      -4.581872    -1.535048    -2.859508     108.24
 H      -4.724366    -2.084390    -1.911272      29.17
 O      -4.888219    -0.127864    -2.842897     280.25
 H      -4.150021     0.552443    -2.292896      20.07
 C      -5.575996    -2.162480    -3.813825     110.40
 O      -5.347241    -3.582026    -3.976952     238.57
 H      -4.480202    -3.650531    -4.232490      36.48
 H      -5.615333    -1.664728    -4.771472      31.16
 H      -6.663571    -2.002763    -3.419313      27.55
55
name = lig-ACN-frame_383
 C       4.507326     2.474216    -0.514031      46.88
 H       4.165876     3.528329    -0.527963      22.02
 C       4.329649     0.271187     0.288709      55.60
 H       3.919326    -0.373326     1.141129      20.36
 C       5.519286    -0.136226    -0.404889      16.85
 O       6.140878    -1.458435    -0.268526     230.31
 C       6.138484    -1.993381     1.109707     100.27
 H       5.086660    -1.923585     1.650833      22.91
 H       6.926394    -1.454586     1.740406      24.27
 H       6.312593    -3.060940     0.836268      24.56
 C       6.048188     0.804263    -1.265099      21.88
 O       7.325533     0.660610    -1.897814     190.36
 H       7.652870    -0.216593    -1.701403      31.70
 C       5.576575     2.135105    -1.381108      55.36
 H       5.996187     2.828348    -2.172749      18.04
 C       3.790086     1.525790     0.274183      18.95
 C       2.639254     1.984137     1.160395      92.25
 H       2.751259     3.127039     1.501642      22.10
 O       2.705916     1.308449     2.378261     223.34
 H       2.166424     0.330868     2.308994      20.27
 C       1.215106     2.028346     0.560292      89.83
 H       1.109938     2.772004    -0.274684      20.81
 C       0.113545     2.449959     1.580167     104.80
 O       0.454507     3.707791     2.172637     298.21
 H       0.592550     4.569403     1.683738      29.01
 H       0.120621     1.671513     2.400306      23.43
 H      -0.896248     2.408390     1.174125      23.76
 C      -1.722955    -1.353083    -1.034156      50.32
 H      -2.527658    -2.188177    -0.748740      22.57
 C      -1.344898     0.210008    -2.830447     147.16
 H      -1.584929     0.676744    -3.818967      16.19
 C      -0.355181     0.818721    -1.974006      10.96
 O       0.273581     2.041474    -2.303579     200.89
 C      -0.355730     2.615823    -3.591632     116.04
 H       0.367970     3.460808    -3.537942      23.08
 H       0.155826     2.360037    -4.637850      24.69
 H      -1.396294     2.703500    -3.668037      27.65
 C       0.004265     0.304275    -0.730895      30.51
 O       1.156649     0.619548     0.046326     205.81
 C      -0.758108    -0.800580    -0.237859      11.68
 H      -0.496175    -1.262380     0.622875      19.01
 C      -2.053480    -1.003117    -2.366619      82.29
 C      -3.093994    -1.568873    -3.225450      41.05
 H      -2.981627    -0.929237    -4.127625      32.86
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 O      -2.790263    -2.982672    -3.530943     187.76
 H      -1.809824    -3.533954    -3.554224      25.14
 C      -4.597086    -1.483187    -2.828086      97.44
 H      -4.765928    -1.854505    -1.801313      30.88
 O      -4.861283    -0.091723    -2.934857     231.16
 H      -4.609728     0.226552    -1.906449      23.06
 C      -5.622697    -2.187935    -3.835741     104.99
 O      -5.442160    -3.601133    -3.899109     205.89
 H      -4.507851    -3.713033    -4.234427      31.84
 H      -5.673187    -1.654565    -4.756295      31.92
 H      -6.626604    -2.117367    -3.281412      28.28
55
name = lig-ACN-frame_384
 C       4.461155     2.506137    -0.580568      55.88
 H       4.099220     3.508666    -0.654328      24.71
 C       4.327702     0.253903     0.347407      45.81
 H       3.977619    -0.583644     1.024029      21.03
 C       5.395496    -0.097285    -0.487051     -13.09
 O       6.115505    -1.452380    -0.265247     234.87
 C       6.212218    -2.006356     1.083384     110.84
 H       5.191909    -2.091105     1.557298      26.80
 H       6.844506    -1.406629     1.798240      27.55
 H       6.716462    -2.982499     1.098469      27.07
 C       6.169581     0.894548    -1.264813      21.66
 O       7.316850     0.644998    -1.853583     145.85
 H       7.729807    -0.157954    -1.562641      17.05
 C       5.594913     2.125409    -1.334818      62.18
 H       6.094032     2.889005    -1.991758      24.73
 C       3.842037     1.603600     0.288202      28.90
 C       2.681217     2.056394     1.161469      81.36
 H       3.020961     3.153371     1.390294      25.02
 O       2.629740     1.401291     2.487838     213.10
 H       2.391506     0.439615     2.381573      25.97
 C       1.179418     1.978431     0.574815      92.25
 H       1.099398     2.695067    -0.317308      22.01
 C       0.097458     2.403363     1.592044     101.70
 O       0.389606     3.702183     2.248147     315.38
 H       0.619753     4.149979     1.553712      35.72
 H      -0.018831     1.739266     2.576346      23.50
 H      -0.838750     2.423321     1.035419      25.46
 C      -1.759069    -1.505780    -1.040884      73.56
 H      -2.288760    -2.235094    -0.411530      19.99
 C      -1.307491     0.235344    -2.776159      29.40
 H      -1.617069     0.576248    -3.778056      21.28
 C      -0.313487     0.910985    -2.035457       5.70
 O       0.242025     2.131098    -2.357330     246.05
 C      -0.252690     2.679617    -3.579054      95.31
 H      -0.122864     3.745044    -3.713909      24.78
 H      -0.158616     1.712954    -4.275169      26.85
 H      -1.334399     2.715252    -3.422252      29.92
 C       0.004523     0.217579    -0.729481      27.64
 O       1.144583     0.677040     0.040253     211.42
 C      -0.753236    -0.825667    -0.246605      43.06
 H      -0.713782    -1.098163     0.790229      18.78
 C      -1.991899    -0.893785    -2.361790      64.55
 C      -3.015996    -1.646285    -3.311679      32.68
 H      -3.051223    -1.141989    -4.286584      30.73
 O      -2.788728    -3.019049    -3.574479     253.75
 H      -1.790929    -2.933126    -3.335649      28.78
 C      -4.599222    -1.453808    -2.837102      89.60
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 H      -4.730026    -1.750104    -1.786749      28.79
 O      -4.893300     0.004597    -2.964503     239.01
 H      -4.694878     0.456065    -2.193368      28.71
 C      -5.665603    -2.190570    -3.708803     111.80
 O      -5.520904    -3.647487    -3.873971     209.37
 H      -4.430451    -3.789659    -3.822699      29.25
 H      -5.621401    -1.771520    -4.691535      30.34
 H      -6.704613    -1.940168    -3.377893      28.56
55
name = lig-ACN-frame_385
 C       4.406924     2.567496    -0.654142      49.56
 H       4.056478     3.559751    -0.686807      24.02
 C       4.339259     0.248209     0.354970      46.05
 H       3.676637    -0.409433     0.930984      22.55
 C       5.481355    -0.179581    -0.424679      11.85
 O       6.050344    -1.355525    -0.312007     251.11
 C       6.269926    -1.951588     1.049327     104.90
 H       5.382437    -2.343070     1.509402      26.84
 H       6.690488    -1.158746     1.637216      27.01
 H       6.960751    -2.740282     0.767116      25.80
 C       6.161242     0.828633    -1.154522      21.09
 O       7.394053     0.587038    -1.883991     149.52
 H       8.046289     0.015584    -1.276130      19.07
 C       5.585636     2.237883    -1.336703      42.83
 H       6.253642     3.019258    -1.766682      23.65
 C       3.828821     1.596487     0.306986       4.53
 C       2.653287     2.147413     1.259105      79.95
 H       2.691495     3.228977     1.534696      25.09
 O       2.600361     1.474718     2.594482     233.02
 H       2.360711     0.620387     2.424139      29.53
 C       1.299920     2.051924     0.563327      67.54
 H       1.288493     2.840603    -0.286629      20.91
 C       0.065976     2.376693     1.645606      88.62
 O       0.314735     3.668102     2.259747     271.29
 H       0.756962     4.356927     1.677303      29.06
 H      -0.095517     1.290775     2.251591      21.39
 H      -0.854587     2.488274     1.110866      24.81
 C      -1.743908    -1.520508    -1.022967      34.43
 H      -2.228714    -2.408769    -0.911188      22.25
 C      -1.300131     0.248791    -2.780924      80.61
 H      -1.533594     0.722035    -3.741001      19.63
 C      -0.307380     0.878148    -1.941006      16.49
 O       0.274836     2.178940    -2.343410     225.78
 C      -0.307021     2.685980    -3.605207     100.93
 H       0.418825     3.474621    -3.882660      25.82
 H      -0.141150     2.122613    -4.681748      25.77
 H      -1.347867     2.909892    -3.468705      28.62
 C       0.048060     0.294909    -0.792408      20.62
 O       1.041461     0.634904     0.019798     191.33
 C      -0.772662    -0.878031    -0.253593      45.02
 H      -0.359724    -1.129805     0.798584      18.15
 C      -2.020638    -0.973347    -2.331537      80.47
 C      -3.109908    -1.558530    -3.409207      43.53
 H      -2.913910    -1.072753    -4.364190      31.83
 O      -2.694794    -3.086413    -3.554329     241.02
 H      -1.832042    -3.268725    -3.548187      32.65
 C      -4.536884    -1.379176    -2.839378      90.97
 H      -4.493301    -1.698907    -1.776295      27.41
 O      -4.930044     0.042543    -3.019258     245.94
 H      -4.283759     0.405059    -2.517387      34.18
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 C      -5.671691    -2.179166    -3.634842     105.29
 O      -5.561474    -3.649408    -3.821707     213.16
 H      -4.643783    -3.936653    -3.503539      31.19
 H      -5.739848    -1.681536    -4.621809      29.77
 H      -6.625121    -2.065901    -3.120745      27.96
55
name = lig-ACN-frame_386
 C       4.379269     2.540439    -0.600318      56.26
 H       4.024793     3.543321    -0.677579      23.21
 C       4.283507     0.340670     0.333737      53.36
 H       3.920652    -0.444265     0.950185      21.04
 C       5.506367    -0.007238    -0.284494     -11.36
 O       6.020511    -1.403528    -0.349204     269.35
 C       6.354788    -1.866957     0.935537     124.64
 H       5.593345    -2.410003     1.340560      28.95
 H       6.638670    -1.163450     1.671161      27.52
 H       7.198696    -2.539649     0.888571      27.15
 C       6.201342     0.917726    -1.169270       6.52
 O       7.379219     0.554485    -1.855023     160.15
 H       8.132580     0.078454    -1.291939      23.30
 C       5.646973     2.150856    -1.272163      54.29
 H       6.103609     2.832940    -2.023947      21.13
 C       3.798234     1.669340     0.303170      21.80
 C       2.643183     2.090520     1.340304      95.15
 H       2.951757     3.112899     1.515383      25.90
 O       2.616899     1.546429     2.640540     242.93
 H       2.154617     0.594580     2.679759      23.19
 C       1.232742     2.090036     0.597957      85.65
 H       1.270126     2.795370    -0.343210      22.07
 C       0.111538     2.400600     1.464924      99.46
 O       0.238515     3.594839     2.335785     187.67
 H       0.596536     4.385082     1.553208      25.56
 H       0.226181     1.780849     2.536736      21.31
 H      -0.829602     2.270309     0.969239      25.97
 C      -1.703218    -1.494621    -1.119579      69.54
 H      -1.999285    -2.315714    -0.715206      22.34
 C      -1.350213     0.205620    -2.749762      33.71
 H      -1.640459     0.604604    -3.737031      21.59
 C      -0.388695     0.926139    -2.024742       7.47
 O       0.259121     2.071918    -2.333676     213.82
 C      -0.264506     2.765552    -3.698295      93.89
 H       0.397459     3.620814    -3.694114      25.22
 H      -0.221756     1.848327    -4.401180      27.19
 H      -1.255343     3.347794    -3.671801      28.14
 C      -0.067348     0.248347    -0.693556      73.85
 O       1.091641     0.678208     0.114117     169.61
 C      -0.706571    -0.854317    -0.315882      28.10
 H      -0.365033    -1.597618     0.551180      18.49
 C      -2.048906    -0.943165    -2.436526      33.23
 C      -2.969226    -1.577661    -3.362467      48.20
 H      -3.004504    -1.060345    -4.341733      30.95
 O      -2.712150    -3.074836    -3.523174     230.99
 H      -1.796524    -3.001439    -3.512554      30.22
 C      -4.507211    -1.378633    -2.925450      88.51
 H      -4.559920    -1.542675    -1.822447      27.42
 O      -4.914822     0.005183    -3.065718     198.17
 H      -4.227477     0.689544    -2.589557      24.29
 C      -5.664062    -2.171135    -3.564703     117.30
 O      -5.558341    -3.600855    -3.746473     278.75
 H      -4.692296    -3.770003    -3.617096      35.67
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 H      -5.972858    -1.738550    -4.554074      28.79
 H      -6.468164    -1.951803    -2.893142      28.23
55
name = lig-ACN-frame_387
 C       4.478816     2.538263    -0.540553      55.91
 H       4.112679     3.543782    -0.794713      24.60
 C       4.327166     0.356088     0.382167      52.96
 H       3.833853    -0.318493     1.014164      23.52
 C       5.545439     0.062704    -0.288803      22.92
 O       5.963577    -1.317810    -0.378980     275.30
 C       6.468642    -1.882481     0.936592     110.23
 H       5.772809    -2.467887     1.322759      29.67
 H       6.588370    -1.052037     1.504221      27.99
 H       7.393834    -2.414351     0.803291      26.56
 C       6.285354     0.890582    -1.095491      11.04
 O       7.327498     0.570588    -1.836795     123.39
 H       7.755831    -0.168857    -1.421082      20.39
 C       5.578329     2.203315    -1.276345      69.31
 H       5.914430     2.894685    -2.079696      24.82
 C       3.734024     1.652767     0.372866       9.26
 C       2.651375     2.135043     1.266313      88.17
 H       2.801170     3.138901     1.467630      26.71
 O       2.652372     1.540444     2.691716     175.14
 H       2.180800     0.551242     2.568405      24.01
 C       1.284929     2.068319     0.557460      85.53
 H       1.366238     2.794053    -0.367703      23.75
 C       0.071713     2.413971     1.536571      91.71
 O       0.177023     3.595030     2.296449     241.03
 H       0.196246     4.566721     1.784423      26.55
 H      -0.065800     1.267988     2.048082      22.97
 H      -0.851054     2.454214     0.942807      24.70
 C      -1.668067    -1.508456    -1.205363      45.55
 H      -2.193374    -2.282405    -0.953250      21.22
 C      -1.419779     0.284497    -2.867897      74.41
 H      -1.642792     0.748524    -3.877737      17.25
 C      -0.467740     0.857929    -1.911387      19.73
 O       0.176495     2.032381    -2.428798     237.05
 C      -0.123841     2.801545    -3.638813      99.90
 H       0.643173     3.456589    -4.112754      25.13
 H      -0.239687     2.180374    -4.588910      26.25
 H      -1.223545     3.041700    -3.371226      25.33
 C      -0.043798     0.408113    -0.658862      65.94
 O       1.080075     0.711382     0.159832     195.38
 C      -0.682489    -0.933115    -0.398355      59.70
 H      -0.432576    -1.240020     0.734310      15.90
 C      -1.975559    -0.942294    -2.385964       9.49
 C      -2.996422    -1.655816    -3.391603      64.09
 H      -2.706265    -1.242669    -4.359434      27.08
 O      -2.735464    -2.989536    -3.482605     266.71
 H      -1.811139    -3.412949    -3.282360      27.39
 C      -4.453096    -1.397077    -2.907500      90.35
 H      -4.424412    -1.770202    -1.843334      28.27
 O      -4.881706    -0.011213    -3.168855     207.69
 H      -4.426207     0.487986    -2.209129      22.33
 C      -5.705143    -2.127780    -3.533699     103.60
 O      -5.508638    -3.558366    -3.645924     205.39
 H      -4.544551    -3.691307    -3.996077      30.80
 H      -5.949113    -1.650814    -4.537464      29.08
 H      -6.536489    -2.006739    -2.903572      29.09
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name = lig-ACN-frame_388
 C       4.458127     2.590813    -0.454807      56.55
 H       3.974072     3.614468    -0.471512      23.52
 C       4.380324     0.347252     0.496345      55.07
 H       3.914695    -0.483604     0.969347      22.21
 C       5.493812    -0.021275    -0.269258      -1.50
 O       5.958354    -1.282860    -0.339650     272.11
 C       6.541223    -1.855478     0.907149     117.08
 H       6.007277    -2.564338     1.293396      31.47
 H       6.834240    -1.241100     1.682833      29.13
 H       7.381932    -2.320941     0.460922      26.44
 C       6.172450     1.024135    -1.058115      11.81
 O       7.348815     0.585391    -1.853303     216.18
 H       7.533985    -0.351411    -1.719969      20.44
 C       5.607175     2.222633    -1.323690      62.14
 H       6.111154     2.992921    -1.940808      23.66
 C       3.893299     1.660295     0.375380      27.41
 C       2.640775     2.199195     1.302922      86.87
 H       2.738265     3.179100     1.459919      28.41
 O       2.674651     1.522921     2.618324     234.89
 H       2.457786     0.587318     2.522872      27.28
 C       1.282723     2.081297     0.577665      77.66
 H       1.260935     2.796697    -0.340811      23.20
 C      -0.007878     2.412220     1.483921      93.06
 O       0.131458     3.620799     2.318553     286.92
 H      -0.018833     4.178129     1.668020      33.94
 H      -0.328192     1.701414     2.430390      22.55
 H      -0.827712     2.566276     0.738458      25.29
 C      -1.605750    -1.534884    -1.183795     114.26
 H      -1.999232    -2.443388    -0.877242      23.96
 C      -1.420427     0.318362    -2.800727      -7.06
 H      -1.590486     0.853414    -3.816379      15.69
 C      -0.492642     0.987792    -2.023576      33.97
 O       0.237580     2.031816    -2.442227     253.25
 C      -0.141655     2.711668    -3.624454     132.25
 H       0.680146     3.462326    -3.348654      23.28
 H      -0.145029     2.098006    -4.505831      29.62
 H      -0.889722     3.635306    -3.692226      26.94
 C      -0.082908     0.321936    -0.722452      76.82
 O       0.999279     0.697774     0.106642     178.13
 C      -0.650231    -0.849947    -0.336522     -15.30
 H      -0.436115    -1.340380     0.650266      18.07
 C      -2.010229    -0.911021    -2.541159      62.38
 C      -2.972363    -1.563200    -3.425368      47.55
 H      -3.110591    -1.056739    -4.397398      32.67
 O      -2.792860    -3.114846    -3.439454     161.04
 H      -1.684925    -3.001899    -3.162390      26.25
 C      -4.495135    -1.408795    -2.909851      87.35
 H      -4.481980    -1.444956    -1.788883      28.36
 O      -4.788773    -0.008597    -3.164156     208.49
 H      -4.675581     0.514120    -2.280132      26.20
 C      -5.668878    -2.130233    -3.537190     107.14
 O      -5.446507    -3.546487    -3.584199     182.47
 H      -4.531594    -3.655281    -4.173764      29.99
 H      -5.854376    -1.675145    -4.571895      29.69
 H      -6.525101    -1.937395    -2.966139      29.68
55
name = lig-ACN-frame_389
 C       4.497350     2.661725    -0.470719      46.92
 H       4.165402     3.760518    -0.463092      21.39
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 C       4.379922     0.348431     0.570145      50.46
 H       3.897375    -0.373993     1.251311      20.05
 C       5.478406     0.066658    -0.282671      10.31
 O       5.994826    -1.332648    -0.279492     297.76
 C       6.660905    -1.917542     0.837696     116.38
 H       5.991142    -2.492817     1.242178      30.52
 H       6.894072    -1.107944     1.492839      26.43
 H       7.557531    -2.453967     0.627689      26.98
 C       6.151410     0.936030    -1.181858      -1.67
 O       7.255769     0.668686    -1.825705     117.20
 H       7.515839    -0.326993    -1.490729      23.16
 C       5.594055     2.334300    -1.235061      71.38
 H       6.126050     3.010906    -1.927832      20.05
 C       3.898651     1.723168     0.507849       6.04
 C       2.703613     2.136217     1.309893      94.98
 H       2.860610     3.082261     1.533131      27.28
 O       2.686827     1.504377     2.528838     275.54
 H       2.545543     0.608483     2.446941      28.40
 C       1.127680     2.061588     0.622604      79.16
 H       1.237681     2.812040    -0.220379      22.86
 C      -0.045783     2.461662     1.455926      95.79
 O       0.083929     3.665664     2.275550     284.83
 H       0.183594     4.554248     1.891897      29.54
 H      -0.179288     1.424487     2.071583      22.70
 H      -1.015824     2.432026     0.837968      23.69
 C      -1.595867    -1.476422    -1.263719      83.92
 H      -1.837478    -2.505417    -0.952408      16.84
 C      -1.465560     0.343388    -2.825161      81.02
 H      -1.914078     0.806004    -3.804447      21.05
 C      -0.443671     0.956500    -1.963861      27.18
 O       0.313396     2.064783    -2.358856     239.49
 C      -0.030503     2.829906    -3.653373      83.23
 H       0.730436     3.510628    -4.179514      23.25
 H       0.017461     2.102755    -4.424820      27.26
 H      -1.230920     2.943785    -3.515361      23.96
 C      -0.088749     0.337942    -0.833624      22.13
 O       0.972849     0.706530     0.030046     194.57
 C      -0.769308    -0.839965    -0.360206      60.05
 H      -0.310866    -1.213432     0.476485      19.09
 C      -1.954267    -0.929334    -2.453999      49.22
 C      -3.114429    -1.647262    -3.416867      34.01
 H      -2.924564    -1.305180    -4.460243      27.98
 O      -2.807111    -3.108437    -3.413659     216.75
 H      -1.762937    -3.458550    -3.505654      27.00
 C      -4.481244    -1.302696    -2.843493     103.91
 H      -4.553512    -1.724826    -1.790583      26.49
 O      -4.743918     0.085128    -3.143385     280.37
 H      -4.400914     0.474322    -2.439447      33.56
 C      -5.591966    -2.158964    -3.577586     106.35
 O      -5.414392    -3.580859    -3.574952     240.30
 H      -4.504252    -3.763396    -3.848476      32.10
 H      -5.764434    -1.805688    -4.647285      29.30
 H      -6.516494    -2.002381    -3.059611      29.01
55
name = lig-ACN-frame_390
 C       4.500093     2.669730    -0.362583      50.73
 H       4.091723     3.710430    -0.526836      21.20
 C       4.415706     0.492329     0.537683      34.53
 H       4.089578    -0.225273     1.352627      19.59
 C       5.520688    -0.020021    -0.244055       2.70
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 O       6.021011    -1.306969    -0.356148     216.14
 C       6.726175    -1.940726     0.892195      99.13
 H       6.193626    -2.544412     1.472671      28.70
 H       7.172868    -1.182923     1.557229      24.54
 H       7.472500    -2.555091     0.405400      25.43
 C       5.988665     0.989307    -1.168749      10.93
 O       7.223077     0.687731    -1.856405     204.52
 H       7.868496     0.058826    -1.370067      27.84
 C       5.625729     2.297229    -1.177687      52.34
 H       6.011448     3.070610    -1.827040      18.63
 C       3.873701     1.772130     0.459025      39.87
 C       2.593982     2.152793     1.263800      84.94
 H       2.603450     3.107557     1.465535      27.47
 O       2.686780     1.413602     2.603665     197.89
 H       2.298113     0.422654     2.421967      20.45
 C       1.197575     2.106960     0.492975      75.04
 H       1.197823     2.814501    -0.362184      22.39
 C      -0.097408     2.466537     1.496622      87.82
 O       0.041059     3.687756     2.251387     188.61
 H       0.553362     4.246968     1.386271      24.26
 H      -0.263850     1.793671     2.406731      22.84
 H      -1.050160     2.590315     0.821367      22.75
 C      -1.643135    -1.554285    -1.237035      50.39
 H      -2.195513    -2.593223    -1.123687      16.20
 C      -1.495169     0.360725    -2.861013      18.72
 H      -1.830579     0.986928    -3.792427      14.00
 C      -0.426152     0.978532    -2.106845       6.71
 O       0.424625     2.210449    -2.334587     222.10
 C       0.006282     2.709758    -3.681211     116.49
 H       0.434911     3.775751    -3.652412      23.76
 H       0.107315     1.992877    -4.441581      30.44
 H      -1.120458     3.231340    -3.592590      26.06
 C      -0.079248     0.375073    -0.747180      45.58
 O       1.002135     0.754158    -0.002796     191.24
 C      -0.765536    -0.802437    -0.413023      32.86
 H      -0.655523    -1.199346     0.477693      21.15
 C      -2.045169    -0.928999    -2.511111      49.16
 C      -2.988229    -1.701139    -3.296440      76.68
 H      -3.078697    -1.212549    -4.337688      27.03
 O      -2.876038    -3.108444    -3.395215     278.86
 H      -1.931042    -3.149577    -3.472566      33.10
 C      -4.508347    -1.352516    -2.876828      75.99
 H      -4.533683    -1.315186    -1.750212      26.21
 O      -4.719609     0.166829    -3.086162     212.68
 H      -4.143726     0.575818    -2.410121      24.81
 C      -5.572901    -2.151452    -3.636783     107.41
 O      -5.374020    -3.643108    -3.562286     246.53
 H      -4.495990    -3.765115    -3.404471      33.31
 H      -5.515796    -1.749564    -4.696582      29.11
 H      -6.583018    -1.925802    -3.264237      27.61
55
name = lig-ACN-frame_391
 C       4.474487     2.769992    -0.358757      59.41
 H       4.059515     3.784800    -0.391829      24.18
 C       4.446432     0.466742     0.574764      42.16
 H       3.947959    -0.233803     1.319061      19.11
 C       5.491869     0.012648    -0.266259       4.43
 O       6.066439    -1.296543    -0.315337     281.59
 C       6.739871    -1.917852     0.859080     103.09
 H       6.007831    -2.319999     1.447547      30.62
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 H       7.438162    -1.192574     1.378651      26.62
 H       7.394632    -2.662005     0.371287      26.00
 C       6.126180     0.945955    -1.110788       7.11
 O       7.183400     0.716165    -1.926342     204.91
 H       7.810462     0.357615    -1.353806      25.55
 C       5.546663     2.299956    -1.133509      45.74
 H       6.195664     2.902551    -1.730203      22.29
 C       3.785585     1.764249     0.411562      -3.68
 C       2.515922     2.157360     1.304007      85.15
 H       2.624270     3.027536     1.698118      27.33
 O       2.608057     1.364560     2.614253     188.46
 H       2.199594     0.338503     2.503621      20.59
 C       1.191736     2.117850     0.508113      84.19
 H       1.288471     2.871508    -0.267758      24.73
 C      -0.069523     2.451890     1.503846      95.77
 O       0.065279     3.761432     2.146100     213.08
 H       0.599081     4.588863     1.615304      24.53
 H      -0.224438     1.559049     2.121027      25.24
 H      -0.989854     2.386623     0.756178      23.85
 C      -1.706054    -1.467762    -1.278003      50.50
 H      -2.067940    -2.385222    -0.593781      15.06
 C      -1.406204     0.410220    -2.859879      82.37
 H      -1.761715     0.693038    -3.899296      20.60
 C      -0.334837     1.014584    -2.064895      10.56
 O       0.349819     2.172660    -2.395673     245.90
 C       0.016629     2.742763    -3.639237     110.96
 H       0.722876     3.580828    -3.815100      24.93
 H       0.487707     2.174580    -4.428589      27.25
 H      -1.167741     2.789532    -3.869475      23.51
 C      -0.142952     0.407372    -0.855975      18.87
 O       1.051157     0.785054    -0.014645     161.42
 C      -0.769776    -0.863707    -0.379691      35.81
 H      -0.548644    -1.128044     0.576762      18.63
 C      -1.981379    -0.869405    -2.447799      39.64
 C      -3.101889    -1.577809    -3.361590      47.39
 H      -2.891587    -1.274308    -4.453116      25.37
 O      -2.844987    -3.130770    -3.348289     260.54
 H      -2.063616    -3.435354    -3.144600      32.58
 C      -4.511791    -1.298631    -2.841002     100.34
 H      -4.761560    -1.767694    -1.833642      28.27
 O      -4.700299     0.122846    -3.098932     228.57
 H      -4.450328     0.557076    -2.066840      21.36
 C      -5.532806    -2.177110    -3.702823     104.25
 O      -5.388565    -3.618159    -3.547226     222.31
 H      -4.372647    -3.720337    -3.303233      27.46
 H      -5.419615    -2.014565    -4.784153      29.97
 H      -6.598299    -1.887380    -3.446701      28.00
55
name = lig-ACN-frame_392
 C       4.403287     2.708453    -0.396935      55.55
 H       4.203982     3.737475    -0.468879      23.47
 C       4.327702     0.445489     0.582875      29.77
 H       3.910672    -0.377666     1.202785      18.19
 C       5.549750     0.034016    -0.250416      -1.72
 O       6.075905    -1.258454    -0.273990     255.41
 C       6.708874    -1.871054     0.806852     108.18
 H       6.103810    -2.086538     1.652570      29.02
 H       7.416824    -1.118809     1.303702      24.89
 H       7.162580    -2.862765     0.569464      25.68
 C       6.151798     1.048994    -1.047137      31.57
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 O       7.192053     0.734319    -1.993062     172.20
 H       7.959589     0.146905    -1.678092      15.54
 C       5.565785     2.320093    -1.123424      39.72
 H       5.972508     3.099343    -1.727309      23.14
 C       3.752954     1.739396     0.479946      14.92
 C       2.597826     2.076579     1.411409     103.43
 H       2.727465     3.002748     1.608343      28.50
 O       2.464387     1.359074     2.566610     278.63
 H       2.407219     0.370341     2.388897      23.27
 C       1.161815     2.123188     0.617397      81.54
 H       1.248251     2.854980    -0.158315      24.68
 C       0.013748     2.491829     1.385403     114.66
 O       0.079273     3.798850     2.070415     284.63
 H       0.395226     4.379108     1.417128      31.72
 H       0.023542     1.938763     2.263921      25.53
 H      -1.049830     2.458479     0.890006      23.93
 C      -1.701321    -1.356750    -1.114439      81.28
 H      -2.419594    -2.322348    -1.140721      17.50
 C      -1.284241     0.354637    -2.884404      18.24
 H      -1.411138     0.817036    -3.852861      18.42
 C      -0.426048     0.950107    -2.047809      18.51
 O       0.267767     2.115769    -2.402248     222.51
 C       0.101609     2.776594    -3.766544     104.44
 H       0.248463     3.822703    -3.656214      25.99
 H       0.463497     2.076077    -4.554719      26.62
 H      -1.060755     2.868913    -3.915172      26.66
 C      -0.014621     0.372998    -0.773648      35.45
 O       1.021810     0.771225    -0.074761     208.06
 C      -0.705227    -0.734767    -0.384953      21.04
 H      -0.318454    -1.289849     0.482064      19.98
 C      -1.997328    -0.804770    -2.472864      74.56
 C      -3.042205    -1.573153    -3.370440      39.27
 H      -3.110588    -1.248016    -4.474079      28.56
 O      -2.836777    -3.065973    -3.292699     272.96
 H      -1.894569    -3.030634    -2.987172      30.29
 C      -4.546383    -1.363545    -2.932125      94.44
 H      -4.465057    -1.488439    -1.822987      27.15
 O      -4.735967     0.054333    -3.060948     214.94
 H      -4.738551     0.580102    -2.026166      21.77
 C      -5.510712    -2.172952    -3.802917     103.22
 O      -5.416922    -3.563385    -3.500824     212.41
 H      -4.374123    -3.847776    -3.632530      26.25
 H      -5.341897    -1.834307    -4.825361      30.20
 H      -6.592908    -1.896675    -3.533129      27.25
55
name = lig-ACN-frame_393
 C       4.356072     2.544105    -0.382759      52.10
 H       3.743300     3.399980    -0.516530      22.28
 C       4.346305     0.371701     0.451740      55.43
 H       3.932969    -0.413313     1.052826      21.15
 C       5.554789     0.133008    -0.132588      20.36
 O       6.019360    -1.201258    -0.342379     268.62
 C       6.680362    -1.804468     0.944911      89.27
 H       5.929847    -1.915587     1.726536      25.65
 H       7.675207    -1.309780     1.147753      24.78
 H       6.951665    -2.756997     0.426169      25.29
 C       6.180676     1.080611    -1.065742      -1.94
 O       7.184200     0.779121    -2.011430     149.75
 H       7.614852    -0.077981    -1.513660      23.76
 C       5.573003     2.383701    -1.119909      54.50
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 H       5.927850     3.114906    -1.836965      21.01
 C       3.836763     1.657881     0.531570      38.78
 C       2.555357     2.120844     1.364477      99.66
 H       2.696291     2.972909     1.751573      28.13
 O       2.354946     1.321516     2.612056     277.29
 H       2.318123     0.418674     2.513278      26.55
 C       1.319859     2.124070     0.505610      80.94
 H       1.459083     2.819926    -0.285673      24.13
 C      -0.056121     2.522026     1.521107     102.61
 O       0.115759     3.862853     1.951284     300.75
 H       0.221097     4.499461     1.337236      31.47
 H      -0.217711     1.845835     2.226408      26.65
 H      -0.878598     2.332392     0.720750      23.80
 C      -1.791116    -1.246977    -1.194211      66.55
 H      -2.093025    -2.133688    -0.495613      15.01
 C      -1.295548     0.228098    -2.985486      53.30
 H      -1.463919     0.655928    -3.948159      21.45
 C      -0.403907     0.973066    -2.039852       8.55
 O       0.257412     2.163844    -2.432045     207.77
 C       0.038294     2.735915    -3.795238     115.95
 H       0.572205     3.591766    -3.601458      26.40
 H       0.850161     2.484068    -4.555592      25.15
 H      -0.983651     2.811320    -4.202001      27.35
 C       0.000097     0.398664    -0.787095      17.74
 O       1.148376     0.825319    -0.006992     179.67
 C      -0.678629    -0.762493    -0.304188      40.62
 H      -0.328441    -1.281111     0.706481      17.05
 C      -2.056427    -0.827892    -2.475502      46.50
 C      -2.985419    -1.596414    -3.330083      68.61
 H      -2.700453    -1.173955    -4.354943      25.81
 O      -2.762605    -2.941965    -3.230184     229.23
 H      -1.786883    -3.470578    -3.385877      24.19
 C      -4.459786    -1.370969    -2.951022      99.70
 H      -4.778733    -1.900324    -2.015864      26.90
 O      -4.858471     0.051672    -3.062425     272.91
 H      -4.446384     0.395042    -2.113559      22.37
 C      -5.513779    -2.115964    -3.819604      99.12
 O      -5.442869    -3.554348    -3.511000     206.21
 H      -4.563730    -3.821916    -3.878964      32.43
 H      -5.347883    -2.046268    -4.875464      30.04
 H      -6.597260    -1.744278    -3.623198      27.67
55
name = lig-ACN-frame_394
 C       4.351066     2.573271    -0.390079      51.16
 H       3.832356     3.507978    -0.618845      23.16
 C       4.398487     0.264311     0.499595      23.08
 H       3.939815    -0.626152     0.892587      19.63
 C       5.651091     0.170148    -0.262595      30.33
 O       6.025855    -1.167730    -0.291620     280.80
 C       6.601582    -1.766398     0.899249      79.86
 H       5.894103    -1.583343     1.810442      25.26
 H       7.430403    -1.138345     1.303643      23.74
 H       6.797928    -2.867930     0.903392      25.71
 C       6.169979     1.134807    -1.085905       6.59
 O       7.161702     0.796322    -1.913731     164.07
 H       7.512450    -0.086091    -1.762412      28.15
 C       5.502136     2.379947    -1.134131      66.16
 H       5.847322     3.116497    -1.884644      20.57
 C       3.802478     1.607549     0.577668      10.58
 C       2.596488     2.075490     1.394901      97.16
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 H       2.740175     2.985101     1.634115      28.00
 O       2.284040     1.341260     2.650195     268.71
 H       2.186087     0.389241     2.350885      23.71
 C       1.264879     2.187968     0.515009      82.51
 H       1.296172     2.931281    -0.238650      25.41
 C       0.026018     2.534915     1.377211     107.95
 O       0.109994     3.927688     1.926328     212.12
 H       0.311479     4.491219     0.984866      25.56
 H      -0.032104     2.038060     2.190804      27.65
 H      -0.984242     2.554539     0.852935      24.38
 C      -1.765735    -1.265827    -1.033044      31.72
 H      -2.521969    -2.015336    -0.816683      18.37
 C      -1.249573     0.273980    -2.958137      49.68
 H      -1.455732     0.416079    -4.009517      20.60
 C      -0.343538     0.961032    -2.179750       1.80
 O       0.219454     2.182983    -2.482918     231.86
 C       0.116648     2.771577    -3.770256     135.13
 H       0.109776     3.793682    -3.807722      27.21
 H       0.558881     1.948918    -4.448576      26.54
 H      -0.888823     2.612614    -4.073549      29.46
 C       0.025266     0.431949    -0.766399      40.70
 O       1.242499     0.790446    -0.005258     146.88
 C      -0.714455    -0.703153    -0.371550      29.91
 H      -0.614781    -1.145072     0.768067      16.96
 C      -2.007233    -0.821068    -2.362413      46.21
 C      -2.960994    -1.532598    -3.362598      49.16
 H      -2.928770    -1.273142    -4.453002      27.07
 O      -2.709823    -3.024254    -3.187949     154.90
 H      -1.620371    -2.998643    -3.535857      23.50
 C      -4.501170    -1.343012    -2.992425      96.23
 H      -4.444582    -1.648448    -1.932224      25.84
 O      -4.939690     0.015676    -3.011392     297.20
 H      -4.479418     0.551883    -2.487710      31.79
 C      -5.475226    -2.137633    -3.865222     104.96
 O      -5.486581    -3.544842    -3.556722     260.52
 H      -4.626348    -3.838727    -3.704298      34.77
 H      -5.413690    -1.893175    -4.925850      28.80
 H      -6.483593    -1.721302    -3.490864      26.59
55
name = lig-ACN-frame_395
 C       4.308409     2.611058    -0.303931      50.62
 H       3.906221     3.655453    -0.226754      22.58
 C       4.452797     0.384931     0.558451      59.31
 H       4.091222    -0.524315     1.072387      20.06
 C       5.525331     0.055897    -0.258621      -3.56
 O       6.134290    -1.227795    -0.332739     272.60
 C       6.505584    -1.648424     0.990456     100.02
 H       5.625100    -1.540618     1.775365      26.51
 H       7.502624    -1.267615     1.195821      25.62
 H       6.658016    -2.735413     0.752114      26.91
 C       6.122572     1.137460    -1.072922      13.92
 O       7.238649     0.834086    -1.898658     179.13
 H       7.531474     0.017463    -1.553393      21.45
 C       5.430351     2.366432    -1.198962      52.82
 H       5.758626     3.230453    -1.839319      23.99
 C       3.801272     1.577256     0.511783      31.52
 C       2.585185     2.070382     1.460522      95.48
 H       2.909404     2.898309     1.805719      27.43
 O       2.266259     1.407327     2.625661     267.87
 H       2.132330     0.295294     2.583553      20.07
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 C       1.270957     2.174284     0.534696      71.15
 H       1.528893     2.755099    -0.308561      24.45
 C       0.040025     2.628539     1.311004     119.12
 O       0.102690     3.935113     1.855375     241.18
 H       0.576112     4.871954     1.307690      22.52
 H       0.068413     1.993472     2.046632      27.30
 H      -0.820950     2.282056     0.700191      25.32
 C      -1.857314    -1.301308    -1.038043      68.21
 H      -2.313759    -2.054514    -0.538797      15.84
 C      -1.234252     0.279022    -2.887518      53.18
 H      -1.338319     0.693357    -3.912240      18.16
 C      -0.195260     0.953519    -2.121425      15.85
 O       0.266109     2.240806    -2.434410     220.16
 C       0.025235     2.684900    -3.866342     126.87
 H       0.459157     3.645469    -3.750910      26.18
 H       0.874842     2.432021    -4.631667      26.37
 H      -0.954205     2.630102    -4.107807      29.20
 C       0.085139     0.448104    -0.870099      32.59
 O       1.150316     0.770997    -0.113207     186.96
 C      -0.713396    -0.586448    -0.272586      73.58
 H      -0.261805    -0.916281     0.837755      18.65
 C      -1.959805    -0.792597    -2.416553      21.28
 C      -2.979878    -1.546775    -3.314272      58.02
 H      -2.710314    -1.151330    -4.291688      27.32
 O      -2.700497    -3.033061    -3.218660     224.76
 H      -1.689209    -3.330789    -3.009647      24.83
 C      -4.462146    -1.345218    -2.935759      99.17
 H      -4.676494    -1.745627    -1.950989      28.31
 O      -5.014862     0.027434    -3.031073     286.69
 H      -4.605508     0.442645    -2.284929      28.81
 C      -5.494178    -2.139516    -3.816334      99.17
 O      -5.504330    -3.564022    -3.640998     224.90
 H      -4.513631    -3.813775    -3.365290      30.24
 H      -5.299464    -1.887920    -4.881902      28.88
 H      -6.558119    -1.861948    -3.602867      26.81
55
name = lig-ACN-frame_396
 C       4.339770     2.641622    -0.298442      65.73
 H       3.788692     3.641705    -0.318642      22.69
 C       4.426936     0.359670     0.623799      38.46
 H       4.047576    -0.132094     1.568435      20.57
 C       5.510629     0.061282    -0.343284       0.46
 O       6.191475    -1.188704    -0.383314     267.65
 C       6.497394    -1.687558     1.068477      84.09
 H       5.576410    -1.336677     1.841520      23.31
 H       7.293705    -1.153072     1.534596      26.15
 H       6.593173    -2.789276     1.141668      26.30
 C       6.049129     1.053522    -1.149019       8.36
 O       7.265260     0.886158    -1.844669     149.94
 H       7.923084     0.228312    -1.341606      21.40
 C       5.357567     2.348778    -1.160793      60.82
 H       5.911940     3.092190    -1.779446      22.27
 C       3.756573     1.676812     0.556255       7.17
 C       2.583462     2.078793     1.386673      97.32
 H       2.603096     3.012526     1.610120      27.50
 O       2.280235     1.405973     2.693555     220.90
 H       2.240685     0.304016     2.466866      19.78
 C       1.412396     2.156510     0.425748      71.02
 H       1.604191     2.956997    -0.293248      24.56
 C       0.035578     2.618971     1.270562     102.34
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 O       0.066445     3.973527     1.821748     249.05
 H       0.749004     4.501918     1.180941      25.51
 H      -0.286197     2.066881     2.041786      26.32
 H      -0.791043     2.745371     0.590317      24.90
 C      -1.709508    -1.167033    -1.013084      64.40
 H      -2.146426    -1.954349    -0.626076      24.04
 C      -1.171666     0.316077    -2.849469      97.81
 H      -1.571665     0.696462    -3.827657      23.92
 C      -0.209920     0.978768    -2.104304      13.87
 O       0.343398     2.233928    -2.466192     219.03
 C       0.044165     2.726192    -3.889905     101.30
 H       0.170067     3.825691    -3.886046      25.55
 H       0.571663     1.915514    -4.525767      25.63
 H      -0.906032     2.645836    -4.264180      28.50
 C       0.064491     0.364361    -0.877334      28.29
 O       1.147363     0.860487    -0.107114     187.67
 C      -0.801276    -0.552924    -0.276891      55.07
 H      -0.543061    -0.965342     0.811061      19.14
 C      -1.972627    -0.835504    -2.360272      53.67
 C      -2.918374    -1.596905    -3.254140      59.10
 H      -2.945359    -1.329536    -4.278857      28.93
 O      -2.764021    -3.002763    -3.267634     332.88
 H      -2.036576    -3.187303    -2.827682      34.20
 C      -4.573884    -1.389723    -2.852820      88.40
 H      -4.601471    -1.728347    -1.839431      26.60
 O      -4.989451     0.027386    -3.027574     214.48
 H      -4.970272     0.582724    -2.080564      22.75
 C      -5.500348    -2.137979    -3.809809     102.39
 O      -5.463545    -3.622829    -3.693817     219.45
 H      -4.433563    -3.793787    -3.435619      27.31
 H      -5.262874    -1.894520    -4.885525      28.93
 H      -6.461860    -1.719533    -3.564676      28.23
55
name = lig-ACN-frame_397
 C       4.308113     2.661533    -0.355471      43.45
 H       3.957531     3.698052    -0.626450      20.34
 C       4.417536     0.419162     0.605831      62.54
 H       4.326136    -0.435333     1.325470      19.48
 C       5.449277     0.044124    -0.274746       2.43
 O       6.233709    -1.159506    -0.251479     237.16
 C       6.461710    -1.680624     1.080851     100.95
 H       5.370950    -1.542788     1.738667      22.49
 H       7.336375    -1.188383     1.418913      26.91
 H       6.689241    -2.756607     1.039779      27.13
 C       5.988817     1.037040    -1.214560      10.74
 O       7.245375     0.956501    -1.785783     173.75
 H       7.839295     0.428408    -1.102325      25.11
 C       5.454070     2.296454    -1.168008      47.71
 H       5.800267     3.126277    -1.786593      19.34
 C       3.879186     1.688142     0.640315      23.06
 C       2.543777     2.123550     1.414760      90.81
 H       2.758876     3.017902     1.737398      26.51
 O       2.343972     1.405780     2.668455     284.29
 H       2.178603     0.434250     2.498237      23.68
 C       1.260354     2.203050     0.457148      88.95
 H       1.500056     2.851820    -0.416771      23.15
 C       0.017722     2.658498     1.118554     112.73
 O       0.084378     3.982467     1.801307     312.14
 H       0.417441     4.658563     1.300519      31.43
 H      -0.206987     1.881133     1.799452      26.01
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 H      -0.667732     2.567194     0.321906      26.71
 C      -1.732587    -1.240648    -0.992227      36.94
 H      -2.427432    -1.985779    -0.686709      16.85
 C      -1.273858     0.298398    -2.914900       1.15
 H      -1.498206     0.653300    -3.943209      16.04
 C      -0.313627     1.010509    -2.147197      12.67
 O       0.388751     2.188133    -2.537667     231.81
 C       0.049785     2.699853    -3.851341     116.02
 H       0.561451     3.684319    -4.076176      24.34
 H       0.614534     2.160630    -4.700734      26.79
 H      -0.996776     2.682248    -3.794703      29.75
 C       0.108756     0.520563    -0.757266      36.83
 O       1.227552     0.870556    -0.084961     213.72
 C      -0.695005    -0.520093    -0.201937      51.16
 H      -0.682162    -0.818828     0.882949      18.27
 C      -1.906207    -0.764136    -2.398249      34.38
 C      -3.085595    -1.546629    -3.235126      54.00
 H      -2.903872    -1.083938    -4.156012      26.36
 O      -2.825082    -3.036945    -3.269149     277.55
 H      -1.865634    -3.284305    -3.152646      29.64
 C      -4.541401    -1.358191    -2.790328     100.98
 H      -4.818845    -1.631226    -1.802132      26.47
 O      -4.949524    -0.011859    -3.001592     258.56
 H      -4.579367     0.501796    -1.994159      18.61
 C      -5.496096    -2.208559    -3.801223      97.07
 O      -5.398028    -3.627595    -3.711673     254.72
 H      -4.499902    -3.869300    -3.797720      33.13
 H      -5.293786    -1.728699    -4.821036      29.43
 H      -6.529594    -2.118595    -3.617151      27.53
55
name = lig-ACN-frame_398
 C       4.345654     2.595118    -0.406362      60.17
 H       3.820117     3.545505    -0.296760      23.89
 C       4.454861     0.415156     0.614043      26.81
 H       3.804929    -0.211781     1.195156      21.19
 C       5.522340     0.077434    -0.267969      17.16
 O       6.196260    -1.094232    -0.133037     264.20
 C       6.461168    -1.715284     1.105799     110.31
 H       5.561631    -1.890303     2.007386      24.64
 H       7.202429    -1.251922     1.730271      26.73
 H       6.762272    -2.698139     0.765749      27.12
 C       6.008000     1.044610    -1.114484      18.15
 O       7.247374     0.963287    -1.747637     180.57
 H       7.766114     0.302873    -1.346838      27.36
 C       5.417540     2.362198    -1.223374      54.11
 H       5.977139     2.982951    -1.873040      19.82
 C       3.866080     1.775591     0.599464      -4.91
 C       2.593796     2.214153     1.485454      91.08
 H       2.737418     3.121915     1.866441      26.93
 O       2.393295     1.396986     2.617887     303.91
 H       2.152289     0.558767     2.382345      27.60
 C       1.363825     2.293278     0.492871      75.19
 H       1.650840     3.024192    -0.341128      23.28
 C      -0.090118     2.731975     1.015814     113.01
 O       0.081779     3.911716     1.785597     289.43
 H       0.202895     4.591014     1.167187      31.22
 H      -0.412197     2.111828     1.858980      24.78
 H      -0.897572     2.809774     0.397588      26.37
 C      -1.682767    -1.190384    -0.989737      49.45
 H      -2.204730    -2.010161    -0.333697      17.12
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 C      -1.302786     0.365781    -2.963174     109.17
 H      -1.403980     0.620672    -4.018689      18.75
 C      -0.294990     1.045998    -2.080696       3.48
 O       0.442368     2.087870    -2.580127     219.93
 C       0.042235     2.676107    -3.847459     106.79
 H       0.574216     3.685749    -3.659984      23.46
 H       0.227033     1.976394    -4.677026      24.96
 H      -0.961102     3.002594    -4.137326      27.12
 C      -0.038763     0.562205    -0.794206      16.48
 O       1.263944     0.863721    -0.073237     131.10
 C      -0.690144    -0.545844    -0.217931      20.66
 H      -0.260317    -0.797825     0.706907      18.05
 C      -2.041517    -0.867776    -2.365774      78.15
 C      -3.071974    -1.513030    -3.197514      58.59
 H      -3.168888    -1.202373    -4.173816      30.57
 O      -2.861486    -3.022122    -3.244525     162.62
 H      -1.844865    -3.107438    -3.731431      23.60
 C      -4.584641    -1.414711    -2.794290     100.14
 H      -4.606354    -1.826949    -1.810346      28.07
 O      -4.916385     0.006764    -2.945907     244.23
 H      -4.336637     0.702384    -2.320946      23.53
 C      -5.493243    -2.219626    -3.727624     106.98
 O      -5.307339    -3.668075    -3.742314     248.16
 H      -4.405147    -3.735046    -4.001462      35.34
 H      -5.345344    -1.940139    -4.820446      30.11
 H      -6.437153    -1.882625    -3.417710      29.51
55
name = lig-ACN-frame_399
 C       4.323545     2.727171    -0.400627      56.01
 H       3.999102     3.703051    -0.660816      22.19
 C       4.361104     0.490216     0.646787      72.04
 H       4.142758    -0.315796     1.264688      21.88
 C       5.513116     0.195263    -0.097633       2.07
 O       6.176878    -1.076668    -0.110259     232.86
 C       6.503944    -1.840206     1.223070      88.80
 H       5.342936    -1.992749     1.605974      23.52
 H       7.173552    -1.163149     1.773047      26.22
 H       7.022513    -2.775403     1.014116      26.37
 C       6.145197     1.177204    -1.031152      14.46
 O       7.282541     0.913228    -1.748019     181.10
 H       7.614041     0.023318    -1.499154      21.90
 C       5.404884     2.333043    -1.293211      58.58
 H       5.720865     3.150092    -1.873741      25.86
 C       3.806140     1.745383     0.543848      35.99
 C       2.684173     2.259397     1.452222      89.95
 H       2.779681     3.209726     1.762430      26.98
 O       2.420804     1.385077     2.610180     262.44
 H       2.143162     0.465852     2.220851      22.78
 C       1.401128     2.283009     0.443479      60.82
 H       1.715104     3.064977    -0.355526      23.86
 C      -0.102632     2.725866     1.054095     103.36
 O       0.042414     3.950769     1.800606     219.10
 H       0.516049     4.751753     1.132138      24.80
 H      -0.601568     1.816508     1.493220      24.46
 H      -0.586500     2.892611     0.178540      27.09
 C      -1.700982    -1.172841    -1.000991      91.95
 H      -2.131888    -2.314408    -0.685598      17.99
 C      -1.326757     0.281799    -2.780046       3.29
 H      -1.552291     0.603619    -3.762296      22.86
 C      -0.387949     0.984055    -2.161999      43.07
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 O       0.462284     1.995907    -2.604894     253.35
 C       0.060606     2.729754    -3.869481     116.75
 H       0.775208     3.542834    -4.238125      24.28
 H       0.317579     2.066904    -4.695041      29.51
 H      -1.012008     2.891910    -3.604606      29.23
 C       0.031044     0.559947    -0.771613      63.36
 O       1.176228     0.950200    -0.109666     195.06
 C      -0.684984    -0.549154    -0.296502      44.75
 H      -0.424936    -1.120046     0.490993      20.05
 C      -2.022331    -0.720564    -2.285764      55.93
 C      -3.067700    -1.612930    -3.234951      79.03
 H      -2.846521    -1.164146    -4.129438      30.15
 O      -2.831141    -2.965252    -3.242367     247.06
 H      -1.868795    -3.240471    -3.728777      25.21
 C      -4.523386    -1.423045    -2.753147     109.36
 H      -4.768702    -1.650378    -1.735963      26.89
 O      -4.929944    -0.002760    -2.918210     323.19
 H      -4.516959     0.376235    -2.188493      28.22
 C      -5.514915    -2.211800    -3.700359      95.55
 O      -5.257068    -3.679597    -3.743546     216.84
 H      -4.182425    -3.776211    -3.739676      26.43
 H      -5.479479    -1.634925    -4.681612      29.10
 H      -6.529055    -2.264062    -3.375706      26.99
55
name = lig-ACN-frame_400
 C       4.325477     2.752360    -0.447155      61.75
 H       3.791632     3.651455    -0.514988      23.61
 C       4.383596     0.521139     0.667917      42.99
 H       4.004622    -0.014647     1.477462      21.12
 C       5.644232     0.289034     0.003599      16.71
 O       6.201928    -1.102764    -0.057331     231.89
 C       6.457476    -1.814492     1.206636     106.68
 H       5.568310    -2.332898     1.854163      23.56
 H       6.939722    -1.220471     2.045021      24.59
 H       7.109887    -2.644801     0.869158      25.14
 C       6.179996     1.214125    -0.936305       4.37
 O       7.319198     0.838854    -1.748009     143.37
 H       7.595283    -0.115844    -1.335158      21.50
 C       5.411069     2.393961    -1.246199      59.08
 H       5.731056     2.893016    -2.136619      23.32
 C       3.787755     1.893457     0.499937      11.88
 C       2.566008     2.173606     1.356480     102.30
 H       2.837948     3.024124     1.822768      25.54
 O       2.459739     1.416280     2.561668     227.56
 H       2.106826     0.357652     2.491936      19.98
 C       1.289566     2.301471     0.475175      93.13
 H       1.517389     2.989325    -0.441103      21.65
 C       0.071388     2.766914     0.970687     107.37
 O      -0.028402     4.002809     1.841557     180.57
 H       0.820689     4.695350     1.375809      24.28
 H      -0.475826     2.098909     1.768141      23.05
 H      -0.604227     2.910140     0.210596      25.68
 C      -1.755561    -1.258182    -1.013539      74.92
 H      -2.204623    -2.424530    -0.593071      15.71
 C      -1.401265     0.356029    -2.841701     125.38
 H      -1.709893     0.676499    -3.814296      19.71
 C      -0.250720     1.003007    -2.050196       4.45
 O       0.514127     1.988209    -2.683396     235.56
 C       0.071919     2.644370    -3.874328     106.34
 H       0.732530     3.562026    -3.793904      23.37
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 H      -0.143801     2.056571    -4.715205      25.77
 H      -0.952105     3.258016    -3.897604      25.56
 C       0.031688     0.505329    -0.833786      21.81
 O       1.164565     1.023244    -0.141178     223.42
 C      -0.633310    -0.625939    -0.277741      12.64
 H      -0.292914    -0.859329     0.679777      17.53
 C      -2.168330    -0.815514    -2.246711      81.55
 C      -2.998351    -1.494705    -3.184140      59.01
 H      -3.024634    -1.170925    -4.144241      32.19
 O      -2.720020    -3.024940    -3.237035     284.09
 H      -1.757449    -3.163711    -3.204628      30.62
 C      -4.555724    -1.394440    -2.770171     102.04
 H      -4.462883    -1.814240    -1.767962      28.21
 O      -4.937730    -0.044542    -2.898868     315.34
 H      -4.937358     0.442562    -2.197446      31.31
 C      -5.538068    -2.268528    -3.634041     101.71
 O      -5.223351    -3.639838    -3.752795     251.89
 H      -4.167132    -3.725414    -3.496230      26.90
 H      -5.570658    -1.865414    -4.688635      29.81
 H      -6.533834    -2.038567    -3.192681      28.42
55
name = lig-ACN-frame_401
 C       4.289956     2.771579    -0.501268      50.41
 H       3.836016     3.691039    -0.813380      23.00
 C       4.536705     0.679354     0.704833      68.52
 H       4.023001    -0.093673     1.249664      21.67
 C       5.702667     0.240620     0.080867      27.55
 O       6.205727    -1.006773     0.035860     231.98
 C       6.433505    -1.798340     1.181230     103.13
 H       5.439700    -2.334797     1.357219      24.45
 H       6.850503    -1.110355     2.036296      22.64
 H       7.268007    -2.518677     0.936719      24.43
 C       6.202864     1.152143    -0.928084      16.65
 O       7.259969     0.788491    -1.679303      81.74
 H       7.849034     0.122177    -1.222505      23.49
 C       5.537766     2.410758    -1.201943      52.03
 H       5.873617     3.031336    -2.062246      20.95
 C       3.831362     1.835934     0.488184      24.21
 C       2.503264     2.198547     1.342358      87.83
 H       2.429616     3.157683     1.538277      27.49
 O       2.454678     1.398725     2.541341     264.27
 H       2.120807     0.470945     2.237464      23.44
 C       1.343721     2.359974     0.356472      65.16
 H       1.806374     3.196551    -0.303418      23.43
 C      -0.097584     2.909715     1.096582     104.71
 O      -0.010660     4.058691     1.846212     255.08
 H       0.595759     4.833376     1.472426      26.89
 H      -0.181587     1.900286     1.766932      22.85
 H      -0.830384     2.875068     0.331061      26.09
 C      -1.673761    -1.332085    -0.943038      82.49
 H      -2.326180    -2.224720    -0.193708      15.07
 C      -1.422814     0.426389    -2.762031      17.59
 H      -1.631901     0.796136    -3.765990      16.90
 C      -0.346416     0.954581    -2.228344      18.36
 O       0.549078     1.954334    -2.688330     236.50
 C       0.034425     2.657409    -3.905578     104.69
 H       0.863609     3.274025    -4.300746      25.05
 H       0.111077     1.958279    -4.694029      29.10
 H      -1.026888     3.112011    -3.567308      25.63
 C       0.032811     0.437434    -0.825875      37.57
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 O       1.182255     0.940976    -0.160875     143.76
 C      -0.653863    -0.694212    -0.269609      19.55
 H      -0.392137    -1.061468     0.755847      17.72
 C      -2.039151    -0.711475    -2.265397      80.98
 C      -3.100636    -1.555156    -3.232751      46.10
 H      -2.890940    -1.144337    -4.145846      27.29
 O      -2.599375    -2.997364    -3.193815     302.14
 H      -1.748419    -3.047464    -2.935920      34.42
 C      -4.517521    -1.471853    -2.762427     108.06
 H      -4.752841    -1.720589    -1.713816      25.94
 O      -5.010050    -0.036590    -2.911871     254.25
 H      -4.621796     0.376487    -2.058307      23.72
 C      -5.538113    -2.228644    -3.595573      98.48
 O      -5.207385    -3.655836    -3.703437     269.73
 H      -4.251508    -3.723463    -3.617729      33.00
 H      -5.654246    -1.742743    -4.595166      29.43
 H      -6.548851    -2.213272    -3.065467      27.12
55
name = lig-ACN-frame_402
 C       4.388375     2.700170    -0.578289      60.07
 H       3.882045     3.633784    -0.885720      23.77
 C       4.585485     0.667546     0.856468      24.24
 H       4.245277    -0.151843     1.546940      18.81
 C       5.686198     0.342959     0.045950      15.08
 O       6.282066    -0.940336     0.040394     226.68
 C       6.405191    -1.791361     1.216294     108.74
 H       5.517842    -2.456471     1.482630      25.87
 H       6.494454    -1.239641     2.238368      25.19
 H       7.264578    -2.512461     1.007022      25.02
 C       6.189200     1.176775    -0.913684      25.53
 O       7.285888     0.750783    -1.672142     188.20
 H       7.859079     0.294436    -1.119786      26.51
 C       5.604712     2.361685    -1.127054      62.90
 H       6.195166     3.151946    -1.678331      22.71
 C       3.818444     1.965174     0.488169     -17.58
 C       2.599713     2.309445     1.304975      73.34
 H       2.853616     3.070135     1.902060      25.36
 O       2.378021     1.385943     2.474798     233.71
 H       2.125199     0.563114     2.247067      26.53
 C       1.261558     2.329686     0.297675      66.24
 H       1.351633     2.793331    -0.760627      18.50
 C      -0.131665     2.834181     1.120555      80.06
 O       0.030698     4.189428     1.888760     266.61
 H       0.227497     4.664995     1.205073      33.81
 H      -0.548735     2.127336     2.042809      21.56
 H      -1.016765     3.007169     0.470743      23.00
 C      -1.648700    -1.244351    -1.031241      39.87
 H      -2.415949    -2.293369    -0.719240      14.26
 C      -1.502938     0.404824    -2.808749     161.60
 H      -2.003353     0.707141    -3.772021      19.08
 C      -0.238219     0.937205    -2.101869      13.09
 O       0.528031     1.921066    -2.693444     244.81
 C       0.083465     2.572647    -3.960998      86.50
 H       0.652631     3.462454    -4.167883      25.37
 H      -0.287637     1.906184    -4.695080      26.15
 H      -1.030478     3.145623    -3.816836      24.71
 C       0.068250     0.423206    -0.883072      17.56
 O       1.169464     0.888934    -0.187837     193.78
 C      -0.601931    -0.651520    -0.249707      38.07
 H      -0.227298    -1.110813     0.780744      16.23
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 C      -2.041945    -0.805573    -2.232808      65.97
 C      -2.972963    -1.600772    -3.167286      63.61
 H      -3.080376    -1.270523    -4.152754      24.82
 O      -2.587907    -2.914662    -3.139094     277.31
 H      -1.541296    -2.926673    -3.345452      25.70
 C      -4.590969    -1.435447    -2.727310      90.38
 H      -4.502088    -1.794161    -1.664242      26.37
 O      -5.039718    -0.075385    -2.890722     246.66
 H      -4.433310     0.753259    -2.346990      21.75
 C      -5.554311    -2.269355    -3.585585     102.24
 O      -5.211369    -3.679084    -3.646658     276.50
 H      -4.327851    -3.755427    -3.858496      37.30
 H      -5.646628    -1.749026    -4.558975      29.42
 H      -6.623541    -2.248882    -3.112793      26.85
55
name = lig-ACN-frame_403
 C       4.395956     2.692780    -0.530474      55.23
 H       3.909923     3.698275    -0.751817      22.94
 C       4.522509     0.742595     0.914348      79.78
 H       4.143365     0.443011     1.960017      20.76
 C       5.626520     0.288410     0.099565       2.87
 O       6.388972    -0.920032     0.074422     217.72
 C       6.331216    -1.782674     1.275884     108.95
 H       5.483378    -2.407434     1.184224      27.15
 H       6.485290    -1.137812     2.237071      24.20
 H       7.325014    -2.341082     1.177749      25.21
 C       6.289961     1.138231    -0.933549       1.06
 O       7.362579     0.754388    -1.690895     114.94
 H       7.897953     0.018290    -1.181658      22.17
 C       5.682984     2.474847    -1.159168      43.66
 H       6.199765     3.169789    -1.922472      19.95
 C       3.930074     1.874791     0.525364      37.00
 C       2.587030     2.339228     1.263547      79.37
 H       2.632908     3.349089     1.555552      25.29
 O       2.289719     1.424521     2.359852     249.01
 H       2.011774     0.564892     1.926828      23.88
 C       1.117095     2.272957     0.378522      88.39
 H       1.181895     3.125499    -0.400661      22.47
 C      -0.075299     2.834483     1.169125      84.80
 O       0.080787     4.193299     1.829244     242.66
 H       0.249922     4.971648     1.243348      28.86
 H      -0.392931     2.060168     2.044990      22.79
 H      -0.895982     2.890668     0.352485      23.02
 C      -1.641813    -1.249524    -1.013750      73.88
 H      -1.797975    -2.469733    -0.533542      14.40
 C      -1.406230     0.371772    -2.770162     -13.31
 H      -1.653811     0.941404    -3.709338      14.66
 C      -0.370137     0.923627    -2.179583      34.95
 O       0.513730     1.931076    -2.725354     231.74
 C       0.018574     2.488933    -3.963487     115.25
 H       0.913604     3.049893    -4.166046      25.60
 H       0.154838     1.829576    -4.790149      29.41
 H      -0.999411     3.132902    -3.716699      26.79
 C       0.127335     0.419600    -0.847838      38.50
 O       1.231875     0.905548    -0.114265     183.80
 C      -0.621673    -0.645614    -0.324457      50.47
 H      -0.206792    -0.995908     0.770766      15.30
 C      -2.061078    -0.731679    -2.319150      61.72
 C      -3.043380    -1.507516    -3.133724      61.02
 H      -2.833677    -1.073141    -4.085138      27.58
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 O      -2.583514    -2.969841    -3.097012     196.56
 H      -1.640702    -3.110375    -3.725877      24.06
 C      -4.534957    -1.420255    -2.658344     101.06
 H      -4.773173    -1.696698    -1.581450      26.19
 O      -5.059564    -0.108758    -2.897238     237.49
 H      -4.489112     0.565381    -2.110586      19.21
 C      -5.555719    -2.324086    -3.568640      93.32
 O      -5.236623    -3.716420    -3.595288     225.95
 H      -4.222661    -3.655966    -3.941142      31.49
 H      -5.534218    -2.008208    -4.610181      30.20
 H      -6.633225    -2.134112    -3.156473      27.42
55
name = lig-ACN-frame_404
 C       4.507666     2.778250    -0.478707      50.94
 H       3.915029     3.721448    -0.747566      22.08
 C       4.614354     0.684524     0.887470      28.46
 H       4.317652    -0.069685     1.748269      19.81
 C       5.709164     0.258869     0.076685       8.30
 O       6.451825    -0.901208     0.191970     232.68
 C       6.307970    -1.743886     1.290750     123.86
 H       5.432202    -2.334067     1.248752      28.73
 H       6.083827    -1.159164     2.231143      25.88
 H       7.131529    -2.489547     1.424875      25.93
 C       6.246121     1.182079    -0.901712      13.13
 O       7.426242     0.771223    -1.674983     153.12
 H       7.789464    -0.186931    -1.391789      20.43
 C       5.687018     2.429078    -1.172142      68.99
 H       5.928235     3.099277    -2.033670      22.68
 C       3.841070     1.973716     0.496690     -19.40
 C       2.461030     2.311103     1.177023      98.06
 H       2.563997     3.326647     1.688947      23.80
 O       2.227468     1.486812     2.293743     224.54
 H       1.800230     0.547247     1.868396      18.74
 C       1.283932     2.369952     0.436739      81.35
 H       1.479707     2.926307    -0.540916      21.04
 C      -0.051991     2.847338     1.222239      96.29
 O       0.121936     4.106074     1.762645     192.10
 H       0.722162     4.605756     0.874742      22.73
 H      -0.260439     2.191019     2.124733      22.92
 H      -1.060569     2.744298     0.570991      21.61
 C      -1.609876    -1.309249    -1.039515      56.38
 H      -2.237917    -2.370544    -0.629120      17.05
 C      -1.373415     0.401994    -2.841466     173.71
 H      -1.673627     0.605658    -3.891198      20.22
 C      -0.211912     0.985554    -2.078364      16.44
 O       0.439291     1.905383    -2.715408     237.51
 C       0.120024     2.456344    -4.008672      95.57
 H       0.682002     3.308665    -4.313500      23.85
 H      -0.141445     1.652472    -4.677074      23.17
 H      -1.035732     2.918721    -4.146718      22.45
 C       0.108582     0.471132    -0.856219      15.55
 O       1.196067     0.960982    -0.061945     201.93
 C      -0.576616    -0.622963    -0.345046      54.61
 H      -0.348649    -1.172843     0.690375      18.23
 C      -2.059257    -0.734313    -2.206509     102.28
 C      -3.097375    -1.533615    -3.153059      32.29
 H      -3.280678    -1.231778    -4.201821      28.35
 O      -2.674936    -2.992484    -3.097701     230.36
 H      -1.673365    -2.985168    -3.485570      28.75
 C      -4.585079    -1.504285    -2.694073      98.59
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 H      -4.502661    -1.786081    -1.596674      25.61
 O      -5.048948    -0.084685    -2.884461     203.82
 H      -5.009614     0.462298    -2.004475      24.27
 C      -5.472456    -2.317928    -3.544948     104.67
 O      -5.255209    -3.773468    -3.534932     212.72
 H      -4.171849    -4.024160    -3.481841      28.39
 H      -5.476959    -1.770489    -4.485880      31.80
 H      -6.560007    -2.294273    -3.147300      27.62
55
name = lig-ACN-frame_405
 C       4.502404     2.851174    -0.395346      60.33
 H       4.179871     3.847535    -0.799359      21.62
 C       4.609734     0.711023     0.721773      72.79
 H       4.019593    -0.126928     1.257083      21.95
 C       5.807221     0.369109     0.069480      20.88
 O       6.546926    -0.863789     0.254930     219.19
 C       6.173005    -1.764977     1.420500     115.31
 H       5.386505    -2.353704     1.181123      29.56
 H       6.125186    -1.222119     2.373983      26.61
 H       7.119418    -2.305675     1.454165      26.50
 C       6.334985     1.139196    -0.955128      14.44
 O       7.393051     0.830854    -1.630907     189.93
 H       7.675518     0.022490    -1.225735      23.53
 C       5.603249     2.347870    -1.174942      51.96
 H       6.207142     2.917132    -1.884597      24.08
 C       3.909323     1.899203     0.504144      17.10
 C       2.621191     2.349849     1.282958      69.23
 H       2.871405     3.358289     1.789798      23.99
 O       2.183690     1.468231     2.348747     248.41
 H       1.787898     0.565951     2.087551      22.70
 C       1.224862     2.412856     0.217723      74.13
 H       1.258413     3.157454    -0.609357      23.31
 C       0.024136     2.727746     1.201786      92.76
 O       0.186311     4.123367     1.681587     175.79
 H       1.037056     4.781962     1.141656      23.70
 H       0.003715     2.043046     1.995852      25.06
 H      -0.975572     2.695791     0.511887      22.83
 C      -1.609279    -1.284857    -1.058347      78.86
 H      -2.288614    -2.170033    -0.482920      17.99
 C      -1.355783     0.299175    -2.765787      26.44
 H      -1.531294     0.689270    -3.765854      19.25
 C      -0.308031     0.927760    -2.163921      10.79
 O       0.548455     2.075515    -2.711053     219.42
 C       0.078642     2.395326    -4.114367     100.27
 H       0.889653     3.114193    -4.314447      25.10
 H       0.373086     1.644835    -4.859387      28.57
 H      -0.985688     2.839693    -3.883029      25.96
 C       0.076609     0.507963    -0.769441      44.59
 O       1.118857     0.990525    -0.038469     178.24
 C      -0.554071    -0.711966    -0.285751      28.43
 H      -0.087358    -0.975672     0.702713      16.59
 C      -2.095514    -0.768007    -2.335650      38.21
 C      -3.080332    -1.588493    -3.116679      67.64
 H      -2.862556    -1.175640    -4.151057      25.23
 O      -2.768593    -2.959233    -3.119821     316.37
 H      -1.881614    -3.084391    -3.021100      35.46
 C      -4.552997    -1.467482    -2.624982     101.05
 H      -4.778440    -1.858079    -1.573517      26.38
 O      -5.053226    -0.109962    -2.847900     289.52
 H      -4.880612     0.344771    -2.145976      32.04
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 C      -5.491978    -2.401047    -3.537653     101.17
 O      -5.261595    -3.819615    -3.482629     268.30
 H      -4.343067    -3.859966    -3.170408      31.82
 H      -5.394250    -2.216261    -4.602467      30.18
 H      -6.549095    -2.109681    -3.200731      27.67
55
name = lig-ACN-frame_406
 C       4.531788     2.805118    -0.406126      64.70
 H       4.096657     3.783484    -0.281493      23.05
 C       4.527011     0.636572     0.581314      52.07
 H       4.048328    -0.037047     1.334042      21.86
 C       5.843747     0.313661     0.137086      18.94
 O       6.572622    -0.810126     0.369265     239.47
 C       6.140289    -1.737894     1.460822     116.59
 H       5.294956    -2.238055     1.186884      28.94
 H       5.871401    -1.144172     2.307543      26.65
 H       6.875219    -2.469513     1.659655      26.45
 C       6.261735     1.193302    -0.919304      12.77
 O       7.470957     0.849607    -1.672455     178.46
 H       8.114672     0.274032    -1.269740      27.62
 C       5.610867     2.409978    -1.208388      69.56
 H       5.946138     3.170077    -1.844240      24.51
 C       3.974786     1.951246     0.515806      23.35
 C       2.725262     2.274207     1.308661      62.54
 H       2.773393     3.388952     1.737669      22.84
 O       2.220555     1.465328     2.441207     276.81
 H       2.059550     0.720976     1.983723      28.51
 C       1.211577     2.417112     0.207012      72.71
 H       1.341089     2.934596    -0.719600      23.00
 C       0.146656     2.792731     1.081463     104.80
 O       0.214963     4.132786     1.653309     233.44
 H       0.948433     4.623847     0.994385      25.00
 H       0.216203     2.139634     1.857911      25.70
 H      -0.993257     2.588915     0.655178      22.96
 C      -1.629236    -1.256888    -0.953461      52.59
 H      -1.991062    -2.288183    -0.535516      19.99
 C      -1.320352     0.310370    -2.876920      82.61
 H      -1.680336     0.666972    -3.828761      16.60
 C      -0.250121     0.985276    -2.106532      -4.38
 O       0.519753     2.068714    -2.703287     220.48
 C       0.160377     2.416795    -4.110292     100.39
 H       0.670398     3.327091    -4.495950      24.82
 H       0.112806     1.427152    -4.684616      26.43
 H      -0.934500     2.707253    -4.462069      25.85
 C      -0.006877     0.456857    -0.836833      35.00
 O       1.089562     1.017003    -0.076673     197.41
 C      -0.574400    -0.686032    -0.320494      34.90
 H      -0.427833    -1.190831     0.556666      19.93
 C      -2.003354    -0.875835    -2.257696      51.25
 C      -3.069543    -1.536280    -3.099808      60.48
 H      -3.189371    -1.132995    -4.173898      26.02
 O      -2.822419    -3.022128    -3.117766     286.96
 H      -1.873500    -3.160752    -2.911174      26.56
 C      -4.580642    -1.468171    -2.665165      87.15
 H      -4.547688    -1.704135    -1.551835      26.47
 O      -5.066416    -0.146878    -2.798509     295.86
 H      -4.528190     0.494712    -2.345862      30.13
 C      -5.522193    -2.433232    -3.570605     100.62
 O      -5.285068    -3.870725    -3.357985     268.72
 H      -4.397141    -3.952227    -3.292807      33.85
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 H      -5.335291    -2.003495    -4.571256      30.47
 H      -6.610090    -2.301056    -3.371478      27.25
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name = lig-ACN-frame_407
 C       4.526678     2.842159    -0.392945      55.12
 H       4.238446     3.837185    -0.640913      22.49
 C       4.481981     0.503419     0.659349      67.73
 H       4.123130    -0.166034     1.400336      22.63
 C       5.751190     0.298680     0.073649       4.57
 O       6.618650    -0.803833     0.502303     219.60
 C       6.053233    -1.660788     1.455756     131.00
 H       5.224912    -2.164843     1.104175      29.32
 H       5.755613    -1.197623     2.381462      27.73
 H       6.828204    -2.307256     1.698928      28.02
 C       6.373544     1.227998    -0.942949      -2.25
 O       7.477145     0.931489    -1.717432     128.67
 H       8.053170     0.303705    -1.077794      22.41
 C       5.681658     2.485466    -1.206126      41.29
 H       6.078058     2.999797    -2.026393      21.84
 C       3.954090     1.852627     0.559728       3.63
 C       2.590619     2.266835     1.241605      79.99
 H       2.805685     3.354328     1.776216      22.74
 O       2.374835     1.483302     2.429367     254.97
 H       2.032670     0.538219     2.415626      24.73
 C       1.474003     2.330050     0.249687      80.92
 H       1.771412     2.960933    -0.531350      25.04
 C       0.104528     2.887804     1.115330      94.06
 O       0.248222     4.178030     1.614874     291.98
 H       0.586701     4.794632     1.029855      31.96
 H       0.028315     2.269338     1.935798      26.48
 H      -0.895339     2.768452     0.378780      23.07
 C      -1.698851    -1.384456    -0.970475      80.29
 H      -2.183488    -2.272233    -0.602569      17.47
 C      -1.289258     0.269221    -2.855836     -21.37
 H      -1.582523     0.484598    -3.886857      18.60
 C      -0.313717     0.998624    -2.219504      29.08
 O       0.403483     2.029888    -2.689831     267.45
 C       0.173494     2.387205    -4.101724      99.38
 H       1.036271     3.133077    -4.288567      24.70
 H       0.508870     1.540932    -4.828096      27.12
 H      -0.858123     2.730817    -3.986507      28.93
 C       0.082309     0.527208    -0.884672      26.18
 O       1.096695     0.961662    -0.135285     220.49
 C      -0.602750    -0.632724    -0.250277      52.09
 H      -0.131687    -0.766328     0.594487      20.96
 C      -1.927679    -0.789829    -2.277541      42.53
 C      -3.096156    -1.593677    -3.115656      48.73
 H      -2.903402    -1.232057    -4.207523      25.10
 O      -2.831252    -3.066202    -3.105230     192.36
 H      -1.728013    -3.121705    -3.378861      25.01
 C      -4.602730    -1.525361    -2.642557      93.61
 H      -4.730572    -2.008695    -1.620971      26.28
 O      -5.127451    -0.133081    -2.799298     214.38
 H      -4.352808     0.503174    -2.233391      21.07
 C      -5.481299    -2.428412    -3.537565     106.64
 O      -5.332941    -3.859544    -3.244314     196.07
 H      -4.380480    -4.084767    -3.598702      30.35
 H      -5.333154    -2.331267    -4.628771      30.42
 H      -6.505474    -2.197729    -3.305012      29.12
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name = lig-ACN-frame_408
 C       4.572485     2.749757    -0.389517      65.75
 H       3.927862     3.576114    -0.539041      24.48
 C       4.534560     0.584971     0.739227      41.50
 H       4.007739    -0.138963     1.267007      21.56
 C       5.784084     0.283987    -0.035062      11.41
 O       6.622661    -0.683323     0.516015     189.80
 C       5.957975    -1.674078     1.510433     107.62
 H       5.234190    -2.214003     0.984951      28.90
 H       5.624420    -1.100402     2.374143      26.25
 H       6.729220    -2.343836     1.743203      27.57
 C       6.348005     1.220654    -0.898588      26.03
 O       7.475937     1.000175    -1.692606     187.96
 H       8.038692     0.148701    -1.475839      21.64
 C       5.722798     2.426222    -1.112831      67.62
 H       6.135642     3.159928    -1.772288      25.02
 C       3.915794     1.808544     0.463567      14.22
 C       2.675836     2.168498     1.255231      83.41
 H       2.648775     3.401719     1.434122      23.42
 O       2.518009     1.483584     2.479781     233.34
 H       1.950765     0.595504     2.090727      20.90
 C       1.403757     2.287129     0.350767      88.63
 H       1.682662     2.914658    -0.430291      24.60
 C       0.177518     2.888152     1.019538      93.33
 O       0.245862     4.300296     1.641283     274.62
 H       0.637572     4.736700     0.997135      33.07
 H      -0.307637     2.270605     1.754065      25.64
 H      -0.613876     2.923195     0.108298      23.32
 C      -1.584360    -1.303783    -0.974909      49.60
 H      -2.120748    -2.009721    -0.539239      21.94
 C      -1.335780     0.206311    -2.899577      84.60
 H      -1.413627     0.517730    -3.969222      18.26
 C      -0.339089     0.918573    -2.195914       4.58
 O       0.357784     2.030171    -2.693645     236.66
 C       0.216474     2.406566    -4.048337     112.91
 H       0.953305     3.287655    -4.207080      23.55
 H       0.193640     1.506848    -4.787555      24.24
 H      -0.668951     2.914062    -4.502308      25.99
 C      -0.005279     0.470063    -0.890549      23.42
 O       1.262143     0.927312    -0.155893     168.17
 C      -0.639445    -0.543326    -0.295890      58.83
 H      -0.468936    -0.873355     0.621552      21.75
 C      -2.109808    -0.927366    -2.299370      51.38
 C      -3.044831    -1.672135    -3.096435      66.86
 H      -3.146519    -1.218934    -4.178708      28.26
 O      -2.750720    -3.065763    -3.099117     215.10
 H      -1.936864    -3.271290    -3.756352      27.53
 C      -4.565930    -1.527541    -2.675290      93.62
 H      -4.714390    -1.738219    -1.588630      26.65
 O      -5.145996    -0.189924    -2.794949     166.66
 H      -4.812804     0.528485    -1.894887      20.64
 C      -5.482238    -2.454527    -3.515578     110.19
 O      -5.402653    -3.826742    -3.146697     189.52
 H      -4.380051    -4.143217    -3.449687      28.95
 H      -5.273602    -2.244269    -4.596169      31.42
 H      -6.457915    -2.128424    -3.352423      30.43
55
name = lig-ACN-frame_409
 C       4.492632     2.706403    -0.425334      62.32
 H       4.215627     3.750070    -0.558080      22.45
```

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 C       4.655149     0.649562     0.659629      84.36
 H       4.260086     0.004038     1.416160      22.20
 C       5.782139     0.284488     0.094709      45.63
 O       6.601856    -0.702890     0.540453     240.73
 C       5.963019    -1.638682     1.455603     122.41
 H       5.115873    -2.149097     0.986752      27.67
 H       5.439525    -1.121271     2.309454      25.49
 H       6.704646    -2.298729     1.875564      27.35
 C       6.346175     1.164073    -0.926527      18.55
 O       7.511347     1.026735    -1.660817     171.37
 H       7.845782     0.181829    -1.481224      29.12
 C       5.711327     2.436442    -1.032718      52.21
 H       6.230158     3.254446    -1.588717      22.47
 C       3.903446     1.770506     0.420772      41.87
 C       2.769038     2.223602     1.265161      64.13
 H       3.248835     3.230973     1.874594      20.91
 O       2.602841     1.436024     2.518924     220.64
 H       2.095488     0.532181     2.425403      23.09
 C       1.399595     2.251244     0.374048      84.64
 H       1.564574     2.831726    -0.461197      24.24
 C       0.104041     2.970609     0.972076      97.16
 O       0.247063     4.273470     1.608630     284.20
 H       1.005754     4.856466     1.352183      29.22
 H      -0.356257     2.310921     1.759302      25.07
 H      -0.610989     3.123692     0.097255      24.61
 C      -1.720019    -1.272955    -1.050682      65.31
 H      -1.939223    -2.058638    -0.471136      18.44
 C      -1.412189     0.127182    -2.926287      19.62
 H      -1.825568     0.363419    -3.935000      18.07
 C      -0.355665     0.859398    -2.185102      10.72
 O       0.300490     2.011400    -2.650489     213.12
 C       0.222269     2.483087    -4.114746      94.14
 H       1.174979     3.095613    -4.365032      24.01
 H       0.446381     1.517881    -4.709374      26.89
 H      -0.732306     2.851098    -4.120268      27.72
 C       0.133545     0.546168    -0.807357      33.62
 O       1.280461     0.869696    -0.229807     216.44
 C      -0.680462    -0.563254    -0.232716      58.29
 H      -0.455255    -0.870894     0.781543      18.70
 C      -2.010347    -0.880823    -2.295546      26.51
 C      -3.124156    -1.698514    -3.149895      46.99
 H      -2.993689    -1.341390    -4.262876      27.91
 O      -2.690212    -3.136042    -3.125862     271.98
 H      -1.955256    -3.138671    -3.609186      33.18
 C      -4.571134    -1.535715    -2.605664      99.65
 H      -4.497283    -1.938745    -1.581045      27.58
 O      -5.128405    -0.228481    -2.811407     236.90
 H      -5.011860     0.317939    -1.929396      25.30
 C      -5.511909    -2.419406    -3.493270     107.09
 O      -5.464614    -3.828176    -3.079036     235.70
 H      -4.530189    -4.049729    -2.925675      32.64
 H      -5.214573    -2.313299    -4.568733      31.19
 H      -6.526182    -2.202502    -3.400352      29.46
55
name = lig-ACN-frame_410
 C       4.455550     2.802786    -0.518820      56.75
 H       4.018773     3.837480    -0.511292      22.14
 C       4.572459     0.584676     0.729277      33.98
 H       4.349276     0.155883     1.739745      19.76
 C       5.954094     0.356036     0.087208      -8.70
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 O       6.642234    -0.820167     0.546931     218.45
 C       5.935420    -1.650753     1.449406     107.25
 H       5.264391    -2.288717     0.855461      26.06
 H       5.569299    -1.095886     2.390764      23.53
 H       6.776748    -2.342186     1.762290      24.79
 C       6.366061     1.179606    -0.947334      22.81
 O       7.536745     0.996981    -1.620374     226.35
 H       8.101881     0.281607    -1.267390      28.46
 C       5.715461     2.443060    -1.043017      49.32
 H       6.293637     3.105276    -1.790259      21.39
 C       3.906915     1.824665     0.399709       0.20
 C       2.693677     2.182161     1.352477      73.52
 H       2.788583     3.442803     1.619514      22.09
 O       2.661930     1.390162     2.555593     263.42
 H       2.342894     0.589920     2.284524      28.04
 C       1.525827     2.349337     0.351918      54.79
 H       1.924100     2.975218    -0.404481      23.11
 C       0.020993     2.983776     0.976161      92.30
 O       0.268262     4.225975     1.611542     201.26
 H       1.194575     4.550820     0.954619      22.43
 H      -0.489047     2.292150     1.759369      23.45
 H      -0.650126     3.001002     0.173203      25.45
 C      -1.776518    -1.292844    -0.856069      22.98
 H      -2.357523    -2.191263    -0.765404      20.80
 C      -1.311510     0.255641    -2.883568      35.31
 H      -1.504363     0.734676    -3.853811      17.65
 C      -0.329767     0.886274    -2.201494      15.87
 O       0.292860     2.025365    -2.660670     226.09
 C       0.213484     2.413141    -4.058283     123.38
 H       0.943935     3.271335    -4.048108      24.70
 H       0.134905     1.678515    -4.902030      27.44
 H      -0.603420     3.005035    -4.368669      28.16
 C      -0.001295     0.406962    -0.885251      19.85
 O       1.296624     0.904767    -0.210065     108.43
 C      -0.692067    -0.543005    -0.224372      43.50
 H      -0.262799    -0.876088     0.797435      18.76
 C      -2.067557    -0.950022    -2.383220      28.86
 C      -3.063533    -1.704194    -3.150589      71.81
 H      -3.206526    -1.342450    -4.250303      25.60
 O      -2.711655    -3.170838    -3.155569     259.52
 H      -1.726724    -3.229402    -3.108533      27.36
 C      -4.597932    -1.628736    -2.609996      88.91
 H      -4.822838    -1.841735    -1.565692      28.96
 O      -5.089206    -0.227202    -2.787239     247.28
 H      -4.679017     0.331518    -2.261597      33.61
 C      -5.540492    -2.471119    -3.437698     119.79
 O      -5.519891    -3.829636    -3.017696     251.62
 H      -4.650275    -3.980985    -2.861642      33.78
 H      -5.253293    -2.416207    -4.513380      30.17
 H      -6.489689    -1.991884    -3.334426      29.32
55
name = lig-ACN-frame_411
 C       4.485168     2.755155    -0.495917      56.40
 H       3.955619     3.691632    -0.880057      22.58
 C       4.673335     0.695891     0.711107      77.77
 H       4.172278    -0.017225     1.461878      21.48
 C       5.840504     0.291770     0.205877      43.37
 O       6.693605    -0.804677     0.455210     216.30
 C       5.989715    -1.796622     1.477233     103.78
 H       4.989062    -2.186522     1.054830      26.00
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 H       5.536445    -1.179651     2.352962      24.55
 H       6.723299    -2.590792     1.896198      25.32
 C       6.401270     1.228959    -0.845507      30.43
 O       7.585249     0.975363    -1.622587      54.79
 H       8.162369     0.212706    -1.126268      20.45
 C       5.703302     2.471721    -1.204985      51.65
 H       6.091654     3.250801    -1.967971      24.52
 C       3.964355     1.885584     0.485496      40.98
 C       2.669295     2.190039     1.316829      71.50
 H       2.739198     3.277606     1.974742      21.92
 O       2.651417     1.371560     2.536606     242.22
 H       2.301909     0.441605     2.406816      24.99
 C       1.359047     2.304337     0.390744      87.60
 H       1.644387     3.030577    -0.366272      24.96
 C       0.139292     2.852836     0.930050     102.79
 O       0.324595     4.195650     1.600717     163.73
 H       0.664525     5.058539     0.844807      24.17
 H      -0.259913     2.113038     1.760200      25.13
 H      -0.525987     2.980070     0.181052      27.24
 C      -1.809422    -1.262610    -0.950411      72.38
 H      -2.273699    -1.869662    -0.088287      17.43
 C      -1.366720     0.211709    -2.868242      58.53
 H      -1.572598     0.439056    -3.896384      21.05
 C      -0.294116     0.927182    -2.127259      15.32
 O       0.330980     2.040059    -2.666513     241.35
 C       0.160218     2.462704    -4.024879     112.93
 H       1.054426     3.050099    -4.293316      25.75
 H       0.405712     1.523807    -4.568821      27.29
 H      -0.761751     2.843478    -4.122546      29.33
 C       0.071124     0.449447    -0.886843      16.50
 O       1.212175     0.966360    -0.206902     196.82
 C      -0.769700    -0.659262    -0.239703      63.69
 H      -0.467891    -0.939646     0.922967      19.16
 C      -2.006603    -0.834739    -2.259641      47.82
 C      -3.087086    -1.770369    -3.100443      40.12
 H      -3.044391    -1.323902    -4.170377      26.88
 O      -2.751668    -3.161479    -3.173403     230.71
 H      -1.714125    -3.259224    -2.771807      24.42
 C      -4.575564    -1.582006    -2.615596      97.80
 H      -4.497877    -1.965066    -1.594351      28.07
 O      -5.031448    -0.243599    -2.774256     252.44
 H      -4.301274     0.289496    -2.464930      31.60
 C      -5.574806    -2.490582    -3.444147     103.70
 O      -5.581662    -3.854870    -2.950136     193.98
 H      -4.620979    -4.268130    -3.163705      29.10
 H      -5.404503    -2.390256    -4.534929      29.86
 H      -6.635498    -2.265987    -3.235214      27.68
55
name = lig-ACN-frame_412
 C       4.530936     2.729094    -0.522379      65.10
 H       3.893749     3.619203    -0.829957      22.89
 C       4.667513     0.729887     0.834279      35.24
 H       4.049602    -0.090676     1.321677      20.72
 C       5.922534     0.371268     0.073020      -5.64
 O       6.606757    -0.865437     0.469636     200.78
 C       6.058461    -1.798035     1.430155      96.25
 H       5.148168    -2.371293     0.931239      25.41
 H       5.970727    -1.292905     2.482935      24.78
 H       6.889736    -2.652264     1.472476      24.97
 C       6.478208     1.289171    -0.813564      13.82
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 O       7.552489     0.975096    -1.553398     189.55
 H       7.966214     0.045995    -1.296644      19.64
 C       5.659059     2.342504    -1.243329      61.88
 H       6.098763     2.942850    -2.088730      24.03
 C       4.011698     1.970794     0.547263      13.94
 C       2.677764     2.201229     1.293510      75.18
 H       2.853520     3.438640     1.612652      22.68
 O       2.575301     1.354127     2.493178     207.28
 H       2.064715     0.369175     2.266252      19.86
 C       1.422016     2.218619     0.342425      81.75
 H       1.654520     2.850165    -0.547702      23.16
 C       0.122733     2.858190     1.035369     104.32
 O       0.357200     4.118883     1.584802     269.94
 H       0.402434     4.797541     0.838196      28.62
 H      -0.290290     2.251446     1.964987      24.28
 H      -0.646181     2.741668     0.312604      26.29
 C      -1.759286    -1.211672    -0.865100      39.58
 H      -2.646816    -2.015168    -0.598326      19.81
 C      -1.354048     0.184920    -2.831669      47.94
 H      -1.591120     0.311851    -3.866251      21.50
 C      -0.369095     0.915183    -2.161268      -5.42
 O       0.417269     2.069088    -2.567256     202.85
 C       0.145147     2.410659    -4.039267     128.69
 H       0.713113     3.284037    -4.261914      26.35
 H       0.081100     1.632851    -4.782979      28.74
 H      -0.786299     2.824558    -4.166958      30.10
 C       0.043534     0.445005    -0.780857      36.20
 O       1.140706     0.957052    -0.175929     219.59
 C      -0.642012    -0.570328    -0.285859      45.86
 H      -0.604739    -0.942641     0.895545      18.83
 C      -2.163997    -0.881068    -2.251697      48.27
 C      -3.069227    -1.681321    -3.103196      69.36
 H      -2.991490    -1.336971    -4.171687      28.24
 O      -2.794360    -3.155491    -3.117847     205.48
 H      -1.693917    -3.237798    -3.122069      27.10
 C      -4.531273    -1.619992    -2.635660      95.85
 H      -4.700145    -1.878959    -1.591803      28.50
 O      -4.967153    -0.249482    -2.773099     191.41
 H      -4.297388     0.543726    -2.256287      22.09
 C      -5.610672    -2.502740    -3.384756     101.71
 O      -5.600758    -3.890179    -2.934692     139.47
 H      -4.724187    -4.357635    -3.419415      27.83
 H      -5.454760    -2.495777    -4.469885      30.11
 H      -6.592782    -1.969982    -3.171998      28.49
55
name = lig-ACN-frame_413
 C       4.495577     2.748272    -0.532769      56.54
 H       4.091136     3.737098    -0.841780      22.25
 C       4.745987     0.715644     0.824239      97.77
 H       4.477559     0.109364     1.701474      23.69
 C       5.861203     0.365367     0.223631      46.74
 O       6.522058    -0.814154     0.389367     222.04
 C       6.167053    -1.810205     1.335309     109.12
 H       5.052883    -2.295253     1.211788      25.48
 H       6.065658    -1.534802     2.460913      24.98
 H       7.042614    -2.592548     1.251720      25.97
 C       6.425798     1.204837    -0.814780      21.75
 O       7.613153     0.965986    -1.554251     138.32
 H       7.971916     0.115414    -1.338963      21.32
 C       5.661638     2.292899    -1.240841      50.01
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 H       5.921873     2.785324    -2.172840      23.62
 C       4.067828     1.910005     0.570516      24.81
 C       2.719302     2.206130     1.252443      80.46
 H       2.468276     3.328003     1.799935      22.10
 O       2.461753     1.411315     2.413794     230.21
 H       1.968427     0.505265     1.988792      22.04
 C       1.486270     2.265772     0.309283      60.29
 H       1.800069     3.002165    -0.518477      24.29
 C       0.085069     2.760490     1.160569      95.07
 O       0.359569     4.128359     1.582680     273.01
 H       0.689793     4.551318     0.925684      35.20
 H      -0.004021     2.044797     2.066935      25.16
 H      -0.818516     2.816071     0.534133      25.97
 C      -1.807447    -1.191844    -0.887961      61.55
 H      -1.978314    -2.224130    -0.200739      19.59
 C      -1.368809     0.179153    -2.844196      57.94
 H      -1.485191     0.613864    -3.819282      21.17
 C      -0.345801     0.927933    -2.099250      20.09
 O       0.406906     1.995898    -2.602595     234.82
 C       0.066483     2.427411    -3.976118     123.73
 H       0.814326     3.167399    -4.139968      27.16
 H       0.360237     1.613840    -4.588516      28.81
 H      -0.886337     2.695202    -3.992975      30.63
 C      -0.062752     0.544576    -0.869110      10.54
 O       1.181965     0.822883    -0.093430     129.90
 C      -0.720655    -0.627801    -0.175992      27.33
 H       0.008043    -0.838924     0.769797      18.66
 C      -2.092115    -0.831905    -2.210420      43.92
 C      -3.112792    -1.714561    -3.125704      69.20
 H      -3.148911    -1.218651    -4.112020      30.21
 O      -2.775325    -3.118479    -3.044854     269.43
 H      -2.025358    -3.271453    -3.555777      31.58
 C      -4.552135    -1.617865    -2.611088      98.96
 H      -4.480446    -1.951572    -1.574051      28.97
 O      -4.952520    -0.209863    -2.811928     177.34
 H      -4.632288     0.251983    -1.783047      23.02
 C      -5.567980    -2.491006    -3.339931     107.95
 O      -5.623459    -3.876847    -2.968466     232.02
 H      -4.802972    -4.221097    -3.234991      33.60
 H      -5.538691    -2.335823    -4.428891      30.58
 H      -6.624521    -2.171668    -2.954229      27.33
55
name = lig-ACN-frame_414
 C       4.520359     2.688774    -0.504068      76.62
 H       3.961550     3.578652    -0.729322      24.94
 C       4.688933     0.752222     0.980823      48.24
 H       4.370690     0.312242     1.889882      22.02
 C       5.908296     0.381460     0.234107      29.02
 O       6.567985    -0.848358     0.286289     226.25
 C       6.239051    -1.860062     1.313177      95.68
 H       5.085687    -2.219381     1.029978      23.06
 H       6.448074    -1.334786     2.291799      21.87
 H       6.922988    -2.778272     1.130903      24.12
 C       6.347340     1.116401    -0.894757      15.90
 O       7.623331     0.947070    -1.557701     227.54
 H       8.087770     0.186144    -1.251860      34.34
 C       5.643289     2.320711    -1.235777      56.42
 H       6.087764     2.880619    -2.011950      23.38
 C       4.007158     1.939772     0.527126      23.33
 C       2.686050     2.280199     1.251696      77.17
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 H       3.167807     3.356083     1.632966      22.11
 O       2.338238     1.443969     2.349770     261.91
 H       2.242328     0.471700     2.211814      24.79
 C       1.352145     2.215799     0.349272      88.13
 H       1.303435     2.770751    -0.679839      23.43
 C       0.263109     2.687786     1.159967     103.29
 O       0.334680     4.156954     1.617006     210.97
 H       1.129717     4.583445     1.108550      27.73
 H       0.209471     2.128715     2.108841      25.02
 H      -0.747416     2.438290     0.664556      25.25
 C      -1.750096    -1.263209    -0.858674      48.39
 H      -2.324472    -2.319737    -0.549989      20.96
 C      -1.357753     0.294182    -2.820527      52.86
 H      -1.805824     0.342158    -3.819377      20.58
 C      -0.377417     0.939149    -2.121195       0.77
 O       0.374083     1.921524    -2.655122     219.78
 C       0.065026     2.430965    -3.916961     142.73
 H       0.567513     3.353163    -4.089289      27.94
 H       0.237715     1.752332    -4.723465      29.20
 H      -0.886503     2.684744    -4.057417      31.67
 C       0.009592     0.476821    -0.641066      43.61
 O       1.204301     0.784090    -0.083519     189.44
 C      -0.766585    -0.517781    -0.203305      51.11
 H      -0.544001    -1.200853     0.688623      20.80
 C      -2.039738    -0.857766    -2.207015      47.08
 C      -3.090145    -1.698000    -3.079477      76.96
 H      -3.028548    -1.499879    -4.131266      28.92
 O      -2.769056    -3.104756    -3.007034     260.08
 H      -2.020492    -3.213857    -3.603574      30.78
 C      -4.554519    -1.563547    -2.546135      96.83
 H      -4.636130    -1.768329    -1.473519      29.29
 O      -4.973649    -0.208394    -2.789627     224.64
 H      -4.953011     0.400703    -2.013807      28.45
 C      -5.626642    -2.438217    -3.298462     104.94
 O      -5.598272    -3.876187    -3.025624     236.75
 H      -4.700003    -4.114858    -2.900274      33.79
 H      -5.535302    -2.236833    -4.380099      30.29
 H      -6.668711    -2.019268    -2.970853      27.73
55
name = lig-ACN-frame_415
 C       4.476734     2.686753    -0.523251      47.07
 H       3.992022     3.550727    -0.887367      23.52
 C       4.745844     0.787007     1.031718      75.98
 H       4.334670     0.081552     1.671619      23.99
 C       5.839278     0.364877     0.172354     -10.66
 O       6.678025    -0.963731     0.234130     181.58
 C       6.300949    -1.833792     1.248146     110.98
 H       5.073767    -2.135753     1.376134      24.50
 H       6.497971    -1.608024     2.330969      25.56
 H       6.901937    -2.772434     1.046399      26.03
 C       6.346386     1.154098    -0.950525       7.11
 O       7.528001     0.922233    -1.544648     157.52
 H       7.904147     0.015808    -1.169145      21.65
 C       5.694375     2.319821    -1.236244      54.04
 H       6.110202     3.086724    -1.845546      23.65
 C       3.936032     1.835569     0.544296      13.63
 C       2.648810     2.284329     1.168952      87.12
 H       2.392109     3.416886     1.624053      23.34
 O       2.307477     1.509936     2.389072     243.66
 H       2.202288     0.668350     2.044521      29.63
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 C       1.398069     2.210376     0.294508      75.14
 H       1.492579     2.927002    -0.657191      24.05
 C       0.250083     2.741119     1.311631     104.43
 O       0.318188     4.104292     1.593451     153.18
 H       1.254909     4.675153     1.143163      23.69
 H       0.325147     2.169052     2.187236      26.52
 H      -0.772242     2.608922     0.735395      25.72
 C      -1.740369    -1.283517    -0.984606      54.14
 H      -2.376087    -2.099366    -0.441711      20.16
 C      -1.476237     0.235860    -2.726650      51.21
 H      -1.427379     0.794849    -3.671120      20.14
 C      -0.363795     0.871732    -1.967826      14.70
 O       0.430230     1.911020    -2.622431     182.59
 C      -0.000257     2.488247    -4.011231     111.93
 H       0.610091     3.376065    -3.911768      26.75
 H       0.298182     1.869369    -4.823211      28.55
 H      -0.958058     2.686912    -3.959775      30.99
 C       0.000699     0.432195    -0.750259      20.45
 O       1.244398     0.820741    -0.029640     159.31
 C      -0.824600    -0.633006    -0.074624      32.90
 H      -0.653726    -0.658288     0.988501      21.22
 C      -2.062264    -0.886309    -2.272398      45.81
 C      -3.033731    -1.671365    -2.988859      71.84
 H      -3.115618    -1.150547    -3.908998      28.67
 O      -2.788852    -3.141010    -2.968102     215.70
 H      -1.689736    -3.371863    -3.152659      25.02
 C      -4.584996    -1.501261    -2.477648      87.04
 H      -4.618428    -1.745314    -1.400044      28.35
 O      -5.047702    -0.155709    -2.787820     250.40
 H      -4.597040     0.337167    -2.238429      34.50
 C      -5.651353    -2.382730    -3.263170     103.10
 O      -5.555907    -3.834210    -3.054657     184.96
 H      -4.457672    -3.904828    -2.922333      28.03
 H      -5.542084    -2.189491    -4.349295      28.88
 H      -6.694785    -2.046791    -2.929019      27.42
55
name = lig-ACN-frame_416
 C       4.428987     2.630109    -0.555268      76.98
 H       3.913179     3.536841    -0.738043      25.44
 C       4.826877     0.662110     0.880515      52.99
 H       4.580964     0.113014     1.764272      23.91
 C       5.871520     0.202956     0.083889      21.03
 O       6.646078    -0.858108     0.202393     199.92
 C       6.350134    -1.912118     1.286664     100.00
 H       5.093054    -1.967178     1.192859      23.85
 H       6.782646    -1.456073     2.168188      26.33
 H       6.763277    -2.885595     1.004538      26.37
 C       6.330465     1.180288    -0.844651       5.98
 O       7.474202     0.844019    -1.571979     143.57
 H       7.892434    -0.105736    -1.303047      19.26
 C       5.626404     2.417189    -1.181575      68.78
 H       6.043644     2.979769    -2.038521      23.39
 C       3.986349     1.885902     0.509837       0.65
 C       2.576113     2.242973     1.218456      80.25
 H       3.006458     3.397558     1.448905      22.39
 O       2.379723     1.580434     2.427839     235.61
 H       1.855673     0.697128     2.392510      24.58
 C       1.379942     2.256463     0.298194      72.70
 H       1.563590     2.962191    -0.643377      23.41
 C       0.152287     2.732832     1.293910      97.69
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 O       0.320800     4.166660     1.604585     172.97
 H       1.009931     4.575627     0.800950      25.03
 H       0.215929     2.208423     2.183933      27.01
 H      -0.973776     2.535853     0.926798      25.31
 C      -1.741417    -1.326191    -0.826919      59.83
 H      -2.297830    -2.151133    -0.390215      22.44
 C      -1.402640     0.343690    -2.685484      77.65
 H      -1.888955     0.549974    -3.645633      24.88
 C      -0.337755     0.887741    -2.037529      11.84
 O       0.437538     1.867524    -2.604891     190.12
 C      -0.028281     2.531366    -3.932207     115.58
 H       0.523842     3.476226    -4.129675      26.65
 H       0.264399     1.814195    -4.708533      27.64
 H      -0.967902     2.736814    -4.089291      30.74
 C       0.038564     0.311024    -0.674804      26.45
 O       1.155953     0.824962    -0.048393     177.29
 C      -0.783876    -0.618000    -0.102307      44.66
 H      -0.784876    -0.870918     0.859525      24.21
 C      -2.051909    -0.905627    -2.206662      47.67
 C      -3.198207    -1.715081    -3.029359      72.55
 H      -3.153903    -1.653988    -4.082877      27.71
 O      -2.804665    -3.133128    -2.943180     231.80
 H      -1.755169    -3.130562    -2.584314      28.41
 C      -4.629327    -1.482549    -2.469381      98.87
 H      -4.680435    -1.647547    -1.375098      28.12
 O      -5.083789    -0.100825    -2.749414     211.46
 H      -4.466083     0.644712    -2.472519      28.51
 C      -5.616285    -2.347855    -3.227423     112.21
 O      -5.462892    -3.735600    -3.031363     182.88
 H      -4.458220    -4.141074    -3.265321      26.48
 H      -5.624895    -1.980070    -4.283689      29.19
 H      -6.639798    -2.160057    -2.822358      27.65
55
name = lig-ACN-frame_417
 C       4.356820     2.682632    -0.537929      35.81
 H       3.735147     3.521861    -0.854720      21.42
 C       4.687279     0.584478     0.775113      79.71
 H       4.417651     0.133143     1.750275      24.16
 C       5.845541     0.292508     0.033620       9.97
 O       6.656112    -0.918465     0.231220     219.35
 C       6.375375    -1.853003     1.230163     117.91
 H       5.169129    -2.102989     1.589631      24.73
 H       6.784121    -1.693321     2.216835      27.66
 H       6.854529    -2.717307     0.827463      28.36
 C       6.378170     1.193985    -0.892737      19.66
 O       7.438064     0.805123    -1.645872     126.87
 H       7.728169    -0.026564    -1.256362      21.54
 C       5.658004     2.340171    -1.163315      36.74
 H       6.000657     2.966210    -2.048307      22.31
 C       4.032848     1.740023     0.516831      22.59
 C       2.781154     2.217685     1.244249      64.21
 H       2.743910     3.428559     1.636473      22.21
 O       2.463214     1.627598     2.563023     192.71
 H       2.105618     0.624349     2.169274      24.13
 C       1.195301     2.237485     0.404762      73.59
 H       1.215527     2.821767    -0.607942      24.05
 C       0.096808     2.776712     1.188215     102.28
 O       0.320880     4.225475     1.584618     246.24
 H       0.500425     4.728411     0.831757      31.63
 H       0.109525     2.292143     2.131054      27.65
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 H      -0.901182     2.528975     0.556654      25.39
 C      -1.812654    -1.348725    -0.795214      58.42
 H      -2.224137    -2.166886    -0.413040      22.64
 C      -1.479210     0.219325    -2.696390      60.27
 H      -1.736117     0.714480    -3.608938      21.39
 C      -0.305444     0.839214    -2.066455      11.51
 O       0.435647     1.933717    -2.618086     225.48
 C      -0.003102     2.472386    -3.810032     121.97
 H       0.625093     3.415269    -3.807991      25.69
 H       0.133840     1.801974    -4.711483      27.98
 H      -0.959706     2.681738    -3.664064      30.94
 C       0.036684     0.404874    -0.772282      21.13
 O       1.128442     0.842037    -0.028142     187.37
 C      -0.737829    -0.672654    -0.084959      37.10
 H      -0.267725    -1.012543     0.695611      23.57
 C      -2.116227    -0.867814    -2.092906      19.13
 C      -3.193362    -1.723060    -3.027431      56.64
 H      -3.229718    -1.237746    -3.991040      29.15
 O      -2.844866    -3.127785    -2.851165     296.21
 H      -1.914158    -3.157600    -2.724406      32.29
 C      -4.628739    -1.393630    -2.478925      93.71
 H      -4.649119    -1.669960    -1.394507      27.92
 O      -5.115016    -0.078172    -2.747376     186.14
 H      -4.486240     0.570396    -1.974824      22.37
 C      -5.661660    -2.294129    -3.189448     109.17
 O      -5.372166    -3.716550    -2.994945     208.27
 H      -4.530820    -3.797551    -3.386160      33.09
 H      -5.663625    -2.106987    -4.301335      29.16
 H      -6.650091    -2.060833    -2.798592      28.97
55
name = lig-ACN-frame_418
 C       4.487572     2.585224    -0.511941      70.65
 H       3.935650     3.526085    -0.780052      25.69
 C       4.592772     0.511093     0.758565      52.31
 H       4.215683    -0.407093     1.333202      21.84
 C       5.841645     0.280529     0.128930       8.90
 O       6.626045    -0.880529     0.208681     210.66
 C       6.415110    -1.885602     1.257756     112.63
 H       5.148333    -2.041246     1.297909      22.99
 H       6.929165    -1.564763     2.135776      26.73
 H       6.770666    -2.832948     0.939131      27.70
 C       6.335768     1.148238    -0.968829       8.65
 O       7.461989     0.787042    -1.743859     171.03
 H       7.902133     0.033775    -1.420197      26.72
 C       5.596218     2.345410    -1.236478      67.53
 H       6.069590     3.125435    -1.902713      23.01
 C       3.854952     1.779117     0.447534      21.05
 C       2.712827     2.269504     1.337458      60.10
 H       2.991953     3.531372     1.441917      23.06
 O       2.562238     1.603405     2.627755     191.12
 H       2.540024     0.562900     2.648024      24.41
 C       1.340020     2.211956     0.416913      67.21
 H       1.556824     2.965771    -0.427227      25.82
 C       0.011657     2.884749     1.208392      98.61
 O       0.286864     4.214801     1.540157     263.46
 H       0.211933     4.740032     0.790737      31.24
 H      -0.421521     2.361631     2.073583      26.52
 H      -0.936019     2.980900     0.481103      25.55
 C      -1.793973    -1.311672    -0.750074      49.04
 H      -2.160351    -2.081231    -0.353698      24.23
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 C      -1.444334     0.161185    -2.699554      61.45
 H      -1.710815     0.313124    -3.710897      23.13
 C      -0.361122     0.802502    -2.092139      16.76
 O       0.453971     1.871994    -2.505076     215.22
 C      -0.033417     2.510631    -3.759690     120.81
 H       0.541794     3.458079    -4.076455      26.36
 H      -0.009386     1.813846    -4.693802      27.04
 H      -0.938169     2.805852    -3.740560      31.51
 C      -0.077997     0.385811    -0.766451      26.07
 O       1.123619     0.855852     0.023200     139.52
 C      -0.630579    -0.712382    -0.199912      42.52
 H      -0.274932    -1.037946     0.709129      21.88
 C      -2.249055    -0.844760    -2.085209      28.31
 C      -3.122965    -1.571471    -2.893477      92.69
 H      -2.890245    -1.470176    -3.949832      28.28
 O      -2.881303    -3.085211    -2.778142     214.23
 H      -2.179038    -3.281570    -3.299159      32.01
 C      -4.662219    -1.416165    -2.485867      91.06
 H      -4.687330    -1.584844    -1.379505      27.94
 O      -5.087862    -0.026556    -2.718631     157.64
 H      -4.918658     0.689128    -1.788491      22.40
 C      -5.718084    -2.304751    -3.177714     124.36
 O      -5.345209    -3.692996    -2.966774     227.69
 H      -4.445462    -3.752423    -3.003419      33.38
 H      -5.788818    -1.976795    -4.265541      30.32
 H      -6.684295    -2.185308    -2.742573      30.26
55
name = lig-ACN-frame_419
 C       4.449955     2.597515    -0.464981      27.86
 H       4.200907     3.703843    -0.430776      22.22
 C       4.531065     0.505690     0.677305      67.95
 H       3.890345    -0.266742     1.235380      22.51
 C       5.812354     0.268909     0.093993      19.13
 O       6.616158    -0.872964     0.188306     216.92
 C       6.409741    -1.886604     1.254714     107.61
 H       5.219578    -2.069018     1.581456      23.84
 H       6.791066    -1.546478     2.201359      26.57
 H       6.945412    -2.756202     0.895812      27.01
 C       6.313326     1.066615    -1.012974      19.38
 O       7.434380     0.806717    -1.787594     151.36
 H       7.871490    -0.052468    -1.356290      23.19
 C       5.670559     2.261074    -1.308719      44.83
 H       6.011576     2.982053    -2.058080      23.46
 C       3.844172     1.688862     0.461735       8.39
 C       2.550064     2.208492     1.366097      75.15
 H       2.764692     3.399380     1.790651      22.46
 O       2.674176     1.621846     2.675812     249.92
 H       2.588585     0.770101     2.430279      32.41
 C       1.360972     2.284610     0.519858      75.08
 H       1.714758     2.778338    -0.399896      25.44
 C      -0.016596     2.904143     1.102251      99.01
 O       0.254223     4.278692     1.574445     164.12
 H       0.443862     4.886135     0.594718      24.65
 H      -0.266290     2.296465     2.027404      26.23
 H      -0.761523     2.723068     0.222648      25.52
 C      -1.761146    -1.303834    -0.731814      64.45
 H      -2.308199    -2.011649    -0.342122      24.81
 C      -1.415643     0.162171    -2.762374      48.90
 H      -1.623330     0.311945    -3.798646      21.47
 C      -0.394865     0.830533    -2.009028      12.40
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 O       0.415882     1.827806    -2.501106     199.82
 C      -0.070589     2.554556    -3.744597     107.05
 H       0.797021     3.287489    -3.838782      25.42
 H      -0.003375     1.673596    -4.517959      25.54
 H      -0.988498     2.865133    -3.643919      31.19
 C       0.035576     0.433854    -0.655785      36.62
 O       1.076681     0.843056     0.013883     178.92
 C      -0.624288    -0.798296    -0.205460      45.27
 H      -0.374837    -1.160783     0.837969      21.21
 C      -2.140359    -0.751349    -2.001521      23.85
 C      -3.258451    -1.625544    -2.871195      62.76
 H      -3.248462    -1.181766    -3.924799      27.54
 O      -2.890981    -3.025167    -2.706538     205.40
 H      -2.358028    -3.321186    -3.604863      25.61
 C      -4.706255    -1.358149    -2.450981     103.75
 H      -4.800352    -1.674608    -1.371372      28.84
 O      -5.088826     0.004217    -2.711696     222.88
 H      -4.603216     0.643076    -1.925560      22.94
 C      -5.712979    -2.333987    -3.152470     124.48
 O      -5.381569    -3.703036    -2.957431     239.18
 H      -4.459178    -3.641965    -2.689477      29.90
 H      -5.862617    -2.117922    -4.256067      30.19
 H      -6.628222    -2.103253    -2.681253      30.45
55
name = lig-ACN-frame_420
 C       4.492108     2.652717    -0.461707      72.04
 H       4.045518     3.687589    -0.588569      24.55
 C       4.508638     0.449616     0.593881      51.21
 H       4.376733    -0.277241     1.450432      22.53
 C       5.745323     0.196868    -0.048974       8.82
 O       6.587347    -0.935579     0.218770     220.69
 C       6.408356    -1.821065     1.268366     119.86
 H       5.292367    -2.292492     1.278303      24.89
 H       6.850694    -1.512900     2.224777      26.88
 H       7.001867    -2.720523     0.972592      26.77
 C       6.270879     1.066057    -1.037506      14.82
 O       7.403386     0.769248    -1.762116     171.45
 H       7.851883    -0.141527    -1.491027      22.54
 C       5.541244     2.233159    -1.223399      72.22
 H       5.943232     2.763381    -2.034412      24.04
 C       3.874894     1.779312     0.461341       4.94
 C       2.709292     2.193541     1.378433      66.61
 H       2.799302     3.429104     1.420258      23.72
 O       2.703721     1.567858     2.701842     234.49
 H       2.224041     0.703082     2.784001      26.45
 C       1.233810     2.233109     0.477075      81.26
 H       1.471742     2.946018    -0.314431      26.41
 C       0.079251     2.906637     1.037519      98.70
 O       0.168741     4.314310     1.536965     154.06
 H       1.062701     4.955691     1.045441      23.35
 H      -0.356547     2.350233     1.980211      25.66
 H      -0.810491     2.931060     0.349131      26.01
 C      -1.782048    -1.296153    -0.780307      54.33
 H      -2.292224    -2.098337    -0.279439      23.31
 C      -1.357330     0.215331    -2.669351      46.04
 H      -1.514379     0.705554    -3.640944      21.60
 C      -0.356300     0.859858    -1.908106      24.63
 O       0.374930     1.879162    -2.536769     244.89
 C      -0.022313     2.489795    -3.685022     136.32
 H       0.580272     3.408940    -3.894096      26.95
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 H      -0.134918     2.039004    -4.780211      26.06
 H      -0.858687     2.935242    -3.603902      33.01
 C      -0.016914     0.317767    -0.677697      23.82
 O       1.147752     0.900530     0.090024     168.68
 C      -0.600318    -0.761193    -0.015162      33.74
 H       0.018071    -1.229856     0.924716      19.76
 C      -2.203899    -0.842664    -2.162727      54.08
 C      -3.279203    -1.546507    -2.807740      70.80
 H      -3.272649    -1.354442    -3.965203      26.94
 O      -2.914706    -2.977094    -2.672209     128.62
 H      -2.323103    -3.362462    -3.521556      25.29
 C      -4.778072    -1.367326    -2.354811     104.71
 H      -4.918758    -1.428930    -1.240748      28.21
 O      -5.096506     0.008245    -2.710941     247.66
 H      -4.454440     0.577652    -2.357787      31.59
 C      -5.759159    -2.287523    -3.124210     113.89
 O      -5.446778    -3.750080    -2.923360     161.83
 H      -4.363519    -3.855417    -2.771054      27.87
 H      -5.678723    -2.071330    -4.225148      29.04
 H      -6.744701    -2.148963    -2.814007      29.75
55
name = lig-ACN-frame_421
 C       4.420237     2.699603    -0.427274      46.53
 H       3.908287     3.604288    -0.814145      23.36
 C       4.553713     0.481881     0.595263      75.31
 H       4.148332    -0.000983     1.492666      24.29
 C       5.667419     0.055375    -0.131138      23.25
 O       6.564495    -0.924922     0.162700     223.01
 C       6.396903    -1.878847     1.309963     104.30
 H       5.288667    -2.173257     1.401470      26.79
 H       6.499322    -1.303333     2.247050      27.04
 H       7.149130    -2.731906     1.176732      25.87
 C       6.198171     1.005485    -1.041506      13.56
 O       7.381077     0.735892    -1.738099     188.29
 H       7.606744    -0.102691    -1.414728      25.13
 C       5.535781     2.286989    -1.267712      42.48
 H       5.911370     3.038600    -1.871222      23.08
 C       3.959088     1.742117     0.502217      27.78
 C       2.778122     2.241369     1.313136      72.20
 H       3.174780     3.206396     1.854756      22.19
 O       2.689077     1.547345     2.693109     186.80
 H       2.015541     0.729386     2.328854      23.60
 C       1.443147     2.251950     0.402693      61.34
 H       1.670969     2.685702    -0.541842      25.47
 C      -0.047148     2.984102     1.153616      92.77
 O       0.155923     4.329357     1.486599     250.60
 H       1.143451     4.482315     1.239661      27.75
 H      -0.463003     2.320404     2.066097      25.25
 H      -0.694832     2.882502     0.286649      26.72
 C      -1.735492    -1.280534    -0.785090      47.68
 H      -2.281549    -2.269481    -0.476662      22.26
 C      -1.422496     0.269879    -2.587946      51.27
 H      -1.799153     0.583391    -3.608827      22.44
 C      -0.336297     0.832171    -1.929442      14.26
 O       0.428144     1.885843    -2.441697     179.16
 C      -0.067895     2.597435    -3.771150     106.60
 H       0.758476     3.288301    -3.834039      26.35
 H       0.075003     1.640983    -4.426906      26.87
 H      -1.031455     2.826124    -3.857190      30.38
 C       0.099888     0.350371    -0.552198      32.64
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 O       1.135293     0.820417     0.106697     193.81
 C      -0.742057    -0.715439    -0.078897      60.33
 H      -0.507137    -1.290787     1.039242      20.63
 C      -2.072213    -0.828050    -2.037306      40.32
 C      -3.295306    -1.587359    -2.839075      47.14
 H      -3.339719    -1.247941    -3.997503      26.28
 O      -2.963737    -3.005088    -2.661423     268.56
 H      -2.133685    -3.063620    -3.094531      31.94
 C      -4.797063    -1.331779    -2.263168      93.10
 H      -4.831975    -1.535345    -1.156649      28.63
 O      -5.148446     0.004956    -2.758499     246.44
 H      -4.751388     0.540300    -2.165192      33.10
 C      -5.757465    -2.330716    -3.093324     105.56
 O      -5.553051    -3.737527    -2.879930     178.66
 H      -4.411931    -3.748330    -3.040572      25.08
 H      -5.595649    -1.966582    -4.135762      29.31
 H      -6.784650    -2.142739    -2.899743      29.48
55
name = lig-ACN-frame_422
 C       4.434690     2.635469    -0.531555      65.84
 H       3.986072     3.603598    -0.367370      24.97
 C       4.553152     0.487088     0.754535      54.68
 H       4.124401    -0.290788     1.321444      23.04
 C       5.611243     0.089022    -0.153972     -13.84
 O       6.566067    -1.042871     0.118281     168.18
 C       6.307133    -1.831241     1.317906     111.87
 H       5.445800    -2.474742     1.219594      27.92
 H       6.435298    -1.255802     2.302274      26.05
 H       7.225847    -2.559324     1.333514      26.03
 C       6.114119     1.037168    -1.129293      12.07
 O       7.326288     0.710289    -1.698413     182.45
 H       7.737822    -0.095910    -1.347880      23.69
 C       5.580200     2.321857    -1.261795      60.39
 H       6.180280     2.910309    -1.921248      22.77
 C       4.000407     1.770829     0.486565      18.99
 C       2.802004     2.249572     1.386020      88.99
 H       2.832894     3.409643     1.430187      25.43
 O       2.584495     1.528912     2.550064     244.61
 H       2.353101     0.476731     2.469717      21.49
 C       1.494718     2.308143     0.502075      63.34
 H       1.654272     2.816715    -0.388663      25.36
 C       0.035212     2.909453     1.096274      92.93
 O       0.179856     4.357757     1.467805     292.85
 H       0.898374     4.708080     1.184421      34.62
 H      -0.170832     2.296019     2.114289      24.40
 H      -0.789301     2.796048     0.438669      26.24
 C      -1.756544    -1.377662    -0.799626      60.15
 H      -2.268531    -2.359128    -0.189972      18.34
 C      -1.485782     0.326942    -2.550515      67.86
 H      -1.786343     0.749657    -3.571585      20.03
 C      -0.267359     0.839621    -1.883892       9.80
 O       0.437069     1.968172    -2.383133     198.50
 C      -0.000847     2.506503    -3.761509     114.28
 H       0.501638     3.416542    -3.970920      27.03
 H       0.236788     1.823143    -4.681871      26.92
 H      -0.940166     2.832838    -3.760454      29.11
 C       0.003079     0.403976    -0.613510      36.84
 O       1.224046     0.737053     0.205073     110.87
 C      -0.742077    -0.632664    -0.041708      46.06
 H      -0.650563    -0.826088     1.233133      18.55
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 C      -2.163185    -0.836604    -2.025449      48.66
 C      -3.243560    -1.590537    -2.718188      60.34
 H      -3.219573    -1.211386    -3.868751      24.79
 O      -3.006681    -3.049286    -2.710305     275.27
 H      -2.130718    -3.217292    -2.497100      34.04
 C      -4.726269    -1.361717    -2.343677      93.60
 H      -4.885333    -1.359826    -1.238534      27.68
 O      -5.218199    -0.013751    -2.737302     182.84
 H      -5.107136     0.742628    -1.986306      25.45
 C      -5.747470    -2.289231    -3.054612     111.21
 O      -5.628272    -3.705308    -2.840936     192.40
 H      -4.676418    -4.065993    -3.020899      30.48
 H      -5.670429    -2.176464    -4.139539      30.15
 H      -6.747127    -2.003122    -2.702826      29.26
55
name = lig-ACN-frame_423
 C       4.496117     2.625946    -0.525418      43.24
 H       4.290581     3.657617    -0.722911      22.69
 C       4.594011     0.467203     0.747645      69.75
 H       4.299945    -0.110985     1.593792      23.56
 C       5.658205     0.120535    -0.050201      22.29
 O       6.433096    -1.067362     0.057066     242.93
 C       6.289338    -1.812208     1.286927     110.23
 H       5.450649    -2.439899     1.186986      28.62
 H       5.967125    -1.102849     2.121823      25.95
 H       7.238301    -2.443324     1.517303      25.67
 C       6.125169     0.957165    -1.101430      14.54
 O       7.302023     0.705658    -1.730160     162.07
 H       7.670125    -0.129951    -1.157318      22.83
 C       5.632131     2.288928    -1.307064      51.84
 H       6.004505     3.094536    -2.004330      21.57
 C       3.932315     1.770000     0.544191       7.47
 C       2.705541     2.275739     1.315497      97.23
 H       3.047388     3.171737     1.877644      24.18
 O       2.499702     1.501874     2.513086     272.27
 H       2.488269     0.647774     2.212829      30.61
 C       1.396300     2.200958     0.511652     104.72
 H       1.632469     2.712871    -0.362501      26.30
 C       0.285112     2.872762     1.114124     108.58
 O       0.193446     4.322737     1.449607     267.91
 H       0.555615     4.856190     0.701324      29.59
 H       0.009710     2.397599     2.149283      25.41
 H      -0.478412     2.634053     0.430532      26.79
 C      -1.703910    -1.314843    -0.700623      62.49
 H      -2.365872    -2.318230    -0.183413      19.61
 C      -1.459550     0.329560    -2.487996      56.03
 H      -1.826821     0.781171    -3.459579      22.88
 C      -0.346441     0.943984    -1.931288       6.33
 O       0.409862     2.027340    -2.417859     227.41
 C       0.087138     2.446843    -3.681757     126.80
 H       0.629785     3.347218    -3.694164      26.45
 H       0.326052     1.678068    -4.502989      27.14
 H      -0.940478     2.507880    -3.792744      29.07
 C       0.039003     0.402435    -0.541956       9.80
 O       1.214570     0.794777     0.236079     162.43
 C      -0.779978    -0.603346     0.022766      34.52
 H      -0.254910    -0.879957     1.144605      19.44
 C      -2.180480    -0.820012    -1.938201      39.74
 C      -3.237321    -1.604895    -2.793725      62.52
 H      -3.033277    -1.352559    -3.951605      25.90
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 O      -3.052488    -3.080466    -2.727144     231.91
 H      -2.020012    -3.293374    -2.395860      27.64
 C      -4.716229    -1.334037    -2.359099      93.23
 H      -4.764326    -1.623874    -1.275567      27.71
 O      -5.271985    -0.037487    -2.722946     171.07
 H      -4.699382     0.651445    -1.920754      21.83
 C      -5.736397    -2.258215    -3.071013     109.20
 O      -5.719160    -3.726033    -2.769326     227.96
 H      -4.851922    -3.854373    -2.872377      35.58
 H      -5.830965    -1.920131    -4.098625      30.10
 H      -6.704285    -1.917899    -2.579459      27.62
55
name = lig-ACN-frame_424
 C       4.526171     2.644914    -0.430952      77.50
 H       3.864076     3.448989    -0.632360      25.00
 C       4.551558     0.587465     0.750411      70.12
 H       4.306755     0.095353     1.700741      23.63
 C       5.725255     0.159687    -0.011413      12.15
 O       6.312503    -1.068971     0.022875     225.40
 C       6.204388    -1.805586     1.271439     110.89
 H       5.581680    -2.583799     1.180662      29.25
 H       5.948953    -1.119711     2.157080      25.58
 H       7.266489    -2.157927     1.530240      25.78
 C       6.223934     0.988564    -1.037282      20.09
 O       7.347783     0.623434    -1.791992     189.04
 H       7.838341    -0.194983    -1.515733      24.05
 C       5.560125     2.164388    -1.273473      63.64
 H       6.126056     2.743767    -2.115526      22.92
 C       3.979596     1.787940     0.472204      31.19
 C       2.728591     2.227026     1.318478      90.58
 H       2.668002     3.313278     1.404358      25.18
 O       2.440895     1.435361     2.552833     275.86
 H       2.114892     0.572743     2.388098      26.47
 C       1.542359     2.229187     0.348980      71.49
 H       1.648535     2.666913    -0.609416      24.38
 C       0.212722     2.874791     1.227856      94.98
 O       0.274145     4.258954     1.408916     179.68
 H       0.292241     4.718336     0.335944      24.92
 H       0.145547     2.356775     2.221738      24.84
 H      -0.700759     2.649624     0.715302      24.68
 C      -1.759608    -1.181456    -0.591208      89.57
 H      -2.198906    -2.333143    -0.092216      19.09
 C      -1.478288     0.307832    -2.475902      62.28
 H      -1.860033     0.538771    -3.484676      19.83
 C      -0.383043     0.959787    -1.733326      27.00
 O       0.376798     1.967817    -2.312090     219.48
 C       0.114975     2.453727    -3.749987     115.58
 H       0.658050     3.357080    -4.002140      26.67
 H       0.625142     1.702426    -4.369412      27.07
 H      -0.821583     2.658409    -4.036676      29.62
 C       0.074153     0.468280    -0.540128      38.49
 O       1.094954     0.840947     0.205034     211.42
 C      -0.658915    -0.593005     0.088031      65.98
 H      -0.423724    -1.299250     1.011121      19.41
 C      -2.083009    -0.785311    -1.884245      55.42
 C      -3.223155    -1.628265    -2.891178      34.08
 H      -3.122105    -1.202550    -4.010052      25.97
 O      -3.077914    -3.067518    -2.689987     246.07
 H      -2.024756    -3.305014    -2.962146      24.79
 C      -4.721542    -1.391249    -2.388286      91.69
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 H      -4.703965    -1.478975    -1.280774      27.98
 O      -5.224772    -0.046947    -2.650693     183.06
 H      -4.559617     0.800701    -2.271085      24.65
 C      -5.847003    -2.273646    -3.039122     109.34
 O      -5.772692    -3.665797    -2.741470     218.09
 H      -4.816862    -3.938809    -2.639444      31.40
 H      -5.754767    -2.266646    -4.110703      29.39
 H      -6.898335    -1.895580    -2.724372      27.72
55
name = lig-ACN-frame_425
 C       4.491910     2.693801    -0.509494      48.41
 H       4.177689     3.706082    -0.784292      23.38
 C       4.658840     0.587014     0.798242      64.22
 H       4.094892    -0.196111     1.390184      22.27
 C       5.691351     0.194336     0.016568      12.67
 O       6.220898    -1.111980     0.064028     245.02
 C       6.183013    -1.828025     1.299842     115.94
 H       5.656145    -2.675420     1.175301      29.75
 H       5.738048    -1.230717     2.145097      27.01
 H       7.205774    -2.190946     1.522331      26.96
 C       6.347013     0.985059    -0.974611      10.05
 O       7.386647     0.561530    -1.868781     203.26
 H       7.592787    -0.265361    -1.523519      23.66
 C       5.573360     2.178293    -1.272199      58.49
 H       5.803694     2.847190    -2.206447      24.90
 C       3.984148     1.847441     0.587215      15.75
 C       2.726150     2.162474     1.281492      95.18
 H       2.987557     3.056423     1.796445      24.63
 O       2.429784     1.477042     2.549660     237.80
 H       1.991294     0.517438     2.248093      21.27
 C       1.400671     2.280058     0.361453      77.76
 H       1.745305     2.915397    -0.452784      24.01
 C       0.188634     2.798232     1.195967     107.18
 O       0.345279     4.251516     1.385149     210.78
 H       0.397103     4.733105     0.380453      26.67
 H       0.441267     2.435143     2.159272      25.16
 H      -0.811527     2.435668     0.950164      25.42
 C      -1.806137    -1.136809    -0.543400      49.23
 H      -2.417775    -2.169472     0.043511      20.46
 C      -1.441475     0.312369    -2.436685      47.15
 H      -1.405870     0.707840    -3.428927      20.14
 C      -0.470262     0.961326    -1.741743       9.09
 O       0.331346     2.013111    -2.272809     201.55
 C       0.208589     2.388977    -3.776395     108.17
 H       0.742430     3.313721    -3.557069      25.25
 H       0.462799     1.699259    -4.545014      28.68
 H      -0.823702     2.556363    -3.874385      28.60
 C      -0.066579     0.417643    -0.452516      21.68
 O       1.150743     0.879943     0.191635     167.23
 C      -0.617915    -0.680023     0.097025      49.02
 H      -0.114363    -0.775311     1.064740      18.50
 C      -2.187058    -0.855139    -1.964736      43.08
 C      -3.204137    -1.587233    -2.749591      93.45
 H      -3.019421    -1.386591    -3.888406      25.73
 O      -3.026263    -3.038594    -2.696843     252.61
 H      -2.444258    -3.316963    -3.355708      30.68
 C      -4.738411    -1.380238    -2.389108      96.64
 H      -4.777314    -1.710353    -1.322138      29.03
 O      -5.152836    -0.031090    -2.630849     269.56
 H      -4.547141     0.531416    -2.058722      28.17
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 C      -5.871717    -2.278700    -3.083592     105.75
 O      -5.837484    -3.670190    -2.662012     162.30
 H      -4.693219    -3.722550    -2.661481      27.07
 H      -5.811324    -2.051489    -4.136175      30.18
 H      -6.906663    -1.840691    -2.766428      28.04
55
name = lig-ACN-frame_426
 C       4.516411     2.617454    -0.528244      61.93
 H       4.109573     3.656186    -0.666004      24.31
 C       4.653479     0.625282     0.819807      38.93
 H       4.074920    -0.192315     1.355287      21.47
 C       5.806486     0.174791     0.002559       1.72
 O       6.160191    -1.161048     0.100526     229.70
 C       6.169888    -1.934588     1.371067     106.11
 H       5.579551    -2.739570     1.193207      28.75
 H       5.663027    -1.351483     2.151880      27.39
 H       7.174259    -2.123980     1.720273      26.76
 C       6.334309     1.046333    -1.029734      13.72
 O       7.332574     0.524575    -1.847164     150.99
 H       7.716007    -0.385345    -1.528805      22.05
 C       5.671562     2.258494    -1.294401      59.19
 H       6.076337     2.851542    -2.185719      22.07
 C       4.047704     1.855163     0.578107      18.14
 C       2.654262     2.308973     1.391332      91.89
 H       2.758678     3.320474     1.632199      26.20
 O       2.424805     1.489426     2.508774     239.13
 H       2.376082     0.385592     2.373821      20.58
 C       1.356584     2.279017     0.493791      90.04
 H       1.267126     2.774176    -0.518981      21.85
 C       0.239014     2.839104     1.260607     118.50
 O       0.336416     4.237151     1.372627     306.30
 H       0.798546     4.612881     0.693207      32.81
 H       0.169370     2.435720     2.212859      27.06
 H      -0.671670     2.574590     0.654353      24.79
 C      -1.866419    -1.260752    -0.598547      63.97
 H      -2.702676    -2.035139     0.042084      18.40
 C      -1.471149     0.238093    -2.498568      35.86
 H      -1.857973     0.375086    -3.479303      17.17
 C      -0.440098     0.965913    -1.751704       0.47
 O       0.279207     2.018229    -2.286690     248.15
 C       0.218894     2.363537    -3.611458     131.28
 H       0.913258     3.175864    -4.032938      24.90
 H       0.609883     1.566087    -4.140663      29.16
 H      -0.671420     2.667547    -4.060793      28.50
 C      -0.025216     0.510841    -0.444308      35.50
 O       1.183497     0.861974     0.084858     208.94
 C      -0.742780    -0.715158     0.113186      30.91
 H      -0.616200    -1.228449     0.980723      21.40
 C      -2.175506    -0.778494    -1.813191      58.66
 C      -3.260800    -1.605158    -2.711912      42.53
 H      -3.193871    -1.072173    -3.726655      27.75
 O      -2.990918    -3.062845    -2.686468     229.04
 H      -2.482401    -3.235260    -3.476655      28.53
 C      -4.771606    -1.395769    -2.339276     102.76
 H      -5.009275    -1.592933    -1.275347      28.67
 O      -5.071297    -0.005362    -2.612729     264.09
 H      -4.897873     0.590623    -1.987814      30.97
 C      -5.827087    -2.211069    -3.132581     101.47
 O      -5.841006    -3.628537    -2.624916     136.53
 H      -4.850274    -4.083903    -2.690956      31.02
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 H      -5.876264    -2.292722    -4.205018      30.74
 H      -6.813219    -1.797489    -2.685957      29.09
55
name = lig-ACN-frame_427
 C       4.605578     2.639860    -0.509556      45.28
 H       3.934033     3.493760    -0.842496      22.26
 C       4.666347     0.635303     0.758169      63.40
 H       4.469471     0.065184     1.692853      22.96
 C       5.760480     0.224160     0.085510      31.87
 O       6.188019    -1.237434     0.122152     236.93
 C       6.115921    -1.971276     1.422975     115.91
 H       5.815800    -2.971213     1.222201      27.13
 H       5.631599    -1.493166     2.249112      26.38
 H       7.103767    -2.176585     1.682756      26.39
 C       6.272103     0.959512    -1.033485      13.90
 O       7.287877     0.523094    -1.836990     144.70
 H       7.768360    -0.268955    -1.305463      24.50
 C       5.757027     2.279618    -1.277178      58.20
 H       6.230888     2.980560    -1.965571      22.67
 C       4.005639     1.885313     0.538223      35.86
 C       2.720588     2.378652     1.332098      91.77
 H       2.655257     3.282268     1.768380      26.27
 O       2.449202     1.508581     2.556351     246.15
 H       2.618313     0.683193     2.175266      27.04
 C       1.456685     2.201268     0.503912      70.28
 H       1.721641     3.015577    -0.291297      21.68
 C       0.089621     2.849507     1.352573      93.76
 O       0.329429     4.314785     1.412024     280.73
 H       1.122838     4.563547     1.073179      32.16
 H      -0.180819     2.465220     2.256786      26.30
 H      -0.807275     2.697102     0.659319      24.39
 C      -1.899560    -1.319258    -0.561039      69.14
 H      -2.379069    -2.409348    -0.126952      17.69
 C      -1.500481     0.204420    -2.473043      65.63
 H      -1.759269     0.659502    -3.421625      23.09
 C      -0.460469     0.871553    -1.806993       5.67
 O       0.240735     2.056629    -2.170009     222.43
 C       0.254864     2.296185    -3.665596     100.29
 H       1.052936     3.090718    -3.568543      23.35
 H       0.368581     1.400892    -4.151795      29.26
 H      -0.760562     2.616065    -3.927402      26.64
 C      -0.096823     0.369881    -0.504382      11.43
 O       1.217138     0.838346     0.037273     162.02
 C      -0.850441    -0.621874     0.138132      46.11
 H      -0.423597    -0.981430     0.938793      22.07
 C      -2.294446    -0.811379    -1.858738      47.15
 C      -3.307493    -1.593899    -2.663480      79.30
 H      -3.267549    -1.379922    -3.748282      29.37
 O      -2.998408    -3.051789    -2.701963     182.32
 H      -2.030313    -3.181231    -3.277071      24.91
 C      -4.775013    -1.362025    -2.263668     101.17
 H      -4.935279    -1.579758    -1.199067      29.29
 O      -5.058570     0.034274    -2.665236     273.79
 H      -4.620248     0.486776    -2.006345      30.74
 C      -5.791196    -2.251985    -3.078910     112.27
 O      -5.849659    -3.562796    -2.633700     244.80
 H      -4.954870    -3.770544    -2.805963      34.41
 H      -5.430712    -2.073231    -4.118402      31.34
 H      -6.841441    -1.802804    -3.060082      28.89
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name = lig-ACN-frame_428
 C       4.608642     2.747908    -0.536941      72.96
 H       4.388836     3.800373    -0.896794      24.05
 C       4.630581     0.687097     0.880018      53.84
 H       4.268457     0.220179     1.794086      21.12
 C       5.717609     0.073944     0.046694      19.29
 O       6.201606    -1.181242     0.201408     235.64
 C       6.153160    -2.002455     1.416311     112.75
 H       5.603139    -2.922427     1.113088      26.75
 H       5.411117    -1.594620     2.057387      28.14
 H       7.059044    -2.041187     1.886007      27.52
 C       6.248333     0.908423    -0.993070      21.11
 O       7.290760     0.492843    -1.820890     198.13
 H       7.784812    -0.221871    -1.433907      25.62
 C       5.752060     2.229477    -1.153204      49.52
 H       6.211759     2.768683    -1.925177      20.01
 C       4.017942     1.912166     0.499315      26.73
 C       2.764079     2.217953     1.357310     103.85
 H       3.102733     3.130396     1.497658      24.70
 O       2.571918     1.559041     2.572773     294.97
 H       2.292181     0.684573     2.543321      27.10
 C       1.330223     2.253798     0.522726      64.86
 H       1.355707     2.756429    -0.533837      19.61
 C       0.107991     2.883495     1.262170     102.12
 O       0.282623     4.368533     1.510984     198.36
 H       1.268803     4.622281     1.051467      25.14
 H       0.109319     2.450247     2.181127      26.27
 H      -0.881362     2.700619     0.686302      24.19
 C      -1.939950    -1.278193    -0.578041      75.93
 H      -2.101933    -2.375377    -0.161683      19.52
 C      -1.585244     0.251234    -2.441537      50.71
 H      -1.881396     0.595400    -3.456892      17.76
 C      -0.479789     0.828347    -1.799497      16.68
 O       0.155829     1.990093    -2.127216     245.09
 C       0.263427     2.244309    -3.618151     119.44
 H       1.018434     3.003505    -3.984784      25.10
 H       0.513901     1.466604    -4.265384      29.61
 H      -0.644065     2.782715    -3.952469      26.38
 C      -0.065291     0.321267    -0.534559      18.78
 O       1.210738     0.795981     0.030268     161.74
 C      -0.839208    -0.599881     0.201019      39.57
 H      -0.517674    -0.778712     1.148913      18.70
 C      -2.294649    -0.912880    -1.886305      43.83
 C      -3.336027    -1.650326    -2.729624      32.11
 H      -3.269772    -1.142971    -3.687989      26.78
 O      -3.026132    -3.049223    -2.704705     254.94
 H      -1.932874    -3.125522    -2.489698      23.47
 C      -4.828087    -1.307152    -2.213650     100.06
 H      -4.904483    -1.344038    -1.131618      29.82
 O      -5.066095     0.022177    -2.704654     239.01
 H      -4.484577     0.858403    -2.381462      23.93
 C      -5.736347    -2.134460    -3.082051     112.07
 O      -5.826084    -3.569389    -2.668132     232.68
 H      -4.974894    -3.902355    -2.585763      35.65
 H      -5.319781    -2.215106    -4.113922      31.00
 H      -6.770106    -1.743954    -3.142889      29.36
55
name = lig-ACN-frame_429
 C       4.601518     2.752396    -0.467607      49.80
 H       4.223127     3.788481    -0.401978      22.01
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 C       4.677176     0.682254     0.887470      70.27
 H       4.099236     0.052065     1.515398      19.97
 C       5.578213     0.064079     0.091731      20.79
 O       6.276429    -1.160544     0.256910     242.80
 C       6.072521    -1.975247     1.407428     122.92
 H       6.065091    -3.073790     1.029803      26.38
 H       5.390789    -1.616473     2.132202      29.27
 H       6.974653    -2.086981     1.906766      28.64
 C       6.239572     0.843214    -0.901873       9.56
 O       7.289918     0.459456    -1.796276     194.10
 H       7.719204    -0.307693    -1.457644      23.28
 C       5.764664     2.157658    -1.135999      45.41
 H       6.311443     2.698258    -1.839985      25.33
 C       4.037767     1.862076     0.470654      23.80
 C       2.709165     2.253867     1.261039      89.07
 H       2.591156     3.139333     1.622113      25.84
 O       2.711503     1.581466     2.644384     196.17
 H       2.066307     0.735235     2.465487      22.41
 C       1.319770     2.274752     0.425770      60.61
 H       1.549820     2.943264    -0.533789      20.60
 C       0.205004     2.934362     1.267561     106.82
 O       0.256924     4.323872     1.578501     181.52
 H       0.945495     4.949635     0.796067      23.65
 H       0.030887     2.414131     2.159316      26.27
 H      -0.799075     2.777032     0.682493      24.14
 C      -1.872256    -1.264885    -0.535680      76.44
 H      -2.617074    -1.901228    -0.007526      19.74
 C      -1.694227     0.239593    -2.435140      13.46
 H      -2.075393     0.576237    -3.435477      15.98
 C      -0.549814     0.809260    -1.764010      17.86
 O       0.130079     1.936260    -2.251925     228.52
 C       0.242697     2.255876    -3.575157     100.97
 H       1.114821     2.895961    -3.464150      24.02
 H       0.308299     1.270050    -3.948619      28.99
 H      -0.718181     2.628708    -4.117378      25.95
 C      -0.015431     0.327580    -0.447595      32.90
 O       1.134773     0.779806     0.099575     193.90
 C      -0.835529    -0.634773     0.169626      55.52
 H      -0.878150    -1.093418     1.154746      20.59
 C      -2.176000    -0.888618    -1.862416      32.92
 C      -3.305450    -1.621793    -2.702423      64.54
 H      -3.341346    -1.449082    -3.750925      23.49
 O      -3.069320    -3.083897    -2.680251     302.69
 H      -2.218786    -3.219373    -2.351561      32.36
 C      -4.746406    -1.244035    -2.268388      98.40
 H      -5.054883    -1.400103    -1.243039      29.24
 O      -5.128377     0.051604    -2.793107     188.53
 H      -4.556332     0.752335    -2.013821      20.43
 C      -5.730401    -2.165741    -3.118031     106.02
 O      -5.830835    -3.550445    -2.694947     187.24
 H      -4.758481    -3.733933    -2.504750      27.58
 H      -5.452941    -1.944727    -4.199234      30.24
 H      -6.716703    -1.768658    -2.971876      29.08
55
name = lig-ACN-frame_430
 C       4.688094     2.612045    -0.372246      60.58
 H       4.351374     3.553260    -0.803378      23.00
 C       4.530579     0.553468     0.856968      43.63
 H       4.184095    -0.005895     1.717256      20.59
 C       5.690904     0.072148     0.097144      18.75
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 O       6.315745    -1.139580     0.292244     250.12
 C       6.074810    -2.011535     1.453863     110.43
 H       5.777759    -3.093737     1.060361      24.78
 H       5.109600    -1.806435     1.944168      25.43
 H       6.889546    -1.867595     2.072555      26.75
 C       6.231409     0.878392    -0.946530      17.01
 O       7.227572     0.419625    -1.713119      94.33
 H       7.774310    -0.355038    -1.255752      22.05
 C       5.742932     2.194215    -1.150720      68.91
 H       6.308039     2.862458    -1.780062      28.29
 C       3.939472     1.886798     0.595821      43.95
 C       2.700266     2.398959     1.251588     100.87
 H       2.888184     3.332400     1.350385      28.32
 O       2.757474     1.595380     2.598947     187.11
 H       2.284128     0.621153     2.534053      20.10
 C       1.486355     2.206060     0.410071      69.82
 H       1.671410     2.749559    -0.632581      21.42
 C       0.164834     2.895723     1.253014      84.63
 O       0.309295     4.313789     1.631126     186.93
 H       0.469423     4.858216     0.669002      26.32
 H       0.142200     2.402229     2.236531      24.88
 H      -0.743514     2.682977     0.573757      22.83
 C      -1.917321    -1.283430    -0.518369      70.15
 H      -2.572867    -1.835804     0.042630      20.67
 C      -1.588262     0.265352    -2.399108      42.21
 H      -1.902821     0.754024    -3.338094      17.44
 C      -0.592363     0.855538    -1.726787      22.11
 O       0.091019     1.901870    -2.175919     242.35
 C       0.238024     2.187118    -3.675456     106.08
 H       0.973681     2.942287    -3.873163      25.86
 H       0.645889     1.528176    -4.460045      26.43
 H      -0.703648     2.809025    -3.951639      23.57
 C      -0.165574     0.339665    -0.481474      17.50
 O       1.087427     0.862887     0.222117     166.18
 C      -0.832915    -0.724801     0.190275      47.44
 H      -0.217742    -0.856324     1.196974      16.81
 C      -2.258739    -0.915060    -1.873386      49.38
 C      -3.223930    -1.614166    -2.651745      64.32
 H      -2.899757    -1.239082    -3.569107      28.01
 O      -3.161771    -3.120747    -2.591193     253.74
 H      -2.264258    -3.312485    -2.712014      30.91
 C      -4.758671    -1.297170    -2.421511      93.61
 H      -4.803824    -1.347016    -1.342890      28.14
 O      -5.141081     0.112938    -2.823919     179.63
 H      -4.893807     0.895465    -2.033966      22.25
 C      -5.800481    -2.160353    -3.121955     119.39
 O      -5.781489    -3.518042    -2.729042     181.14
 H      -4.728385    -3.868551    -2.666433      28.37
 H      -5.666897    -2.173945    -4.264473      29.74
 H      -6.747204    -1.759394    -2.907986      30.86
55
name = lig-ACN-frame_431
 C       4.630331     2.616158    -0.345459      50.99
 H       4.172219     3.593699    -0.425535      23.79
 C       4.450311     0.462969     0.785024      84.00
 H       4.151732    -0.106390     1.699019      21.71
 C       5.659182     0.154337     0.185224       6.07
 O       6.351849    -1.159457     0.329732     257.24
 C       6.015844    -2.006111     1.473134      98.46
 H       6.198802    -3.112001     1.038279      23.40
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 H       5.040604    -1.677121     1.898408      24.04
 H       6.693180    -2.096616     2.324538      24.03
 C       6.208803     0.900842    -0.930107      12.69
 O       7.234777     0.373160    -1.711381     181.03
 H       7.785306    -0.358823    -1.104221      23.11
 C       5.775639     2.175822    -1.132119      51.97
 H       6.110297     2.838989    -1.985171      21.25
 C       4.062780     1.761437     0.593480      35.23
 C       2.849639     2.347396     1.368713      96.56
 H       2.838449     3.282207     1.686084      25.02
 O       2.694560     1.700509     2.531742     298.12
 H       2.522262     0.858786     2.219219      28.10
 C       1.363157     2.274315     0.487169      72.12
 H       1.556529     2.722452    -0.557553      20.76
 C       0.253034     2.859087     1.185440     105.74
 O       0.351700     4.264801     1.624932     278.72
 H       0.410673     4.742702     0.896791      33.95
 H       0.095500     2.182703     2.136411      23.92
 H      -0.764434     2.751481     0.713030      24.28
 C      -1.989197    -1.336087    -0.426707      44.61
 H      -2.128564    -2.298189    -0.303456      21.01
 C      -1.582992     0.163863    -2.401123      35.53
 H      -1.812116     0.360986    -3.440398      18.62
 C      -0.549439     0.904010    -1.647681      -3.18
 O       0.186173     1.994482    -2.222169     201.92
 C       0.220644     2.229291    -3.732272      79.54
 H       0.935524     2.991601    -3.614754      24.24
 H       0.258359     1.164869    -4.118895      25.76
 H      -0.890558     2.481528    -4.151770      23.76
 C      -0.138902     0.446306    -0.357970      30.91
 O       0.986482     0.806424     0.303530     211.83
 C      -0.771136    -0.703952     0.148936      50.81
 H      -0.490408    -1.393869     1.171955      16.13
 C      -2.266713    -0.821572    -1.703402      27.21
 C      -3.289175    -1.669178    -2.810307      81.10
 H      -3.147507    -1.600102    -3.836192      29.44
 O      -3.199040    -3.102260    -2.484045     217.98
 H      -2.353127    -3.462955    -3.080325      24.96
 C      -4.771375    -1.217289    -2.490554     100.38
 H      -5.042562    -1.434617    -1.456552      29.15
 O      -5.116931     0.126206    -2.851022     259.93
 H      -4.658512     0.697202    -2.186549      28.21
 C      -5.869777    -2.142888    -3.186825     104.67
 O      -5.751704    -3.566085    -2.728507     191.50
 H      -4.794389    -3.700450    -2.919739      31.62
 H      -5.814521    -1.972039    -4.333912      29.83
 H      -6.816502    -1.821739    -2.845090      30.27
55
name = lig-ACN-frame_432
 C       4.616695     2.673734    -0.383191      63.31
 H       4.345999     3.715863    -0.318734      25.26
 C       4.519675     0.411186     0.803158      52.53
 H       3.829521    -0.317164     1.348004      19.36
 C       5.704984    -0.002918     0.175376      21.70
 O       6.343632    -1.105927     0.402714     244.61
 C       5.976333    -2.015622     1.468063     108.35
 H       6.022489    -3.113888     1.045295      25.22
 H       4.869129    -2.073288     1.780873      25.87
 H       6.720211    -1.745312     2.226567      25.10
 C       6.248517     0.859376    -0.838991      30.19
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 O       7.227125     0.363696    -1.724798      65.04
 H       7.772215    -0.432583    -1.273996      21.81
 C       5.688967     2.205334    -1.119783      65.59
 H       6.240804     2.686871    -2.023670      21.92
 C       4.036274     1.777465     0.550993      31.14
 C       2.845162     2.324276     1.296454      86.84
 H       3.150021     3.299499     1.375007      25.29
 O       2.571733     1.678758     2.628046     246.84
 H       2.447220     0.746529     2.667127      26.83
 C       1.428715     2.272100     0.486327      68.03
 H       1.508671     2.787493    -0.504431      21.80
 C       0.181150     2.882275     1.269520      96.03
 O       0.400371     4.208418     1.633815     260.12
 H       0.807957     4.682850     0.878454      30.42
 H       0.014471     2.344083     2.338554      23.06
 H      -0.623445     2.707573     0.535649      24.38
 C      -1.889528    -1.361927    -0.462517      78.72
 H      -2.189427    -2.258403    -0.107071      22.85
 C      -1.518772     0.183227    -2.299157      49.09
 H      -1.597002     0.287936    -3.365251      20.63
 C      -0.488024     0.953277    -1.676777      -6.71
 O       0.253831     2.061257    -2.246146     254.92
 C       0.146876     2.189461    -3.637644     117.15
 H       0.930613     2.725255    -4.188340      24.95
 H       0.544882     1.290246    -4.259462      25.95
 H      -0.858098     2.781520    -4.036835      25.36
 C      -0.185493     0.457802    -0.293117      32.84
 O       1.009362     0.816574     0.424346     155.08
 C      -0.872266    -0.733889     0.158424      28.12
 H      -0.206012    -1.264908     1.142274      14.54
 C      -2.393179    -0.882923    -1.802154      42.63
 C      -3.360797    -1.651152    -2.757097      60.10
 H      -2.994587    -1.427362    -3.704410      31.07
 O      -3.211845    -3.088586    -2.417578     190.87
 H      -2.269926    -3.430530    -2.929760      25.04
 C      -4.871045    -1.265765    -2.524674      99.41
 H      -4.886298    -1.317776    -1.424359      27.32
 O      -5.037151     0.155126    -2.878140     262.65
 H      -4.473747     0.685099    -2.494214      32.79
 C      -5.920029    -2.162925    -3.210607     123.37
 O      -5.749372    -3.542231    -2.794836     240.82
 H      -4.879659    -3.686254    -2.715978      36.59
 H      -5.923134    -2.095205    -4.366068      29.44
 H      -6.910811    -1.840868    -2.896403      29.77
55
name = lig-ACN-frame_433
 C       4.664316     2.660039    -0.361604      49.19
 H       4.365346     3.626172    -0.769235      22.59
 C       4.519019     0.507081     0.772917      56.58
 H       3.879862    -0.245462     1.317791      19.53
 C       5.662491     0.036231     0.110772       9.91
 O       6.377817    -1.199836     0.453091     258.89
 C       5.945598    -2.088917     1.449227     102.13
 H       6.276288    -3.114544     1.050297      25.10
 H       4.868275    -1.825609     1.748704      25.76
 H       6.492347    -2.111710     2.495649      24.57
 C       6.270852     0.874910    -0.848923      22.38
 O       7.176193     0.411779    -1.737222     180.71
 H       7.735589    -0.260274    -1.272449      22.30
 C       5.717215     2.074653    -1.126811      56.92
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 H       6.258857     2.846138    -1.779697      26.51
 C       3.957893     1.737548     0.534576      40.04
 C       2.704998     2.219604     1.286408      97.85
 H       2.765897     3.249104     1.604817      24.35
 O       2.517321     1.712246     2.714090     199.94
 H       2.328022     0.659482     2.420954      22.48
 C       1.422193     2.187942     0.556095      88.72
 H       1.594030     2.573218    -0.434296      21.95
 C       0.183580     2.872664     1.306395      91.67
 O       0.454884     4.284117     1.664203     167.74
 H       1.288100     4.559059     0.898923      23.85
 H      -0.109051     2.210201     2.307659      23.20
 H      -0.738273     2.829329     0.743585      24.35
 C      -1.910020    -1.402503    -0.625358      75.85
 H      -2.597466    -1.966287    -0.049628      18.82
 C      -1.512612     0.239596    -2.317294      75.65
 H      -1.774537     0.700852    -3.257633      20.59
 C      -0.468915     0.915420    -1.593013       3.61
 O       0.266531     2.000755    -2.168101     224.17
 C       0.161939     2.170752    -3.706725      65.76
 H       0.913029     2.982556    -3.708308      21.94
 H      -0.133521     1.183099    -4.157640      23.82
 H      -0.955802     2.680495    -3.752418      23.46
 C      -0.140637     0.459776    -0.342801      16.72
 O       1.025964     0.834388     0.478299     193.41
 C      -0.849213    -0.641873     0.189675      42.22
 H      -0.440628    -1.093763     1.345826      19.49
 C      -2.265193    -0.873313    -1.806284      41.28
 C      -3.351147    -1.621579    -2.628580      64.01
 H      -3.237500    -1.439011    -3.664263      29.20
 O      -3.203627    -3.081858    -2.404867     250.28
 H      -2.220801    -3.218788    -2.337762      33.87
 C      -4.867251    -1.253904    -2.476509      96.21
 H      -5.311011    -1.385279    -1.459229      28.45
 O      -4.995251     0.145367    -2.956099     215.59
 H      -4.327055     0.619032    -2.302087      27.39
 C      -5.955654    -2.166964    -3.227807     113.96
 O      -5.794816    -3.527913    -2.849339     230.15
 H      -4.857299    -3.600325    -2.539184      31.70
 H      -5.790531    -2.029211    -4.361335      29.96
 H      -6.971729    -1.826498    -2.943642      29.59
55
name = lig-ACN-frame_434
 C       4.622648     2.556901    -0.376469      60.74
 H       4.109543     3.533734    -0.480817      23.68
 C       4.465023     0.496713     0.764625      58.47
 H       4.202692    -0.001118     1.704559      22.92
 C       5.664316     0.020781     0.169745       5.85
 O       6.383972    -1.191625     0.423420     235.74
 C       5.888785    -2.196545     1.493507     101.71
 H       5.923869    -3.212651     1.086015      25.41
 H       4.746597    -2.182309     1.574523      23.81
 H       6.519983    -1.946147     2.469913      23.13
 C       6.221030     0.798296    -0.899997      18.94
 O       7.235662     0.424414    -1.788164     216.89
 H       7.770306    -0.226936    -1.409346      29.95
 C       5.755771     2.142709    -1.088577      56.27
 H       6.264010     2.667193    -1.917118      22.99
 C       3.898699     1.815395     0.531597      26.05
 C       2.630712     2.252850     1.450508      91.28
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 H       2.815284     3.359888     1.479636      24.10
 O       2.547003     1.670959     2.672699     257.30
 H       2.159263     0.700952     2.780552      22.48
 C       1.246773     2.151461     0.599288      91.65
 H       1.400863     2.645456    -0.315870      24.43
 C       0.232997     2.948966     1.320787     104.18
 O       0.528128     4.328724     1.673279     137.83
 H       1.373328     4.891123     1.010525      23.30
 H       0.053040     2.422401     2.403835      23.97
 H      -0.654223     2.916062     0.734078      26.16
 C      -1.841242    -1.254893    -0.480175      86.09
 H      -2.346718    -2.235773    -0.150349      24.99
 C      -1.539505     0.341823    -2.387966      10.57
 H      -2.086766     0.789490    -3.249994      17.99
 C      -0.481729     0.894906    -1.628134      15.67
 O       0.269383     1.861203    -2.128491     207.37
 C       0.066636     2.228598    -3.557679      88.04
 H       1.056323     2.585230    -4.072555      24.32
 H       0.250314     1.347114    -4.202365      26.74
 H      -0.830484     2.922621    -3.898427      24.42
 C      -0.048924     0.339475    -0.282428      29.34
 O       0.977422     0.725986     0.444852     224.57
 C      -0.900792    -0.656283     0.164057      44.62
 H      -0.926306    -0.985463     1.378159      17.90
 C      -2.145063    -0.808023    -1.882634      77.96
 C      -3.344285    -1.627094    -2.617566      62.56
 H      -3.159019    -1.487971    -3.674368      28.38
 O      -3.164219    -3.056172    -2.370495     301.64
 H      -2.372786    -3.212422    -2.039542      34.23
 C      -4.905956    -1.199057    -2.379132      93.21
 H      -5.101172    -1.124172    -1.272197      28.18
 O      -4.957748     0.093309    -2.996942     181.20
 H      -4.642798     0.952067    -2.250451      22.99
 C      -5.875219    -2.094874    -3.269648     105.82
 O      -5.866838    -3.539418    -2.849665     161.04
 H      -4.778971    -3.746813    -2.699105      27.84
 H      -5.747617    -1.935695    -4.383532      29.93
 H      -6.928755    -1.730525    -3.041716      28.96
55
name = lig-ACN-frame_435
 C       4.476209     2.610563    -0.418489      44.86
 H       4.430887     3.706893    -0.627828      22.77
 C       4.479049     0.449699     0.901615      60.32
 H       4.086443    -0.036575     1.760895      21.70
 C       5.657079    -0.014084     0.183814       6.15
 O       6.294158    -1.214692     0.447903     228.28
 C       5.810307    -2.201293     1.405572     106.77
 H       6.271745    -3.084110     1.085659      25.99
 H       4.753096    -2.020561     1.654529      25.91
 H       6.375331    -2.014755     2.496264      23.76
 C       6.186894     0.791210    -0.954797      13.29
 O       7.302575     0.396828    -1.805963     199.66
 H       7.744121    -0.358014    -1.322493      26.46
 C       5.732348     2.133426    -1.056190      35.33
 H       6.115761     2.760464    -1.814767      21.95
 C       3.869741     1.711738     0.619538      16.26
 C       2.646803     2.299736     1.322102      80.10
 H       2.833176     3.349388     1.809032      21.58
 O       2.603548     1.582648     2.736875     233.00
 H       2.200346     0.851703     2.426795      28.92
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 C       1.317146     2.186055     0.628069      78.08
 H       1.383848     2.520759    -0.373628      21.52
 C       0.134827     3.054921     1.409604      95.82
 O       0.632600     4.390898     1.668877     182.44
 H       1.070384     4.688524     0.664866      25.06
 H      -0.172536     2.666013     2.497883      23.87
 H      -0.787403     3.020206     0.856980      25.13
 C      -1.959646    -1.212364    -0.599892      72.30
 H      -2.307805    -2.257322    -0.119297      18.87
 C      -1.624433     0.352378    -2.348730      50.70
 H      -1.660369     0.870350    -3.361291      13.68
 C      -0.484838     0.783743    -1.652900      16.81
 O       0.348136     1.857751    -2.162723     251.78
 C       0.122337     2.218316    -3.479044      82.63
 H       0.997862     3.027173    -3.599804      21.73
 H      -0.258160     1.387888    -4.045406      27.73
 H      -0.846113     2.920825    -3.446056      25.51
 C      -0.166055     0.255205    -0.423595      15.88
 O       1.014324     0.691597     0.470316     137.18
 C      -0.879428    -0.653790     0.368844      35.35
 H      -0.421715    -0.965929     1.449831      16.72
 C      -2.268254    -0.851166    -1.855463      36.70
 C      -3.261885    -1.609167    -2.633406      55.70
 H      -3.148563    -1.385861    -3.710870      23.29
 O      -3.173845    -3.045345    -2.291761     235.71
 H      -2.112331    -3.215333    -2.384542      27.02
 C      -4.775808    -1.179790    -2.373099      86.26
 H      -5.088917    -1.218594    -1.290899      28.48
 O      -4.957192     0.128518    -3.021447     175.97
 H      -4.945793     0.944244    -2.282045      25.21
 C      -5.786334    -2.075463    -3.162931     102.61
 O      -5.923105    -3.465671    -2.855462     182.64
 H      -4.922406    -3.865540    -2.916592      31.18
 H      -5.340900    -1.985382    -4.189012      30.65
 H      -6.869419    -1.660413    -3.176997      28.59
55
name = lig-ACN-frame_436
 C       4.495759     2.512262    -0.373555      64.87
 H       3.896674     3.441225    -0.455794      23.38
 C       4.550328     0.487999     0.974370      56.84
 H       4.118736    -0.277958     1.545970      19.28
 C       5.581176     0.018183     0.139790      12.13
 O       6.220874    -1.219410     0.415706     240.47
 C       5.785953    -2.148146     1.369298     118.48
 H       6.008129    -3.098422     1.044731      27.08
 H       4.705232    -2.339724     1.280270      28.16
 H       6.170738    -1.940278     2.512299      25.04
 C       6.193119     0.787727    -0.900973       7.31
 O       7.251389     0.366555    -1.710190     156.77
 H       7.855013    -0.391374    -1.218066      21.27
 C       5.586251     2.069275    -1.087611      70.89
 H       6.174714     2.756816    -1.563026      27.98
 C       3.934736     1.727438     0.556280      33.36
 C       2.749101     2.202415     1.419539      74.77
 H       2.845755     3.424130     1.414645      23.33
 O       2.615100     1.512825     2.684914     238.77
 H       2.272080     0.587295     2.624264      24.63
 C       1.270824     2.194783     0.651614      72.18
 H       1.441451     2.786433    -0.249737      23.06
 C       0.122132     3.081025     1.468473     101.94
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 O       0.712571     4.450121     1.613944     241.07
 H       0.906614     4.794713     0.792200      32.34
 H      -0.088014     2.625547     2.424588      26.48
 H      -0.808937     3.126381     0.868401      25.63
 C      -1.991672    -1.316782    -0.421761      53.59
 H      -2.826536    -2.123507    -0.146907      18.24
 C      -1.631493     0.285810    -2.341876      39.61
 H      -2.061482     0.447183    -3.373637      18.42
 C      -0.441194     0.789166    -1.682885       2.81
 O       0.432729     1.735497    -2.070391     208.47
 C       0.094262     2.335594    -3.455744      99.50
 H       1.009360     2.883442    -4.016621      23.65
 H       0.107870     1.633695    -4.244656      27.42
 H      -0.906228     2.893816    -3.350732      26.32
 C      -0.089130     0.335940    -0.245405      29.95
 O       1.010202     0.749832     0.431611     199.18
 C      -0.993546    -0.686140     0.232112      47.08
 H      -0.635177    -1.288946     1.113771      22.55
 C      -2.344213    -0.732648    -1.756098      34.47
 C      -3.291255    -1.632098    -2.665372      64.25
 H      -3.005700    -1.643682    -3.758844      26.58
 O      -3.147387    -3.024625    -2.247180     173.53
 H      -2.282443    -3.475620    -2.868209      24.25
 C      -4.669902    -1.180597    -2.401444      97.69
 H      -4.783184    -1.099614    -1.282041      27.67
 O      -4.973949     0.180456    -2.997678     218.52
 H      -4.744167     0.731516    -2.336972      32.18
 C      -5.658393    -2.045279    -3.161773     109.81
 O      -5.960509    -3.416068    -2.820026     243.50
 H      -5.155811    -3.812629    -2.854274      37.95
 H      -5.432885    -1.977191    -4.258040      30.91
 H      -6.656593    -1.430878    -3.039163      28.35
55
name = lig-ACN-frame_437
 C       4.470004     2.466231    -0.372561      46.15
 H       4.052777     3.378898    -0.825412      23.09
 C       4.580157     0.474641     0.913653      80.31
 H       4.167668     0.004687     1.799725      22.44
 C       5.598737    -0.024378     0.159512      37.82
 O       6.221197    -1.197936     0.298529     212.78
 C       5.659336    -2.193715     1.324762     106.21
 H       6.325848    -2.950423     1.202668      27.11
 H       4.604062    -2.205515     1.281417      27.90
 H       5.890613    -1.747856     2.448254      25.77
 C       6.150408     0.803857    -0.820591      18.41
 O       7.176824     0.346762    -1.575565     119.44
 H       7.738768    -0.344861    -1.034743      21.34
 C       5.606042     2.044520    -1.190565      50.11
 H       6.022798     2.587476    -2.001424      25.69
 C       3.889570     1.655682     0.694755      35.93
 C       2.669459     2.110006     1.443142      94.71
 H       3.055263     3.128591     2.048311      21.59
 O       2.615328     1.464352     2.680176     214.85
 H       2.382516     0.387234     2.415234      21.65
 C       1.300506     2.231497     0.726123      95.28
 H       1.373151     2.650111    -0.313579      22.04
 C       0.281792     3.087372     1.430244     117.34
 O       0.699052     4.446408     1.602585     285.40
 H       1.160606     4.726696     0.928212      34.95
 H       0.097825     2.891837     2.429440      26.86
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 H      -0.710557     2.975473     0.899195      26.23
 C      -2.154856    -1.280241    -0.413557      46.50
 H      -2.425841    -2.143718     0.251228      20.34
 C      -1.521437     0.220706    -2.285457      52.86
 H      -1.658826     0.686050    -3.266481      18.34
 C      -0.431468     0.787870    -1.530909       2.24
 O       0.519571     1.688451    -2.153940     218.57
 C       0.113170     2.362278    -3.429131      90.30
 H       0.920178     3.205244    -3.339252      23.34
 H       0.049454     1.575583    -4.093904      26.86
 H      -0.872095     2.915028    -3.435880      26.95
 C      -0.236996     0.374175    -0.267771      28.82
 O       0.994128     0.849081     0.412932     211.91
 C      -0.937849    -0.754114     0.228984      61.72
 H      -0.786754    -1.029487     1.225701      18.49
 C      -2.365454    -0.802815    -1.681431      26.76
 C      -3.179012    -1.604854    -2.614081      81.32
 H      -2.835390    -1.339508    -3.684591      26.17
 O      -3.160224    -3.044148    -2.248594     223.02
 H      -2.272253    -3.421261    -2.728604      25.41
 C      -4.668261    -1.154587    -2.459959      96.13
 H      -4.973495    -1.275488    -1.365043      28.46
 O      -4.952757     0.197516    -2.912860     254.48
 H      -4.298984     0.769313    -2.561004      31.68
 C      -5.718012    -1.991489    -3.242493     103.34
 O      -5.972415    -3.375220    -2.758543     205.56
 H      -5.103594    -3.775327    -2.541806      33.58
 H      -5.464371    -1.940470    -4.318558      30.38
 H      -6.767986    -1.519611    -3.037000      28.00
55
name = lig-ACN-frame_438
 C       4.405897     2.451990    -0.468219      70.94
 H       3.914311     3.402055    -0.583377      23.93
 C       4.473175     0.394127     1.018465      52.41
 H       4.396712    -0.208812     1.949255      21.64
 C       5.613357     0.006807     0.206259       0.33
 O       6.234519    -1.339788     0.262223     235.01
 C       5.631233    -2.117931     1.244597     118.85
 H       6.113869    -3.071276     1.357378      25.77
 H       4.711395    -2.498492     0.879022      27.16
 H       5.610878    -1.584476     2.300293      25.18
 C       6.134018     0.827845    -0.841731      22.19
 O       7.219875     0.299594    -1.508695     217.92
 H       7.578950    -0.406722    -1.040105      27.81
 C       5.540266     2.031774    -1.159828      73.74
 H       5.727621     2.473660    -2.150630      22.47
 C       3.925573     1.717782     0.609388      24.80
 C       2.692188     2.159370     1.515564      61.64
 H       2.715553     3.418757     1.646792      21.58
 O       2.543517     1.283023     2.771608     205.16
 H       2.231085     0.301531     2.479017      19.42
 C       1.410338     2.253345     0.657413      70.48
 H       1.784754     2.879313    -0.222134      21.69
 C       0.360958     3.052582     1.497377     111.36
 O       0.673179     4.490228     1.578807     229.17
 H       1.400121     4.630124     0.928140      29.19
 H       0.276619     2.545310     2.340223      27.22
 H      -0.623291     2.961138     0.933794      25.26
 C      -2.061238    -1.202370    -0.296690      43.66
 H      -2.684497    -2.041780    -0.199731      21.49
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 C      -1.445752     0.155545    -2.204225      41.70
 H      -1.506157     0.275826    -3.265968      20.22
 C      -0.428083     0.883501    -1.561175      19.43
 O       0.507834     1.629696    -2.186978     254.08
 C       0.159099     2.346410    -3.345204     123.27
 H       0.953913     3.129975    -3.612812      24.72
 H       0.231248     1.965778    -4.309057      27.32
 H      -0.864523     2.678797    -3.133106      28.11
 C      -0.222536     0.418535    -0.195096      25.41
 O       0.891462     0.836562     0.457347     177.71
 C      -0.944359    -0.706050     0.411833      34.52
 H      -0.561428    -0.981820     1.263317      17.15
 C      -2.230881    -0.812084    -1.692447      43.13
 C      -3.248305    -1.610321    -2.621394      77.78
 H      -2.885791    -1.573039    -3.735435      25.02
 O      -3.161042    -3.046145    -2.310436     312.10
 H      -2.282054    -3.247305    -2.194303      32.91
 C      -4.762884    -1.172902    -2.490035      86.97
 H      -4.992340    -1.346317    -1.381933      27.63
 O      -4.892842     0.216269    -2.846628     221.97
 H      -4.048763     0.798136    -2.359264      22.69
 C      -5.845140    -2.009796    -3.319295     114.37
 O      -5.954535    -3.306706    -2.712329     180.24
 H      -4.892891    -3.419240    -2.376574      27.28
 H      -5.554387    -2.135678    -4.375863      29.35
 H      -6.827712    -1.413687    -3.336403      28.64
55
name = lig-ACN-frame_439
 C       4.297158     2.440843    -0.451375      49.71
 H       3.860561     3.354368    -0.788493      23.01
 C       4.524252     0.440516     0.982200      62.04
 H       3.806608    -0.022541     1.709093      18.99
 C       5.593551    -0.049763     0.248617      20.82
 O       6.229415    -1.306969     0.236279     259.57
 C       5.560465    -2.214812     1.203824     109.32
 H       6.346158    -2.949539     1.451676      25.67
 H       4.594905    -2.454877     0.865847      28.97
 H       5.283846    -1.632432     2.174570      26.61
 C       6.144537     0.736798    -0.814438      -0.18
 O       7.294509     0.292792    -1.513820     156.07
 H       7.596063    -0.544525    -1.084279      24.49
 C       5.460784     1.999113    -1.213451      44.53
 H       6.086823     2.704496    -1.897475      27.06
 C       3.914996     1.641490     0.714228      32.12
 C       2.765187     2.081694     1.566126      70.39
 H       3.097527     3.019661     2.321784      20.23
 O       2.465539     1.219265     2.761834     278.32
 H       2.059373     0.485486     2.437393      27.75
 C       1.447649     2.217829     0.656682      80.02
 H       1.488958     2.509195    -0.452953      17.71
 C       0.390068     3.013683     1.470035      96.63
 O       0.647620     4.483758     1.600377     198.20
 H       1.154847     4.963958     0.688048      23.89
 H       0.481518     2.796138     2.434991      26.09
 H      -0.694608     2.857744     1.150312      23.44
 C      -1.950100    -1.203667    -0.242360      88.27
 H      -2.478114    -1.829070     0.335185      19.41
 C      -1.401600     0.156301    -2.356694      28.83
 H      -1.466142     0.165644    -3.412442      16.92
 C      -0.449224     0.819309    -1.516767       0.80
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 O       0.575946     1.566075    -2.147340     220.65
 C       0.144421     2.400412    -3.380950     102.66
 H       0.823081     3.218064    -3.258008      24.49
 H       0.174437     1.656138    -4.089117      25.74
 H      -0.824760     2.926201    -3.320996      27.53
 C      -0.193667     0.484007    -0.145930      19.61
 O       0.932733     0.878967     0.598690     205.11
 C      -0.981081    -0.516992     0.532835      41.94
 H      -0.719251    -1.054430     1.270489      23.71
 C      -2.175240    -0.828565    -1.634045      24.20
 C      -3.338612    -1.682034    -2.662960      29.31
 H      -3.036117    -1.339843    -3.758092      23.86
 O      -3.179489    -3.057301    -2.343725     300.90
 H      -2.301125    -3.189854    -2.042415      31.10
 C      -4.838042    -1.184213    -2.505890      86.90
 H      -5.214415    -1.330863    -1.436074      26.19
 O      -4.829816     0.236440    -2.824677     188.67
 H      -4.406635     0.838525    -1.883709      19.62
 C      -5.842287    -1.989435    -3.383027     111.47
 O      -5.945095    -3.249353    -2.656037     186.88
 H      -4.981919    -3.585519    -2.372008      28.76
 H      -5.536518    -2.103790    -4.434887      30.68
 H      -6.879755    -1.571326    -3.306801      29.12
55
name = lig-ACN-frame_440
 C       4.340526     2.339004    -0.411740      61.80
 H       3.750136     3.182168    -0.695280      24.24
 C       4.560573     0.403316     0.956319      57.01
 H       4.241761    -0.416392     1.624233      19.88
 C       5.603235    -0.061060     0.131603      28.00
 O       6.174716    -1.306887     0.317887     235.49
 C       5.505485    -2.291638     1.191710     122.37
 H       6.287453    -3.147359     1.341207      25.76
 H       4.756473    -2.850691     0.683024      28.15
 H       5.328335    -1.815141     2.152200      28.69
 C       6.146371     0.754323    -0.855962      22.48
 O       7.292246     0.345722    -1.511201     143.95
 H       7.772722    -0.494512    -1.042727      20.93
 C       5.461363     1.884406    -1.123707      71.92
 H       5.924369     2.672799    -1.888636      27.27
 C       3.917962     1.653331     0.697482      33.74
 C       2.746097     1.991921     1.631768      89.69
 H       3.070554     3.179216     1.946839      22.01
 O       2.399588     1.188990     2.694460     315.09
 H       1.921112     0.396104     2.410039      23.46
 C       1.424590     2.252261     0.768077      80.21
 H       1.787206     2.698586    -0.225213      21.16
 C       0.418472     3.096840     1.506397     110.79
 O       0.600927     4.462151     1.612817     196.90
 H       0.875971     4.830430     0.490547      22.84
 H       0.377467     2.616979     2.424560      26.25
 H      -0.589677     2.790690     1.067052      24.12
 C      -1.940969    -1.157358    -0.235014      70.25
 H      -2.374038    -1.977659     0.197508      20.76
 C      -1.401761     0.058835    -2.306813      30.93
 H      -1.464200     0.544634    -3.260529      18.21
 C      -0.353000     0.731944    -1.548608       8.98
 O       0.584078     1.598538    -2.117840     233.04
 C       0.170449     2.388953    -3.313570     120.64
 H       0.937495     3.044317    -3.575302      25.94
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 H       0.124130     1.934658    -4.329118      26.03
 H      -0.847086     2.707470    -3.126276      27.25
 C      -0.154776     0.547922    -0.097619      21.89
 O       0.995722     0.848614     0.740345     170.45
 C      -1.019513    -0.399425     0.553382      24.22
 H      -0.833007    -0.307599     1.527128      18.34
 C      -2.310690    -0.902245    -1.754161      46.19
 C      -3.290944    -1.611039    -2.534648      71.48
 H      -2.999714    -1.507765    -3.676568      28.62
 O      -3.234504    -3.105395    -2.364191     197.02
 H      -2.138900    -3.402144    -2.479057      24.38
 C      -4.810309    -1.131115    -2.481968      97.34
 H      -5.203623    -1.334344    -1.426186      27.60
 O      -4.815367     0.258301    -2.826809     252.75
 H      -4.803426     0.838221    -1.955155      24.40
 C      -5.781422    -1.977576    -3.350895     116.16
 O      -5.972127    -3.244523    -2.647309     216.97
 H      -5.126265    -3.555028    -2.670853      35.42
 H      -5.437928    -2.101574    -4.397730      31.86
 H      -6.749051    -1.477706    -3.401805      31.47
55
name = lig-ACN-frame_441
 C       4.367935     2.291700    -0.361500      64.14
 H       3.971721     3.259889    -0.674185      23.69
 C       4.554384     0.297101     0.955617      59.93
 H       4.338382    -0.138724     1.905300      22.20
 C       5.578261    -0.125572     0.096503      21.43
 O       6.164542    -1.380979     0.404075     262.80
 C       5.528032    -2.405077     1.154287     112.54
 H       6.410588    -3.173460     1.265764      24.33
 H       4.623263    -2.693306     0.621971      27.53
 H       5.096233    -2.239216     2.127905      27.39
 C       6.184473     0.698365    -0.876621      24.44
 O       7.329056     0.414941    -1.558823     204.85
 H       7.790478    -0.255285    -0.997470      25.36
 C       5.509400     1.957125    -1.125336      52.92
 H       5.729948     2.432302    -2.179133      21.41
 C       3.903686     1.494610     0.748989      34.16
 C       2.718642     2.084189     1.593880      87.33
 H       2.899298     3.143017     2.242415      20.63
 O       2.400286     1.163448     2.732819     226.75
 H       2.152535     0.179519     2.241298      17.72
 C       1.499584     2.269809     0.872414      75.48
 H       1.610735     2.731383    -0.153371      20.07
 C       0.318760     3.025754     1.592364      93.04
 O       0.555221     4.519132     1.622123     181.04
 H       1.069776     4.821972     0.654851      24.87
 H       0.103676     2.856022     2.643970      24.32
 H      -0.562729     2.929558     0.922999      22.87
 C      -2.062037    -1.112065    -0.292454      45.70
 H      -2.617544    -1.964691     0.102422      19.46
 C      -1.373666     0.062665    -2.197749      73.02
 H      -1.723230     0.214878    -3.237406      15.31
 C      -0.205653     0.682643    -1.520461       4.38
 O       0.587718     1.634964    -2.138173     248.99
 C       0.173113     2.352169    -3.268711     100.64
 H       0.801152     3.122636    -3.300082      27.22
 H       0.034269     1.607781    -4.087313      23.68
 H      -0.711787     3.008358    -3.024124      25.77
 C      -0.099099     0.523752    -0.101807      44.47
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 O       0.913685     0.848827     0.706745     178.62
 C      -1.105738    -0.317099     0.467377      49.85
 H      -1.301762    -0.504409     1.490722      20.60
 C      -2.181758    -0.876410    -1.594897      30.23
 C      -3.277902    -1.652932    -2.535769      58.91
 H      -2.931585    -1.357073    -3.621039      23.08
 O      -3.277669    -3.131479    -2.348205     208.73
 H      -2.397158    -3.477606    -3.001417      22.38
 C      -4.714607    -1.108454    -2.369218      96.42
 H      -4.983164    -1.117012    -1.264252      27.67
 O      -4.855814     0.290858    -2.873319     275.65
 H      -4.556589     0.845872    -2.254436      31.25
 C      -5.704753    -1.948964    -3.286828     114.55
 O      -6.015797    -3.239284    -2.714474     220.74
 H      -5.182434    -3.684863    -2.654494      34.29
 H      -5.221430    -2.142885    -4.272510      31.42
 H      -6.585348    -1.389661    -3.428990      31.02
55
name = lig-ACN-frame_442
 C       4.407786     2.300511    -0.331215      57.05
 H       3.843965     3.246405    -0.427253      20.52
 C       4.490873     0.241440     1.025796      41.90
 H       4.258729    -0.347970     1.867185      18.23
 C       5.575626    -0.260035     0.172939      28.16
 O       6.281552    -1.421339     0.435133     242.55
 C       5.487127    -2.548062     1.117390     118.23
 H       6.207840    -3.477882     1.174600      25.08
 H       4.662823    -2.944260     0.485514      25.61
 H       5.351329    -2.176894     2.046770      29.89
 C       6.139543     0.682303    -0.856653      18.52
 O       7.391944     0.442174    -1.599992     198.73
 H       7.948319    -0.208957    -1.260864      24.52
 C       5.522716     1.924028    -1.137311      50.74
 H       6.045745     2.705901    -1.792118      28.80
 C       3.873855     1.515403     0.728584      29.61
 C       2.816677     1.999441     1.727333      77.14
 H       3.350101     3.041473     2.108337      22.61
 O       2.468098     1.190122     2.788665     274.61
 H       2.304163     0.142548     2.504850      18.53
 C       1.278654     2.264851     0.864495      75.01
 H       1.467358     2.731616    -0.121713      19.61
 C       0.231586     3.086868     1.606269      97.29
 O       0.523260     4.552249     1.640668     280.35
 H       1.235267     4.715393     1.016030      30.30
 H       0.133144     2.642725     2.685845      23.54
 H      -0.739761     2.750856     1.170806      24.72
 C      -2.168778    -1.095215    -0.195046      54.79
 H      -2.861755    -1.604979     0.595421      16.81
 C      -1.279605     0.123774    -2.209079      52.94
 H      -1.146680     0.362534    -3.319634      15.80
 C      -0.221764     0.707879    -1.531761       3.33
 O       0.675409     1.623524    -2.066256     233.07
 C       0.110915     2.400893    -3.255668     109.15
 H       0.891838     2.858742    -3.620759      27.62
 H      -0.051796     1.761999    -4.245085      23.88
 H      -0.908887     2.826504    -3.072523      26.62
 C      -0.171760     0.393448    -0.149535      10.68
 O       0.898995     0.903235     0.670555     205.86
 C      -1.248345    -0.332528     0.477941      56.71
 H      -0.803916    -0.524711     1.512279      19.44
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 C      -2.161433    -0.918757    -1.626218      39.03
 C      -3.165593    -1.631309    -2.520364      65.49
 H      -2.976146    -1.485429    -3.654939      25.16
 O      -3.302630    -3.095785    -2.350708     240.31
 H      -2.682983    -3.526776    -2.921121      29.20
 C      -4.654900    -1.081413    -2.311886      92.16
 H      -5.003884    -1.211009    -1.235689      27.21
 O      -4.862598     0.274505    -2.912640     247.11
 H      -4.274361     0.900719    -2.541124      29.44
 C      -5.593563    -1.908772    -3.196379     114.16
 O      -6.077987    -3.242832    -2.792966     162.14
 H      -5.135736    -3.682944    -2.404052      29.40
 H      -5.099957    -1.872818    -4.192750      31.64
 H      -6.489364    -1.411141    -3.312042      30.98
55
name = lig-ACN-frame_443
 C       4.398105     2.305735    -0.280009      55.96
 H       4.064270     3.320334    -0.588520      21.42
 C       4.501961     0.192761     0.969708      40.27
 H       3.985208    -0.461688     1.628992      14.67
 C       5.609428    -0.209145     0.205953      33.69
 O       6.366148    -1.555431     0.457495     262.69
 C       5.552219    -2.603167     1.048037     117.56
 H       6.246547    -3.511404     1.017937      25.04
 H       4.556961    -2.668900     0.491799      26.12
 H       5.172066    -2.510928     1.987818      29.92
 C       6.172696     0.591904    -0.820829      16.97
 O       7.333912     0.461345    -1.568484     171.08
 H       7.795406    -0.375827    -1.137158      27.74
 C       5.523026     1.847426    -1.003824      70.65
 H       6.112621     2.572606    -1.546842      30.98
 C       3.911770     1.442396     0.732175      43.48
 C       2.734624     1.962572     1.661718      85.08
 H       2.981506     3.042548     2.127205      23.08
 O       2.583713     1.201125     2.920016     271.62
 H       2.195713     0.379043     2.662034      24.75
 C       1.236749     2.287570     0.846354      67.57
 H       1.524068     2.802762    -0.058751      21.23
 C       0.154629     3.140629     1.667286     105.32
 O       0.490357     4.516759     1.662615     313.84
 H       1.104605     4.688512     1.104578      36.17
 H       0.285673     2.784759     2.793019      22.99
 H      -0.879484     3.208503     1.345268      24.35
 C      -2.248127    -0.990435    -0.201026      44.67
 H      -3.184503    -1.782664     0.020449      19.28
 C      -1.263882    -0.003092    -2.287442      53.31
 H      -1.399616     0.051786    -3.445804      14.84
 C      -0.278506     0.786531    -1.513934       2.65
 O       0.699437     1.642030    -2.066152     229.01
 C       0.121551     2.366337    -3.272048     105.49
 H       0.682280     3.195463    -3.464709      25.47
 H      -0.212383     1.574790    -4.077020      22.35
 H      -0.694236     2.973852    -2.790804      25.71
 C      -0.215533     0.446309    -0.072208      24.13
 O       0.846045     0.857675     0.651882     212.03
 C      -1.134193    -0.378803     0.601777      43.31
 H      -1.162099    -0.384593     1.812020      16.92
 C      -2.145591    -0.893566    -1.658869      14.98
 C      -3.155447    -1.585264    -2.541424      75.18
 H      -2.777789    -1.373337    -3.588332      22.54
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 O      -3.312929    -3.044165    -2.317095     270.96
 H      -2.534937    -3.410770    -2.615411      30.29
 C      -4.577358    -1.073269    -2.332433      95.52
 H      -4.739565    -0.975514    -1.221123      27.82
 O      -4.829841     0.199259    -2.921010     226.00
 H      -4.235473     0.962043    -2.299176      22.29
 C      -5.612915    -1.887175    -3.201033     113.28
 O      -6.065950    -3.218494    -2.844293     184.15
 H      -5.227558    -3.672757    -2.374384      30.42
 H      -5.188869    -2.028756    -4.215567      30.22
 H      -6.417480    -1.227849    -3.238478      30.80
55
name = lig-ACN-frame_444
 C       4.434115     2.244680    -0.218314      63.44
 H       4.023803     3.253343    -0.362928      24.17
 C       4.498478     0.131246     0.878767      37.90
 H       4.105918    -0.577937     1.643794      20.56
 C       5.765937    -0.375633     0.246556       1.91
 O       6.359581    -1.521514     0.462619     305.31
 C       5.576434    -2.644960     0.962833     115.77
 H       6.119852    -3.584806     0.757502      23.95
 H       4.682584    -2.775508     0.263083      24.74
 H       5.486732    -2.508101     1.966663      26.00
 C       6.174884     0.589262    -0.719530      46.69
 O       7.272302     0.381257    -1.481873     212.91
 H       7.883674    -0.427197    -1.221016      29.85
 C       5.581642     1.837720    -0.895130      63.70
 H       5.823989     2.294571    -1.783223      21.16
 C       3.811200     1.448090     0.780996      27.70
 C       2.590912     1.999381     1.605995      81.70
 H       2.964139     3.099004     1.854566      20.59
 O       2.656763     1.233410     2.957012     267.61
 H       2.155611     0.472992     2.903525      25.61
 C       1.297726     2.201467     0.916234      80.58
 H       1.376063     2.636556    -0.047335      19.49
 C       0.183359     3.100076     1.739687      85.85
 O       0.501040     4.568852     1.706372     239.69
 H       0.974584     4.687369     0.787777      26.86
 H      -0.010843     2.836116     2.904752      22.27
 H      -0.681074     2.686967     1.248124      23.62
 C      -2.152125    -0.879382    -0.274251      44.73
 H      -2.866125    -1.684161     0.399223      18.75
 C      -1.171336    -0.072952    -2.303205      34.74
 H      -1.233385    -0.018440    -3.448845      17.71
 C      -0.376643     0.753193    -1.543969      -4.21
 O       0.630572     1.627661    -2.093136     244.89
 C       0.123552     2.403819    -3.163342     116.23
 H       0.955209     2.874170    -3.588579      24.89
 H      -0.047568     1.747687    -4.176340      21.98
 H      -0.932931     2.795757    -3.005885      24.11
 C      -0.327868     0.543115    -0.020471      25.83
 O       0.846561     0.867477     0.697157     188.82
 C      -1.215629    -0.429644     0.560314      28.59
 H      -1.326102    -0.683114     1.780861      15.90
 C      -2.151887    -0.810811    -1.587429      44.39
 C      -3.148215    -1.597037    -2.579150      75.31
 H      -2.926477    -1.475520    -3.671569      25.65
 O      -3.259417    -2.991962    -2.275231     250.78
 H      -2.252115    -3.371579    -2.030765      24.82
 C      -4.586143    -1.103486    -2.400995      99.61
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 H      -4.884371    -1.274541    -1.340936      27.37
 O      -4.739803     0.233795    -2.926193     204.91
 H      -4.576299     1.023150    -2.044189      20.76
 C      -5.664647    -1.883531    -3.259534     113.76
 O      -6.046262    -3.198092    -2.831498     240.69
 H      -5.249976    -3.561998    -2.660478      36.72
 H      -5.237259    -1.794936    -4.285743      31.12
 H      -6.623549    -1.384051    -3.292443      29.82
55
name = lig-ACN-frame_445
 C       4.431428     2.232287    -0.113055      51.46
 H       3.977006     3.167618    -0.400503      18.77
 C       4.427141     0.048365     0.933596      44.61
 H       4.029672    -0.635882     1.749818      16.29
 C       5.602127    -0.265484     0.324211      30.10
 O       6.412836    -1.533928     0.443052     263.94
 C       5.612296    -2.709804     0.860074     117.59
 H       6.277549    -3.503503     0.620267      25.59
 H       4.526599    -2.750948     0.511237      25.83
 H       5.365507    -2.705279     1.877119      28.41
 C       6.258450     0.586534    -0.597661      10.17
 O       7.324865     0.247373    -1.468326     211.01
 H       7.766399    -0.442569    -1.037261      21.40
 C       5.579975     1.822974    -0.888723      66.42
 H       5.975795     2.435727    -1.616454      34.16
 C       3.833647     1.307173     0.737869      59.93
 C       2.738240     1.960743     1.693367      99.27
 H       3.033834     3.053515     1.965099      23.30
 O       2.645508     1.362711     2.906615     274.65
 H       2.268957     0.363793     2.685914      20.24
 C       1.276925     2.159801     1.044942      86.71
 H       1.543854     2.715953     0.195489      21.46
 C       0.300962     3.037500     1.738447      93.24
 O       0.485537     4.523894     1.731345     170.31
 H       0.843190     4.850312     0.633987      23.87
 H       0.154189     2.723769     2.914942      22.30
 H      -0.633716     3.068864     1.234241      22.50
 C      -2.210772    -1.001473    -0.239362      83.78
 H      -3.156009    -1.680808     0.268799      19.00
 C      -1.152952    -0.045532    -2.292561      14.48
 H      -0.805764     0.018933    -3.338485      15.65
 C      -0.311567     0.721116    -1.422434      10.61
 O       0.508341     1.562150    -2.025930     224.36
 C       0.123539     2.414604    -3.232607      83.03
 H       0.856982     3.274484    -3.199289      22.08
 H      -0.045311     1.685640    -4.144062      20.60
 H      -0.722438     3.143214    -2.952458      23.38
 C      -0.350179     0.603572    -0.058577      40.25
 O       0.770534     0.829209     0.756792     218.36
 C      -1.222691    -0.257881     0.522439      18.44
 H      -0.702436    -0.737232     1.565509      17.91
 C      -2.230993    -0.812320    -1.812035      36.96
 C      -3.161202    -1.603236    -2.564753      76.80
 H      -2.749137    -1.494750    -3.572809      26.22
 O      -3.151252    -3.012800    -2.191415     174.17
 H      -2.115897    -3.327381    -1.793591      24.84
 C      -4.717270    -1.124212    -2.475809      92.32
 H      -5.041792    -1.196839    -1.435280      28.61
 O      -4.648640     0.321854    -2.902237     213.91
 H      -4.557309     1.022197    -2.031293      21.04
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 C      -5.718544    -1.843000    -3.374711     111.39
 O      -5.988720    -3.210819    -2.811376     162.70
 H      -5.132311    -3.685947    -2.890023      32.50
 H      -5.515703    -1.995464    -4.442468      30.44
 H      -6.623517    -1.198043    -3.227349      30.29
55
name = lig-ACN-frame_446
 C       4.476496     2.158031    -0.155161      60.19
 H       4.053580     3.138566    -0.244741      21.22
 C       4.325183    -0.023415     1.089792      28.47
 H       3.805216    -0.755404     1.773156      12.61
 C       5.638258    -0.307253     0.321799      15.18
 O       6.328907    -1.495354     0.440638     260.12
 C       5.665465    -2.738261     0.812509     118.59
 H       6.157706    -3.585637     0.441755      25.76
 H       4.783336    -2.712559     0.130356      26.56
 H       5.615069    -2.877070     1.878484      28.36
 C       6.283077     0.628758    -0.607911      19.80
 O       7.347273     0.117921    -1.382331     190.89
 H       7.894481    -0.519816    -0.884266      22.00
 C       5.611223     1.834260    -0.866012      69.15
 H       6.127854     2.591734    -1.399020      34.73
 C       3.822184     1.282903     0.782165      40.26
 C       2.841069     1.964412     1.663317      96.51
 H       3.318436     2.980970     1.822370      23.21
 O       2.605674     1.365910     2.994478     225.95
 H       2.343249     0.279863     2.877949      19.27
 C       1.426320     2.193232     0.998850      60.12
 H       1.489284     2.486678    -0.015606      19.22
 C       0.276205     3.072933     1.774702      85.88
 O       0.515352     4.443863     1.772499     209.79
 H       1.071013     4.781727     0.777725      23.08
 H       0.339995     2.787848     2.969204      21.34
 H      -0.646770     2.593395     1.456111      23.95
 C      -2.250155    -0.981810    -0.360717      62.05
 H      -2.998296    -1.837695     0.051145      18.53
 C      -1.235466    -0.037202    -2.261312      36.30
 H      -1.161003    -0.017987    -3.327131      19.31
 C      -0.339759     0.735371    -1.459520      13.82
 O       0.553024     1.653241    -2.025125     227.63
 C       0.129380     2.445063    -3.172414      97.70
 H       1.101845     3.039225    -3.366356      21.81
 H       0.092236     2.045899    -4.280562      23.09
 H      -0.963898     2.831325    -2.994882      23.21
 C      -0.306799     0.588787    -0.034621      38.21
 O       0.739610     0.834740     0.861464     173.99
 C      -1.344979    -0.309423     0.463633      51.62
 H      -1.282141    -0.522860     1.707221      15.87
 C      -2.213766    -0.815464    -1.650417      29.15
 C      -3.262236    -1.681666    -2.652712      44.66
 H      -3.094075    -1.663881    -3.730301      26.30
 O      -3.074101    -3.069247    -2.083838     246.19
 H      -2.056010    -3.168024    -2.232532      25.96
 C      -4.663510    -1.032083    -2.575616     100.63
 H      -5.044676    -1.189392    -1.576817      28.37
 O      -4.617781     0.343408    -2.902332     286.71
 H      -4.192686     0.790732    -2.190097      26.84
 C      -5.787827    -1.880953    -3.432383      99.75
 O      -5.935675    -3.187363    -2.831447     125.52
 H      -4.877055    -3.586963    -2.869087      28.79
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 H      -5.421713    -1.864286    -4.481220      29.60
 H      -6.868231    -1.467954    -3.430303      28.31
55
name = lig-ACN-frame_447
 C       4.459469     2.075538    -0.157619      75.81
 H       4.132555     3.110738    -0.209957      24.70
 C       4.477850    -0.009651     1.016052      59.42
 H       4.072918    -0.750214     1.697773      19.67
 C       5.556054    -0.352928     0.366485      10.43
 O       6.300394    -1.499355     0.458434     310.47
 C       5.677564    -2.757748     0.705571     119.72
 H       6.446265    -3.361053     0.324964      25.00
 H       4.638718    -2.953387     0.433261      27.46
 H       5.518695    -2.848085     1.807646      25.39
 C       6.214585     0.493205    -0.591822      15.53
 O       7.341601     0.069279    -1.273945     209.41
 H       7.971026    -0.540572    -0.643492      25.75
 C       5.743109     1.829103    -0.839676      47.80
 H       5.999337     2.505397    -1.710385      17.41
 C       3.892848     1.258131     0.841413      31.71
 C       2.744622     1.974920     1.683835      80.08
 H       3.112708     2.949150     2.004230      21.38
 O       2.595530     1.339477     3.082392     273.60
 H       2.171944     0.473073     2.899882      23.26
 C       1.408155     2.209392     0.907547      72.63
 H       1.617417     2.727480    -0.039786      16.56
 C       0.393788     2.963205     1.836704      86.34
 O       0.546684     4.456560     1.783137     270.68
 H       1.233676     4.574591     1.051088      27.81
 H       0.461649     2.568475     2.974138      20.28
 H      -0.605978     2.873496     1.375932      22.46
 C      -2.313974    -0.997211    -0.262759      58.80
 H      -2.920856    -1.757359     0.308764      21.75
 C      -1.323595     0.049983    -2.300412      44.31
 H      -1.487189     0.350794    -3.310741      20.39
 C      -0.336911     0.811580    -1.477250       8.33
 O       0.643083     1.724771    -2.027033     250.33
 C       0.151168     2.464896    -3.166968      94.86
 H       0.724769     3.574654    -3.295323      20.26
 H       0.139855     1.638710    -3.910484      22.69
 H      -0.857459     3.007917    -2.967029      24.37
 C      -0.336968     0.445124    -0.025145      23.06
 O       0.751886     0.858760     0.967417     141.52
 C      -1.395487    -0.338182     0.504169      21.44
 H      -1.820891    -0.328855     1.607665      16.23
 C      -2.304844    -0.897775    -1.849306      49.96
 C      -3.198682    -1.709331    -2.631836      88.74
 H      -2.765342    -1.783695    -3.594184      30.00
 O      -3.060615    -3.086735    -2.059634     241.35
 H      -2.442957    -3.493172    -2.507781      28.80
 C      -4.722110    -1.089539    -2.571541     102.04
 H      -4.982095    -1.135472    -1.530856      30.04
 O      -4.612307     0.337832    -2.993790     280.26
 H      -4.196989     0.801173    -2.362559      30.71
 C      -5.727288    -1.854453    -3.440495     124.25
 O      -5.850436    -3.182900    -2.893559     146.87
 H      -4.864139    -3.478577    -2.501524      29.96
 H      -5.470259    -1.981989    -4.514454      29.81
 H      -6.774061    -1.333294    -3.351192      29.18
55
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name = lig-ACN-frame_448
 C       4.542968     2.126333    -0.141518      58.23
 H       3.997409     3.012339    -0.520243      20.74
 C       4.451767     0.018246     1.086547      45.53
 H       4.107292    -0.568840     1.896072      18.42
 C       5.632844    -0.382737     0.265751      34.63
 O       6.307635    -1.567253     0.476128     310.40
 C       5.677928    -2.843551     0.708947     120.14
 H       6.285302    -3.662381     0.353909      25.13
 H       4.830551    -2.866571     0.061418      27.40
 H       5.632334    -3.127049     1.817806      25.55
 C       6.230277     0.455123    -0.625984       7.23
 O       7.353758     0.053730    -1.198837     135.09
 H       7.865664    -0.639205    -0.621701      19.38
 C       5.637878     1.688806    -0.802854      75.92
 H       6.267924     2.208468    -1.651963      23.39
 C       3.921577     1.334898     0.874533      55.89
 C       2.728481     1.904082     1.786865     101.11
 H       2.992898     2.938017     1.922087      24.51
 O       2.560229     1.326093     3.032083     333.87
 H       2.083557     0.585647     2.971391      28.34
 C       1.323039     2.113236     1.006152      77.40
 H       1.460305     2.469857    -0.063740      18.54
 C       0.470258     2.999427     1.815206      97.79
 O       0.617729     4.456102     1.810557     319.16
 H       1.278581     4.733747     1.369802      35.37
 H       0.551554     2.542313     2.908146      22.67
 H      -0.598886     2.745798     1.562584      25.49
 C      -2.373603    -1.058074    -0.357792      56.36
 H      -3.247268    -1.514392    -0.028769      19.16
 C      -1.392904     0.234613    -2.299931      30.45
 H      -1.351591     0.566427    -3.331927      15.62
 C      -0.361258     0.767601    -1.421385       0.78
 O       0.641793     1.716950    -1.914274     199.47
 C       0.120755     2.507647    -3.178298      74.37
 H       1.041584     3.364484    -3.380138      21.40
 H       0.095392     2.124209    -4.212265      24.10
 H      -0.993068     2.693818    -2.943914      24.80
 C      -0.252311     0.443415    -0.037490       5.78
 O       0.658508     0.815960     0.880477     228.60
 C      -1.411503    -0.285256     0.548328      45.31
 H      -1.091822    -0.351492     1.622559      19.42
 C      -2.199925    -0.803139    -1.706855      21.69
 C      -3.150742    -1.754423    -2.650415      63.34
 H      -2.982049    -1.699304    -3.690130      26.97
 O      -3.178065    -3.115501    -2.071817     231.04
 H      -2.402209    -3.616945    -2.534049      25.63
 C      -4.624796    -1.123602    -2.571103      96.45
 H      -5.050640    -1.169160    -1.581899      30.00
 O      -4.640856     0.252130    -3.122966     185.88
 H      -4.453354     0.911927    -2.308013      24.59
 C      -5.638066    -1.842078    -3.423531     122.76
 O      -5.778160    -3.223341    -2.936741     177.00
 H      -4.972479    -3.336085    -2.434982      33.23
 H      -5.309496    -1.722103    -4.496171      30.60
 H      -6.646407    -1.256570    -3.300235      28.84
55
name = lig-ACN-frame_449
 C       4.487131     2.197271    -0.099069      38.54
 H       4.105183     3.204277    -0.434076      20.20
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 C       4.500401     0.080045     1.131723      50.67
 H       4.089511    -0.527792     1.884890      16.61
 C       5.521680    -0.511722     0.383972      22.02
 O       6.379446    -1.677383     0.518963     293.65
 C       5.644714    -2.963711     0.689223     103.67
 H       6.382366    -3.670064     0.259482      24.87
 H       4.707887    -2.990824     0.232450      29.21
 H       5.260848    -3.071025     1.777196      25.88
 C       6.220689     0.391342    -0.575029      -2.36
 O       7.447437     0.068595    -1.249702     176.18
 H       7.891579    -0.639861    -0.817279      21.72
 C       5.606184     1.631943    -0.930344      40.63
 H       6.007941     2.547192    -1.559256      28.52
 C       3.922315     1.368609     0.919721      31.04
 C       2.750041     1.885644     1.688147     103.34
 H       3.043330     2.867628     1.988514      23.95
 O       2.518018     1.269501     3.029782     267.84
 H       2.164108     0.307593     2.807152      20.98
 C       1.375827     1.990973     1.005586      64.18
 H       1.603461     2.528592    -0.010933      16.71
 C       0.372623     3.061137     1.914098      85.52
 O       0.700658     4.473832     1.845704     301.20
 H       1.362293     4.516264     1.143609      29.57
 H       0.528914     2.863982     3.008684      21.76
 H      -0.706036     2.868761     1.592493      22.64
 C      -2.256781    -0.910903    -0.282179      74.98
 H      -2.897416    -1.575159     0.035457      21.12
 C      -1.355944     0.321806    -2.161822      94.50
 H      -1.416170     0.348685    -3.272972      16.27
 C      -0.338236     0.824816    -1.450622      16.01
 O       0.529608     1.691348    -1.916228     261.16
 C       0.136938     2.490948    -3.105727      53.78
 H       0.868841     3.541021    -2.891142      21.67
 H       0.291799     1.803915    -3.904144      23.29
 H      -0.843089     3.066702    -2.944430      24.37
 C      -0.393174     0.447502    -0.062686      38.37
 O       0.638675     0.723079     0.842136     219.36
 C      -1.371355    -0.351718     0.477949      31.13
 H      -1.439195    -0.774014     1.398305      19.09
 C      -2.179720    -0.719999    -1.741523      57.94
 C      -3.139113    -1.648349    -2.612796      74.98
 H      -2.686512    -1.835869    -3.555794      24.00
 O      -3.312903    -3.115109    -2.132657     189.27
 H      -2.191847    -3.428409    -2.150986      22.37
 C      -4.518199    -1.099156    -2.573770     109.20
 H      -4.703009    -1.034272    -1.500963      29.83
 O      -4.649041     0.155196    -3.202644     194.94
 H      -4.468740     1.039899    -2.433368      23.48
 C      -5.562663    -1.903714    -3.401916     121.88
 O      -5.744597    -3.255576    -3.008328     211.28
 H      -4.926470    -3.527482    -2.763963      36.58
 H      -5.268824    -1.905904    -4.500432      30.41
 H      -6.623424    -1.453861    -3.342457      29.11
55
name = lig-ACN-frame_450
 C       4.515418     2.113692    -0.154751      57.66
 H       4.207123     3.173060    -0.062232      21.94
 C       4.518219     0.036737     1.203038      41.65
 H       4.000757    -0.526415     1.968735      14.27
 C       5.656143    -0.493544     0.388118      28.59
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 O       6.311829    -1.765725     0.599418     317.49
 C       5.575456    -3.022869     0.688242     121.26
 H       6.322113    -3.895373     0.520699      25.69
 H       4.821234    -3.092159    -0.007094      29.32
 H       5.447054    -3.272655     1.820304      26.93
 C       6.174943     0.379559    -0.594226      23.38
 O       7.400466     0.132059    -1.305977     218.72
 H       7.956272    -0.459616    -0.798298      25.99
 C       5.536179     1.651480    -0.896367      55.28
 H       6.074799     2.010281    -1.849608      20.64
 C       3.979305     1.332816     0.887048      24.11
 C       2.694888     1.865894     1.738865      96.24
 H       2.847950     2.903951     1.925844      22.66
 O       2.513862     1.174297     2.992348     228.90
 H       2.159951     0.103761     2.806502      17.19
 C       1.285580     2.062748     1.012175      69.91
 H       1.380497     2.531349    -0.060526      15.90
 C       0.359495     2.993792     1.974850      86.86
 O       0.794410     4.481643     1.853731     234.87
 H       1.255952     4.785197     0.879800      24.03
 H       0.262161     2.564794     2.944753      23.95
 H      -0.665999     3.090673     1.513697      22.72
 C      -2.349166    -0.970054    -0.386612      68.16
 H      -2.715438    -1.758146     0.013453      22.51
 C      -1.403666     0.200725    -2.282247      42.37
 H      -1.308918     0.685544    -3.304565      15.30
 C      -0.449860     0.878962    -1.348476       1.29
 O       0.528354     1.760002    -1.909934     247.62
 C       0.194514     2.540361    -2.991123      99.13
 H       1.092095     3.415041    -3.168644      21.30
 H       0.299486     2.132038    -4.004402      24.44
 H      -0.911224     2.759546    -3.077829      25.23
 C      -0.349084     0.559679     0.033408      18.93
 O       0.747561     0.675290     0.873666     202.93
 C      -1.256430    -0.408113     0.572932      42.61
 H      -1.128535    -0.494266     1.549855      16.66
 C      -2.301871    -0.736884    -1.705954      31.50
 C      -3.031533    -1.599518    -2.606125      71.06
 H      -2.650509    -1.479723    -3.620146      25.66
 O      -3.317477    -3.007906    -2.169967     213.74
 H      -2.462777    -3.506245    -1.741788      26.34
 C      -4.555994    -1.101300    -2.585804      85.16
 H      -4.955950    -1.033599    -1.560432      29.94
 O      -4.636368     0.200208    -3.292131     178.44
 H      -4.188709     0.900677    -2.495770      22.72
 C      -5.512307    -1.985008    -3.399424     115.43
 O      -5.744711    -3.368823    -3.069657     143.38
 H      -4.790784    -3.763269    -3.149500      31.35
 H      -5.133052    -1.843048    -4.459656      29.92
 H      -6.451118    -1.384793    -3.295070      29.61
55
name = lig-ACN-frame_451
 C       4.493078     2.072363    -0.122382      44.26
 H       4.082754     2.995878    -0.573201      19.40
 C       4.584873    -0.035143     1.152091      45.67
 H       4.285724    -0.726386     1.982643      19.19
 C       5.693950    -0.481674     0.463692      22.70
 O       6.238570    -1.750116     0.654879     294.13
 C       5.542517    -3.069679     0.737628      88.67
 H       6.399004    -3.757503     0.372356      22.57
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 H       4.752531    -3.114277     0.017775      28.39
 H       4.951806    -3.219108     1.683631      23.31
 C       6.188461     0.360962    -0.632249      41.73
 O       7.288995     0.182244    -1.349579     101.93
 H       7.977053    -0.395743    -0.765135      26.91
 C       5.603195     1.561958    -0.914902      47.07
 H       5.916812     2.244569    -1.718635      27.12
 C       3.913969     1.231984     0.937487      44.66
 C       2.695167     1.871843     1.768532     102.68
 H       3.109578     2.724600     2.180294      25.51
 O       2.523528     1.083900     2.944752     277.04
 H       1.945690     0.188783     2.735270      18.04
 C       1.271215     2.111510     1.104796      79.03
 H       1.340412     2.603116     0.047092      18.36
 C       0.365519     3.017214     1.846525     112.05
 O       0.815289     4.379387     1.961744     204.69
 H       1.513658     4.522615     0.986646      23.74
 H       0.431736     2.854669     2.842246      24.87
 H      -0.694635     2.769161     1.527597      24.83
 C      -2.250783    -1.087056    -0.201214      59.11
 H      -3.009589    -1.675856    -0.000464      20.22
 C      -1.361280     0.222249    -2.234918      36.33
 H      -1.507218     0.310678    -3.354313      21.02
 C      -0.540171     0.916670    -1.364174      -5.55
 O       0.549348     1.761808    -1.775963     177.27
 C       0.210705     2.643556    -3.110821      81.47
 H       0.791949     3.666230    -2.829279      21.57
 H       0.395361     2.008370    -3.982079      24.07
 H      -0.751736     3.098575    -2.853337      25.14
 C      -0.328756     0.511652     0.097574      17.65
 O       0.853893     0.752978     0.881653     204.56
 C      -1.296893    -0.405088     0.547290      30.97
 H      -1.157039    -0.873916     1.438849      22.14
 C      -2.272847    -0.727232    -1.686583      27.66
 C      -3.184905    -1.613051    -2.663659      71.63
 H      -2.803413    -1.677156    -3.720316      26.58
 O      -3.239435    -2.912302    -2.177211     296.68
 H      -2.418332    -3.126932    -1.952780      35.16
 C      -4.573279    -1.096760    -2.659061     101.73
 H      -4.870654    -1.000636    -1.581846      27.77
 O      -4.613248     0.247821    -3.318407     231.91
 H      -4.229477     0.869799    -2.729046      30.20
 C      -5.530344    -2.005301    -3.490488     102.47
 O      -5.740790    -3.465990    -3.145880      80.68
 H      -4.723142    -3.963235    -3.105534      28.80
 H      -5.239465    -1.979771    -4.581569      29.60
 H      -6.561206    -1.723582    -3.446855      30.33
55
name = lig-ACN-frame_452
 C       4.406005     1.939012    -0.125262      61.51
 H       3.775606     2.782184    -0.364847      20.27
 C       4.520914    -0.015306     1.189499      34.14
 H       4.137960    -0.696361     2.023929      14.42
 C       5.649451    -0.507503     0.407650      36.29
 O       6.260123    -1.730011     0.714481     333.48
 C       5.465513    -2.972212     0.710742     119.82
 H       6.261804    -3.840818     0.710628      25.39
 H       4.733976    -3.115595    -0.107206      26.85
 H       5.199543    -3.167560     1.762901      28.20
 C       6.187883     0.348052    -0.571703      18.07
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 O       7.338948     0.107297    -1.427685     145.28
 H       7.997668    -0.655428    -1.043688      18.52
 C       5.515825     1.601774    -0.857461      61.93
 H       6.014706     2.191658    -1.526182      31.02
 C       3.874826     1.205741     0.884681      44.62
 C       2.805874     1.813843     1.822400     103.52
 H       3.094089     2.778233     2.095987      25.74
 O       2.510606     1.003628     2.961832     326.64
 H       2.008172     0.279783     2.681094      26.08
 C       1.467849     2.148515     1.054755      55.00
 H       1.829660     2.693438     0.126913      18.42
 C       0.341284     2.981926     1.934830      97.63
 O       0.818591     4.312437     2.005917     257.63
 H       1.667306     4.667333     1.316043      24.88
 H       0.139991     2.464899     2.770397      26.17
 H      -0.622773     3.160265     1.332285      22.79
 C      -2.219674    -1.090484    -0.310102      79.37
 H      -2.732366    -1.666456     0.349356      17.74
 C      -1.402382     0.228359    -2.086428      74.15
 H      -1.214608     0.439694    -3.158636      16.18
 C      -0.379888     0.933848    -1.280532      12.26
 O       0.500978     1.842119    -1.782065     259.00
 C       0.212294     2.711825    -2.977131     101.93
 H       1.070271     3.440361    -3.066432      23.13
 H       0.444102     2.123207    -3.927848      24.84
 H      -0.793887     2.934274    -3.240849      27.47
 C      -0.352233     0.452757     0.001058      15.70
 O       0.795945     0.805633     0.824551     179.19
 C      -1.280912    -0.490020     0.650216      48.33
 H      -1.153267    -0.831924     1.689335      18.03
 C      -2.242913    -0.809799    -1.635692      39.02
 C      -3.200079    -1.518924    -2.642075      43.63
 H      -2.729497    -1.373734    -3.684566      26.04
 O      -3.142534    -2.953691    -2.135665     231.16
 H      -2.248888    -3.245375    -2.424451      26.91
 C      -4.692060    -1.043771    -2.752918      93.52
 H      -5.137691    -1.012108    -1.706548      29.26
 O      -4.618545     0.252252    -3.330642     255.10
 H      -4.429659     0.774582    -2.663490      33.75
 C      -5.645923    -2.101593    -3.630293     122.24
 O      -5.697192    -3.481906    -3.222660     165.82
 H      -4.692264    -3.602856    -2.865289      30.54
 H      -5.244563    -1.997670    -4.678404      30.38
 H      -6.570921    -1.610344    -3.548466      31.39
55
name = lig-ACN-frame_453
 C       4.246658     1.948379    -0.219739      67.13
 H       4.039814     2.994826    -0.345501      23.49
 C       4.486673    -0.097716     1.221672      47.28
 H       4.047466    -0.621137     2.134329      18.45
 C       5.557767    -0.527998     0.384091      16.65
 O       6.300171    -1.700562     0.720061     299.73
 C       5.466191    -2.879463     0.774104     102.37
 H       6.155115    -3.759834     0.525552      24.58
 H       4.718338    -2.763325    -0.115042      26.01
 H       4.788751    -2.895614     1.610906      28.58
 C       6.249167     0.364757    -0.609665       6.47
 O       7.329887    -0.004512    -1.429862     180.68
 H       7.679510    -0.753495    -0.938740      23.20
 C       5.537407     1.568564    -0.813886      53.59
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 H       5.813633     2.155795    -1.576138      21.89
 C       3.840281     1.140840     0.936993      20.24
 C       2.800109     1.726577     1.843535      99.48
 H       3.244572     2.578101     2.273509      22.65
 O       2.529948     0.977855     3.019496     312.79
 H       2.086864     0.205551     2.865856      28.90
 C       1.487964     2.123735     1.049614      70.18
 H       1.573993     2.603254     0.069098      18.11
 C       0.452059     2.895260     1.828461      97.77
 O       0.843617     4.361357     2.155863     263.43
 H       1.397977     4.452410     1.371867      29.66
 H       0.179195     2.563390     2.755584      25.57
 H      -0.434712     2.757201     1.129043      24.18
 C      -2.206293    -1.123305    -0.165136      25.21
 H      -2.768965    -2.012596    -0.233622      16.86
 C      -1.352192     0.279211    -2.071598      38.26
 H      -1.530963     0.637111    -3.068236      19.70
 C      -0.419853     0.825150    -1.287974      -1.44
 O       0.482046     1.969260    -1.761636     211.87
 C       0.241471     2.651088    -2.940281     107.67
 H       0.770406     3.596275    -2.794288      24.29
 H       0.494476     2.052365    -3.903352      24.16
 H      -0.714573     3.131670    -2.826610      25.83
 C      -0.251507     0.460902     0.117247      31.67
 O       0.779469     0.834019     0.793937     215.22
 C      -1.171232    -0.493980     0.541250      54.36
 H      -1.143366    -0.560227     1.711905      20.22
 C      -2.250732    -0.747821    -1.624694      54.89
 C      -3.141953    -1.534279    -2.541966      70.98
 H      -2.824939    -1.419855    -3.656451      25.63
 O      -3.071073    -2.991686    -2.169454     155.90
 H      -2.277908    -3.547338    -2.776155      23.58
 C      -4.800298    -1.148001    -2.803458      80.61
 H      -5.391668    -1.098998    -1.830226      29.40
 O      -4.676502     0.263905    -3.357549     178.96
 H      -4.628693     0.884494    -2.499957      25.29
 C      -5.675582    -2.034879    -3.757951     128.73
 O      -5.605562    -3.420602    -3.251492     180.33
 H      -4.834089    -3.473401    -2.709940      35.10
 H      -5.390734    -2.026716    -4.839776      30.62
 H      -6.706528    -1.831079    -3.735731      32.00
55
name = lig-ACN-frame_454
 C       4.326484     1.881598    -0.190540      55.41
 H       3.751230     2.763366    -0.473865      22.21
 C       4.486418    -0.140628     1.150860      37.68
 H       4.410465    -0.848089     1.998731      19.99
 C       5.636168    -0.494805     0.414122       2.66
 O       6.328933    -1.637155     0.697463     270.64
 C       5.408725    -2.785479     0.763896      94.92
 H       5.982661    -3.749617     0.805767      24.01
 H       4.677584    -2.834851    -0.185834      25.13
 H       4.953274    -2.838230     1.721569      24.78
 C       6.115653     0.309770    -0.591381      16.19
 O       7.246465    -0.126162    -1.332774     199.18
 H       7.823496    -0.683118    -0.846039      28.48
 C       5.491953     1.568822    -0.887735      57.56
 H       5.898592     2.196758    -1.598768      21.94
 C       3.824025     1.122119     0.870510      25.66
 C       2.739395     1.697969     1.855048      91.90
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 H       3.096448     2.652568     2.161533      24.66
 O       2.541388     0.956070     3.112742     279.07
 H       2.016450     0.074169     2.893841      22.14
 C       1.474898     2.064865     1.055930      98.60
 H       1.887543     2.511521     0.194176      22.40
 C       0.495316     2.993780     1.805767     109.08
 O       0.869112     4.297472     2.231044     332.64
 H       1.076892     4.895839     1.681198      36.04
 H       0.449684     2.403341     2.712546      25.00
 H      -0.509150     3.076826     1.335771      25.11
 C      -2.125115    -1.131943    -0.253461      85.92
 H      -2.550279    -1.857251     0.484707      18.28
 C      -1.447776     0.288418    -2.193147      70.12
 H      -1.713520     0.677185    -3.123001      23.65
 C      -0.347643     0.940479    -1.343933       2.00
 O       0.464587     1.920757    -1.571153     190.09
 C       0.179059     2.720327    -2.945075      92.63
 H       0.911485     3.457525    -2.973138      24.79
 H       0.374415     2.068344    -3.926447      24.33
 H      -0.860347     2.882864    -3.096551      26.79
 C      -0.251638     0.480895     0.003043      15.62
 O       0.922886     0.782903     0.925232     175.14
 C      -1.142427    -0.512576     0.592945      44.92
 H      -0.904662    -1.063539     1.675964      16.62
 C      -2.270698    -0.653310    -1.504134      24.37
 C      -3.241767    -1.637193    -2.572402      33.08
 H      -2.609997    -1.497904    -3.545377      25.64
 O      -3.074514    -3.028422    -2.227791     196.61
 H      -2.055812    -3.198934    -2.724139      21.02
 C      -4.763212    -1.132873    -2.828500      95.34
 H      -5.227983    -1.253908    -1.790399      28.47
 O      -4.787585     0.205020    -3.347123     173.78
 H      -4.560087     0.913146    -2.414153      21.78
 C      -5.610784    -2.006743    -3.817469     137.85
 O      -5.527482    -3.337599    -3.271122     207.98
 H      -4.692414    -3.407497    -2.981774      35.28
 H      -5.223028    -1.874154    -4.845836      30.73
 H      -6.590897    -1.613605    -3.718972      32.04
55
name = lig-ACN-frame_455
 C       4.365358     1.872705    -0.151649      54.25
 H       3.768848     2.745770    -0.504550      21.95
 C       4.502541    -0.128551     1.136678      59.10
 H       3.973575    -0.594315     1.944415      19.11
 C       5.663105    -0.447720     0.479442      11.31
 O       6.343657    -1.660426     0.668459     260.85
 C       5.411829    -2.768111     0.805875      89.60
 H       6.086284    -3.587758     0.801078      24.51
 H       4.595298    -2.856656    -0.122673      25.90
 H       4.811883    -2.635550     1.683553      25.26
 C       6.089018     0.300331    -0.669417      14.11
 O       7.169617    -0.196258    -1.259082      87.80
 H       7.679660    -0.682391    -0.467728      20.69
 C       5.471604     1.492794    -0.990337      60.87
 H       5.915076     2.112381    -1.804129      23.22
 C       3.817749     1.048788     0.896319      20.05
 C       2.778104     1.725291     1.905673      92.76
 H       3.180983     2.649146     2.239172      25.05
 O       2.559862     0.979981     3.128408     246.07
 H       1.890742     0.077917     2.929726      19.64
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 C       1.541198     2.055466     1.054643      65.60
 H       1.741398     2.408264     0.102187      21.17
 C       0.440031     3.028284     1.882037      98.31
 O       0.946857     4.307363     2.352276     265.99
 H       0.979349     4.709134     1.377549      27.07
 H       0.044696     2.535111     2.820773      24.27
 H      -0.452803     3.102612     1.273839      25.04
 C      -2.026710    -1.090057    -0.188285      99.00
 H      -2.883456    -1.840689     0.052169      20.54
 C      -1.482966     0.373465    -2.122537      53.16
 H      -1.492083     0.581519    -3.148093      20.44
 C      -0.489463     0.901819    -1.326066      -4.58
 O       0.468729     2.032650    -1.637888     208.16
 C       0.165218     2.682345    -2.889872     106.92
 H       0.677373     3.533758    -2.900705      26.50
 H       0.520304     1.829222    -3.607427      23.35
 H      -0.829233     3.096792    -2.878262      27.12
 C      -0.184098     0.416256     0.081267      20.08
 O       0.879743     0.631301     0.901326     162.80
 C      -1.014213    -0.510368     0.570976      21.40
 H      -0.608548    -1.029157     1.631209      18.76
 C      -2.412829    -0.733644    -1.647110      53.70
 C      -3.207979    -1.534451    -2.607522      55.34
 H      -2.841851    -1.344395    -3.711499      25.81
 O      -3.101928    -3.047948    -2.299996     223.59
 H      -2.158288    -3.246972    -2.120276      29.11
 C      -4.666911    -1.147286    -2.789764     107.35
 H      -5.235224    -1.201119    -1.813884      27.92
 O      -4.877630     0.179356    -3.287044     179.34
 H      -4.374623     0.928489    -2.537012      22.18
 C      -5.451643    -1.951437    -3.760564     125.46
 O      -5.492969    -3.301639    -3.328227     160.01
 H      -4.574948    -3.644194    -3.332166      32.66
 H      -5.081253    -1.906684    -4.782993      31.28
 H      -6.482352    -1.628290    -3.816060      30.91
55
name = lig-ACN-frame_456
 C       4.328443     1.909941    -0.212922      62.78
 H       4.122987     3.015285    -0.239651      23.13
 C       4.443829    -0.134928     1.272098      49.13
 H       4.211465    -0.885345     1.967753      18.89
 C       5.602944    -0.485946     0.497273      -9.73
 O       6.330836    -1.670835     0.652001     267.64
 C       5.448398    -2.807196     0.868346     102.36
 H       5.922869    -3.738898     0.925486      25.39
 H       4.767231    -2.791851    -0.164721      24.67
 H       4.865744    -2.747867     1.797242      25.54
 C       6.095226     0.267733    -0.612879      14.85
 O       7.230985    -0.251017    -1.280346     122.99
 H       7.679419    -1.105338    -0.806658      21.11
 C       5.387901     1.441111    -1.022167      56.71
 H       5.572371     2.052478    -2.011278      21.38
 C       3.872198     1.176408     0.909567      19.73
 C       2.871376     1.727823     1.878626      87.57
 H       3.331451     2.598580     2.246332      25.27
 O       2.566547     1.020263     3.097839     233.76
 H       1.888299     0.208387     2.894864      22.22
 C       1.420859     2.032790     1.205121      81.67
 H       1.575050     2.518408     0.278030      22.91
 C       0.414170     2.906084     1.927756      87.40
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 O       1.018498     4.318730     2.383999     139.26
 H       1.605805     4.974473     1.581184      24.61
 H      -0.093472     2.473209     2.892544      24.23
 H      -0.275115     3.176880     1.181500      25.54
 C      -2.169241    -1.092299    -0.308912      57.80
 H      -2.525282    -2.051853     0.214367      20.31
 C      -1.539291     0.367346    -2.040594      54.07
 H      -1.512849     0.723741    -3.054589      18.90
 C      -0.468473     0.992963    -1.170185      11.12
 O       0.369534     2.024919    -1.641700     223.66
 C       0.160469     2.688838    -2.917859     115.19
 H       0.810485     3.448752    -2.890081      27.10
 H       0.240974     2.202393    -3.946932      26.07
 H      -0.911462     2.855786    -2.984285      27.00
 C      -0.147403     0.401557     0.034393      22.47
 O       0.925274     0.641943     0.866067     199.28
 C      -1.041629    -0.672582     0.497701      74.08
 H      -1.008076    -0.939820     1.694517      17.40
 C      -2.220525    -0.684842    -1.610893      37.54
 C      -3.119247    -1.507358    -2.654567      63.59
 H      -2.608951    -1.340764    -3.656859      24.69
 O      -3.152838    -2.960669    -2.356505     295.10
 H      -2.320463    -3.159755    -2.147189      33.11
 C      -4.671962    -1.111945    -2.646284      94.26
 H      -5.048149    -1.354951    -1.618133      29.41
 O      -4.881637     0.240396    -3.228029     232.65
 H      -4.571068     0.898902    -2.461572      25.83
 C      -5.337135    -1.974948    -3.763383     111.69
 O      -5.505592    -3.362343    -3.394807     120.50
 H      -4.450536    -3.744478    -3.318834      28.04
 H      -4.804911    -1.742997    -4.669701      30.78
 H      -6.361768    -1.556633    -3.805739      30.02
55
name = lig-ACN-frame_457
 C       4.343320     1.927160    -0.186727      51.29
 H       3.824747     2.912926    -0.442447      22.60
 C       4.473543    -0.077456     1.245506      77.78
 H       4.035513    -0.423650     2.149090      21.97
 C       5.545181    -0.544697     0.467837      13.26
 O       6.297206    -1.704645     0.704027     272.70
 C       5.467450    -2.891689     0.893504     111.74
 H       6.228767    -3.621222     0.943631      25.11
 H       4.572283    -3.163925     0.090295      25.48
 H       4.983485    -2.765997     1.913610      26.23
 C       6.113456     0.219940    -0.587655       2.05
 O       7.249111    -0.241892    -1.344616     152.88
 H       7.436887    -1.045224    -0.841376      19.60
 C       5.353481     1.353407    -1.016342      38.04
 H       5.867059     1.875202    -1.988142      20.41
 C       3.939061     1.185491     0.987212      18.71
 C       2.778846     1.826701     1.891950      98.91
 H       3.022286     2.812714     2.131168      26.68
 O       2.602964     1.025044     3.077792     291.78
 H       2.105294     0.325585     2.802764      30.39
 C       1.442421     2.020984     1.240631      84.38
 H       1.704954     2.607229     0.354644      23.06
 C       0.435690     2.998609     1.988048     103.92
 O       1.056482     4.213171     2.394469     222.53
 H       1.836319     4.248266     1.577066      26.52
 H       0.062911     2.539799     3.029601      23.66
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 H      -0.457479     3.126546     1.421163      26.54
 C      -2.175024    -1.232557    -0.307635      30.99
 H      -2.903306    -2.000335    -0.025717      16.19
 C      -1.406308     0.505560    -2.002245      79.50
 H      -1.745905     0.931660    -2.963511      21.68
 C      -0.487646     1.039924    -1.191846      20.73
 O       0.332352     1.988697    -1.596085     178.76
 C       0.054897     2.751163    -3.042996      81.92
 H       0.713897     3.561728    -2.909205      26.06
 H       0.468326     1.932504    -3.594227      24.71
 H      -0.907021     3.266447    -3.115097      26.20
 C      -0.247468     0.308007     0.099882      27.12
 O       1.014538     0.704653     0.890045     173.13
 C      -1.117176    -0.672141     0.456222      49.16
 H      -0.955243    -1.255479     1.458046      20.88
 C      -2.199675    -0.756933    -1.630652      65.93
 C      -3.078670    -1.436298    -2.608023      78.62
 H      -2.795121    -1.248195    -3.671663      26.52
 O      -3.159980    -2.838091    -2.372466     211.06
 H      -2.212512    -3.310995    -2.615383      26.16
 C      -4.574202    -1.065189    -2.645677     106.32
 H      -5.019650    -1.109946    -1.646472      29.74
 O      -4.844144     0.277752    -3.106096     285.58
 H      -4.829537     0.826648    -2.375110      30.95
 C      -5.318903    -1.992606    -3.700676     118.53
 O      -5.513646    -3.426603    -3.490329     162.22
 H      -4.576174    -3.635746    -2.988071      30.72
 H      -4.700462    -1.955431    -4.569550      31.72
 H      -6.311684    -1.571983    -4.054661      29.81
55
name = lig-ACN-frame_458
 C       4.391013     1.871109    -0.186918      59.06
 H       3.765717     2.590632    -0.760218      23.31
 C       4.493449     0.007124     1.228213      26.81
 H       4.284289    -0.678004     2.071579      19.45
 C       5.564264    -0.587351     0.435210      12.25
 O       6.214652    -1.764620     0.748010     256.73
 C       5.538810    -3.007348     1.004092     106.85
 H       6.242416    -3.854286     0.900777      24.35
 H       4.814054    -3.123193     0.036441      26.05
 H       4.972742    -3.108443     2.021347      25.45
 C       6.073716     0.162118    -0.664932      20.71
 O       7.159910    -0.205133    -1.344969     145.39
 H       7.726960    -0.795915    -0.911306      23.56
 C       5.425630     1.338692    -0.963948      57.22
 H       5.745905     2.022493    -1.907918      22.35
 C       3.884104     1.321470     0.998417       8.95
 C       2.783925     1.872854     1.947899      93.67
 H       3.138127     2.729257     2.380896      25.42
 O       2.653734     1.030725     3.097672     270.48
 H       2.049956     0.320322     2.958794      27.60
 C       1.427274     2.107953     1.107133      62.30
 H       1.543981     2.562749     0.082045      21.01
 C       0.405240     2.942231     2.101347     102.86
 O       1.156054     4.146420     2.361369     284.13
 H       1.677541     4.470497     1.671457      32.78
 H       0.204656     2.380834     3.114306      24.20
 H      -0.485317     3.181382     1.539023      25.68
 C      -2.109446    -1.305699    -0.368566      53.59
 H      -2.780131    -2.049236    -0.085766      20.29
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 C      -1.521255     0.394630    -2.030988      40.30
 H      -1.620880     0.999561    -2.972234      18.41
 C      -0.486254     0.949349    -1.145087      -7.93
 O       0.352888     2.168542    -1.633299     201.66
 C       0.071203     2.729794    -2.950348     111.73
 H       0.740257     3.563136    -3.144499      25.16
 H       0.175601     2.166889    -3.883541      26.63
 H      -1.005873     2.922994    -3.160534      26.14
 C      -0.206482     0.438790     0.171679      13.24
 O       0.924976     0.642544     0.866280     170.99
 C      -1.119822    -0.724609     0.623842      35.86
 H      -0.677523    -1.248960     1.460813      19.80
 C      -2.211880    -0.653068    -1.678190      31.28
 C      -3.112455    -1.327487    -2.669696      70.73
 H      -2.668117    -1.107705    -3.640332      25.78
 O      -3.097438    -2.823421    -2.373527     165.86
 H      -2.128170    -3.108090    -2.966470      22.28
 C      -4.603954    -1.056837    -2.645594     106.30
 H      -4.961022    -1.348847    -1.658309      29.43
 O      -4.804357     0.302176    -3.048170     315.74
 H      -4.592404     0.910013    -2.432345      31.34
 C      -5.285063    -1.987603    -3.727736     112.86
 O      -5.518448    -3.438694    -3.504427     213.29
 H      -4.894837    -3.694679    -2.908745      38.56
 H      -4.738659    -1.772095    -4.631941      31.45
 H      -6.347326    -1.522666    -3.785426      28.26
55
name = lig-ACN-frame_459
 C       4.318411     1.907605    -0.269364      46.29
 H       4.009012     2.938981    -0.469899      21.94
 C       4.515059     0.023138     1.240260      63.58
 H       4.121196    -0.530627     2.157353      19.47
 C       5.482827    -0.577634     0.445780       6.57
 O       6.209335    -1.799451     0.807438     280.85
 C       5.571472    -3.122567     1.015519      93.54
 H       6.494514    -3.834993     0.952361      22.96
 H       4.661698    -3.386586     0.313913      26.07
 H       5.199339    -3.123561     2.089149      24.72
 C       6.013802     0.107032    -0.649293      17.97
 O       7.173750    -0.207042    -1.425250     182.48
 H       7.791549    -0.728367    -0.745064      22.21
 C       5.472895     1.418806    -0.949272      31.32
 H       5.808381     1.905395    -1.964164      21.34
 C       3.919595     1.237406     0.976148      25.40
 C       2.849189     1.859724     1.899581      84.40
 H       3.084774     2.781199     2.169202      26.14
 O       2.656389     1.039497     3.143724     220.89
 H       1.958070     0.222202     2.840674      21.68
 C       1.339960     2.073392     1.151125      83.41
 H       1.471410     2.689894     0.164195      20.23
 C       0.488283     2.835029     2.021858     106.80
 O       1.245520     4.174639     2.377325     255.61
 H       1.209122     4.549377     1.596095      33.87
 H       0.431846     2.367520     3.025137      25.32
 H      -0.572789     3.071055     1.800798      25.19
 C      -1.942883    -1.212603    -0.319504      74.34
 H      -2.162738    -2.196047    -0.072014      18.93
 C      -1.448891     0.490657    -2.022935      86.12
 H      -1.550633     0.656487    -3.125149      19.61
 C      -0.436371     1.053201    -1.209470      -3.88
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 O       0.323052     2.207902    -1.605927     203.19
 C       0.021229     2.677670    -2.913632      98.67
 H       0.575590     3.683683    -2.966430      23.83
 H       0.299172     1.902150    -3.575531      26.48
 H      -0.986650     3.090991    -2.831628      26.01
 C      -0.336875     0.393917     0.153579      27.61
 O       0.874101     0.671520     0.908620     166.13
 C      -1.026362    -0.677323     0.590232      30.39
 H      -1.091163    -1.104669     1.491085      20.18
 C      -2.309603    -0.684604    -1.573645      68.57
 C      -3.130078    -1.403950    -2.712526      58.20
 H      -2.877128    -1.134594    -3.720762      26.30
 O      -2.985776    -2.795328    -2.446153     252.74
 H      -1.986581    -3.180581    -2.613645      25.10
 C      -4.632709    -1.119061    -2.657400     104.25
 H      -5.064856    -1.286141    -1.691153      28.49
 O      -4.824935     0.286969    -3.104570     269.82
 H      -4.518824     0.739323    -2.300893      28.09
 C      -5.352031    -1.934644    -3.762327     112.31
 O      -5.530182    -3.363167    -3.472665     225.60
 H      -4.647187    -3.568786    -3.110491      34.12
 H      -4.926242    -1.818293    -4.770598      30.33
 H      -6.436340    -1.537773    -3.844718      28.06
55
name = lig-ACN-frame_460
 C       4.337044     1.974724    -0.238359      66.14
 H       3.990287     2.976576    -0.327966      24.04
 C       4.468300    -0.074708     1.290934      35.86
 H       4.129800    -0.408109     2.347555      19.25
 C       5.501714    -0.692584     0.459927       4.13
 O       6.197088    -1.773669     0.827600     242.44
 C       5.614049    -3.135299     1.026856     100.14
 H       6.527966    -3.876951     0.754681      23.51
 H       4.869759    -3.304393     0.188583      27.94
 H       5.203716    -3.379909     1.977746      28.64
 C       6.022513     0.193587    -0.680795       4.89
 O       7.157063    -0.242103    -1.438785      88.52
 H       7.718199    -1.012125    -0.939063      19.79
 C       5.423331     1.421188    -0.987999      60.37
 H       6.037891     1.992114    -1.712548      22.46
 C       3.908980     1.198689     0.847252      17.25
 C       2.798032     1.780362     1.814448     102.87
 H       3.088862     2.656258     2.081101      26.96
 O       2.642751     1.094799     3.107521     230.71
 H       2.032454     0.200375     2.881690      22.72
 C       1.478795     1.947645     1.177576      75.81
 H       1.725173     2.442186     0.125531      19.95
 C       0.576662     2.915018     2.160049     104.49
 O       1.217551     4.126722     2.345522     239.60
 H       1.164171     4.920990     1.586243      26.17
 H       0.516209     2.420449     3.078526      26.16
 H      -0.403753     2.952843     1.605688      24.67
 C      -1.921753    -1.260783    -0.310418     118.99
 H      -2.614157    -2.169005    -0.117453      20.85
 C      -1.465976     0.482598    -2.014995      56.12
 H      -1.559917     0.903405    -3.032983      21.11
 C      -0.505829     1.076756    -1.174445      22.97
 O       0.313036     2.135611    -1.468676     224.34
 C      -0.061741     2.724547    -2.884897      97.57
 H       0.788808     3.538312    -3.077975      22.76
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 H       0.231435     2.037003    -3.660313      26.66
 H      -1.083927     2.823491    -3.210621      25.77
 C      -0.209332     0.565663     0.061646      17.85
 O       0.805002     0.751406     0.971760     205.25
 C      -1.015743    -0.616812     0.526372      14.12
 H      -0.694172    -0.816601     1.451124      20.72
 C      -2.206174    -0.572417    -1.614277      57.83
 C      -3.098320    -1.451555    -2.616139      62.96
 H      -2.644831    -1.112407    -3.539648      26.82
 O      -2.874318    -2.880332    -2.532662     306.27
 H      -1.973488    -2.941249    -2.438387      33.05
 C      -4.688973    -1.129030    -2.754038     102.91
 H      -5.119381    -1.307732    -1.796980      28.01
 O      -4.842243     0.215997    -3.161700     237.94
 H      -4.841457     1.034844    -2.394204      22.85
 C      -5.518972    -1.911137    -3.793815     112.16
 O      -5.515563    -3.270141    -3.411345     175.35
 H      -4.465712    -3.605061    -3.542748      28.00
 H      -4.919402    -1.751735    -4.724881      29.72
 H      -6.554335    -1.468639    -3.920700      29.25
55
name = lig-ACN-frame_461
 C       4.432171     1.925721    -0.173652      42.45
 H       3.938133     2.779251    -0.569772      23.74
 C       4.456835    -0.102701     1.181315      52.22
 H       4.295169    -0.800829     2.071295      17.68
 C       5.491800    -0.597924     0.430101      12.50
 O       6.264216    -1.791541     0.860292     303.99
 C       5.658111    -3.094467     0.913688      99.86
 H       6.572001    -3.901483     0.766893      22.71
 H       4.890172    -3.196663     0.139154      28.65
 H       5.240853    -3.267530     1.857509      28.25
 C       6.030617     0.115374    -0.623178      14.03
 O       7.079155    -0.268462    -1.405172     183.87
 H       7.443011    -1.032493    -0.956601      23.05
 C       5.439564     1.432503    -1.013778      45.17
 H       5.782857     2.094749    -1.734267      24.01
 C       3.834140     1.090484     0.885549      40.23
 C       2.880021     1.687761     1.806295     117.21
 H       3.192537     2.591612     1.990500      27.15
 O       2.643188     1.105158     3.052211     320.45
 H       2.148775     0.329060     3.050998      29.31
 C       1.518992     2.061325     1.183967      67.68
 H       1.588823     2.653930     0.161258      20.02
 C       0.657687     2.875528     2.142065     109.25
 O       1.198868     4.208230     2.379472     166.77
 H       1.238910     4.582179     1.247417      24.35
 H       0.462343     2.527066     3.068211      26.82
 H      -0.396165     3.030120     1.723980      23.99
 C      -1.981452    -1.195709    -0.351285      85.72
 H      -2.680830    -2.014591     0.233175      18.15
 C      -1.510039     0.513898    -2.046779      66.81
 H      -1.810426     1.056458    -2.952750      19.57
 C      -0.519798     1.127175    -1.103975       9.83
 O       0.254380     2.209682    -1.557336     220.40
 C       0.017319     2.692195    -2.823488     101.47
 H       0.440986     3.854817    -2.874174      22.02
 H       0.219335     1.968205    -3.606808      24.89
 H      -0.973085     3.095974    -2.660973      25.53
 C      -0.232077     0.489187     0.098606      26.01
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 O       0.770659     0.774434     1.052136     203.66
 C      -0.955682    -0.533182     0.476311      52.18
 H      -0.759009    -1.165262     1.298472      19.89
 C      -2.196020    -0.724482    -1.626959      49.36
 C      -3.067093    -1.387646    -2.656524      56.46
 H      -2.779496    -1.146768    -3.673886      27.08
 O      -2.812009    -2.966068    -2.568623     227.79
 H      -1.951256    -3.073407    -2.761979      27.83
 C      -4.695625    -1.098912    -2.737244      95.74
 H      -5.160139    -1.312698    -1.801873      28.13
 O      -4.860465     0.253014    -3.242122     219.06
 H      -4.829859     0.908727    -2.307648      23.35
 C      -5.517639    -1.881511    -3.822651     106.36
 O      -5.532340    -3.273910    -3.383227     187.57
 H      -4.545933    -3.619911    -3.597029      30.68
 H      -5.342942    -1.719353    -4.941090      29.50
 H      -6.578374    -1.599494    -3.649346      29.68
55
name = lig-ACN-frame_462
 C       4.397935     1.789505    -0.152628      70.25
 H       3.968072     2.782875    -0.233142      22.98
 C       4.437818    -0.236702     1.127385      47.65
 H       3.847611    -0.751520     1.915558      18.77
 C       5.600524    -0.655760     0.425344       0.50
 O       6.350403    -1.689685     0.830126     294.99
 C       5.651068    -3.047704     0.806628      96.61
 H       6.578671    -3.812144     0.701884      23.01
 H       4.953761    -3.242594     0.030331      29.67
 H       5.198473    -3.183572     1.754874      26.89
 C       6.027454     0.172941    -0.685729      21.31
 O       7.052561    -0.344855    -1.392308     201.36
 H       7.560648    -0.948307    -0.885287      22.35
 C       5.487543     1.370914    -0.934818      78.01
 H       5.731915     1.621276    -1.866912      22.62
 C       3.889141     1.034711     0.871389      29.33
 C       2.888308     1.799450     1.831440      90.95
 H       3.382991     2.571072     2.137855      25.88
 O       2.681271     1.042016     3.098371     312.51
 H       2.131428     0.381200     2.809693      28.18
 C       1.439622     2.132558     1.169760      79.37
 H       1.568133     2.612783     0.137564      18.04
 C       0.610918     2.918866     2.152520     102.28
 O       1.182077     4.319204     2.361408     234.20
 H       1.825218     4.637950     1.527546      26.09
 H       0.765637     2.328207     2.975698      25.56
 H      -0.451687     2.913345     1.745387      24.48
 C      -2.038992    -1.099376    -0.290514      56.89
 H      -2.420602    -2.276975    -0.032022      19.79
 C      -1.546560     0.494965    -1.953404      48.28
 H      -1.754871     0.869211    -2.959742      18.64
 C      -0.550623     1.145053    -1.191034       6.32
 O       0.264061     2.240725    -1.514988     241.11
 C      -0.043420     2.842829    -2.840446      98.19
 H       0.970732     3.543834    -3.012733      21.47
 H       0.208085     2.090885    -3.660839      25.27
 H      -1.036178     3.042458    -3.169195      26.09
 C      -0.208688     0.518793     0.143872      -6.24
 O       0.799951     0.818277     1.090649     169.82
 C      -1.065504    -0.742513     0.504965      60.52
 H      -0.877513    -1.088292     1.582835      18.06
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 C      -2.217424    -0.710711    -1.734944      32.82
 C      -3.103031    -1.509313    -2.808201      76.96
 H      -2.725716    -1.100885    -3.765160      24.67
 O      -2.859621    -2.922143    -2.618453     284.11
 H      -1.900755    -3.127398    -2.941252      26.04
 C      -4.615591    -1.071568    -2.787837      96.65
 H      -4.999406    -1.106010    -1.787234      28.50
 O      -4.859468     0.347788    -3.241222     249.72
 H      -4.611731     0.973950    -2.514244      27.61
 C      -5.528236    -1.930167    -3.699249     117.70
 O      -5.545331    -3.334548    -3.432568     264.30
 H      -4.693045    -3.526876    -3.192326      35.19
 H      -5.201951    -1.737901    -4.795625      28.86
 H      -6.520021    -1.498165    -3.550671      29.07
55
name = lig-ACN-frame_463
 C       4.355175     1.800814    -0.197008      39.50
 H       4.077378     2.878914    -0.341048      21.80
 C       4.356049    -0.349459     1.132279      56.10
 H       4.171807    -1.076767     1.905155      20.96
 C       5.575375    -0.631104     0.486468      -6.95
 O       6.440692    -1.721103     0.757040     309.52
 C       5.714234    -2.965908     0.757669      89.95
 H       6.497510    -3.800629     0.629628      22.24
 H       5.152291    -2.851060    -0.117941      29.05
 H       5.081842    -3.214684     1.632654      24.51
 C       6.091536     0.061525    -0.613911       6.16
 O       7.121939    -0.422272    -1.474638     199.26
 H       7.832136    -0.959345    -0.884851      22.63
 C       5.460204     1.347301    -1.000687      40.63
 H       5.774547     2.067755    -1.661131      22.73
 C       3.880218     1.026895     0.921322      18.84
 C       2.876220     1.824527     1.867137      90.10
 H       3.194515     2.691066     2.152009      24.63
 O       2.707500     0.987353     3.086306     280.75
 H       1.970800     0.184688     3.038261      18.27
 C       1.494508     2.138887     1.174937      70.44
 H       1.609996     2.576447     0.176998      18.40
 C       0.622412     3.081055     2.185996     112.93
 O       1.118600     4.374078     2.324778     326.58
 H       1.804044     4.437057     1.822206      35.35
 H       0.554301     2.736028     3.188403      24.10
 H      -0.489687     3.231495     2.016377      23.92
 C      -2.143190    -1.277694    -0.411749     104.58
 H      -2.884537    -2.269537    -0.203776      15.00
 C      -1.536396     0.529057    -2.029564      40.39
 H      -1.424590     0.983262    -3.011498      12.63
 C      -0.520370     1.031753    -1.052771       4.64
 O       0.193536     2.265055    -1.495262     167.20
 C       0.005405     2.909087    -2.962320      65.45
 H       0.696704     3.934102    -2.950749      21.93
 H       0.190353     1.999776    -3.666646      23.84
 H      -0.909172     3.489153    -2.916151      25.09
 C      -0.289020     0.460585     0.171776      13.49
 O       0.778107     0.830048     1.029722     226.80
 C      -1.023196    -0.631185     0.566378      85.04
 H      -0.854645    -1.127082     1.630272      19.37
 C      -2.283313    -0.652657    -1.682939      26.81
 C      -3.030040    -1.435997    -2.889402      56.98
 H      -2.556224    -1.309321    -3.887017      23.99
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 O      -2.978180    -2.880910    -2.700781     198.26
 H      -1.832380    -3.113082    -2.631784      22.06
 C      -4.567688    -1.025121    -2.769797      89.32
 H      -4.710494    -1.164055    -1.695833      26.99
 O      -4.793553     0.344408    -3.215095     287.76
 H      -4.496905     0.845521    -2.554357      32.58
 C      -5.539519    -1.929385    -3.618367     110.50
 O      -5.550437    -3.409293    -3.452171     244.04
 H      -4.795707    -3.616715    -2.919345      33.70
 H      -5.140893    -1.752223    -4.691546      28.06
 H      -6.565491    -1.624196    -3.634013      28.78
55
name = lig-ACN-frame_464
 C       4.399169     1.748841    -0.172983      55.19
 H       3.890403     2.721862    -0.486575      21.03
 C       4.368435    -0.265731     1.169459      37.05
 H       3.961405    -0.730032     2.032042      19.35
 C       5.623124    -0.650584     0.446146      -9.95
 O       6.493278    -1.743590     0.756697     319.10
 C       5.743588    -2.970316     0.660509     109.72
 H       6.456500    -3.803262     0.694495      23.60
 H       5.061918    -3.137644    -0.119291      30.81
 H       5.141841    -2.953107     1.626304      25.83
 C       6.131434     0.113136    -0.694317      -4.38
 O       7.144684    -0.438257    -1.498858     119.03
 H       7.923127    -1.014384    -0.946158      21.91
 C       5.430922     1.272735    -0.998336      60.09
 H       6.025140     1.842092    -1.721034      23.84
 C       3.820775     1.035663     0.925874      29.65
 C       2.818836     1.641563     1.880709     112.58
 H       3.278464     2.458940     2.111197      24.54
 O       2.714852     0.983419     3.092852     295.77
 H       1.926005     0.223406     2.804935      18.36
 C       1.426505     2.142373     1.285002      68.75
 H       1.627582     2.692500     0.417499      20.56
 C       0.587020     3.103216     2.207683     100.46
 O       1.120986     4.523862     2.297316     277.84
 H       1.616183     4.789620     1.521175      30.25
 H       0.538538     2.572098     3.155674      24.70
 H      -0.308314     3.050720     1.563110      24.09
 C      -2.029020    -1.267867    -0.427642      66.32
 H      -2.650664    -2.109895     0.117767      20.47
 C      -1.419523     0.514276    -1.995459      52.82
 H      -1.674817     0.916240    -2.978034      20.11
 C      -0.561306     1.123964    -1.206623       8.66
 O       0.107386     2.268392    -1.509210     224.23
 C       0.028580     2.892418    -2.842837      95.93
 H       0.978992     3.580738    -2.885934      22.22
 H       0.112509     2.397912    -3.923156      23.00
 H      -1.033003     3.223005    -3.008302      24.10
 C      -0.316332     0.468033     0.205663       1.07
 O       0.764383     0.814027     0.992690     176.56
 C      -1.250936    -0.681341     0.474392      40.50
 H      -0.978562    -1.270058     1.454909      17.83
 C      -2.262516    -0.647246    -1.719956      45.78
 C      -2.994995    -1.303269    -2.842916      51.96
 H      -2.690750    -0.799969    -3.812895      24.58
 O      -3.055117    -2.850112    -2.748297     163.96
 H      -2.023470    -3.205310    -2.378267      24.18
 C      -4.519075    -1.068869    -2.740198      93.48
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 H      -4.922717    -1.147870    -1.708005      26.21
 O      -4.713974     0.286224    -3.172299     256.95
 H      -4.635952     0.980881    -2.385024      24.47
 C      -5.498766    -1.953015    -3.653211     106.10
 O      -5.570107    -3.420400    -3.421920     189.54
 H      -4.586725    -3.659393    -2.927887      25.31
 H      -5.380840    -1.754690    -4.773574      28.85
 H      -6.440266    -1.576100    -3.320835      29.79
55
name = lig-ACN-frame_465
 C       4.382545     1.734106    -0.205948      62.64
 H       3.896533     2.739474    -0.463530      19.08
 C       4.587425    -0.166346     1.178926      43.26
 H       4.274182    -0.799790     1.975888      11.95
 C       5.645593    -0.650216     0.418670      13.91
 O       6.449287    -1.709738     0.726996     310.60
 C       5.739978    -3.081207     0.693726     103.92
 H       6.494170    -3.759859     0.721348      23.36
 H       5.284387    -3.059521    -0.278930      29.02
 H       5.015029    -3.293980     1.588635      24.79
 C       6.091621     0.040213    -0.690695      22.18
 O       7.116223    -0.368924    -1.502212     212.38
 H       7.689757    -1.020813    -0.857836      21.03
 C       5.488272     1.268200    -0.995083      60.91
 H       5.424099     1.748794    -2.031958      19.29
 C       3.833078     0.956289     0.804849      36.53
 C       2.803560     1.665499     1.851096      93.22
 H       3.233447     2.479937     2.133934      25.32
 O       2.638126     0.901353     3.143819     298.70
 H       2.122421     0.025818     3.188215      21.20
 C       1.438985     2.105151     1.326128      75.50
 H       1.570075     2.534364     0.414099      19.24
 C       0.554734     3.104344     2.122013     100.64
 O       1.113568     4.560736     2.284760     197.89
 H       1.263843     4.902520     1.219368      25.13
 H       0.399687     3.015574     3.234371      22.89
 H      -0.477901     3.231391     1.845905      23.67
 C      -2.070131    -1.234770    -0.502860      71.24
 H      -2.495960    -2.251062    -0.453304      15.02
 C      -1.483942     0.445178    -2.113364      82.92
 H      -1.645088     0.936572    -3.062823      14.68
 C      -0.575915     1.136477    -1.122081      16.78
 O       0.113567     2.283100    -1.503553     247.85
 C       0.007203     2.859651    -2.765992      85.45
 H       0.747141     3.714391    -2.719218      22.05
 H       0.331329     1.896069    -3.325793      21.20
 H      -0.868077     3.567664    -2.983102      23.60
 C      -0.408323     0.570619     0.058011      28.79
 O       0.704376     0.781333     1.007488     187.74
 C      -1.150359    -0.573205     0.522572      54.81
 H      -1.137817    -1.034523     1.550096      18.26
 C      -2.106231    -0.733617    -1.729963       2.82
 C      -3.082310    -1.346865    -2.740516      83.99
 H      -2.671569    -1.129206    -3.787129      21.67
 O      -3.013388    -2.757326    -2.791764     312.08
 H      -2.199641    -3.108540    -2.537196      29.39
 C      -4.558920    -1.108290    -2.739608      92.12
 H      -4.839482    -1.392488    -1.668237      27.58
 O      -4.679576     0.288577    -3.149569     244.26
 H      -4.877563     0.858689    -2.159186      21.68
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 C      -5.492662    -1.972514    -3.633224     112.23
 O      -5.562053    -3.366684    -3.374997     198.88
 H      -4.473859    -3.599655    -3.321803      24.92
 H      -5.313318    -1.727735    -4.728346      29.39
 H      -6.474401    -1.570112    -3.433305      29.69
55
name = lig-ACN-frame_466
 C       4.321018     1.751197    -0.311519      64.68
 H       3.901134     2.751090    -0.610874      20.48
 C       4.680644    -0.178703     1.256224      35.64
 H       4.613080    -0.699425     2.216674      15.74
 C       5.702094    -0.638579     0.397724       3.63
 O       6.380906    -1.828437     0.768175     298.64
 C       5.801865    -3.106027     0.698750     104.93
 H       6.554955    -3.753988     0.810402      20.59
 H       5.221850    -3.344273    -0.228067      29.45
 H       4.981264    -3.278245     1.524817      24.86
 C       6.038934     0.089703    -0.765393      12.02
 O       7.083170    -0.310120    -1.513712     165.76
 H       7.667885    -0.998856    -1.204961      26.39
 C       5.397634     1.324823    -1.072183      56.78
 H       5.902720     1.814256    -2.059895      18.62
 C       3.851815     0.982451     0.862915      54.29
 C       2.811176     1.605473     1.927159     106.31
 H       3.177981     2.453903     2.205762      26.00
 O       2.593052     0.861235     3.156583     356.66
 H       2.185525     0.158905     2.827055      26.41
 C       1.388749     2.042729     1.187228      59.98
 H       1.635671     2.485243     0.301573      19.04
 C       0.529610     3.223559     2.162681      98.92
 O       1.061893     4.472448     2.221682     229.42
 H       1.426243     4.894362     1.156255      22.50
 H       0.588833     2.575449     3.123712      22.60
 H      -0.386683     3.154611     1.644039      24.38
 C      -1.980028    -1.237454    -0.374029      61.40
 H      -2.452435    -2.084108     0.009895      19.25
 C      -1.448294     0.539736    -2.185027      48.34
 H      -1.499435     0.859964    -3.206315      15.57
 C      -0.685638     1.139594    -1.269980      16.43
 O       0.122456     2.305152    -1.332450     218.68
 C       0.067552     2.859391    -2.785271     109.95
 H       0.824677     3.567694    -2.925837      23.93
 H       0.191150     2.257036    -3.789218      24.41
 H      -1.067731     2.979896    -2.951750      25.08
 C      -0.392895     0.574568     0.184776      20.74
 O       0.607880     0.812894     1.036750     176.74
 C      -1.154277    -0.537839     0.467908      37.61
 H      -0.894273    -0.728945     1.482127      16.06
 C      -2.107918    -0.760940    -1.842780      64.27
 C      -3.037298    -1.437822    -2.863413      46.42
 H      -2.839696    -0.844633    -3.841699      24.80
 O      -2.906651    -2.868672    -2.787505     275.84
 H      -2.039042    -2.972430    -2.933559      29.11
 C      -4.634339    -1.066315    -2.654581      85.70
 H      -5.045905    -1.086221    -1.586578      26.60
 O      -4.740745     0.284859    -3.112262     262.40
 H      -4.601011     1.012431    -2.200355      18.61
 C      -5.531500    -1.897773    -3.650960     108.31
 O      -5.514441    -3.336427    -3.320869     240.66
 H      -4.686529    -3.652057    -3.497508      35.13
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 H      -5.070811    -1.805495    -4.660502      31.28
 H      -6.585416    -1.620833    -3.694515      30.14
55
name = lig-ACN-frame_467
 C       4.196293     1.714898    -0.298823      58.00
 H       3.560681     2.581517    -0.499658      20.21
 C       4.652700    -0.098061     1.297621      37.15
 H       4.387824    -0.445349     2.329289      18.77
 C       5.657443    -0.680756     0.427769       5.00
 O       6.412735    -1.833673     0.776571     302.12
 C       5.777212    -3.194543     0.714863     109.05
 H       6.547543    -3.842077     0.902551      22.55
 H       5.345827    -3.422188    -0.310661      27.74
 H       5.082508    -3.262621     1.618453      26.22
 C       6.018727     0.125023    -0.777213      11.56
 O       7.081065    -0.253268    -1.631298     164.31
 H       7.625815    -0.748980    -1.041577      25.23
 C       5.316011     1.298794    -1.160048      48.04
 H       5.887554     2.163184    -1.773827      26.27
 C       3.962080     1.057001     0.979707      13.67
 C       2.778579     1.615270     1.899567     100.91
 H       3.158988     2.429452     2.265470      21.23
 O       2.561204     0.843363     3.069635     384.88
 H       2.053395     0.094968     3.137880      25.90
 C       1.412253     2.080657     1.180123      65.58
 H       1.603465     2.418668     0.179813      15.76
 C       0.548866     3.015015     2.030641      96.79
 O       1.049720     4.452987     2.175417     237.14
 H       1.795086     4.545484     1.344136      24.40
 H       0.444292     2.810758     3.199914      20.90
 H      -0.476355     3.115411     1.802427      23.49
 C      -1.955366    -1.211107    -0.472508      65.54
 H      -2.552448    -1.931061    -0.125047      18.30
 C      -1.476063     0.424747    -2.194944      59.04
 H      -1.507822     0.790406    -3.212826      17.94
 C      -0.572028     1.194970    -1.108355       5.96
 O       0.123857     2.344265    -1.403979     248.31
 C       0.073205     2.847846    -2.767113      83.06
 H       0.548259     3.725067    -2.713455      24.88
 H       0.566551     1.948746    -3.255191      21.75
 H      -0.981204     3.335640    -2.999236      23.56
 C      -0.448291     0.605564     0.053181      18.45
 O       0.557418     0.919922     1.099195     220.46
 C      -1.158731    -0.558253     0.537181      30.49
 H      -1.090529    -1.155129     1.335894      17.00
 C      -2.145523    -0.707244    -1.798483      27.22
 C      -3.086341    -1.431172    -2.877870      28.54
 H      -2.825115    -1.247094    -3.990609      23.40
 O      -2.743704    -3.028222    -2.816634     158.34
 H      -1.772769    -3.223178    -3.248214      22.39
 C      -4.630582    -1.034703    -2.652824      98.74
 H      -4.823243    -1.305734    -1.541316      23.60
 O      -4.845268     0.324005    -3.114259     262.13
 H      -4.382435     0.935631    -2.379138      22.91
 C      -5.485956    -1.894294    -3.642902     113.70
 O      -5.517337    -3.294312    -3.283891     251.71
 H      -4.607678    -3.486686    -3.260212      33.81
 H      -5.108921    -1.682327    -4.649586      31.41
 H      -6.512451    -1.464753    -3.641151      29.63
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name = lig-ACN-frame_468
 C       4.148884     1.670836    -0.259371      53.51
 H       3.615003     2.492269    -0.652528      22.43
 C       4.680194    -0.065674     1.336023      29.85
 H       4.473947    -0.779258     2.198410      14.07
 C       5.581069    -0.642678     0.424238      39.79
 O       6.434693    -1.763587     0.731974     287.91
 C       5.770014    -3.199115     0.776483      86.50
 H       6.665808    -3.872937     0.838451      24.17
 H       5.294376    -3.283582    -0.278326      26.23
 H       4.923713    -3.413652     1.448187      27.75
 C       5.982693     0.109352    -0.761284      10.69
 O       7.038280    -0.214855    -1.645793     214.98
 H       7.875890    -0.737429    -1.309266      21.86
 C       5.194976     1.280241    -1.037741      52.74
 H       5.234897     1.770291    -2.124609      19.50
 C       3.913245     1.142290     0.974777      37.15
 C       2.777572     1.682621     1.850056     113.17
 H       3.030144     2.543883     2.195516      20.63
 O       2.552092     0.849513     3.038420     333.87
 H       1.929259     0.167040     2.562354      19.88
 C       1.454070     2.083172     1.183977      67.85
 H       1.636726     2.685763     0.239444      14.94
 C       0.570081     2.997673     2.007355      92.25
 O       1.057520     4.378199     2.110585     307.09
 H       1.725695     4.609730     1.492873      31.20
 H       0.593367     2.386177     3.030234      20.62
 H      -0.317336     2.911078     1.431521      24.40
 C      -2.082197    -1.221605    -0.535363      46.96
 H      -2.372066    -2.177142    -0.435615      16.82
 C      -1.348661     0.481843    -2.061004      52.35
 H      -1.504692     0.909701    -3.056469      20.75
 C      -0.615955     1.143135    -1.231591      14.76
 O       0.102191     2.380930    -1.442726     264.76
 C       0.105953     2.906826    -2.757604     129.17
 H       0.718889     3.682036    -2.785717      24.93
 H       0.622570     2.279891    -3.599297      24.77
 H      -0.881650     2.806630    -3.322303      23.85
 C      -0.375855     0.540020     0.228948       6.48
 O       0.475462     0.936650     1.124766     186.08
 C      -1.185782    -0.623837     0.428318      35.05
 H      -0.987801    -0.847080     1.376373      17.12
 C      -2.193113    -0.696444    -1.816591      70.45
 C      -2.998325    -1.501036    -2.798588      60.06
 H      -2.642157    -1.105736    -3.834145      23.84
 O      -2.690539    -3.063149    -2.844915     167.68
 H      -1.546720    -2.853551    -3.019191      18.52
 C      -4.530080    -1.123784    -2.762564     103.26
 H      -4.939167    -1.185555    -1.697045      25.30
 O      -4.909568     0.297096    -3.153752     246.29
 H      -4.844026     0.857798    -2.311890      24.42
 C      -5.468525    -1.881786    -3.603968     115.29
 O      -5.508276    -3.254468    -3.271162     219.90
 H      -4.591101    -3.556424    -2.778086      29.06
 H      -5.206180    -1.799076    -4.643445      30.42
 H      -6.516725    -1.524811    -3.426958      29.01
55
name = lig-ACN-frame_469
 C       4.110868     1.736090    -0.263140      31.84
 H       3.496719     2.522501    -0.603390      18.38
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 C       4.630416    -0.057127     1.321674      25.24
 H       4.457491    -0.482257     2.367023      14.04
 C       5.655518    -0.600236     0.413579      45.39
 O       6.360843    -1.745131     0.713680     338.21
 C       5.791214    -3.024039     0.734616     113.60
 H       6.714186    -3.766975     0.973292      22.01
 H       5.221296    -3.398778    -0.211159      27.58
 H       5.275910    -3.066380     1.666213      29.21
 C       5.964600     0.115958    -0.740258       9.96
 O       6.945895    -0.174832    -1.625454     145.05
 H       7.468888    -0.891238    -0.987008      20.15
 C       5.149567     1.169732    -1.079661      74.31
 H       5.285609     1.367411    -2.193965      23.25
 C       3.835760     1.039628     1.034932      52.13
 C       2.804357     1.754126     1.907417     115.68
 H       3.194235     2.578917     2.218752      26.55
 O       2.538186     0.932334     2.968912     335.38
 H       2.059005    -0.089315     2.886343      13.83
 C       1.435101     2.072420     1.122263      52.14
 H       1.593047     2.247008    -0.032243      11.96
 C       0.592996     3.041072     1.986065     106.44
 O       1.067471     4.332057     2.110034     349.24
 H       1.356242     4.482609     1.325473      35.02
 H       0.320054     2.746417     3.081167      22.00
 H      -0.433221     3.158624     1.622660      22.70
 C      -2.096825    -1.271919    -0.461073      84.84
 H      -2.526669    -2.172715    -0.095056      10.74
 C      -1.428227     0.479554    -2.155169     133.87
 H      -1.428054     0.963369    -3.144549       6.22
 C      -0.494303     1.136824    -1.078107      64.68
 O       0.052041     2.339330    -1.414607     226.59
 C       0.174398     2.931893    -2.932394      71.75
 H       0.379364     3.897794    -2.749242      25.40
 H       0.865715     2.237595    -3.403745      24.10
 H      -0.903728     3.177177    -3.163971      23.36
 C      -0.420638     0.500709     0.070110      11.82
 O       0.506629     0.888506     1.198883     226.13
 C      -1.198250    -0.662057     0.392338      -0.42
 H      -1.169994    -1.238050     1.240690      13.86
 C      -2.131346    -0.695128    -1.797992      60.42
 C      -2.886315    -1.476990    -2.903591      37.92
 H      -2.568812    -1.105671    -3.946969      28.91
 O      -2.674044    -2.901867    -2.840726     252.04
 H      -1.711114    -3.300837    -2.522282      20.44
 C      -4.485195    -1.122083    -2.771124      70.75
 H      -4.692573    -1.343414    -1.680795      25.95
 O      -4.883418     0.208347    -3.212829     241.84
 H      -4.879022     0.665031    -2.463185      29.20
 C      -5.491247    -1.945889    -3.656441     103.63
 O      -5.521219    -3.344676    -3.233059     199.62
 H      -4.527975    -3.437837    -2.681332      26.20
 H      -5.348645    -1.780063    -4.704481      31.02
 H      -6.484896    -1.453787    -3.426292      30.23
55
name = lig-ACN-frame_470
 C       4.117074     1.674904    -0.269295      56.35
 H       3.585525     2.571703    -0.528574      20.50
 C       4.591570    -0.092797     1.322108      42.25
 H       4.536730    -0.543219     2.340844      20.40
 C       5.596357    -0.530349     0.525617       1.80
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 O       6.414297    -1.647785     0.667770     297.64
 C       5.775261    -2.943932     0.818484      85.72
 H       6.759240    -3.706199     0.740140      21.69
 H       5.098459    -3.145805    -0.131919      26.55
 H       5.131462    -3.114036     1.632755      27.61
 C       5.870313     0.144920    -0.703669       3.32
 O       6.925341    -0.226684    -1.569768     211.53
 H       7.547592    -0.975086    -1.404852      23.19
 C       5.018794     1.192892    -1.213692      73.71
 H       5.355291     1.921740    -1.932402      29.05
 C       3.840763     1.079932     0.882410      35.87
 C       2.779517     1.704850     1.850718     106.96
 H       3.092494     2.555354     2.196156      24.74
 O       2.510265     1.002008     3.107083     332.14
 H       2.036705     0.122940     2.719382      19.95
 C       1.329776     2.006370     1.173295      68.68
 H       1.475598     2.485777     0.085674      14.58
 C       0.468945     3.038021     1.934227      89.05
 O       1.155283     4.430563     2.117467     236.16
 H       1.382402     4.994874     1.261310      27.28
 H       0.622486     2.538922     2.922275      22.83
 H      -0.553248     3.006265     1.525675      24.33
 C      -2.062760    -1.256766    -0.531943      76.29
 H      -2.924175    -1.957672    -0.284647      18.76
 C      -1.419438     0.465395    -2.083061      17.65
 H      -1.529277     0.712967    -3.138151      14.79
 C      -0.592262     1.105937    -1.291217      10.60
 O       0.074966     2.394465    -1.463370     259.60
 C       0.133834     2.922064    -2.845695     137.71
 H       0.719853     3.796353    -2.759869      24.96
 H       0.854540     2.400752    -3.481379      28.54
 H      -0.660386     2.756289    -3.572619      27.87
 C      -0.319681     0.441228     0.186533      15.06
 O       0.522774     0.755798     1.186089     190.40
 C      -1.145219    -0.685967     0.499508      37.32
 H      -0.837577    -1.048154     1.500497      16.02
 C      -2.079914    -0.745723    -1.838946      22.52
 C      -2.848855    -1.342708    -3.033601      56.58
 H      -2.462852    -1.032362    -4.052793      23.81
 O      -2.736559    -2.783247    -2.814485     302.07
 H      -1.920961    -2.805365    -2.464480      31.83
 C      -4.458393    -1.184520    -2.853622      88.87
 H      -4.666940    -1.324698    -1.776854      26.64
 O      -4.795731     0.149841    -3.232475     315.86
 H      -4.378051     0.814158    -2.681284      27.31
 C      -5.479203    -2.062080    -3.632470     109.73
 O      -5.530176    -3.449290    -3.207621     227.67
 H      -4.587235    -3.664921    -3.005527      30.92
 H      -5.204517    -2.063157    -4.668204      30.00
 H      -6.540511    -1.679625    -3.498710      29.18
55
name = lig-ACN-frame_471
 C       4.034034     1.713671    -0.398667      80.67
 H       3.599414     2.725185    -0.574940      22.31
 C       4.501605    -0.066719     1.385965      10.26
 H       4.129585    -0.606529     2.242632      12.09
 C       5.581262    -0.481311     0.445305      23.94
 O       6.514705    -1.544601     0.702921     305.22
 C       5.733500    -2.902705     0.853175      82.76
 H       6.579709    -3.868666     0.808032      22.86
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 H       5.004398    -2.917316    -0.030046      25.07
 H       5.339635    -2.930817     1.839933      26.63
 C       5.820258     0.149656    -0.830670      17.14
 O       6.898647    -0.262025    -1.542155     225.13
 H       7.257842    -0.782930    -0.863865      25.80
 C       5.075429     1.272198    -1.236775      32.27
 H       5.367393     1.730020    -2.131650      18.86
 C       3.752730     1.029063     0.980517      47.18
 C       2.650240     1.693553     1.819635     100.54
 H       3.014551     2.609183     1.914653      22.93
 O       2.490265     1.034995     3.202972     307.77
 H       1.931778     0.302862     3.166071      26.25
 C       1.304281     1.983906     1.185810      59.26
 H       1.486544     2.264768     0.048673      11.28
 C       0.503856     3.112115     1.982712      98.88
 O       1.147232     4.427699     2.147314     179.87
 H       1.488404     4.640090     1.009311      22.32
 H       0.187269     2.925639     2.991617      23.30
 H      -0.477255     3.342306     1.481282      21.89
 C      -2.018214    -1.221778    -0.529004      83.19
 H      -2.642987    -2.218732    -0.196182      14.94
 C      -1.358757     0.464243    -2.191884     128.57
 H      -1.488511     1.053349    -3.086413      14.11
 C      -0.511050     1.118566    -1.121352      31.26
 O       0.024395     2.373807    -1.508560     263.90
 C       0.218261     2.842841    -2.826474      89.39
 H       0.298681     3.922567    -2.773713      23.43
 H       0.907763     2.203306    -3.292900      25.09
 H      -0.806682     2.975859    -3.171775      22.23
 C      -0.345720     0.424661     0.066629      29.24
 O       0.607510     0.698360     1.135927     223.81
 C      -1.114369    -0.691033     0.459207       9.64
 H      -1.249858    -1.134394     1.537443      13.70
 C      -2.091369    -0.731463    -1.884443      57.78
 C      -2.967832    -1.341395    -2.990388      55.50
 H      -2.615045    -0.844945    -3.923601      28.90
 O      -2.771688    -2.746111    -2.833607     293.87
 H      -1.884024    -3.060775    -2.798015      28.45
 C      -4.420314    -1.176321    -2.906720      94.43
 H      -4.617027    -1.371249    -1.858663      28.27
 O      -4.749972     0.174702    -3.290165     270.23
 H      -4.042148     0.716817    -2.578640      23.14
 C      -5.383634    -2.212430    -3.665612     111.54
 O      -5.519858    -3.572391    -3.170327     247.63
 H      -4.722279    -3.892320    -3.305179      35.95
 H      -5.218155    -2.161174    -4.736132      31.27
 H      -6.386422    -1.709340    -3.511859      30.44
55
name = lig-ACN-frame_472
 C       3.956825     1.707738    -0.322871      58.69
 H       3.279855     2.544729    -0.708325      19.50
 C       4.483794    -0.059333     1.257460      40.79
 H       4.393853    -0.571848     2.182843      20.00
 C       5.523256    -0.468418     0.415072     -13.59
 O       6.496684    -1.497162     0.768238     304.37
 C       5.770561    -2.740768     0.899210      83.50
 H       6.602250    -3.687410     0.684214      21.90
 H       4.846563    -2.923239     0.272650      27.49
 H       5.392041    -2.790394     1.948548      23.77
 C       5.773159     0.157508    -0.830086      15.69
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 O       6.900606    -0.319812    -1.523292     232.26
 H       7.573890    -0.867804    -1.040551      25.54
 C       5.094377     1.350494    -1.206381      54.85
 H       5.151442     1.657344    -2.193717      19.11
 C       3.635096     1.079322     0.858175      19.37
 C       2.600660     1.693168     1.943258     109.59
 H       2.950848     2.557211     2.287635      20.50
 O       2.483165     1.125505     3.207217     340.69
 H       1.903159     0.407168     3.053495      26.23
 C       1.280620     1.981729     1.211228      68.91
 H       1.496808     2.514760     0.227669      14.67
 C       0.445977     3.175920     2.011141     105.59
 O       1.172172     4.379399     2.126817     210.20
 H       1.913696     4.596655     1.211842      23.23
 H       0.187126     2.776423     2.923462      24.58
 H      -0.416583     3.272043     1.287939      22.23
 C      -2.025637    -1.262770    -0.625877      94.88
 H      -2.472707    -2.418214    -0.297334      16.96
 C      -1.274526     0.491676    -2.144167      34.91
 H      -1.367325     0.925754    -3.121862      22.65
 C      -0.512892     1.077839    -1.202815      18.66
 O       0.020079     2.335753    -1.330818     214.69
 C       0.176170     2.796867    -2.877926     107.46
 H       0.768138     3.728496    -2.654798      23.27
 H       0.915115     2.346159    -3.485705      27.30
 H      -0.676811     2.696405    -3.490952      24.65
 C      -0.299359     0.443982     0.112723      12.02
 O       0.632214     0.707894     1.040548     218.55
 C      -1.151176    -0.649758     0.329054      41.02
 H      -0.970864    -1.170023     1.432511      14.26
 C      -2.089839    -0.590256    -1.872831     102.97
 C      -2.917904    -1.402813    -2.934710      54.83
 H      -2.684943    -1.174068    -3.968704      26.25
 O      -2.779372    -2.871722    -2.904315     197.59
 H      -1.749786    -2.869458    -3.348413      23.03
 C      -4.518202    -1.197775    -2.832795      97.81
 H      -4.942699    -1.274469    -1.858343      29.02
 O      -4.727042     0.197454    -3.361497     247.12
 H      -4.579164     0.903575    -2.487380      20.17
 C      -5.314826    -2.242116    -3.725119     102.45
 O      -5.488260    -3.645881    -3.163801     120.54
 H      -4.528392    -4.146832    -3.274442      29.23
 H      -5.027530    -2.321172    -4.784979      32.03
 H      -6.374132    -1.906366    -3.646278      31.12
55
name = lig-ACN-frame_473
 C       3.928314     1.727244    -0.366122      57.21
 H       3.220847     2.530565    -0.780618      17.26
 C       4.420611    -0.002010     1.156405      45.79
 H       4.393839    -0.306428     2.172727      18.91
 C       5.526778    -0.458956     0.402733      19.68
 O       6.375799    -1.391395     0.801337     308.13
 C       5.803007    -2.673057     1.030360      93.25
 H       6.690673    -3.502338     0.681023      22.49
 H       5.012058    -2.716655     0.255373      28.03
 H       5.504614    -2.983434     2.096206      24.55
 C       5.883988     0.191510    -0.780262       4.27
 O       6.875421    -0.311646    -1.598847     157.69
 H       7.468226    -0.949304    -0.962820      19.30
 C       4.973369     1.303633    -1.130961      73.98
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 H       5.251564     2.002368    -1.891188      31.25
 C       3.599795     1.039693     0.890903      39.11
 C       2.678891     1.809352     1.938074      90.36
 H       3.145947     2.709435     2.013789      25.59
 O       2.432801     1.100266     3.227385     290.20
 H       2.016313     0.102422     3.054302      19.77
 C       1.277582     2.126090     1.273784      81.33
 H       1.558528     2.506059     0.298261      17.84
 C       0.366680     3.058908     1.913005     109.77
 O       1.242036     4.362994     2.128504     181.72
 H       1.784353     4.492600     1.221039      27.46
 H       0.216024     2.887011     2.914976      25.30
 H      -0.662123     3.319883     1.541259      23.71
 C      -1.993396    -1.264793    -0.682425      61.78
 H      -2.793566    -2.308330    -0.665429      17.43
 C      -1.323263     0.481047    -2.193556      75.91
 H      -1.273579     0.845842    -3.221524      15.83
 C      -0.463249     1.087499    -1.176454      20.66
 O       0.085484     2.367277    -1.357211     253.35
 C       0.222091     2.761335    -2.778782      95.65
 H       0.553569     3.887932    -2.886062      22.83
 H       0.729836     1.894530    -3.050300      26.07
 H      -0.734866     2.911216    -3.201122      26.22
 C      -0.360134     0.468163     0.044923      23.48
 O       0.659565     0.769669     1.011063     195.52
 C      -1.130724    -0.695852     0.352692      62.45
 H      -0.733260    -1.352515     1.307898      17.76
 C      -2.151072    -0.707065    -1.927137      37.77
 C      -2.990968    -1.443898    -2.940864      46.23
 H      -2.721567    -0.948387    -3.850442      24.78
 O      -2.708669    -2.985687    -2.977232     161.17
 H      -1.622134    -3.261252    -3.214931      21.93
 C      -4.538717    -1.194978    -2.819204      94.59
 H      -4.798506    -1.221378    -1.786641      28.58
 O      -4.752371     0.165002    -3.385737     233.75
 H      -5.109623     0.628368    -2.671988      29.07
 C      -5.327696    -2.274927    -3.720723     111.97
 O      -5.420972    -3.624225    -3.208319     133.36
 H      -4.291775    -3.827809    -2.964112      26.21
 H      -4.616413    -2.233627    -4.587883      32.95
 H      -6.305406    -1.956637    -4.075817      31.51
55
name = lig-ACN-frame_474
 C       3.824227     1.707866    -0.365001      77.56
 H       3.522297     2.757653    -0.634496      23.53
 C       4.380605     0.007575     1.281120      21.99
 H       4.204286    -0.612418     2.163855      17.33
 C       5.466961    -0.338473     0.384740      17.69
 O       6.372429    -1.341204     0.917933     304.18
 C       5.827976    -2.735741     1.099246      98.49
 H       6.764328    -3.488155     0.876200      23.96
 H       4.928790    -3.071406     0.579288      28.16
 H       5.611611    -2.696590     2.265244      25.69
 C       5.856508     0.294247    -0.815735       1.59
 O       6.846404    -0.241293    -1.673156     162.01
 H       7.420253    -0.863234    -1.125796      19.18
 C       5.014759     1.274893    -1.153785      73.19
 H       5.332899     1.812462    -2.093759      23.60
 C       3.557922     1.143240     0.876629      26.87
 C       2.665622     1.814871     1.896639      96.53
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 H       3.149997     2.619444     2.384726      22.49
 O       2.420506     1.083238     3.192633     232.64
 H       2.097591     0.090472     2.777764      20.13
 C       1.329073     2.135843     1.145646      85.33
 H       1.466829     2.618604     0.254307      20.84
 C       0.395617     3.139630     2.025238     114.61
 O       1.223722     4.293821     2.081992     290.64
 H       1.352244     4.587338     1.294711      35.85
 H       0.088011     2.680637     2.947590      25.68
 H      -0.435064     3.294431     1.306067      25.24
 C      -1.998168    -1.288972    -0.609183      72.48
 H      -2.513229    -2.336288     0.046191      16.04
 C      -1.384011     0.431943    -2.258292      15.76
 H      -1.537467     0.942591    -3.227836      16.12
 C      -0.570379     1.122872    -1.252225      -1.01
 O       0.147086     2.381240    -1.374338     268.55
 C       0.230584     2.727115    -2.712396     128.59
 H       1.012346     3.617384    -2.732734      23.50
 H       0.717347     2.249616    -3.464049      29.59
 H      -0.768199     2.873886    -3.118479      26.51
 C      -0.346396     0.466271     0.078699      12.35
 O       0.652947     0.836410     1.008443     168.13
 C      -1.068390    -0.801080     0.330916      57.65
 H      -1.094585    -1.366413     1.375365      16.12
 C      -2.078855    -0.752956    -1.979750      67.15
 C      -3.015356    -1.489032    -3.044303      58.00
 H      -2.854410    -1.250426    -4.069500      27.68
 O      -2.678473    -2.986996    -3.042642     223.59
 H      -1.714433    -2.923563    -2.695764      23.59
 C      -4.552530    -1.240103    -2.830368     107.18
 H      -4.841558    -1.304048    -1.785115      30.54
 O      -4.816147     0.065191    -3.384601     266.57
 H      -5.108976     0.675532    -2.720151      30.07
 C      -5.252789    -2.234845    -3.765704     116.74
 O      -5.317761    -3.564078    -3.223461     192.00
 H      -4.389449    -3.680119    -2.707952      27.89
 H      -4.716159    -2.312013    -4.764095      31.34
 H      -6.260689    -1.882183    -3.976331      30.85
55
name = lig-ACN-frame_475
 C       3.924555     1.749226    -0.402231      59.20
 H       3.286989     2.616316    -0.622801      22.02
 C       4.364138     0.065248     1.275377      52.06
 H       4.154637    -0.531838     2.210961      20.30
 C       5.467955    -0.367287     0.551036       1.32
 O       6.360228    -1.346782     0.956009     293.96
 C       5.911522    -2.718747     1.247786      89.18
 H       6.821736    -3.434325     1.029965      22.83
 H       5.166610    -2.885915     0.451620      28.57
 H       5.534470    -2.989119     2.358372      22.59
 C       5.765659     0.231272    -0.789842       3.14
 O       6.798684    -0.125738    -1.692868     239.95
 H       7.467125    -0.617010    -1.294712      30.24
 C       4.951317     1.424989    -1.269571      44.82
 H       4.876575     1.809212    -2.376702      19.33
 C       3.634048     1.157808     0.907521      26.60
 C       2.583628     1.784821     1.899429      97.30
 H       2.904625     2.833448     2.044057      21.11
 O       2.409106     1.024851     3.049625     331.41
 H       1.852569     0.226550     2.938808      24.52
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 C       1.275438     2.148891     1.152236      89.71
 H       1.537852     2.536891     0.272953      21.17
 C       0.466444     3.093258     1.938468     110.00
 O       1.203170     4.343504     2.122219     231.79
 H       1.142900     4.805090     1.228791      28.35
 H       0.328703     2.840233     3.045772      23.91
 H      -0.560756     3.318057     1.565313      24.52
 C      -1.963199    -1.319450    -0.637291      73.43
 H      -2.709851    -2.441314    -0.517112      17.89
 C      -1.406480     0.452308    -2.219439     115.64
 H      -1.647025     0.889503    -3.212776      17.39
 C      -0.656172     1.056776    -1.193735      14.34
 O       0.130999     2.205624    -1.376093     205.17
 C       0.270980     2.847967    -2.841348      83.78
 H       0.846677     3.833297    -2.555489      22.86
 H       0.642813     2.012423    -3.264568      26.64
 H      -0.623734     3.311418    -3.276573      24.80
 C      -0.315142     0.436741     0.021835      10.43
 O       0.586763     0.861519     0.976667     218.00
 C      -0.980774    -0.722038     0.336037      88.78
 H      -0.818628    -1.040261     1.394042      17.70
 C      -2.058627    -0.847302    -1.926295      72.58
 C      -2.937610    -1.522213    -3.072443      69.87
 H      -2.716980    -0.970749    -3.980095      26.73
 O      -2.686032    -2.900612    -3.041392     311.69
 H      -1.867716    -3.081797    -2.788069      31.97
 C      -4.489742    -1.304655    -2.899230      94.54
 H      -4.916784    -1.581047    -1.894671      28.40
 O      -4.913712     0.015019    -3.378483     234.13
 H      -4.492346     0.662017    -2.531765      24.39
 C      -5.233835    -2.213998    -3.819827     120.68
 O      -5.239331    -3.531582    -3.192641     201.51
 H      -4.424876    -3.679678    -2.929674      34.17
 H      -4.872547    -2.074255    -4.893165      31.43
 H      -6.281269    -1.947925    -3.762399      31.23
55
name = lig-ACN-frame_476
 C       3.936396     1.901144    -0.352108      55.95
 H       3.201249     2.468871    -0.847087      22.17
 C       4.406962     0.064516     1.316684      44.03
 H       4.152068    -0.154123     2.408488      19.37
 C       5.537309    -0.376718     0.473580       2.02
 O       6.415705    -1.359643     1.013169     306.40
 C       5.995152    -2.685706     1.288100     104.27
 H       6.950191    -3.278414     1.226768      22.01
 H       5.259071    -3.133386     0.586275      28.60
 H       5.559803    -2.711769     2.389956      24.27
 C       5.668716     0.271617    -0.799022      10.86
 O       6.715685    -0.016800    -1.650511     186.54
 H       7.440787    -0.509811    -1.123878      24.10
 C       4.895378     1.311873    -1.225983      56.52
 H       5.264874     1.743701    -2.284144      22.68
 C       3.684589     1.235107     0.863654      29.13
 C       2.571930     1.783129     1.746413      98.65
 H       2.999575     2.671097     2.300469      22.38
 O       2.374187     0.949361     2.985836     307.47
 H       1.794850     0.370653     2.667052      27.58
 C       1.247593     2.065874     1.080273      93.00
 H       1.409261     2.532618     0.163641      22.65
 C       0.422284     3.116304     1.967247      88.35
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 O       1.179095     4.475548     2.162654      97.16
 H       1.313478     5.014717     1.097641      24.30
 H       0.481631     2.560453     3.007185      24.13
 H      -0.607275     3.240588     1.606726      25.03
 C      -1.822200    -1.379342    -0.632819      71.36
 H      -2.425310    -2.483701    -0.202016      19.62
 C      -1.487763     0.398655    -2.137947      31.63
 H      -1.432193     0.947395    -3.083685      19.32
 C      -0.609536     1.037804    -1.254610      16.52
 O       0.079808     2.170775    -1.525541     261.39
 C       0.277200     2.896156    -2.781297     111.68
 H       1.105853     3.571295    -2.635526      25.74
 H       0.721018     2.397782    -3.617889      27.51
 H      -0.742260     3.194907    -3.215840      24.75
 C      -0.348132     0.411669    -0.030572      24.05
 O       0.510215     0.852580     0.971701     213.02
 C      -1.069217    -0.760689     0.325269      53.27
 H      -0.794446    -1.360512     1.128172      20.87
 C      -2.070845    -0.767792    -1.906414      62.05
 C      -2.848550    -1.388264    -2.975621      72.51
 H      -2.497107    -1.038123    -3.943726      27.81
 O      -2.697838    -2.907930    -3.044458     223.24
 H      -1.753072    -2.997128    -3.287140      28.24
 C      -4.426261    -1.293202    -2.997688      91.78
 H      -4.571782    -1.482455    -1.884830      26.63
 O      -4.947381     0.019006    -3.270224     225.71
 H      -4.254151     0.788375    -2.869549      25.52
 C      -5.327897    -2.278146    -3.821054     122.00
 O      -5.183266    -3.551916    -3.219201     188.85
 H      -4.277480    -3.663400    -3.288012      32.63
 H      -4.949905    -2.435207    -4.877172      30.14
 H      -6.322769    -1.836239    -3.881232      31.27
55
name = lig-ACN-frame_477
 C       3.887867     1.922352    -0.401356      57.59
 H       3.526738     2.895256    -0.550220      22.78
 C       4.521292     0.207226     1.273772      52.55
 H       4.487987    -0.403149     2.222101      19.48
 C       5.452308    -0.388509     0.490752      22.47
 O       6.516889    -1.267374     0.946827     286.79
 C       6.086310    -2.694749     1.340158     104.48
 H       6.937659    -3.286534     1.516633      25.29
 H       5.436281    -3.163720     0.535315      27.94
 H       5.501702    -2.616398     2.311686      27.36
 C       5.707680     0.217907    -0.728763       9.43
 O       6.719975     0.022567    -1.613826     149.21
 H       7.435669    -0.648689    -1.177349      20.61
 C       4.827169     1.294280    -1.155102      49.89
 H       5.214198     1.841781    -2.130643      23.43
 C       3.693803     1.252549     0.844073      36.57
 C       2.633985     1.753382     1.761395      86.58
 H       2.889390     2.847240     2.119464      23.28
 O       2.306817     0.903793     2.878460     262.19
 H       2.023962    -0.075064     2.684813      23.16
 C       1.216464     2.135673     0.986175      54.07
 H       1.232432     2.502156    -0.084330      18.58
 C       0.477685     3.211597     2.031061      97.22
 O       1.076353     4.500988     2.167337     141.58
 H       1.538756     4.686642     1.091592      24.83
 H       0.236844     2.841385     3.148857      24.66
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 H      -0.496161     3.399041     1.558651      25.69
 C      -1.827819    -1.487811    -0.649296      52.79
 H      -2.138666    -2.702003    -0.391569      18.10
 C      -1.480057     0.506120    -2.199915      64.25
 H      -1.768350     0.771608    -3.194998      20.06
 C      -0.534057     1.020997    -1.330229       3.77
 O       0.118656     2.225001    -1.603244     236.50
 C       0.232293     2.901042    -2.820251     108.43
 H       0.716693     3.776632    -2.460438      25.58
 H       0.695756     2.259374    -3.592101      26.53
 H      -0.686371     3.503647    -3.091673      25.81
 C      -0.401028     0.406208     0.034714      14.77
 O       0.449837     0.812606     1.013289     161.77
 C      -1.041179    -0.850597     0.318872      51.11
 H      -0.879179    -1.186689     1.288558      18.78
 C      -2.142962    -0.795658    -1.815501      79.73
 C      -2.902732    -1.421701    -3.062799      48.46
 H      -2.565251    -0.881978    -3.999573      26.51
 O      -2.660194    -2.881987    -3.058389     182.63
 H      -1.554861    -3.093961    -3.275024      23.47
 C      -4.428713    -1.216462    -2.930899      94.17
 H      -4.813214    -1.618988    -1.935435      27.46
 O      -4.944447     0.086304    -3.208059     280.99
 H      -4.449447     0.717030    -2.806798      32.80
 C      -5.292325    -2.291376    -3.833331     102.19
 O      -5.188391    -3.630891    -3.253253      98.06
 H      -4.108605    -3.866986    -3.322527      27.77
 H      -5.071976    -2.174401    -4.913274      30.98
 H      -6.361606    -2.120974    -3.633564      30.62
55
name = lig-ACN-frame_478
 C       3.882762     1.855124    -0.357101      60.62
 H       3.523371     2.842178    -0.609206      22.42
 C       4.539534     0.245073     1.332510      51.65
 H       4.208873     0.035509     2.377208      20.94
 C       5.559725    -0.416717     0.466635      23.10
 O       6.564754    -1.253502     0.857798     314.82
 C       6.173380    -2.598574     1.378028     125.79
 H       7.056519    -3.023559     1.648709      25.65
 H       5.797865    -3.060634     0.425506      28.06
 H       5.449693    -2.639586     2.175561      30.86
 C       5.692034     0.260513    -0.810779      11.34
 O       6.809908    -0.021184    -1.593124     176.43
 H       7.417224    -0.678344    -1.204214      21.63
 C       4.904047     1.355991    -1.215699      42.86
 H       5.101301     1.787796    -2.235074      20.35
 C       3.654724     1.272758     0.897838      24.75
 C       2.503810     1.774557     1.762823      98.95
 H       3.025062     2.640168     2.388243      21.86
 O       2.267073     0.898195     2.830166     225.19
 H       2.210869    -0.101440     2.293264      20.53
 C       1.187808     2.176101     1.164787      84.24
 H       1.399099     2.628628     0.077160      19.46
 C       0.411677     3.209861     1.941113     106.45
 O       1.062207     4.523515     2.124194     224.59
 H       1.611535     4.777465     1.328091      29.18
 H       0.444181     2.704089     3.046087      23.85
 H      -0.640526     3.287947     1.625278      25.92
 C      -1.867518    -1.548102    -0.673547      55.78
 H      -2.326230    -2.637843    -0.774344      17.31
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 C      -1.542860     0.416764    -2.214633      37.75
 H      -1.694453     1.088098    -3.012209      14.83
 C      -0.548449     1.013436    -1.322914       9.95
 O       0.184460     2.217637    -1.503973     198.23
 C       0.157773     3.047702    -2.924367      93.24
 H       0.881948     3.749383    -2.930296      25.46
 H       0.559024     2.246098    -3.673612      26.01
 H      -0.881309     3.068023    -3.343452      25.47
 C      -0.422564     0.417920    -0.043665      13.98
 O       0.436021     0.884215     1.077510     154.72
 C      -0.977347    -0.868437     0.317792      46.98
 H      -0.774797    -1.278931     1.310596      19.50
 C      -2.149097    -0.781935    -1.946095      18.58
 C      -2.984881    -1.459916    -3.014867      75.97
 H      -2.776891    -0.991532    -4.037550      25.54
 O      -2.623940    -2.847852    -3.120165     198.28
 H      -1.532594    -2.884399    -2.705404      21.32
 C      -4.557922    -1.312674    -2.857893      82.81
 H      -4.702586    -1.398964    -1.725223      27.01
 O      -4.919808     0.159579    -3.185534     228.20
 H      -4.822290     0.531312    -2.341745      28.69
 C      -5.269733    -2.254846    -3.732722     119.67
 O      -5.179873    -3.703154    -3.345133     109.45
 H      -4.043391    -3.823115    -3.103582      23.98
 H      -5.026709    -2.202397    -4.786783      29.95
 H      -6.341614    -1.932922    -3.669513      29.68
55
name = lig-ACN-frame_479
 C       3.937143     1.842676    -0.391746      51.31
 H       3.052596     2.305673    -0.854300      19.64
 C       4.531742     0.179434     1.379323      45.60
 H       4.692186    -0.231285     2.372500      20.20
 C       5.519588    -0.200704     0.474589      -6.32
 O       6.599667    -1.244257     0.810374     265.70
 C       6.281390    -2.505991     1.338431     108.14
 H       7.076010    -2.835816     1.854518      24.73
 H       5.950899    -3.400868     0.727581      27.91
 H       5.503127    -2.327459     2.029988      30.05
 C       5.785577     0.284193    -0.877775       0.16
 O       6.872834    -0.080580    -1.614603     202.94
 H       7.431020    -0.555163    -1.034522      24.75
 C       4.975345     1.383218    -1.259074      60.30
 H       5.186857     1.843665    -2.189527      23.18
 C       3.646766     1.255348     0.878732      19.50
 C       2.521839     1.826909     1.876968      77.90
 H       2.768887     2.923477     2.360745      22.20
 O       2.248269     0.840659     2.885456     256.16
 H       1.695223    -0.049605     2.577585      17.75
 C       1.159607     2.193113     1.163494      76.03
 H       1.393883     2.682104     0.064930      18.46
 C       0.330808     3.188444     1.971169      96.60
 O       1.065770     4.533412     2.062280     239.40
 H       1.297568     4.688383     1.258088      34.92
 H       0.146995     2.879838     3.128061      24.01
 H      -0.644984     3.323517     1.428528      24.77
 C      -1.844604    -1.418322    -0.760755      52.57
 H      -2.263848    -2.235284    -0.229508      19.69
 C      -1.484828     0.467140    -2.198360      50.49
 H      -1.825772     0.816493    -3.140464      19.53
 C      -0.627458     1.048364    -1.288166      -3.29
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 O       0.209740     2.289853    -1.547023     188.87
 C       0.069187     2.909187    -2.928260      98.11
 H       0.426066     3.855237    -2.755058      25.39
 H       0.602782     2.270757    -3.783176      23.94
 H      -1.000548     3.320160    -2.992576      24.72
 C      -0.314323     0.376978     0.021209      15.19
 O       0.356675     0.969990     1.056787     175.89
 C      -0.999886    -0.859433     0.158697      58.72
 H      -0.686276    -1.571686     0.997268      18.91
 C      -2.120585    -0.849598    -1.978797      65.38
 C      -3.070891    -1.419990    -2.995933      50.16
 H      -2.913878    -0.890951    -4.008267      26.55
 O      -2.637423    -2.864250    -3.146868     182.78
 H      -1.573900    -2.966533    -2.920368      23.29
 C      -4.568753    -1.280805    -2.702607      96.18
 H      -4.992640    -1.551829    -1.678090      27.03
 O      -4.864610     0.101494    -3.121210     183.54
 H      -5.255071     0.716112    -2.304099      24.45
 C      -5.375623    -2.305596    -3.680623     113.62
 O      -5.164986    -3.701126    -3.422673     194.32
 H      -4.159752    -3.721416    -3.039600      27.20
 H      -4.846899    -2.053600    -4.569585      32.47
 H      -6.485292    -2.117696    -3.814738      30.18
55
name = lig-ACN-frame_480
 C       3.890794     1.733968    -0.444017      66.01
 H       3.223506     2.535702    -0.920271      21.50
 C       4.557262     0.214930     1.301558      53.83
 H       4.241415    -0.326089     2.174076      21.58
 C       5.639948    -0.197690     0.448398      18.58
 O       6.575815    -1.090011     0.704943     269.12
 C       6.304744    -2.470435     1.435148     100.32
 H       7.139660    -2.628690     2.031268      26.15
 H       6.228918    -3.090838     0.513554      26.48
 H       5.466165    -2.503808     2.031101      31.05
 C       5.886074     0.398166    -0.809996      12.77
 O       6.876043    -0.121018    -1.653543     137.71
 H       7.587891    -0.655365    -1.243924      18.10
 C       5.005722     1.400877    -1.264340      60.82
 H       5.147227     1.796521    -2.194726      23.12
 C       3.680945     1.238511     0.936508      24.81
 C       2.531984     1.728356     1.882202      68.04
 H       3.052513     2.705752     2.464264      20.82
 O       2.249085     0.858688     3.031135     279.18
 H       1.685808     0.278469     2.621364      27.36
 C       1.157313     2.188042     1.126111      68.83
 H       1.231056     2.654205     0.009558      18.18
 C       0.292877     3.287071     1.995349      98.71
 O       1.018923     4.467281     1.996859     216.40
 H       1.181836     4.829110     1.026178      26.55
 H      -0.056891     2.992433     3.082337      24.56
 H      -0.678411     3.498311     1.434118      24.57
 C      -1.903383    -1.394057    -0.779727      46.78
 H      -2.378055    -2.257958    -0.697185      20.61
 C      -1.457104     0.465764    -2.258293      59.49
 H      -1.450962     1.026504    -3.171341      15.88
 C      -0.554614     1.160444    -1.244067      20.23
 O       0.129909     2.241550    -1.615059     240.78
 C      -0.072184     2.856690    -2.798669     106.65
 H       0.573854     3.694134    -2.884553      24.75
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 H       0.371059     2.198445    -3.751481      25.09
 H      -1.146008     2.806221    -3.194520      25.38
 C      -0.282199     0.460582    -0.090760      25.25
 O       0.288020     0.997683     1.084085     171.36
 C      -0.836777    -0.810369     0.153264      50.03
 H      -0.693791    -1.327380     1.229507      17.48
 C      -2.097262    -0.724519    -1.992977      13.46
 C      -3.042111    -1.453059    -2.973936      53.20
 H      -3.022364    -0.904061    -3.981314      25.82
 O      -2.722082    -2.871811    -3.163679     246.76
 H      -1.810512    -2.951509    -3.291952      30.15
 C      -4.653678    -1.313835    -2.611663      87.77
 H      -4.668757    -1.422176    -1.488609      27.00
 O      -4.867791     0.005999    -3.064452     218.51
 H      -4.858340     0.720856    -2.150012      21.93
 C      -5.388854    -2.279487    -3.700036     111.69
 O      -5.165751    -3.694739    -3.432851     203.70
 H      -4.249948    -3.774074    -3.390130      31.78
 H      -5.229959    -2.002839    -4.713006      31.32
 H      -6.512967    -2.164872    -3.521164      28.91
55
name = lig-ACN-frame_481
 C       3.816915     1.722113    -0.431707      71.22
 H       3.324867     2.737746    -0.622688      21.67
 C       4.575394     0.204139     1.238203      55.83
 H       4.375165    -0.390765     2.114868      21.22
 C       5.664866    -0.141900     0.437795      13.30
 O       6.622334    -1.131093     0.774162     266.83
 C       6.343306    -2.331017     1.438483     117.94
 H       7.204629    -2.473586     2.116554      25.90
 H       6.440568    -3.195163     0.774240      28.34
 H       5.403577    -2.409986     1.912511      31.82
 C       5.982682     0.504644    -0.799340      -8.93
 O       6.821811    -0.087972    -1.728515      55.85
 H       7.504888    -0.598762    -1.093451      15.24
 C       4.995996     1.381830    -1.218921      57.27
 H       5.044182     1.693712    -2.241250      23.05
 C       3.675880     1.219090     0.813084      29.50
 C       2.524870     1.681270     1.843160      66.02
 H       3.016527     2.763615     2.294398      21.54
 O       2.245745     0.942385     3.102614     267.45
 H       2.011667     0.044080     3.029806      26.59
 C       1.123041     2.170036     1.257056      86.34
 H       1.528369     2.542313     0.225108      20.78
 C       0.281506     3.262701     1.856550     106.21
 O       1.019863     4.524322     1.979763     132.41
 H       1.357328     4.923629     0.878360      22.30
 H       0.342691     2.950642     2.954741      24.58
 H      -0.781585     3.249757     1.471658      25.01
 C      -1.800464    -1.341227    -0.726120      63.10
 H      -2.104585    -2.268430    -0.562577      21.95
 C      -1.367250     0.543415    -2.319927      56.70
 H      -1.524732     0.890977    -3.333865      21.25
 C      -0.583108     1.082050    -1.406761       9.90
 O       0.103946     2.255679    -1.537384     207.29
 C      -0.190869     2.842773    -2.946653      80.92
 H       0.264095     3.883397    -2.923996      23.97
 H       0.253984     2.012091    -3.660811      23.58
 H      -1.294487     3.179093    -2.943173      25.16
 C      -0.309451     0.461934    -0.043976      10.50
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 O       0.270379     1.011450     1.117944     165.62
 C      -0.848132    -0.806673     0.132388      55.55
 H      -0.602299    -1.168390     1.261079      17.15
 C      -2.123162    -0.662877    -1.989286      51.05
 C      -3.057742    -1.448838    -2.988375      73.22
 H      -2.895279    -1.008970    -4.031755      25.45
 O      -2.770425    -2.880025    -3.160996     245.62
 H      -1.878463    -3.024353    -3.218129      31.76
 C      -4.521159    -1.418576    -2.716334     111.80
 H      -4.945191    -1.738175    -1.756758      27.26
 O      -4.958493     0.004864    -2.973085     254.45
 H      -4.338553     0.523711    -2.347399      26.67
 C      -5.458040    -2.250247    -3.556428     114.72
 O      -5.189176    -3.689395    -3.451788     212.20
 H      -4.339922    -3.709259    -3.754437      33.71
 H      -5.256940    -1.909302    -4.546635      31.23
 H      -6.524839    -2.008142    -3.277995      29.63
55
name = lig-ACN-frame_482
 C       3.863053     1.861952    -0.454726      52.08
 H       3.042153     2.457925    -0.986914      20.92
 C       4.575685     0.146050     1.226978      50.01
 H       4.623922    -0.268956     2.252925      20.70
 C       5.736815    -0.119971     0.458720       6.01
 O       6.693223    -1.084898     0.813561     275.32
 C       6.378886    -2.342977     1.528472      82.84
 H       6.926643    -2.354104     2.525072      22.92
 H       6.419190    -3.184593     0.867289      25.74
 H       5.385892    -2.181860     1.896170      29.19
 C       5.915272     0.481631    -0.818563      -5.64
 O       6.786144     0.004513    -1.765110     154.48
 H       7.618144    -0.598636    -1.436669      18.60
 C       4.908439     1.441664    -1.242419      48.63
 H       5.081503     1.874118    -2.298006      22.36
 C       3.543545     1.094843     0.841244      17.15
 C       2.484530     1.714748     1.885148      81.84
 H       2.959088     2.852018     2.188898      22.51
 O       2.288176     1.027018     3.136192     227.74
 H       2.497570     0.026698     2.755100      22.52
 C       1.212991     2.089804     1.149722      83.72
 H       1.336543     2.480469     0.123872      20.50
 C       0.394196     3.227829     1.911850      96.51
 O       0.989178     4.612624     1.933093     161.57
 H       1.572163     4.736393     0.872645      22.14
 H      -0.024655     3.034464     2.923026      25.08
 H      -0.506336     3.380335     1.234755      23.88
 C      -1.730985    -1.331961    -0.808215      61.44
 H      -2.193861    -2.226853    -0.451892      19.73
 C      -1.493914     0.385226    -2.446423      63.76
 H      -1.699344     0.900097    -3.395487      20.61
 C      -0.455286     1.066025    -1.304730      -1.67
 O       0.077133     2.400992    -1.594612     202.55
 C      -0.261494     2.886500    -2.951249      79.35
 H       0.527222     3.793054    -3.067890      22.56
 H      -0.113869     2.361971    -4.000747      24.61
 H      -1.402381     3.002323    -3.003174      25.24
 C      -0.328079     0.517806    -0.025737      24.67
 O       0.241215     0.983114     1.113553     176.98
 C      -0.903836    -0.785484     0.226885      41.22
 H      -0.626579    -1.619723     1.001036      18.36
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 C      -2.116722    -0.761933    -1.973118      22.69
 C      -2.977534    -1.438669    -3.069258      51.61
 H      -2.795797    -0.850061    -4.021323      25.64
 O      -2.724981    -2.903730    -3.133739     241.20
 H      -1.683155    -3.056797    -2.874849      24.88
 C      -4.511751    -1.371440    -2.708023      96.19
 H      -4.325768    -1.695107    -1.690211      26.43
 O      -5.029734    -0.055558    -2.890981     303.24
 H      -4.712928     0.552669    -2.326792      31.49
 C      -5.505622    -2.263725    -3.547128     113.96
 O      -5.281453    -3.665420    -3.490168     187.79
 H      -4.214177    -3.846657    -3.687285      26.90
 H      -5.674292    -1.950858    -4.561332      29.76
 H      -6.490703    -2.136039    -3.039936      28.62
55
name = lig-ACN-frame_483
 C       3.792556     1.810851    -0.363130      55.89
 H       3.023022     2.465338    -0.840229      20.52
 C       4.555070     0.183780     1.258489      47.81
 H       4.386201    -0.180288     2.318598      20.30
 C       5.735702    -0.168588     0.462862      -6.54
 O       6.789354    -0.986054     0.847154     232.59
 C       6.287869    -2.316538     1.689167      84.94
 H       7.119017    -2.496344     2.511465      22.79
 H       6.650335    -3.014044     0.998127      26.83
 H       5.204514    -2.471725     1.849802      27.22
 C       5.758846     0.421664    -0.872275      19.55
 O       6.778375     0.128396    -1.812234     192.55
 H       7.396638    -0.431541    -1.252619      23.37
 C       4.925359     1.470197    -1.231476      33.28
 H       5.173437     1.946732    -2.323672      20.47
 C       3.569346     1.096797     0.836573      29.53
 C       2.550416     1.739025     1.811348      76.94
 H       3.093081     2.844525     2.157772      21.95
 O       2.378608     1.073313     3.101716     196.40
 H       2.191421    -0.053518     3.012852      20.35
 C       1.199794     2.102211     1.105313      88.66
 H       1.429781     2.376051     0.138688      22.41
 C       0.439912     3.306810     1.857689     106.31
 O       0.961658     4.614319     1.921310     229.96
 H       1.628915     4.823146     1.019998      23.15
 H       0.191982     2.947628     2.855702      25.52
 H      -0.512723     3.316816     1.229630      24.57
 C      -1.782140    -1.476173    -0.738699      72.78
 H      -2.230421    -2.527784    -0.683717      19.66
 C      -1.359929     0.408824    -2.225626      36.35
 H      -1.578820     0.891917    -3.192716      20.40
 C      -0.549493     1.104627    -1.446743      17.63
 O       0.024074     2.401099    -1.703230     237.57
 C      -0.323504     2.986199    -2.950870      92.79
 H       0.336774     4.018358    -3.183544      22.33
 H      -0.079542     2.067346    -3.546334      24.91
 H      -1.366635     3.462797    -2.982072      26.02
 C      -0.347147     0.507524    -0.055633       4.74
 O       0.286582     0.981662     1.141581     154.69
 C      -0.969673    -0.823530     0.174797      29.30
 H      -0.637880    -1.158172     1.197212      18.46
 C      -2.043874    -0.826834    -2.135300      38.31
 C      -2.934915    -1.497651    -3.141680      81.02
 H      -2.722721    -1.199618    -4.196755      26.25
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 O      -2.625428    -2.899489    -3.116566     206.73
 H      -1.507770    -3.070442    -2.808474      22.57
 C      -4.482004    -1.352960    -2.669504     100.96
 H      -4.716712    -1.617530    -1.680298      29.20
 O      -5.119474    -0.079516    -2.856042     286.15
 H      -5.060847     0.347142    -2.024142      29.47
 C      -5.570694    -2.266941    -3.499661     105.73
 O      -5.362570    -3.706308    -3.547723     176.83
 H      -4.218016    -3.802075    -3.343631      25.22
 H      -5.662693    -1.785678    -4.463742      30.64
 H      -6.479476    -2.113851    -2.920792      29.79
55
name = lig-ACN-frame_484
 C       3.752768     1.729643    -0.443094      68.90
 H       3.346641     2.708400    -0.429105      22.22
 C       4.597612     0.203107     1.297661      52.14
 H       4.567449    -0.355981     2.302234      18.87
 C       5.594270    -0.168744     0.431437      -0.30
 O       6.727647    -0.984261     0.996033     280.98
 C       6.377595    -2.226091     1.660897      79.62
 H       6.733437    -2.156410     2.812058      22.98
 H       6.511651    -3.145482     1.146338      24.90
 H       5.250293    -2.085422     1.897821      26.20
 C       5.739090     0.368136    -0.887544      22.37
 O       6.768583     0.213250    -1.772840     239.52
 H       7.461059    -0.319365    -1.480306      27.36
 C       4.841485     1.463508    -1.147478      37.37
 H       4.963063     2.088743    -2.149235      21.54
 C       3.672146     1.162019     0.854616      23.30
 C       2.599543     1.717207     1.753222      78.86
 H       3.086100     2.872132     2.083424      21.07
 O       2.470543     1.085300     3.046123     249.13
 H       1.770237     0.395534     2.816331      25.38
 C       1.222511     2.194958     1.110508      83.44
 H       1.383486     2.464711     0.161843      22.39
 C       0.366581     3.276289     1.751195     112.77
 O       0.986254     4.633714     1.933556     245.93
 H       1.345785     4.986668     1.057010      26.92
 H       0.400414     2.974812     2.784619      25.43
 H      -0.721109     3.320059     1.531331      24.90
 C      -1.834921    -1.533730    -0.841323      56.98
 H      -2.106502    -2.604562    -0.394558      17.08
 C      -1.355051     0.434703    -2.294429      82.14
 H      -1.521917     0.893280    -3.284865      17.73
 C      -0.553862     1.178136    -1.261709      17.86
 O      -0.034453     2.357443    -1.695799     190.31
 C      -0.379053     3.045353    -3.028490      69.96
 H       0.649061     3.743819    -2.991989      21.09
 H      -0.401775     2.668384    -4.074624      24.25
 H      -1.450431     3.425290    -2.898347      24.57
 C      -0.377521     0.469959    -0.105294      17.90
 O       0.312964     0.953964     1.084991     170.06
 C      -1.012256    -0.781302     0.095337      49.78
 H      -1.045831    -1.129400     1.082675      19.21
 C      -1.872655    -0.904550    -1.991596      44.07
 C      -2.946066    -1.545924    -3.131748      43.71
 H      -2.960148    -1.019752    -4.101809      26.53
 O      -2.557945    -2.975266    -3.109255     200.42
 H      -1.425724    -3.029346    -3.113848      21.63
 C      -4.548294    -1.471548    -2.688795      83.47
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 H      -4.366357    -1.772016    -1.713752      28.47
 O      -5.166605    -0.069072    -2.851644     202.49
 H      -4.785050     0.649269    -2.098588      22.36
 C      -5.579467    -2.250862    -3.417010     117.47
 O      -5.393255    -3.730658    -3.590031     234.64
 H      -4.431462    -3.923871    -3.302840      32.31
 H      -5.591259    -1.920826    -4.459962      29.42
 H      -6.568416    -2.068466    -3.036818      29.45
55
name = lig-ACN-frame_485
 C       3.748391     1.794279    -0.374037      47.02
 H       3.190503     2.572675    -0.800894      23.11
 C       4.587715     0.211154     1.304412      38.36
 H       4.504908    -0.067904     2.415194      19.80
 C       5.655138    -0.282716     0.430323      25.07
 O       6.617048    -0.922150     1.034740     276.71
 C       6.318738    -2.120789     1.709143     103.79
 H       7.021436    -2.251559     2.686530      22.16
 H       6.763779    -2.933336     1.086795      24.06
 H       5.184608    -2.370351     1.844177      26.85
 C       5.758889     0.405867    -0.825315       2.61
 O       6.797735     0.249477    -1.743236     156.35
 H       7.474383    -0.350237    -1.291894      23.96
 C       4.833077     1.367227    -1.261711      37.38
 H       5.227757     1.970804    -2.136770      22.32
 C       3.627933     1.165615     0.913080      26.64
 C       2.602589     1.866031     1.794393      80.45
 H       3.055976     3.041132     2.094780      22.19
 O       2.479555     1.083212     2.971663     270.16
 H       1.940529     0.387254     2.879903      29.92
 C       1.219118     2.160849     0.974441      70.20
 H       1.406668     2.504589     0.019820      21.94
 C       0.347049     3.282471     1.884759     105.55
 O       0.955433     4.597827     1.943171     289.59
 H       1.161684     4.829864     1.129102      33.58
 H       0.037894     2.961577     2.870529      25.96
 H      -0.486796     3.354224     1.167263      24.32
 C      -1.703334    -1.482329    -0.792373      34.71
 H      -2.396892    -2.452568    -0.683325      17.00
 C      -1.384591     0.346472    -2.311062      51.16
 H      -1.544846     0.829377    -3.293206      21.53
 C      -0.689023     1.108551    -1.388257       7.84
 O      -0.041989     2.370101    -1.700053     230.19
 C      -0.408866     3.095416    -2.992294      86.09
 H       0.410545     4.020619    -3.122389      22.55
 H      -0.405852     2.320981    -3.742815      25.11
 H      -1.329352     3.748066    -2.810859      24.97
 C      -0.359963     0.488503    -0.017623       6.06
 O       0.354508     0.937914     1.022970     162.30
 C      -1.063634    -0.796168     0.213330      51.13
 H      -0.864811    -1.274220     1.066351      23.05
 C      -1.994104    -0.849932    -2.183378      44.20
 C      -2.912141    -1.559820    -3.032088      74.96
 H      -2.698482    -1.184343    -4.029948      26.24
 O      -2.570811    -3.031308    -3.165436     240.74
 H      -1.586297    -3.099558    -3.176270      29.31
 C      -4.498170    -1.463039    -2.594993      92.35
 H      -4.754799    -1.661099    -1.615345      27.17
 O      -5.114173    -0.146804    -2.844403     224.97
 H      -4.405676     0.571191    -2.275702      22.27
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 C      -5.579508    -2.347391    -3.507589     110.65
 O      -5.411428    -3.733530    -3.572896     282.00
 H      -4.560654    -3.888710    -3.493225      35.96
 H      -5.659946    -1.784937    -4.469295      29.75
 H      -6.481030    -2.205961    -2.937004      29.16
55
name = lig-ACN-frame_486
 C       3.864421     1.814208    -0.434905      68.43
 H       3.005385     2.299320    -0.768398      22.89
 C       4.490394     0.268860     1.281234      54.12
 H       4.605744    -0.105273     2.316376      20.60
 C       5.513451    -0.139691     0.471193       9.75
 O       6.663268    -0.876625     1.039566     234.76
 C       6.320542    -2.208913     1.759759      85.75
 H       6.909031    -2.172529     2.752533      23.68
 H       6.653658    -2.994537     0.999841      23.43
 H       5.188266    -2.416178     2.055715      25.84
 C       5.803208     0.418779    -0.809613       3.71
 O       6.877871     0.220926    -1.667592     173.87
 H       7.688148    -0.369233    -1.271909      21.93
 C       4.811772     1.307771    -1.270698      55.56
 H       4.895260     1.690906    -2.251235      23.23
 C       3.608986     1.276260     0.819825      30.97
 C       2.553466     1.900006     1.740833      73.91
 H       2.904899     3.040859     2.225816      22.43
 O       2.408397     1.122327     2.997602     209.95
 H       2.458383     0.194399     2.523949      24.03
 C       1.179669     2.190188     1.105799      95.62
 H       1.258488     2.588100     0.086726      21.91
 C       0.313903     3.225583     1.812024     110.38
 O       0.908002     4.518952     2.014880     245.39
 H       1.421119     4.872630     1.187601      26.96
 H       0.018504     2.845457     2.819891      25.72
 H      -0.675724     3.335194     1.339530      25.82
 C      -1.741420    -1.392637    -0.853368      61.91
 H      -2.086650    -2.439339    -0.529161      20.31
 C      -1.432736     0.407194    -2.453261      67.21
 H      -1.634577     0.881878    -3.448318      20.78
 C      -0.677274     1.067465    -1.429235      -1.80
 O      -0.081547     2.356409    -1.684489     246.91
 C      -0.424104     3.095708    -2.829660     109.59
 H       0.551746     3.556516    -3.267342      24.50
 H      -0.524962     2.426791    -3.723153      24.56
 H      -1.479400     3.501512    -2.906097      26.35
 C      -0.484437     0.474110    -0.110113      -1.83
 O       0.463825     0.966431     0.986875     139.43
 C      -0.978007    -0.766314     0.320203      29.31
 H      -0.666335    -1.183490     1.177620      20.89
 C      -2.055253    -0.906552    -2.025032      61.81
 C      -2.991360    -1.668156    -3.083173      46.22
 H      -3.095776    -1.133825    -4.018571      27.49
 O      -2.638169    -3.049487    -3.210584     314.16
 H      -1.845195    -3.188371    -2.922732      34.44
 C      -4.510508    -1.515774    -2.606714     104.65
 H      -4.460856    -1.869330    -1.630272      28.34
 O      -4.962795    -0.215320    -2.863875     257.71
 H      -4.729668     0.568709    -2.096742      22.64
 C      -5.530934    -2.316586    -3.488384     105.59
 O      -5.382974    -3.801529    -3.564266     202.65
 H      -4.386882    -3.967700    -3.831186      29.17
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 H      -5.541878    -1.968615    -4.561777      29.59
 H      -6.515536    -2.104325    -3.097416      29.54
55
name = lig-ACN-frame_487
 C       3.775154     1.818759    -0.554743      57.31
 H       3.381235     2.703026    -1.054293      21.81
 C       4.414536     0.350697     1.290397      57.02
 H       4.170932    -0.060005     2.238768      22.92
 C       5.621594    -0.047995     0.528923       0.62
 O       6.618964    -0.909371     1.067559     298.93
 C       6.366549    -2.208001     1.732658      76.54
 H       6.964291    -2.354257     2.647760      23.52
 H       6.473375    -3.261119     1.175479      24.23
 H       5.260321    -2.036307     1.939183      25.99
 C       5.843676     0.408565    -0.822494      13.65
 O       6.966376     0.154146    -1.555802     188.07
 H       7.572361    -0.430508    -1.004862      23.73
 C       4.867327     1.313482    -1.353054      52.75
 H       4.921286     1.525740    -2.324849      24.33
 C       3.590791     1.401924     0.831721      18.99
 C       2.477761     1.887653     1.766133      75.96
 H       3.052275     3.042495     1.990116      21.11
 O       2.336320     1.157412     2.963338     173.39
 H       2.524921     0.030700     2.952365      19.41
 C       1.136067     2.257797     1.083034      83.99
 H       1.555211     2.800550     0.188911      23.44
 C       0.190539     3.167082     1.836876     106.92
 O       0.887406     4.464562     2.091685     146.28
 H       1.424564     4.871794     1.099814      23.25
 H       0.132542     2.786815     2.885246      24.71
 H      -0.740087     3.215221     1.260849      25.36
 C      -1.800373    -1.475852    -0.604134      49.75
 H      -2.006305    -2.505284    -0.438338      22.08
 C      -1.533937     0.387199    -2.426266      38.95
 H      -1.726941     0.746601    -3.478485      17.76
 C      -0.656067     1.073979    -1.459525      22.28
 O      -0.119853     2.281153    -1.575265     226.20
 C      -0.444346     3.000745    -2.845339     110.98
 H       0.269124     3.859445    -2.743549      24.78
 H      -0.550220     2.401467    -3.761732      26.04
 H      -1.230692     3.655130    -2.453750      25.56
 C      -0.419806     0.585062    -0.105259      27.87
 O       0.470226     0.907560     0.881230     160.25
 C      -0.928234    -0.712309     0.133069      45.24
 H      -0.735047    -1.170945     1.083353      19.90
 C      -2.071742    -0.808589    -2.091271      16.80
 C      -3.074782    -1.668250    -3.105705      77.47
 H      -2.835377    -1.243653    -4.051576      26.15
 O      -2.712972    -3.091954    -3.245502     255.50
 H      -1.757788    -3.135620    -2.927949      27.32
 C      -4.489002    -1.680412    -2.636089     109.40
 H      -4.672994    -1.877761    -1.614692      30.20
 O      -4.837968    -0.175549    -2.861232     239.00
 H      -4.792196     0.154649    -2.007458      30.08
 C      -5.486054    -2.386769    -3.505810     108.62
 O      -5.333593    -3.829549    -3.531828     147.12
 H      -4.306783    -4.061678    -4.010969      26.79
 H      -5.241263    -1.880227    -4.497958      30.16
 H      -6.519847    -2.183704    -3.217575      29.83
55
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name = lig-ACN-frame_488
 C       3.769165     1.844856    -0.642607      47.21
 H       3.114779     2.729954    -0.947106      23.14
 C       4.503598     0.421411     1.227484      48.45
 H       4.330186    -0.009732     2.162326      22.64
 C       5.660769    -0.036490     0.619524      11.50
 O       6.623254    -0.935321     1.057333     266.37
 C       6.275107    -2.155132     1.724528     109.42
 H       7.070541    -2.243680     2.392408      25.70
 H       6.476687    -2.813731     0.745537      24.02
 H       5.362570    -2.404474     2.325180      26.05
 C       5.840063     0.438700    -0.736822       1.82
 O       7.031210     0.065142    -1.434873     178.89
 H       7.575752    -0.515424    -0.966614      25.34
 C       4.907842     1.309311    -1.381262      69.24
 H       5.232979     1.745347    -2.235530      23.76
 C       3.563353     1.415000     0.705046      15.84
 C       2.463522     1.954556     1.754585      73.44
 H       2.644904     3.047751     2.398215      20.59
 O       2.273688     1.192755     2.990820     195.73
 H       1.873510     0.226543     2.604002      21.58
 C       1.137184     2.208741     0.978118      75.78
 H       1.122883     2.682227    -0.091320      20.02
 C       0.169786     3.167627     1.933435     100.76
 O       0.829148     4.411769     2.149552     130.12
 H       1.044530     4.656770     0.984106      23.02
 H      -0.313233     2.709600     2.878842      25.41
 H      -0.758597     3.414498     1.398460      25.95
 C      -1.883983    -1.425881    -0.779255      45.64
 H      -2.278424    -2.254761    -0.377008      23.61
 C      -1.553209     0.353842    -2.267219     133.38
 H      -1.746565     0.901786    -3.233936      21.25
 C      -0.728963     1.032290    -1.402923      12.44
 O      -0.098419     2.300664    -1.607294     258.75
 C      -0.455394     3.086684    -2.716918     136.02
 H       0.360979     3.674513    -3.030195      26.79
 H      -0.417137     2.415401    -3.637733      26.83
 H      -1.490467     3.359224    -2.854463      29.00
 C      -0.382223     0.503830    -0.198887      13.51
 O       0.525221     0.962922     0.771817     178.51
 C      -0.944215    -0.746057     0.103720      55.26
 H      -0.455263    -1.089027     1.088691      19.38
 C      -2.181690    -1.020886    -1.979921      73.98
 C      -2.954293    -1.663080    -3.042234      39.87
 H      -3.085149    -1.161735    -3.959344      30.34
 O      -2.702372    -3.127160    -3.229740     148.34
 H      -1.576966    -3.361153    -3.385456      22.66
 C      -4.514435    -1.579452    -2.631868      88.51
 H      -4.625274    -2.013496    -1.627394      28.55
 O      -4.782052    -0.215193    -2.829410     300.68
 H      -4.522428     0.388194    -2.199309      31.78
 C      -5.440531    -2.474418    -3.624160     105.68
 O      -5.295937    -3.879724    -3.519153     212.47
 H      -4.266874    -4.026410    -3.678679      28.43
 H      -5.486842    -2.172173    -4.733935      29.67
 H      -6.469856    -2.261578    -3.223033      29.65
55
name = lig-ACN-frame_489
 C       3.841718     1.843591    -0.638482      56.90
 H       3.056051     2.359012    -1.336385      21.89
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 C       4.528288     0.505820     1.283926      67.01
 H       4.381685     0.318341     2.317989      21.59
 C       5.612530    -0.013040     0.544874      21.44
 O       6.600819    -0.852820     1.081773     275.00
 C       6.283941    -2.202028     1.689145      96.73
 H       7.078981    -2.537030     2.235309      26.04
 H       5.929045    -3.185562     1.018038      25.14
 H       5.369166    -1.949279     2.230306      28.38
 C       5.933547     0.463468    -0.715314      11.86
 O       6.976562     0.045265    -1.352448     146.18
 H       7.649027    -0.524080    -0.845569      18.02
 C       4.978587     1.366052    -1.307698      40.59
 H       5.218966     1.753414    -2.293764      21.50
 C       3.600052     1.351767     0.680914      18.16
 C       2.467002     2.026451     1.640186      52.57
 H       3.019354     3.166246     1.799552      22.45
 O       2.183975     1.188399     2.924423     216.90
 H       1.663367     0.498209     2.618357      29.03
 C       1.019150     2.276513     1.010727      79.85
 H       1.347781     3.013555     0.110540      22.28
 C       0.113945     3.105420     1.874558     104.46
 O       0.785269     4.385747     2.195507     199.55
 H       1.029007     5.051281     1.427725      27.45
 H       0.187862     2.595452     2.939269      24.47
 H      -0.856749     3.189326     1.359138      26.00
 C      -1.887903    -1.500581    -0.687866      48.75
 H      -2.366886    -2.334908    -0.385186      21.77
 C      -1.642081     0.280384    -2.260429      71.17
 H      -1.977565     0.713302    -3.237495      24.97
 C      -0.757645     1.106284    -1.366041      15.13
 O      -0.103099     2.318972    -1.612733     222.25
 C      -0.467786     3.105369    -2.829675     114.92
 H       0.096976     3.926512    -2.619573      26.95
 H      -0.282029     2.512579    -3.768635      27.39
 H      -1.463570     3.488241    -2.599474      28.75
 C      -0.324792     0.348136    -0.182376      29.53
 O       0.561551     0.895963     0.695917     177.06
 C      -0.978120    -0.853607     0.164785      51.06
 H      -0.856203    -1.622419     1.099497      20.36
 C      -2.112527    -0.920385    -2.005481      20.19
 C      -3.003797    -1.766495    -3.030689      73.90
 H      -2.622959    -1.290888    -3.895326      27.13
 O      -2.637694    -3.133465    -3.201904     186.66
 H      -1.488557    -3.116314    -3.409302      23.39
 C      -4.461879    -1.598822    -2.724241      96.31
 H      -4.722205    -1.861060    -1.656810      26.22
 O      -4.853390    -0.186203    -2.827760     233.16
 H      -4.189902     0.266734    -2.124898      25.38
 C      -5.451815    -2.442702    -3.656003      95.79
 O      -5.222444    -3.967150    -3.508937     247.23
 H      -4.416272    -4.062750    -3.209018      35.06
 H      -5.228395    -2.152420    -4.744744      28.43
 H      -6.547631    -2.249987    -3.386513      27.41
55
name = lig-ACN-frame_490
 C       3.873258     1.740656    -0.614118      43.92
 H       3.095897     2.404149    -1.203705      20.93
 C       4.524443     0.566183     1.388497      47.82
 H       4.415818     0.277865     2.453164      22.27
 C       5.574275    -0.032153     0.604053       4.32
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 O       6.620442    -0.852969     1.120328     247.40
 C       6.187459    -2.163027     1.681889     105.69
 H       7.077982    -2.533175     2.100963      26.28
 H       5.744814    -2.806747     0.738003      24.13
 H       5.561141    -2.073929     2.572537      27.35
 C       5.888513     0.525418    -0.690142       1.36
 O       7.014310     0.043333    -1.430358     155.75
 H       7.541052    -0.494236    -0.667706      18.16
 C       5.110517     1.476677    -1.288894      61.85
 H       5.175290     1.582644    -2.435676      22.36
 C       3.538104     1.390645     0.714428      29.08
 C       2.424516     1.952756     1.538088      97.33
 H       2.867566     2.981972     2.177103      22.01
 O       2.153348     1.305209     2.756620     237.35
 H       2.003813     0.403542     2.516531      29.10
 C       1.132556     2.347576     0.916321      64.63
 H       1.041685     2.782269    -0.224668      18.13
 C       0.116234     3.066880     1.878811     100.69
 O       0.708202     4.388988     2.262989     264.92
 H       0.807347     4.738239     1.505957      35.97
 H      -0.053073     2.486530     2.921953      24.53
 H      -0.949399     3.171932     1.556325      25.94
 C      -1.895574    -1.601895    -0.631346      49.68
 H      -2.232437    -2.618433    -0.521668      22.84
 C      -1.622573     0.447782    -2.333989      68.38
 H      -1.818323     0.857094    -3.334950      19.28
 C      -0.775432     1.004998    -1.378808       5.24
 O      -0.153151     2.257105    -1.610010     194.29
 C      -0.499699     3.152934    -2.866272     111.39
 H       0.094922     3.981577    -2.772409      26.92
 H      -0.305887     2.907863    -3.942395      26.30
 H      -1.591974     3.297989    -2.854548      27.24
 C      -0.374564     0.336990    -0.174197       4.23
 O       0.636540     0.797328     0.703893      96.45
 C      -1.002008    -0.988192     0.248213      46.34
 H      -0.602489    -1.184942     1.417416      17.42
 C      -2.121585    -0.992570    -1.932152      36.84
 C      -2.929393    -1.708990    -3.099474      59.34
 H      -3.011794    -1.291336    -4.075889      28.01
 O      -2.535706    -3.156516    -3.126041     204.49
 H      -1.504652    -3.205072    -2.845248      24.03
 C      -4.537298    -1.658130    -2.782528      76.22
 H      -4.617075    -2.088010    -1.706324      27.73
 O      -4.937490    -0.182943    -2.872643     167.36
 H      -4.472878     0.440905    -1.997937      21.91
 C      -5.363511    -2.507931    -3.681708     114.94
 O      -5.211721    -3.931820    -3.486296     219.65
 H      -4.277414    -4.071427    -3.049680      28.71
 H      -5.126421    -2.202295    -4.764169      28.95
 H      -6.478120    -2.242339    -3.532167      28.09
55
name = lig-ACN-frame_491
 C       3.836344     1.766056    -0.625497      48.67
 H       3.106725     2.557131    -1.015828      20.53
 C       4.532029     0.548589     1.397910      68.58
 H       4.377135     0.198945     2.474898      22.17
 C       5.630213     0.062605     0.691271      10.63
 O       6.582506    -0.850896     1.184901     270.60
 C       6.132189    -2.094596     1.684513     108.83
 H       6.983521    -2.743337     1.636021      26.10
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 H       5.453332    -2.662275     0.816173      25.66
 H       5.496350    -2.132439     2.554035      27.37
 C       5.956769     0.477504    -0.666540       1.17
 O       6.989782     0.071872    -1.447951     159.32
 H       7.731963    -0.535542    -1.170955      21.26
 C       5.061668     1.490570    -1.266613      17.74
 H       5.375092     2.000695    -2.330354      23.34
 C       3.626454     1.377579     0.746185      19.12
 C       2.450930     2.074587     1.501218      75.20
 H       2.793731     3.293152     1.694201      23.82
 O       2.138591     1.287874     2.680742     164.41
 H       2.297135     0.217679     2.468323      22.40
 C       1.085117     2.192081     0.758347      77.96
 H       1.144172     2.785259    -0.305015      20.19
 C       0.148040     3.057272     1.917317      99.56
 O       0.586963     4.356795     2.306508     226.75
 H       0.941487     4.833416     1.481147      29.07
 H       0.044819     2.284305     2.786723      24.27
 H      -0.718811     3.204579     1.237347      25.61
 C      -1.832995    -1.607160    -0.724754      68.71
 H      -2.205580    -2.670722    -0.444161      20.51
 C      -1.655915     0.273218    -2.279120      14.29
 H      -1.758937     0.786745    -3.213328      16.93
 C      -0.722124     0.967598    -1.406654      17.45
 O      -0.205600     2.228210    -1.702096     210.58
 C      -0.555395     3.126298    -2.814897     100.06
 H       0.028532     4.008832    -2.512045      25.69
 H      -0.107292     2.463065    -3.509738      26.96
 H      -1.648255     3.353204    -2.945449      28.22
 C      -0.447770     0.317368    -0.088299      34.74
 O       0.654345     0.760251     0.686438     141.07
 C      -0.972619    -0.885596     0.244891      47.90
 H      -0.619821    -1.503057     1.262777      19.27
 C      -2.158003    -0.934053    -1.999224      31.63
 C      -2.917805    -1.667811    -3.038928      63.01
 H      -2.555790    -1.176389    -3.930158      27.69
 O      -2.466510    -3.139044    -3.036131     249.30
 H      -1.619945    -3.163631    -2.744647      32.43
 C      -4.484657    -1.594921    -2.726382      77.57
 H      -4.762786    -1.981051    -1.639650      26.35
 O      -5.024210    -0.300944    -2.927514     201.43
 H      -4.816205     0.274826    -2.037124      24.66
 C      -5.320636    -2.538009    -3.806769      93.47
 O      -5.208135    -3.899569    -3.424332     152.50
 H      -4.056908    -4.115751    -3.419072      25.14
 H      -5.071209    -2.418537    -4.911071      28.15
 H      -6.425276    -2.289429    -3.620812      27.98
55
name = lig-ACN-frame_492
 C       3.881197     1.876517    -0.573168      66.42
 H       3.269821     2.558565    -1.152243      24.78
 C       4.563436     0.514068     1.359694       2.76
 H       4.373859     0.279696     2.471238      20.80
 C       5.773526     0.117526     0.662158      19.09
 O       6.573463    -0.795750     1.282318     249.05
 C       6.022187    -2.151700     1.615830      98.86
 H       6.885821    -2.865342     1.772205      24.95
 H       5.086338    -2.453311     0.996883      26.96
 H       5.868040    -1.983462     2.672702      23.80
 C       5.937825     0.528925    -0.651145      18.94
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 O       6.967664     0.113358    -1.504863     158.19
 H       7.524328    -0.431863    -1.002136      25.43
 C       5.017124     1.379093    -1.199105      44.78
 H       5.426802     2.010125    -2.173147      20.33
 C       3.649475     1.451355     0.723315      21.20
 C       2.485034     2.067311     1.399564      73.82
 H       2.763015     3.155774     1.933625      23.71
 O       2.179915     1.273928     2.721683     141.76
 H       2.110395     0.229708     2.237430      21.66
 C       1.062960     2.107990     0.832186     102.80
 H       1.073253     2.595517    -0.241148      20.64
 C       0.133830     2.946185     1.690176     101.77
 O       0.514879     4.317370     2.340851     123.72
 H       1.105087     4.979835     1.540968      24.75
 H       0.103372     2.476557     2.705627      25.23
 H      -0.963906     2.957033     1.518486      26.18
 C      -1.739878    -1.516445    -0.741914      61.15
 H      -2.222812    -2.608991    -0.497748      21.50
 C      -1.570502     0.266377    -2.259203      62.44
 H      -1.976583     0.586065    -3.175944      25.35
 C      -0.763664     0.946619    -1.387915      19.81
 O      -0.242393     2.176945    -1.668087     254.54
 C      -0.560149     2.971096    -2.794258     125.11
 H      -0.113880     4.043330    -2.598630      25.15
 H      -0.316373     2.953494    -3.815814      28.61
 H      -1.680945     3.129826    -2.793205      28.17
 C      -0.398191     0.440858    -0.138132      26.65
 O       0.620596     0.792390     0.658162     208.68
 C      -1.026248    -0.896962     0.136998      55.68
 H      -0.677995    -1.535927     1.037340      22.48
 C      -2.161039    -1.005419    -1.928342      59.13
 C      -2.938585    -1.730158    -2.953979      82.75
 H      -2.826688    -1.356607    -3.989755      28.97
 O      -2.499592    -3.068633    -2.964775     257.57
 H      -1.604727    -3.105307    -3.146763      32.83
 C      -4.470055    -1.660698    -2.855807      98.52
 H      -4.637605    -2.094593    -1.756667      26.16
 O      -5.111071    -0.356605    -2.954430     250.78
 H      -4.790395     0.186218    -2.326212      33.51
 C      -5.257479    -2.495755    -3.796816     105.57
 O      -5.173014    -3.942687    -3.379688     168.81
 H      -4.177113    -4.191653    -3.660062      28.59
 H      -4.767935    -2.258551    -4.790866      29.49
 H      -6.346460    -2.197925    -3.884674      28.38
55
name = lig-ACN-frame_493
 C       3.964491     1.980195    -0.574956      76.83
 H       3.307114     2.663959    -0.969956      26.16
 C       4.583726     0.618448     1.269935      65.06
 H       4.427320     0.163750     2.286906      22.88
 C       5.718596     0.108259     0.700711       3.52
 O       6.659820    -0.821811     1.336693     243.65
 C       5.955514    -2.110259     1.689862     103.39
 H       6.611985    -2.867882     1.117264      24.64
 H       5.099712    -2.243438     0.981161      26.94
 H       5.500694    -2.340170     2.673982      26.14
 C       5.968763     0.536243    -0.677427       5.75
 O       6.955623     0.144725    -1.516623     129.17
 H       7.699100    -0.441957    -1.110591      20.22
 C       5.031053     1.423893    -1.283501      33.32
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 H       5.068127     1.432145    -2.507776      20.16
 C       3.650726     1.483440     0.739976      19.32
 C       2.424920     1.926083     1.609025      95.18
 H       2.723034     3.116343     1.936652      23.95
 O       2.282483     1.257213     2.735259     262.66
 H       1.768276     0.387178     2.597258      25.75
 C       1.136191     2.263371     0.772057      75.47
 H       1.285768     2.714521    -0.229068      23.36
 C       0.049148     2.896408     1.741333     104.71
 O       0.464590     4.216599     2.258182     158.21
 H       0.966129     4.838944     1.399825      25.50
 H      -0.056450     2.149711     2.510248      27.08
 H      -0.786969     3.021171     0.988900      25.55
 C      -1.833084    -1.620690    -0.709828      61.62
 H      -2.065036    -2.803837    -0.398232      20.69
 C      -1.606479     0.283842    -2.354221      49.74
 H      -1.654213     0.839353    -3.242494      20.19
 C      -0.811811     0.991195    -1.397843      29.61
 O      -0.164440     2.170565    -1.650918     238.05
 C      -0.672852     2.963022    -2.823430      89.37
 H      -0.177631     4.046177    -2.564824      23.32
 H      -0.299477     2.335280    -3.542863      28.35
 H      -1.827281     2.939477    -2.801917      29.21
 C      -0.417722     0.378144    -0.222311      17.54
 O       0.599465     0.790653     0.706403     152.89
 C      -0.896859    -0.848204     0.208135      52.38
 H      -0.522503    -1.045685     1.197814      19.95
 C      -2.125451    -0.962669    -1.971993      57.80
 C      -2.980545    -1.693882    -3.046136      60.65
 H      -2.745558    -1.155040    -3.974926      30.64
 O      -2.565060    -3.132198    -2.918787     157.82
 H      -1.494708    -3.164530    -3.242193      24.75
 C      -4.539343    -1.728567    -2.759568      83.22
 H      -4.903216    -2.209340    -1.733794      26.86
 O      -5.138072    -0.364087    -2.969377     226.97
 H      -4.562139     0.209781    -2.477748      31.71
 C      -5.156797    -2.612138    -3.860875     112.29
 O      -5.166866    -3.945839    -3.411524     254.43
 H      -4.376932    -4.266049    -3.475916      36.06
 H      -4.772744    -2.591399    -4.908425      29.78
 H      -6.231096    -2.290248    -3.839009      29.14
55
name = lig-ACN-frame_494
 C       3.969474     2.048970    -0.587761      68.45
 H       3.400501     2.704219    -1.115172      24.51
 C       4.587375     0.620869     1.360518      38.05
 H       4.231457     0.284152     2.324910      21.14
 C       5.779991     0.100211     0.626795       2.20
 O       6.623944    -0.829239     1.368559     260.66
 C       5.888822    -2.069617     1.581857     101.25
 H       6.496381    -3.062419     1.338139      24.38
 H       4.937982    -1.927043     1.166619      26.41
 H       5.952787    -2.136080     2.738735      24.31
 C       5.973783     0.529863    -0.697047       4.64
 O       7.006457     0.129985    -1.530571     155.25
 H       7.748709    -0.552167    -1.123188      21.41
 C       5.031082     1.452642    -1.359369       0.44
 H       5.036556     1.537455    -2.539849      19.83
 C       3.672185     1.552928     0.727765      -5.71
 C       2.489297     2.031947     1.613762      67.71
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 H       2.834890     3.100194     2.167847      23.52
 O       2.319599     1.144718     2.905402     219.24
 H       1.935091     0.431599     2.571773      30.60
 C       1.160272     2.208607     0.878377      86.12
 H       1.410468     2.817108     0.055961      25.31
 C       0.015523     2.901422     1.659103     115.81
 O       0.414700     4.117158     2.170802     268.81
 H       0.768247     4.561603     1.370754      31.84
 H      -0.423851     2.421046     2.482226      27.68
 H      -0.942116     3.041999     1.045148      26.13
 C      -1.802532    -1.536612    -0.664770      60.81
 H      -2.304640    -2.632928    -0.487644      21.96
 C      -1.628391     0.317374    -2.357526      83.71
 H      -1.822183     0.440525    -3.405594      14.29
 C      -0.765359     1.027680    -1.438076       9.53
 O      -0.122312     2.271077    -1.674988     247.76
 C      -0.725321     2.879195    -2.795176     126.67
 H      -0.245350     3.990996    -3.110497      24.18
 H      -0.464645     2.559512    -3.769639      28.37
 H      -1.877626     2.986959    -2.835588      30.71
 C      -0.346378     0.344163    -0.178776      15.76
 O       0.571132     0.873621     0.661522     188.46
 C      -0.941553    -0.980095     0.207410      27.35
 H      -0.709696    -1.504729     1.054299      20.59
 C      -2.114771    -0.987439    -1.988040      73.06
 C      -2.997459    -1.690577    -2.967106      60.13
 H      -2.870572    -1.502047    -4.050475      27.75
 O      -2.638239    -3.205888    -2.976618     135.62
 H      -1.497835    -3.168607    -2.679084      22.96
 C      -4.550266    -1.685505    -2.780143      81.10
 H      -4.749039    -2.051818    -1.678462      27.28
 O      -5.098564    -0.413484    -2.954063     210.93
 H      -4.570106     0.354107    -2.318423      25.80
 C      -5.185369    -2.705925    -3.921524     102.01
 O      -5.201630    -4.076193    -3.443796     216.08
 H      -4.236659    -4.206453    -3.127881      28.73
 H      -4.543733    -2.470328    -4.810360      30.72
 H      -6.215437    -2.449721    -4.191576      29.36
55
name = lig-ACN-frame_495
 C       3.964188     2.003930    -0.616691      60.83
 H       3.302782     2.712745    -1.025753      25.14
 C       4.633814     0.628342     1.316065      43.68
 H       4.612122     0.358374     2.321849      24.44
 C       5.721526     0.166006     0.663903       9.89
 O       6.548146    -0.771662     1.248674     236.85
 C       5.858968    -2.049665     1.596718      98.59
 H       6.392919    -2.858510     0.894735      24.75
 H       4.873613    -2.112927     1.342079      29.74
 H       5.848609    -2.226887     2.752583      24.40
 C       5.961109     0.539484    -0.776240      -1.22
 O       7.059924     0.096578    -1.537255     142.11
 H       7.485352    -0.575366    -0.951911      23.56
 C       5.048750     1.427321    -1.294289      63.53
 H       5.418293     1.972738    -2.190346      21.55
 C       3.771203     1.601750     0.766260      12.95
 C       2.565090     2.055848     1.727567      65.49
 H       2.654098     3.175064     2.186775      22.90
 O       2.339693     1.111369     2.953298     208.49
 H       2.351789     0.192452     2.558397      24.91
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 C       1.092848     2.138305     0.997636      91.64
 H       1.278036     2.595973     0.097066      24.33
 C      -0.087076     2.863266     1.581353     110.93
 O       0.403769     4.182635     2.123020     289.35
 H       0.778569     4.711339     1.547766      35.16
 H      -0.284508     2.271724     2.415424      27.37
 H      -0.849278     2.886056     0.754199      26.36
 C      -1.859471    -1.496152    -0.776933      72.26
 H      -2.432116    -2.405680    -0.387354      21.95
 C      -1.553406     0.298828    -2.282926     104.21
 H      -1.822728     0.874058    -3.187572      20.19
 C      -0.673953     0.945254    -1.430644      15.42
 O      -0.155430     2.286483    -1.707733     232.60
 C      -0.753976     2.926821    -2.943071      84.30
 H      -0.254935     4.040155    -2.726050      22.34
 H      -0.700113     2.221499    -3.729781      27.21
 H      -1.799054     2.987885    -2.499055      26.95
 C      -0.348648     0.332055    -0.184094      30.86
 O       0.626593     0.853377     0.630534     204.01
 C      -0.923488    -0.932231     0.157195      39.01
 H      -0.554914    -1.400680     1.041570      18.56
 C      -2.142180    -0.972677    -1.947258      41.24
 C      -2.993466    -1.853060    -2.943123      54.63
 H      -2.700854    -1.219959    -3.811799      28.16
 O      -2.681371    -3.222739    -3.006142     223.61
 H      -1.819261    -3.469050    -2.495284      28.11
 C      -4.556256    -1.766644    -2.831920      87.57
 H      -4.884974    -2.229750    -1.806694      27.19
 O      -5.072930    -0.381471    -2.957078     202.83
 H      -4.690277     0.125510    -2.014398      22.87
 C      -5.186512    -2.693237    -3.870661     110.37
 O      -5.215775    -4.200328    -3.501016     100.61
 H      -4.289038    -4.268416    -2.809491      26.78
 H      -4.517370    -2.811576    -4.732959      29.72
 H      -6.144517    -2.403936    -4.217808      30.24
55
name = lig-ACN-frame_496
 C       3.933887     1.926309    -0.508337      34.36
 H       3.344810     2.709816    -1.047785      22.37
 C       4.665886     0.742679     1.331172      45.23
 H       4.570539     0.432243     2.330072      26.37
 C       5.706973     0.171216     0.521396      41.20
 O       6.509980    -0.766380     1.127625     249.88
 C       5.856308    -2.038053     1.572925      97.10
 H       6.387696    -2.877597     0.934915      24.87
 H       4.878134    -1.893394     1.265545      28.66
 H       6.112471    -2.392748     2.664939      24.22
 C       5.982087     0.500351    -0.750424      12.10
 O       7.029688     0.081153    -1.468342     190.79
 H       7.639134    -0.567319    -1.219430      24.68
 C       5.101015     1.537660    -1.311235      36.87
 H       5.300675     1.886703    -2.279811      25.00
 C       3.706521     1.641879     0.863591       3.00
 C       2.455166     1.944155     1.829359      91.33
 H       2.744586     2.981339     2.355654      21.48
 O       2.407283     1.153337     2.886876     215.83
 H       2.435502     0.062377     2.533238      21.03
 C       1.156894     2.143646     0.889345      91.97
 H       1.435173     2.695791     0.055738      23.57
 C      -0.061079     2.919209     1.640158     109.18
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 O       0.320139     4.238470     2.099883     263.83
 H       0.894443     4.483918     1.265234      28.24
 H      -0.676492     2.499295     2.385439      25.47
 H      -0.866152     3.124851     0.888930      24.08
 C      -1.876648    -1.554705    -0.645452      56.25
 H      -2.237049    -2.525721    -0.381216      22.78
 C      -1.536889     0.261282    -2.299927      49.57
 H      -1.899879     0.860406    -3.190132      21.22
 C      -0.611428     0.971209    -1.442181      13.02
 O      -0.189402     2.185462    -1.750541     227.02
 C      -0.823715     2.968626    -2.885094     108.93
 H      -0.102252     3.847543    -3.305657      23.98
 H      -0.520197     2.510710    -3.836496      26.03
 H      -1.874234     3.309365    -3.047765      27.04
 C      -0.290558     0.377288    -0.205643      33.95
 O       0.749165     0.650022     0.691971     177.18
 C      -0.881652    -0.818139     0.103872      37.99
 H      -0.633883    -1.193607     1.161137      18.11
 C      -2.213753    -0.954548    -2.007386      74.60
 C      -2.991968    -1.779554    -3.004616      69.57
 H      -2.881382    -1.646823    -4.112338      29.24
 O      -2.681546    -3.297204    -2.994978     240.02
 H      -1.876155    -3.330771    -2.696496      33.36
 C      -4.565210    -1.855590    -2.794082      82.12
 H      -4.960312    -2.201834    -1.789331      27.51
 O      -5.024384    -0.406348    -2.942628     252.26
 H      -4.761931     0.028904    -2.122284      27.48
 C      -5.144968    -2.819831    -3.919491     114.48
 O      -5.272153    -4.189437    -3.515873     197.10
 H      -4.331310    -4.426887    -3.012793      26.90
 H      -4.735476    -2.527142    -4.902179      30.95
 H      -6.151086    -2.507883    -3.873412      29.91
55
name = lig-ACN-frame_497
 C       3.943396     1.988728    -0.489469      57.26
 H       3.113596     2.580646    -1.063872      21.53
 C       4.709367     0.797492     1.421482      65.38
 H       4.658853     0.399588     2.432504      24.12
 C       5.633818     0.135004     0.580978     -34.40
 O       6.569565    -0.842336     1.066607     251.05
 C       5.902800    -2.028426     1.465599     116.13
 H       6.202398    -2.992293     0.939615      25.67
 H       4.815016    -2.035499     1.536986      26.27
 H       6.114979    -1.961781     2.582155      24.95
 C       5.926878     0.622594    -0.791226       1.40
 O       7.037043     0.077649    -1.520264     148.63
 H       7.374356    -0.568320    -0.799192      19.75
 C       5.059349     1.575002    -1.263465      82.80
 H       4.920124     1.743129    -2.233720      25.48
 C       3.654569     1.604317     0.864243      -2.00
 C       2.454396     2.035100     1.686140      90.60
 H       2.490708     3.119365     2.164862      23.57
 O       2.433974     1.059473     2.906506     178.92
 H       1.971428     0.094830     2.452276      20.22
 C       1.150154     2.041034     0.964520      91.25
 H       1.263056     2.364007    -0.045418      21.40
 C      -0.063423     2.967667     1.601182     102.78
 O       0.282979     4.293004     2.046193     232.12
 H       1.146323     4.906760     1.572301      24.98
 H      -0.251807     2.381249     2.490524      25.70
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 H      -0.814680     2.954082     0.803225      25.20
 C      -1.848084    -1.495388    -0.674107      51.83
 H      -2.048805    -2.412912    -0.377814      22.39
 C      -1.595351     0.224861    -2.334857      43.64
 H      -1.746276     0.435362    -3.428322      17.78
 C      -0.713194     0.936089    -1.516289       7.36
 O      -0.212652     2.263605    -1.849260     225.95
 C      -0.723710     2.972009    -2.954787      85.10
 H      -0.119780     3.906432    -2.652426      23.28
 H      -0.841080     2.333881    -3.872345      26.28
 H      -1.722850     3.161252    -2.493090      27.28
 C      -0.171969     0.350205    -0.232597      23.47
 O       0.887976     0.632441     0.717101     186.10
 C      -0.974178    -0.850804     0.153161      48.74
 H      -0.604226    -1.447541     1.169937      19.36
 C      -2.149367    -1.055811    -1.915829      24.85
 C      -3.068303    -1.831314    -3.058708      38.78
 H      -2.836363    -1.192095    -4.001999      26.65
 O      -2.623672    -3.323470    -2.931578     201.96
 H      -1.630369    -3.342065    -3.131678      26.69
 C      -4.507726    -1.838028    -2.798730     101.45
 H      -4.563690    -2.296993    -1.800026      27.90
 O      -5.001939    -0.523795    -2.941357     300.96
 H      -4.604678    -0.022718    -2.343545      35.14
 C      -5.281693    -2.784909    -3.892385     106.25
 O      -5.276582    -4.182264    -3.515606     244.12
 H      -4.456408    -4.468200    -3.632243      34.97
 H      -4.733670    -2.784183    -4.859110      30.98
 H      -6.290021    -2.511207    -4.115058      30.47
55
name = lig-ACN-frame_498
 C       3.862543     2.077603    -0.489135      63.31
 H       2.964791     2.697304    -0.973444      18.53
 C       4.702502     0.729338     1.448770      72.18
 H       4.524470     0.571134     2.557844      22.51
 C       5.703229     0.210336     0.598939       2.61
 O       6.597292    -0.849930     0.936867     206.45
 C       5.935197    -2.094243     1.531554     100.56
 H       6.337176    -2.827882     0.830671      26.02
 H       4.884313    -1.866457     1.120064      23.87
 H       6.175884    -2.515512     2.526356      25.55
 C       5.902982     0.662639    -0.718656      -3.29
 O       6.932414     0.124327    -1.501760     157.85
 H       7.535644    -0.655469    -1.039074      19.35
 C       4.900643     1.589750    -1.296260      45.34
 H       5.177242     1.895495    -2.227907      21.25
 C       3.775299     1.593824     0.828426      16.07
 C       2.531106     2.025804     1.703211      84.75
 H       2.737881     3.010724     2.245615      24.41
 O       2.384549     1.066817     2.856921     253.26
 H       2.015550     0.204647     2.409538      22.39
 C       1.122825     2.058850     0.909471      93.11
 H       1.382625     2.672431     0.037321      20.54
 C       0.022911     2.873126     1.561647     103.81
 O       0.257862     4.349111     2.025001     214.54
 H       1.078205     4.542472     1.173986      23.99
 H      -0.388367     2.526196     2.533037      24.16
 H      -0.903265     2.859356     1.006104      24.61
 C      -1.843442    -1.569219    -0.671783      48.67
 H      -2.318971    -2.374197    -0.390184      21.24
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 C      -1.611673     0.149663    -2.360031      42.91
 H      -1.674838     0.620889    -3.341497      18.97
 C      -0.687652     0.945181    -1.472399       9.62
 O      -0.138867     2.163263    -1.840440     223.33
 C      -0.753911     3.043826    -2.934764     108.95
 H      -0.211383     3.946424    -3.240449      25.55
 H      -0.510305     2.617276    -3.984836      25.37
 H      -1.821711     3.304684    -2.913183      28.50
 C      -0.236259     0.238090    -0.259799      34.63
 O       0.837438     0.649097     0.632610     214.31
 C      -0.896011    -0.819620     0.217674      33.13
 H      -0.500676    -1.396003     1.310869      19.56
 C      -2.155622    -1.079530    -2.028947      19.40
 C      -2.872765    -1.942839    -2.955155      54.77
 H      -2.643878    -1.627721    -4.079196      25.01
 O      -2.554167    -3.261384    -2.943491     175.49
 H      -1.430549    -3.343233    -3.223834      23.24
 C      -4.551190    -1.933262    -2.827942      99.33
 H      -4.883915    -2.300582    -1.879314      28.18
 O      -5.033022    -0.573994    -2.939488     250.14
 H      -4.440237     0.040582    -2.317130      25.72
 C      -5.334384    -2.710938    -3.845472     107.15
 O      -5.306413    -4.193186    -3.502939     188.27
 H      -4.448701    -4.452402    -3.910659      31.48
 H      -4.828395    -2.504749    -4.817903      30.57
 H      -6.347741    -2.311793    -3.907529      30.37
55
name = lig-ACN-frame_499
 C       3.834337     2.068087    -0.510941      36.49
 H       3.205760     2.993118    -0.892818      21.65
 C       4.693151     0.686427     1.376580      36.89
 H       4.558273     0.205147     2.420648      25.16
 C       5.814562     0.239401     0.657880      32.16
 O       6.630551    -0.865702     0.920512     253.33
 C       5.983160    -2.130881     1.407596     108.50
 H       6.388681    -2.977578     0.911288      27.24
 H       4.808882    -2.241737     1.527585      26.28
 H       6.210388    -2.054217     2.452602      24.69
 C       5.814880     0.692809    -0.691037      -3.63
 O       6.785358     0.226493    -1.515672     161.80
 H       7.315204    -0.504129    -1.077772      23.37
 C       4.919540     1.568891    -1.325926      63.36
 H       5.030287     1.987611    -2.314455      21.07
 C       3.748869     1.656637     0.884143      16.29
 C       2.555449     1.923817     1.755750     100.03
 H       2.754208     2.950940     2.271937      19.08
 O       2.301111     1.112232     2.797484     330.13
 H       2.363071     0.244717     2.519586      27.07
 C       1.265301     2.198466     0.848889      48.82
 H       1.304732     2.635454    -0.221084      15.80
 C      -0.029378     2.849465     1.669758      97.13
 O       0.260731     4.255546     1.918420     275.76
 H       0.933602     4.811518     1.265643      25.64
 H      -0.243827     2.189982     2.574477      22.87
 H      -0.760186     2.846700     0.899776      23.26
 C      -1.821329    -1.594799    -0.651552      47.00
 H      -2.234088    -2.544250    -0.426277      20.56
 C      -1.493392     0.225495    -2.346006      81.01
 H      -1.922675     0.615821    -3.211843      22.40
 C      -0.689944     0.860837    -1.490518       8.12
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 O      -0.076570     2.097867    -1.835147     226.12
 C      -0.734687     3.047399    -2.995239      85.79
 H      -0.155025     3.763373    -2.584547      25.45
 H      -0.509159     2.348446    -3.875494      23.15
 H      -1.807973     3.182505    -2.841055      27.13
 C      -0.290250     0.328720    -0.263061      37.25
 O       0.725362     0.725916     0.496788     167.05
 C      -0.940920    -0.990599     0.124559      64.49
 H      -0.638364    -1.245040     1.381245      14.23
 C      -2.067045    -1.063796    -1.931011      71.25
 C      -2.919904    -1.954337    -2.993031      26.84
 H      -2.874551    -1.390252    -4.050222      26.12
 O      -2.410848    -3.389260    -2.963769     165.43
 H      -1.311756    -3.411912    -2.581948      19.79
 C      -4.507112    -1.942203    -2.746355      92.46
 H      -4.700693    -2.385189    -1.813926      28.66
 O      -5.042315    -0.573831    -2.948425     238.23
 H      -4.590156     0.035404    -2.059922      21.26
 C      -5.320651    -2.734201    -3.843968     106.82
 O      -5.356267    -4.117047    -3.547984     129.30
 H      -4.333863    -4.672674    -3.650658      28.13
 H      -5.255166    -2.468332    -4.911608      30.44
 H      -6.348059    -2.539959    -3.500819      29.59
55
name = lig-ACN-frame_500
 C       3.916019     2.073292    -0.438913      66.58
 H       3.193581     2.811099    -0.889788      23.05
 C       4.672944     0.662463     1.371142      52.84
 H       4.413706     0.134337     2.335383      24.37
 C       5.748330     0.244588     0.602636      11.49
 O       6.643302    -0.882317     0.913619     243.73
 C       6.079769    -2.106972     1.402267     112.04
 H       6.534623    -2.913983     0.892878      27.67
 H       4.925956    -2.033565     1.044009      24.55
 H       6.280264    -2.315191     2.437368      26.80
 C       5.797954     0.712842    -0.762130       1.57
 O       6.737198     0.270301    -1.603506     170.98
 H       7.242420    -0.396158    -1.171111      24.64
 C       4.873326     1.632038    -1.232434      71.80
 H       4.956871     1.628062    -2.378201      21.20
 C       3.758006     1.598570     0.857217      29.16
 C       2.482361     2.057363     1.644926      78.55
 H       2.570433     3.056234     2.212558      23.50
 O       2.210647     1.050957     2.850879     271.90
 H       2.145327     0.229537     2.459052      27.00
 C       1.152133     2.173901     0.852771     104.13
 H       1.565044     2.932392    -0.011733      21.05
 C       0.068302     2.820793     1.556663     115.91
 O       0.208727     4.180605     1.916266     325.05
 H       0.904005     4.441391     1.362329      32.79
 H       0.011814     2.389906     2.634112      22.97
 H      -0.882406     2.555155     1.180690      26.88
 C      -1.829737    -1.672111    -0.728164      44.11
 H      -2.126673    -2.745467    -0.433505      17.55
 C      -1.570646     0.123828    -2.359511      71.31
 H      -1.725848     0.527437    -3.314141      15.82
 C      -0.636887     0.907315    -1.533592      13.45
 O      -0.063644     2.096972    -1.864235     249.53
 C      -0.609979     2.889788    -2.878644     130.00
 H      -0.313929     3.856305    -2.915601      28.10
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 H      -0.485060     2.874651    -3.986835      25.70
 H      -1.668970     2.935771    -2.633486      28.25
 C      -0.387739     0.294543    -0.224646      59.79
 O       0.751168     0.865820     0.475405     201.98
 C      -0.864645    -0.915188     0.142686      74.41
 H      -0.638428    -1.619823     1.208391      15.68
 C      -2.093859    -1.112908    -1.994985      11.73
 C      -2.932934    -1.881377    -2.970372      60.47
 H      -2.645911    -1.486758    -4.044308      25.38
 O      -2.343557    -3.467460    -2.978803     176.04
 H      -1.467585    -3.280073    -2.561729      25.61
 C      -4.428558    -1.919075    -2.744971     102.98
 H      -4.621723    -2.231713    -1.769676      30.66
 O      -4.983932    -0.588260    -2.896049     240.66
 H      -4.859964     0.011728    -2.003566      24.72
 C      -5.395619    -2.724299    -3.710965     107.75
 O      -5.357310    -4.166003    -3.611101     180.56
 H      -4.270224    -4.282852    -3.351395      29.45
 H      -5.027756    -2.442898    -4.719925      30.56
 H      -6.417715    -2.266199    -3.613168      29.97
55
name = lig-ACN-frame_501
 C       3.854364     2.182952    -0.364509      40.55
 H       3.012546     2.656572    -0.780565      19.59
 C       4.619219     0.610378     1.421256      51.87
 H       4.498063     0.314688     2.466211      22.10
 C       5.663023     0.131291     0.518057       3.19
 O       6.659280    -0.756310     0.895772     244.97
 C       6.131233    -2.111338     1.369975     104.22
 H       6.753833    -2.775292     0.824281      26.54
 H       4.998935    -2.268832     1.009123      24.66
 H       6.036145    -2.260945     2.414041      27.30
 C       5.865773     0.687488    -0.758417       8.62
 O       6.792493     0.234094    -1.747120     176.24
 H       7.442156    -0.469763    -1.355480      21.73
 C       4.913693     1.631478    -1.278589      29.86
 H       4.821619     2.047131    -2.377913      20.94
 C       3.661816     1.581925     0.916656       4.57
 C       2.390030     1.984855     1.734121      94.21
 H       2.653511     2.938103     2.196057      23.95
 O       2.158206     1.120976     2.810671     292.44
 H       1.720751     0.229414     2.432774      21.13
 C       1.130707     2.186959     0.760521      77.62
 H       1.121672     2.785728    -0.317622      15.18
 C      -0.008816     2.742540     1.666187      97.21
 O       0.163959     4.203710     1.906796     308.74
 H       0.838113     4.669320     1.455134      31.66
 H       0.027109     2.088226     2.593782      23.27
 H      -0.911937     2.698943     1.106097      24.31
 C      -1.699735    -1.648145    -0.734799      77.48
 H      -2.110338    -2.742157    -0.408457      19.76
 C      -1.576048     0.115248    -2.406083      42.99
 H      -1.653084     0.364536    -3.451481      19.24
 C      -0.731195     0.809668    -1.532441      -1.20
 O       0.042605     2.044398    -1.851249     258.15
 C      -0.635793     2.893043    -2.856848     107.56
 H      -0.195506     3.750192    -2.600868      25.85
 H      -0.323550     2.249079    -3.658374      23.58
 H      -1.723956     2.833728    -2.849190      27.53
 C      -0.316168     0.419036    -0.257604      19.65
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 O       0.789375     0.819448     0.454346     196.25
 C      -0.917264    -0.943623     0.132898      44.95
 H      -0.182475    -1.321260     1.058518      17.19
 C      -2.126953    -1.143624    -2.005878      41.25
 C      -2.829611    -2.048190    -3.050746      38.06
 H      -2.798108    -1.628281    -4.144862      24.14
 O      -2.448229    -3.365327    -2.997751     291.18
 H      -1.581164    -3.514396    -3.055777      33.38
 C      -4.492760    -1.921789    -2.659943      97.94
 H      -4.559586    -2.283175    -1.673425      28.25
 O      -4.912805    -0.541979    -2.830239     308.56
 H      -4.613061    -0.120571    -2.070357      27.64
 C      -5.359730    -2.665461    -3.657313     100.79
 O      -5.297426    -4.200296    -3.610020     234.49
 H      -4.452007    -4.399199    -3.316128      36.11
 H      -5.075839    -2.349998    -4.681432      30.63
 H      -6.479269    -2.420189    -3.493711      28.25
55
name = lig-ACN-frame_502
 C       3.850569     2.100741    -0.382654      69.37
 H       3.369550     2.912210    -0.744624      25.79
 C       4.572184     0.603577     1.356117      52.47
 H       4.663202     0.183233     2.313027      24.52
 C       5.584963     0.124117     0.486288     -14.35
 O       6.627484    -0.714421     0.960781     304.10
 C       6.182349    -2.071507     1.282721     113.82
 H       6.897618    -2.895061     1.133143      26.70
 H       5.153398    -2.328109     0.863134      25.26
 H       6.203559    -1.960633     2.342497      27.94
 C       5.819114     0.684014    -0.870602     -14.21
 O       6.843722     0.193293    -1.811619     132.76
 H       7.384500    -0.515692    -1.206101      20.79
 C       4.889652     1.680663    -1.160386      60.96
 H       5.215068     2.054865    -2.224887      19.46
 C       3.624037     1.561544     0.940928      26.20
 C       2.416696     1.994660     1.703042     100.11
 H       2.483439     2.966675     2.192885      23.49
 O       2.047544     1.180272     2.816918     238.14
 H       1.997396     0.068871     2.442298      18.83
 C       1.078044     2.186138     0.822236      57.58
 H       1.307900     2.857628    -0.201596      18.08
 C      -0.103570     2.802482     1.687393     106.24
 O       0.096622     4.208983     1.969683     276.48
 H       0.931934     4.305166     1.291128      25.91
 H      -0.235418     2.364846     2.690500      23.59
 H      -1.040252     2.555501     1.195807      25.00
 C      -1.647181    -1.614463    -0.736955      96.71
 H      -1.874293    -2.783917    -0.420553      16.28
 C      -1.545742     0.105542    -2.439894      57.34
 H      -1.842079     0.541928    -3.430627      21.31
 C      -0.706158     0.885165    -1.523746      44.74
 O       0.034135     1.921581    -1.822351     216.74
 C      -0.598798     2.840207    -2.910930     136.09
 H      -0.265546     3.789035    -2.853339      27.13
 H      -0.495824     2.714491    -3.941292      29.01
 H      -1.648385     2.956457    -2.649875      30.35
 C      -0.324415     0.291838    -0.285023      37.89
 O       0.806021     0.672567     0.412972     168.00
 C      -0.824551    -0.863419     0.115263      29.10
 H      -0.619184    -1.423219     1.076797      18.35
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 C      -2.021214    -1.159231    -2.005616      76.68
 C      -2.975671    -2.003086    -3.058979      30.87
 H      -2.792647    -1.510433    -4.080786      29.56
 O      -2.562546    -3.435538    -3.026074     270.20
 H      -1.635805    -3.391733    -3.171823      27.89
 C      -4.422819    -1.931861    -2.626221     104.77
 H      -4.675758    -2.318096    -1.653274      26.33
 O      -4.822333    -0.513199    -2.749460     322.27
 H      -4.511169    -0.007632    -2.081874      29.81
 C      -5.336330    -2.746773    -3.656568     112.00
 O      -5.228367    -4.143750    -3.583261     251.08
 H      -4.330057    -4.362881    -3.536593      34.43
 H      -5.268470    -2.320439    -4.677861      31.32
 H      -6.422014    -2.574812    -3.273727      29.01
55
name = lig-ACN-frame_503
 C       3.861235     2.080753    -0.388392      52.24
 H       3.336269     2.935522    -0.573427      22.62
 C       4.572218     0.551550     1.267954      57.98
 H       4.369703     0.152814     2.211624      25.67
 C       5.634830     0.168396     0.404375      23.25
 O       6.578415    -0.692235     0.976636     258.58
 C       6.228219    -2.035343     1.357426     118.71
 H       7.127658    -2.570978     0.960590      26.37
 H       5.422814    -2.328740     0.627379      27.00
 H       5.776538    -2.359088     2.264797      27.50
 C       5.775971     0.546201    -0.903759      19.32
 O       6.773440     0.202969    -1.696502     204.05
 H       7.352343    -0.522948    -1.309003      25.11
 C       4.979048     1.735140    -1.225552      54.12
 H       5.029192     2.399230    -2.061877      22.43
 C       3.618756     1.535722     0.851792      12.42
 C       2.328508     2.075432     1.698414      86.49
 H       2.652173     2.990956     2.059310      23.54
 O       1.981953     1.164079     2.871562     248.96
 H       2.286166     0.172791     2.534285      21.69
 C       1.007395     2.054357     0.954975      92.96
 H       1.169198     2.805929    -0.008271      18.96
 C      -0.186449     2.781694     1.680138      95.57
 O       0.086206     4.195298     1.975480     230.19
 H       0.660734     5.045622     1.452800      24.36
 H      -0.228139     2.275065     2.609165      24.32
 H      -1.135609     2.794426     1.116057      23.36
 C      -1.683173    -1.701095    -0.789831     109.89
 H      -2.076443    -2.803204    -0.463439      16.33
 C      -1.535303     0.113637    -2.395230      24.12
 H      -1.867781     0.650864    -3.352010      16.45
 C      -0.674847     0.807932    -1.541277      18.78
 O       0.019581     2.012326    -1.985498     261.05
 C      -0.568110     2.839758    -2.886275     126.68
 H       0.042221     3.693967    -2.806863      24.91
 H      -0.550600     2.307267    -3.749764      27.26
 H      -1.623435     2.917321    -2.621389      27.66
 C      -0.260575     0.255728    -0.310407      27.72
 O       0.860047     0.718281     0.430134     173.54
 C      -0.844999    -1.006727     0.176168      29.30
 H      -0.573186    -1.233019     1.141477      17.81
 C      -1.969515    -1.176581    -2.112463      54.78
 C      -2.953716    -1.852880    -2.916207      63.10
 H      -2.930757    -1.570350    -3.980224      25.34
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 O      -2.648538    -3.526100    -3.088705     120.17
 H      -1.589560    -3.689173    -2.755457      24.65
 C      -4.455180    -1.911229    -2.659026     102.34
 H      -4.471793    -2.326018    -1.627292      29.55
 O      -4.768420    -0.530799    -2.738372     330.29
 H      -4.757799    -0.200943    -1.794843      27.12
 C      -5.378927    -2.704489    -3.582726     109.61
 O      -5.130141    -4.165943    -3.564252     158.92
 H      -4.073730    -4.095413    -3.787366      28.86
 H      -5.188578    -2.367025    -4.618923      31.71
 H      -6.442740    -2.392806    -3.292498      30.24
55
name = lig-ACN-frame_504
 C       3.906229     2.202746    -0.455697      51.72
 H       3.236009     2.865605    -0.960185      23.23
 C       4.462177     0.527345     1.234711      52.57
 H       4.536844     0.024089     2.176213      22.42
 C       5.584984     0.119869     0.494630       3.02
 O       6.608266    -0.657646     1.038300     249.44
 C       6.195922    -2.093257     1.296011     111.32
 H       7.137403    -2.713467     1.608029      25.52
 H       5.599471    -2.548570     0.542021      26.99
 H       5.806966    -1.964164     2.318813      25.51
 C       5.682353     0.638105    -0.865531      -0.68
 O       6.786039     0.162055    -1.658760     190.86
 H       7.260639    -0.442027    -1.129839      23.29
 C       4.962580     1.732640    -1.299157      58.73
 H       5.441135     2.028915    -2.141589      19.41
 C       3.527004     1.481605     0.822758      17.26
 C       2.316907     1.942185     1.774645     101.81
 H       2.371063     2.875216     2.164997      25.62
 O       2.033201     1.193254     2.912448     324.92
 H       2.015803     0.302139     2.696977      27.90
 C       0.969266     2.129077     0.873093      69.09
 H       1.087095     2.777375    -0.152129      19.95
 C      -0.194580     2.779389     1.671182     105.63
 O       0.069724     4.192330     2.053463     230.07
 H       0.440538     4.342244     1.016318      25.85
 H      -0.573135     2.390283     2.565870      25.70
 H      -1.039291     2.658714     0.917295      23.95
 C      -1.679274    -1.778988    -0.789705      69.21
 H      -2.328194    -2.699372    -0.556930      17.59
 C      -1.525973     0.144098    -2.395880      52.03
 H      -1.827124     0.489772    -3.446984      13.92
 C      -0.539600     0.797749    -1.577450       5.62
 O       0.063788     1.964768    -1.948887     210.25
 C      -0.636889     2.882977    -2.993957     119.46
 H      -0.004612     3.755597    -3.145287      26.34
 H      -0.679319     2.496875    -3.929326      27.08
 H      -1.583504     3.329427    -2.772373      27.67
 C      -0.185505     0.197162    -0.261435      26.65
 O       0.834392     0.725233     0.476398     183.89
 C      -0.867135    -1.048127     0.096447      38.08
 H      -0.580752    -1.519870     0.871071      24.82
 C      -1.973248    -1.219615    -1.990963      46.88
 C      -2.866591    -2.063888    -3.056866      49.44
 H      -2.728889    -1.511137    -3.968702      24.60
 O      -2.678490    -3.448206    -3.126722     226.10
 H      -1.794406    -3.880227    -2.518084      24.55
 C      -4.455859    -1.892719    -2.540438      88.63
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 H      -4.780427    -2.268179    -1.517577      26.13
 O      -4.822798    -0.505689    -2.753817     235.81
 H      -4.881378     0.134187    -1.807065      20.07
 C      -5.362754    -2.683481    -3.570106     101.38
 O      -5.071040    -4.129195    -3.572552     158.11
 H      -3.920475    -4.356905    -3.492851      23.00
 H      -5.302433    -2.196158    -4.571892      31.45
 H      -6.440084    -2.733378    -3.251562      29.81
55
name = lig-ACN-frame_505
 C       3.838561     2.216292    -0.489060      55.29
 H       3.217714     3.121291    -0.822964      22.36
 C       4.351934     0.490029     1.293516      43.33
 H       4.015864     0.269775     2.323834      18.40
 C       5.467690     0.120931     0.509031       8.08
 O       6.634985    -0.700999     1.063262     209.96
 C       6.184799    -2.073642     1.368763     112.13
 H       7.124506    -2.655155     1.751853      25.25
 H       5.836755    -2.565254     0.491479      26.84
 H       5.214369    -2.158229     1.944363      25.76
 C       5.807079     0.648346    -0.745487       7.81
 O       6.748775     0.145513    -1.599799     163.86
 H       7.396158    -0.435117    -1.123682      20.85
 C       4.913981     1.684709    -1.291892      56.96
 H       5.001321     2.112521    -2.229861      21.96
 C       3.497245     1.551527     0.729615      -2.77
 C       2.304323     1.967366     1.686317      90.16
 H       2.709343     2.818206     2.022889      25.48
 O       2.103188     1.143895     2.970670     293.46
 H       1.750029     0.335703     2.772980      26.88
 C       1.039237     2.164849     0.879250      67.86
 H       1.381632     2.873756     0.004114      21.41
 C      -0.267325     2.776277     1.603990      99.39
 O       0.075588     4.114169     2.019871     303.10
 H       0.498625     4.721118     1.453372      31.89
 H      -0.373773     2.064665     2.489578      24.11
 H      -1.219239     2.864192     0.979050      24.03
 C      -1.713722    -1.794280    -0.752851     119.52
 H      -1.872135    -2.764649    -0.295408      19.07
 C      -1.476867    -0.001975    -2.355468      50.20
 H      -1.673567     0.473388    -3.338870      17.08
 C      -0.518510     0.730952    -1.585566       8.33
 O       0.075153     1.996795    -1.942604     191.64
 C      -0.638644     2.909014    -3.096029      92.58
 H       0.190732     3.684221    -3.198034      24.48
 H      -0.899522     2.330193    -3.888115      27.15
 H      -1.459211     3.077580    -2.471731      26.74
 C      -0.237394     0.158736    -0.355214      24.98
 O       0.750239     0.670496     0.553639     130.07
 C      -0.746054    -1.058684     0.083269      21.21
 H      -0.504292    -1.444071     0.917886      18.98
 C      -2.057020    -1.236638    -2.091046      59.37
 C      -2.936136    -2.025209    -3.022409      61.00
 H      -2.925629    -1.763875    -4.035959      28.93
 O      -2.589277    -3.471909    -3.136568     226.46
 H      -1.803694    -3.645144    -2.536708      25.85
 C      -4.409164    -1.851997    -2.608392      91.48
 H      -4.290251    -2.145621    -1.488538      28.29
 O      -4.923308    -0.468968    -2.778947     247.96
 H      -4.372905     0.019966    -1.898263      21.16
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 C      -5.339563    -2.729395    -3.505727     120.69
 O      -5.067095    -4.101741    -3.624143     192.87
 H      -3.936928    -4.069886    -3.211558      22.60
 H      -5.259261    -2.239358    -4.518746      30.66
 H      -6.362599    -2.499020    -3.131687      30.12
55
name = lig-ACN-frame_506
 C       3.781559     2.105537    -0.473332      61.22
 H       3.268922     3.120299    -0.846538      22.86
 C       4.270901     0.553732     1.249945      55.45
 H       4.038221     0.012554     2.205559      23.28
 C       5.517177     0.096889     0.634264      -5.46
 O       6.494188    -0.712668     1.086944     285.60
 C       6.156554    -2.076223     1.372185     119.04
 H       6.917328    -2.405370     2.179548      25.67
 H       6.299693    -2.648523     0.516791      27.82
 H       5.168703    -2.171170     1.983956      25.37
 C       5.754846     0.700403    -0.694533      -6.58
 O       6.740501     0.148177    -1.548849     128.33
 H       7.365415    -0.552227    -1.038218      16.84
 C       4.868447     1.655258    -1.209832      59.01
 H       5.038968     1.934877    -2.278132      21.24
 C       3.479331     1.530364     0.759209      56.62
 C       2.361740     2.045164     1.693910      97.62
 H       2.431782     2.964796     2.060297      26.03
 O       2.187075     1.156149     2.915347     260.64
 H       1.768839     0.255057     2.433698      20.17
 C       0.991044     2.080496     0.869763      87.41
 H       1.164317     2.463130    -0.158408      22.19
 C      -0.163008     2.783651     1.452610     107.14
 O       0.058450     4.078256     2.075964     299.08
 H       0.628903     4.450409     1.457999      31.86
 H      -0.448385     2.243929     2.468950      23.71
 H      -1.098433     2.624729     0.791726      25.02
 C      -1.662860    -1.774668    -0.744841      41.36
 H      -1.970268    -2.733757    -0.624609      22.75
 C      -1.410094    -0.054264    -2.477176      63.50
 H      -1.753135     0.299756    -3.441869      21.41
 C      -0.566837     0.746253    -1.634604      11.98
 O       0.035902     1.985753    -2.015564     248.69
 C      -0.606642     2.770402    -2.959264     136.13
 H       0.090378     3.686448    -3.331223      24.88
 H      -0.714754     2.264736    -3.891299      26.88
 H      -1.480454     3.374428    -2.851504      27.93
 C      -0.174092     0.238865    -0.323951      12.29
 O       0.656402     0.681024     0.614732     182.44
 C      -0.737404    -1.135253     0.032349      41.57
 H      -0.358048    -1.350339     0.962854      19.29
 C      -2.033798    -1.320249    -2.018652      51.29
 C      -2.977209    -1.853302    -3.079193      55.67
 H      -2.789365    -1.322844    -3.950656      29.17
 O      -2.481801    -3.526132    -3.096678     174.46
 H      -1.699510    -3.600249    -2.720503      28.56
 C      -4.437129    -1.839904    -2.648501     100.25
 H      -4.690836    -2.161066    -1.573653      26.12
 O      -4.942330    -0.503021    -2.805286     273.83
 H      -4.707004     0.139578    -2.033585      25.69
 C      -5.371072    -2.654251    -3.466837     113.95
 O      -5.061947    -4.114765    -3.635118     176.25
 H      -4.023038    -4.355609    -3.404230      26.07
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 H      -5.373548    -2.241998    -4.520608      29.53
 H      -6.393973    -2.601573    -3.058106      30.16
55
name = lig-ACN-frame_507
 C       3.736343     2.074613    -0.456819      50.86
 H       2.925044     2.791490    -1.023635      22.24
 C       4.360800     0.464067     1.303444      47.38
 H       4.193259    -0.030928     2.291500      23.76
 C       5.476095     0.224719     0.603994      30.49
 O       6.386625    -0.706408     1.168387     264.06
 C       6.152226    -2.147175     1.441445     101.62
 H       6.756918    -2.324710     2.374485      24.67
 H       6.298955    -2.875628     0.715239      27.37
 H       4.983650    -2.218659     1.555116      25.78
 C       5.695704     0.631220    -0.673342      15.30
 O       6.716885     0.189243    -1.479293     149.14
 H       7.303530    -0.470572    -0.926671      20.95
 C       4.861648     1.612100    -1.201250      59.16
 H       5.273166     1.995628    -2.230129      20.48
 C       3.460584     1.561351     0.857751      -8.31
 C       2.285292     2.059884     1.723256     111.09
 H       2.455711     2.967982     2.089900      25.86
 O       2.236746     1.221403     2.772148     268.76
 H       2.170479     0.099090     2.530055      19.95
 C       1.050887     2.025794     0.753775      92.06
 H       1.262918     2.496723    -0.150398      24.09
 C      -0.186475     2.737090     1.497786      91.51
 O       0.077055     4.073378     2.068199     189.33
 H       0.723128     4.758381     1.439618      25.13
 H      -0.774370     1.951468     2.173426      23.95
 H      -0.801780     3.081644     0.601665      23.22
 C      -1.637721    -1.875960    -0.793159      51.05
 H      -2.092933    -2.615567    -0.320644      17.58
 C      -1.360092    -0.052363    -2.529123      50.70
 H      -1.557399     0.291744    -3.522884      24.36
 C      -0.585241     0.748954    -1.640848      22.76
 O      -0.009094     1.895468    -1.980590     218.88
 C      -0.604183     2.750092    -3.042093      95.82
 H       0.318631     3.511559    -3.011687      22.73
 H      -0.725059     2.156992    -3.979955      25.20
 H      -1.550038     2.958752    -2.530703      25.82
 C      -0.263402     0.147754    -0.371625      28.56
 O       0.601387     0.678002     0.717666     168.26
 C      -0.688969    -1.042876     0.023205      42.85
 H      -0.433970    -1.730670     0.864593      20.71
 C      -1.925276    -1.172076    -2.062348      33.40
 C      -2.842010    -1.964779    -2.997657      58.55
 H      -2.818282    -1.641581    -3.995036      29.40
 O      -2.478767    -3.390956    -3.107287     200.91
 H      -1.445347    -3.432470    -3.135668      27.93
 C      -4.508925    -1.844094    -2.601129      86.25
 H      -4.459639    -2.202453    -1.524178      26.54
 O      -4.964337    -0.471169    -2.841163     272.56
 H      -5.041053    -0.148242    -2.037247      32.71
 C      -5.444688    -2.733698    -3.572026     119.27
 O      -5.083945    -4.107287    -3.625773     224.31
 H      -4.150601    -4.062183    -3.619685      32.89
 H      -5.594631    -2.124330    -4.530702      30.87
 H      -6.401427    -2.704133    -3.043225      30.65
55
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name = lig-ACN-frame_508
 C       3.743898     2.005334    -0.441000      51.66
 H       2.932475     2.757146    -0.907196      21.98
 C       4.305384     0.581233     1.437364      47.70
 H       4.260409     0.275731     2.484853      25.23
 C       5.448579     0.086910     0.640300     -14.50
 O       6.418282    -0.733255     1.238002     257.79
 C       6.038920    -2.160657     1.511957     110.11
 H       6.477733    -2.465317     2.454045      26.92
 H       6.673223    -2.536319     0.782994      26.57
 H       4.942488    -2.516345     1.569206      26.68
 C       5.658894     0.625539    -0.719975       2.96
 O       6.776738     0.200508    -1.445218     191.88
 H       7.351659    -0.357342    -0.959578      22.76
 C       4.799934     1.634076    -1.228603      63.20
 H       4.808982     2.147198    -2.282123      21.05
 C       3.547831     1.560905     0.843366      52.27
 C       2.322491     2.018330     1.573302     100.15
 H       2.448578     2.967265     1.857858      25.88
 O       2.185574     1.207029     2.838037     266.94
 H       2.302844     0.276000     2.484002      26.64
 C       0.983139     2.095257     0.836393      82.18
 H       1.203288     2.435140    -0.075183      24.63
 C      -0.218111     2.847630     1.355845      99.39
 O       0.120432     4.043630     2.115072     173.80
 H       0.631406     4.717049     1.281092      24.33
 H      -0.623000     2.225847     2.288660      23.59
 H      -1.118810     2.853848     0.629165      24.22
 C      -1.584296    -1.749910    -0.856705      68.08
 H      -1.974228    -2.694769    -0.711298      25.14
 C      -1.320040     0.015762    -2.533025      52.80
 H      -1.396769     0.413593    -3.537585      21.29
 C      -0.564774     0.646155    -1.582419      19.45
 O       0.052107     1.886507    -1.933064     210.78
 C      -0.597782     2.711127    -3.067951     101.75
 H      -0.140168     3.847546    -3.244099      24.18
 H      -0.612791     2.291906    -4.159449      24.37
 H      -1.646882     3.074580    -2.892450      26.42
 C      -0.241490     0.159446    -0.305303       9.09
 O       0.541450     0.609618     0.677751     146.22
 C      -0.780816    -1.232589     0.022702      42.87
 H      -0.282260    -1.308563     1.094734      17.75
 C      -1.947293    -1.294723    -2.118538      39.79
 C      -2.899153    -1.997174    -2.998681      81.06
 H      -2.837676    -1.405867    -3.886356      27.80
 O      -2.479136    -3.313167    -3.105986     181.32
 H      -1.359268    -3.452317    -3.339697      24.26
 C      -4.450786    -1.898180    -2.666996      93.32
 H      -4.757971    -2.091310    -1.632615      28.20
 O      -4.972569    -0.478170    -2.827292     236.46
 H      -4.884309     0.022637    -1.962986      27.45
 C      -5.486614    -2.734193    -3.530757     117.68
 O      -5.086709    -4.125315    -3.652753     208.80
 H      -4.223926    -4.110603    -3.808468      36.90
 H      -5.332236    -2.410663    -4.614092      29.79
 H      -6.529187    -2.674558    -3.250978      31.69
55
name = lig-ACN-frame_509
 C       3.709173     2.029000    -0.482593      53.32
 H       3.081365     2.926163    -0.833011      22.66
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 C       4.472698     0.671059     1.467706      50.73
 H       4.287755     0.506260     2.503950      21.36
 C       5.375207     0.017017     0.669213       4.13
 O       6.406650    -0.763181     1.308926     282.63
 C       6.054581    -2.160764     1.523708     106.10
 H       6.160729    -2.349270     2.570093      27.35
 H       6.405761    -2.975902     0.945855      26.57
 H       4.995677    -2.151949     1.153345      26.51
 C       5.646402     0.587031    -0.635795     -15.36
 O       6.839487     0.222747    -1.462112     170.53
 H       7.414952    -0.381972    -0.938611      23.00
 C       4.795252     1.560633    -1.268245      47.83
 H       5.031506     1.701407    -2.353730      19.15
 C       3.508550     1.508523     0.839259      12.63
 C       2.280519     2.019340     1.668151      92.04
 H       2.481514     2.945799     2.039204      26.08
 O       2.098026     1.231904     2.891100     316.08
 H       1.935598     0.386559     2.776237      31.48
 C       0.898765     2.028970     0.748144      89.95
 H       1.039015     2.410990    -0.177731      24.52
 C      -0.272239     2.883141     1.425786      92.81
 O       0.170234     4.081851     2.081101     247.25
 H       0.590968     4.815463     1.482093      28.03
 H      -0.767413     2.169426     2.234664      24.94
 H      -1.030124     3.129030     0.571545      24.82
 C      -1.665844    -1.882868    -0.916540      62.51
 H      -1.907516    -2.954404    -0.777194      18.92
 C      -1.362950    -0.061374    -2.484382      51.43
 H      -1.650582     0.363513    -3.457124      20.95
 C      -0.479362     0.668822    -1.588068       0.36
 O       0.096867     1.992461    -1.982499     176.20
 C      -0.607190     2.690078    -3.042021      82.71
 H       0.126666     3.639095    -2.884984      22.01
 H      -0.154891     2.040991    -3.951894      23.07
 H      -1.729008     2.635722    -2.911754      25.88
 C      -0.279761     0.040327    -0.251791      29.96
 O       0.572816     0.663948     0.686824     176.01
 C      -0.735015    -1.155321     0.092970      48.96
 H      -0.797833    -1.937016     0.980657      17.72
 C      -1.954652    -1.199011    -2.182847      20.80
 C      -3.025432    -1.815465    -3.135499      57.24
 H      -3.005641    -1.458410    -4.164121      27.50
 O      -2.498496    -3.439228    -3.167847     104.04
 H      -1.450782    -3.228103    -3.011499      25.17
 C      -4.520123    -1.882973    -2.635158     104.91
 H      -4.446368    -2.355281    -1.664890      29.45
 O      -4.938593    -0.540229    -2.803129     248.29
 H      -4.402136     0.024070    -1.966749      23.64
 C      -5.357266    -2.710416    -3.606125     119.76
 O      -5.113715    -4.176743    -3.675706     153.72
 H      -4.048136    -4.319894    -3.694129      27.23
 H      -5.422672    -2.108996    -4.554755      29.80
 H      -6.312565    -2.617202    -3.109558      29.69
55
name = lig-ACN-frame_510
 C       3.724641     2.017571    -0.517960      56.52
 H       3.051735     2.703106    -1.018173      23.89
 C       4.484014     0.733776     1.457280      34.14
 H       4.522098     0.415599     2.480297      21.68
 C       5.532164     0.073574     0.661180       4.61
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 O       6.428475    -0.787728     1.307332     274.46
 C       5.937649    -2.162773     1.516038     109.73
 H       5.968573    -2.363247     2.554790      27.10
 H       6.761100    -2.735361     1.052855      25.42
 H       4.912666    -2.348202     1.188835      28.75
 C       5.750826     0.464221    -0.657747      18.45
 O       6.782096     0.262802    -1.398633     176.04
 H       7.487650    -0.425579    -1.006096      21.68
 C       4.808344     1.391632    -1.209412      51.60
 H       5.112314     1.866438    -2.100921      21.23
 C       3.439091     1.550769     0.840399      -9.19
 C       2.146131     2.023637     1.760448      96.77
 H       2.307760     3.018461     2.078545      25.87
 O       1.997149     1.281816     2.958474     275.51
 H       1.571746     0.411426     2.562760      25.53
 C       0.940523     2.073464     0.780452      81.25
 H       1.244828     2.474981    -0.177710      24.22
 C      -0.276647     2.868312     1.466379      98.48
 O       0.216745     4.159745     2.084272     275.03
 H       0.543929     4.516855     1.378893      34.76
 H      -0.960650     2.335094     2.221707      25.84
 H      -1.007906     3.212751     0.648266      25.87
 C      -1.657159    -1.939405    -0.944232      62.22
 H      -2.138769    -2.913593    -0.518008      22.01
 C      -1.345812     0.069240    -2.460164      46.42
 H      -1.585653     0.622740    -3.396454      22.86
 C      -0.422901     0.708723    -1.604600      20.85
 O       0.079879     1.922096    -1.897839     233.55
 C      -0.479683     2.615457    -3.039578     110.50
 H      -0.490364     3.813009    -3.113328      24.39
 H      -0.390086     2.332496    -4.206520      24.96
 H      -1.634028     2.601759    -2.930578      26.38
 C      -0.217101     0.137690    -0.308939      -4.23
 O       0.580659     0.626460     0.719664     146.80
 C      -0.939978    -1.308132    -0.030124      37.47
 H      -0.432049    -1.628648     0.963729      21.70
 C      -2.073966    -1.260893    -2.147782      33.60
 C      -2.974019    -1.930387    -3.190474      72.51
 H      -2.957245    -1.529755    -4.245282      27.49
 O      -2.574851    -3.401049    -3.274853     217.44
 H      -1.783535    -3.625972    -2.940814      33.08
 C      -4.380309    -1.924055    -2.657607     108.32
 H      -4.542043    -2.203541    -1.648970      29.43
 O      -4.939507    -0.563844    -2.715521     217.31
 H      -4.535098     0.120681    -1.926804      24.34
 C      -5.319906    -2.756608    -3.625992     113.29
 O      -5.117742    -4.144951    -3.730787     132.40
 H      -3.966647    -4.305809    -3.410397      23.29
 H      -5.153606    -2.400015    -4.670546      28.59
 H      -6.382008    -2.644266    -3.402321      30.01
55
name = lig-ACN-frame_511
 C       3.708367     1.854876    -0.447998      58.08
 H       3.144369     2.430005    -1.070530      24.62
 C       4.431068     0.716260     1.381078      45.56
 H       4.232578     0.483238     2.438393      23.15
 C       5.600143     0.209543     0.797454       6.03
 O       6.447699    -0.788328     1.280627     244.52
 C       5.879637    -2.166735     1.519643     101.62
 H       5.777204    -2.383579     2.605707      24.22
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 H       6.655860    -2.865342     1.049620      24.74
 H       5.091550    -2.432119     0.899979      30.34
 C       5.689666     0.480754    -0.641695      -5.03
 O       6.888258     0.204478    -1.437677     170.42
 H       7.497185    -0.426762    -0.912507      23.69
 C       4.806394     1.366164    -1.172021      62.85
 H       4.998131     1.679624    -2.122440      23.80
 C       3.458117     1.614132     0.909026      44.08
 C       2.222761     2.077404     1.721251      91.79
 H       2.321604     3.099334     2.090938      24.17
 O       1.859867     1.304499     2.999637     204.98
 H       1.653451     0.191136     2.715744      19.80
 C       0.910177     2.104544     0.992081      70.33
 H       1.162092     2.524663    -0.048649      22.19
 C      -0.251882     2.928425     1.457041     111.72
 O       0.234196     4.175199     2.047403     247.90
 H       0.746947     4.871192     1.497674      27.21
 H      -0.529877     2.366178     2.342534      25.77
 H      -1.057564     2.894845     0.657712      26.08
 C      -1.756456    -1.903954    -0.998282      72.77
 H      -2.307626    -2.988235    -0.924281      17.66
 C      -1.454562     0.001855    -2.427420      56.05
 H      -1.641629     0.374551    -3.469310      20.64
 C      -0.516125     0.641993    -1.570574      12.18
 O       0.129412     1.920931    -1.876466     171.75
 C      -0.532981     2.635968    -3.061197      85.27
 H       0.026671     3.582714    -2.778155      23.97
 H       0.150962     2.092523    -3.914674      23.84
 H      -1.675235     2.449270    -3.053076      25.26
 C      -0.248631     0.019806    -0.327347      30.21
 O       0.536541     0.549101     0.686910     140.16
 C      -0.822489    -1.120624    -0.083045      64.93
 H      -0.611728    -1.656785     0.857984      24.22
 C      -1.977988    -1.219138    -2.180450      42.34
 C      -2.831787    -2.035300    -3.123582      80.06
 H      -2.730496    -1.421552    -4.071506      27.44
 O      -2.656855    -3.394362    -3.411494     247.51
 H      -1.834101    -3.619135    -2.936562      30.25
 C      -4.400373    -1.952500    -2.694270      91.12
 H      -4.345464    -2.485252    -1.774026      29.73
 O      -4.942102    -0.584703    -2.641478     257.27
 H      -4.782616    -0.260385    -1.771698      30.29
 C      -5.313688    -2.723204    -3.701646     119.43
 O      -5.097338    -4.191832    -3.732936     100.83
 H      -3.915915    -4.231226    -3.473340      20.76
 H      -5.054702    -2.222636    -4.651476      28.82
 H      -6.360370    -2.474830    -3.443757      29.59
55
name = lig-ACN-frame_512
 C       3.590230     1.826273    -0.485271      44.29
 H       2.860110     2.419257    -0.815914      23.87
 C       4.410772     0.645103     1.583084      38.89
 H       4.224202     0.153539     2.596275      21.45
 C       5.557990     0.223292     0.779442      -2.32
 O       6.455882    -0.792772     1.293942     273.91
 C       5.884094    -2.134028     1.441775      92.24
 H       5.410045    -2.164713     2.470948      25.55
 H       6.661037    -3.012996     1.365222      24.20
 H       5.066816    -2.106296     0.830647      30.91
 C       5.879428     0.557386    -0.595619      -6.29
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 O       6.886448     0.122318    -1.403386     214.64
 H       7.531521    -0.372258    -0.937419      25.31
 C       4.778650     1.381926    -1.229872      45.93
 H       4.699625     1.416369    -2.272293      22.42
 C       3.506359     1.578630     0.942690       5.30
 C       2.251918     2.038931     1.822307      80.67
 H       2.587038     3.053872     2.201345      23.17
 O       1.805809     1.327549     2.986112     232.99
 H       2.109448     0.301806     2.796641      23.29
 C       0.924714     2.025275     0.860967      68.26
 H       1.050215     2.488095    -0.234287      20.65
 C      -0.213381     2.907459     1.610351     104.47
 O       0.213778     4.224901     2.001149     161.75
 H       0.761054     4.845597     1.105407      23.26
 H      -0.734731     2.550212     2.443939      26.61
 H      -0.996536     3.182821     0.855944      24.97
 C      -1.698926    -1.756238    -0.907227      66.07
 H      -1.917329    -2.873140    -0.433909      23.39
 C      -1.475385    -0.004055    -2.520559      56.27
 H      -1.687295     0.473872    -3.516204      20.98
 C      -0.605043     0.697151    -1.606420      15.93
 O       0.050830     1.841549    -1.871484     243.15
 C      -0.370797     2.611832    -2.987586     116.55
 H      -0.221759     3.695294    -3.088087      25.57
 H      -0.143024     2.137276    -4.114142      24.58
 H      -1.543313     2.710938    -3.112705      26.14
 C      -0.245988     0.088741    -0.340032      -1.48
 O       0.543168     0.584527     0.722987     129.26
 C      -0.837390    -1.290096    -0.013347      47.86
 H      -0.746166    -1.671396     0.910062      21.88
 C      -1.926108    -1.340933    -2.212179      49.21
 C      -2.947801    -1.857293    -3.198874      59.38
 H      -2.872904    -1.465851    -4.271648      25.69
 O      -2.598074    -3.478129    -3.506484     106.81
 H      -1.592461    -3.881900    -3.132634      24.11
 C      -4.411593    -1.979958    -2.719855     103.21
 H      -4.604532    -2.500522    -1.810938      30.99
 O      -4.919689    -0.659528    -2.554399     274.77
 H      -4.870438    -0.310915    -1.724576      31.88
 C      -5.263799    -2.696104    -3.794112     106.83
 O      -5.110029    -4.172768    -3.726255     101.39
 H      -4.002225    -4.347373    -3.806151      24.78
 H      -5.270587    -2.341928    -4.818184      30.26
 H      -6.315911    -2.646156    -3.387229      29.87
55
name = lig-ACN-frame_513
 C       3.641997     1.791372    -0.427210      48.07
 H       2.934854     2.167688    -1.088771      22.25
 C       4.519730     0.598741     1.592074      53.22
 H       4.462812     0.203179     2.681706      22.04
 C       5.562458     0.118943     0.768545      -7.02
 O       6.498024    -0.762809     1.297380     258.60
 C       5.775934    -2.035818     1.397458     112.22
 H       5.208981    -2.209282     2.385814      26.60
 H       6.751632    -2.715789     1.400748      23.81
 H       5.341110    -2.456016     0.586108      29.96
 C       5.806561     0.739805    -0.529043      -2.97
 O       6.833629     0.064659    -1.334934     167.60
 H       7.516370    -0.393134    -0.791655      21.43
 C       4.715875     1.345477    -1.200430      42.49
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 H       4.859649     1.538768    -2.288721      20.68
 C       3.483191     1.408119     1.045235      19.52
 C       2.204816     1.985008     1.732823      92.39
 H       2.191555     3.108940     2.035932      24.27
 O       1.875317     1.289519     2.987147     281.62
 H       2.045352     0.424264     2.896338      32.18
 C       0.944026     2.022442     0.857412      74.82
 H       1.191361     2.536908    -0.217701      21.60
 C      -0.229075     2.900111     1.639290     100.70
 O       0.241667     4.304806     1.976728     182.53
 H       0.523108     4.534929     0.865653      24.49
 H      -0.392722     2.357492     2.503025      27.91
 H      -1.126873     2.796502     0.978973      26.48
 C      -1.667848    -1.905959    -0.861548      47.87
 H      -2.397074    -2.886294    -0.695604      20.08
 C      -1.402947    -0.021067    -2.584601      50.03
 H      -1.700510     0.504545    -3.528377      23.22
 C      -0.655244     0.617494    -1.563760       8.56
 O       0.000920     1.858701    -1.884347     178.22
 C      -0.341602     2.645381    -3.044040      99.11
 H       0.340740     3.428639    -2.824841      25.32
 H       0.036171     2.066686    -4.087169      24.13
 H      -1.477631     2.776326    -2.907763      25.81
 C      -0.297226     0.087015    -0.253964      16.92
 O       0.538911     0.668450     0.716951     163.93
 C      -0.742635    -1.146287     0.111362      42.85
 H      -0.402203    -1.519758     0.919363      25.71
 C      -1.984634    -1.289654    -2.273296      30.96
 C      -2.967864    -1.994498    -3.267842      58.60
 H      -3.065599    -1.230956    -4.143486      28.30
 O      -2.531748    -3.463878    -3.591001     142.32
 H      -1.477953    -3.318019    -3.279364      25.34
 C      -4.420411    -2.020313    -2.752961      95.70
 H      -4.334431    -2.676630    -1.884759      29.91
 O      -4.951364    -0.676240    -2.514583     235.42
 H      -4.456606    -0.284460    -1.627547      25.79
 C      -5.334729    -2.773916    -3.809078     126.76
 O      -5.115295    -4.136882    -3.765761     169.95
 H      -4.162805    -4.245812    -3.870090      29.00
 H      -5.019288    -2.363972    -4.771441      30.03
 H      -6.413874    -2.432843    -3.612359      29.47
55
name = lig-ACN-frame_514
 C       3.656070     1.681037    -0.296657      71.42
 H       2.760059     2.227952    -0.637991      23.42
 C       4.530665     0.622274     1.548038      30.52
 H       4.579070     0.426817     2.668824      19.91
 C       5.604163     0.230988     0.781279      18.36
 O       6.484425    -0.749181     1.264846     256.09
 C       5.844134    -2.089391     1.378184      78.04
 H       4.935799    -1.876626     2.060524      25.84
 H       6.554565    -2.899592     1.873261      21.72
 H       5.416675    -2.167568     0.437700      31.39
 C       5.765916     0.560903    -0.520870      18.70
 O       6.723857     0.107745    -1.251519      92.90
 H       7.401981    -0.323408    -0.547094      19.80
 C       4.760084     1.365524    -1.095033      60.40
 H       4.852253     1.780525    -2.185826      21.94
 C       3.444984     1.333811     0.956839       7.23
 C       2.200719     1.906888     1.700245      70.28
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 H       2.671752     2.941212     1.975138      23.05
 O       1.992143     1.245933     3.001379     275.88
 H       1.777736     0.381323     2.663006      28.27
 C       0.885968     2.116324     0.904209      88.89
 H       1.137946     2.676929    -0.123744      22.17
 C      -0.154626     2.844912     1.636196     112.93
 O       0.221729     4.257304     1.870369     286.84
 H       0.510402     5.008518     1.320355      28.18
 H      -0.114945     2.551663     2.666182      26.35
 H      -1.171936     2.880968     1.304287      26.67
 C      -1.606564    -1.861369    -0.959481      70.39
 H      -1.966667    -2.932938    -0.521930      21.67
 C      -1.375324    -0.114010    -2.515468      59.18
 H      -1.411125     0.324292    -3.545027      24.36
 C      -0.593357     0.651180    -1.567034      13.82
 O      -0.015032     1.842727    -1.832094     211.03
 C      -0.306733     2.668632    -3.053124     112.84
 H       0.352974     3.437801    -3.120713      27.71
 H      -0.189554     1.954431    -4.076865      24.19
 H      -1.193042     3.337262    -3.284190      26.80
 C      -0.365289     0.151673    -0.247533      13.11
 O       0.496992     0.701339     0.663189     164.71
 C      -0.865323    -1.201834     0.031101      52.33
 H      -0.541030    -1.637249     0.816638      25.84
 C      -2.017192    -1.344082    -2.123185      50.56
 C      -2.899777    -2.072464    -3.249671      58.55
 H      -2.814609    -1.538843    -4.276925      26.39
 O      -2.438929    -3.312324    -3.646435     257.94
 H      -1.523510    -3.456826    -3.652180      31.62
 C      -4.469788    -2.105190    -2.733416      95.96
 H      -4.603851    -2.622375    -1.760617      27.70
 O      -4.962196    -0.744810    -2.508472     201.64
 H      -4.308763    -0.143672    -1.773092      23.21
 C      -5.343764    -2.686123    -3.818013     106.73
 O      -5.152597    -4.210305    -3.818597     198.98
 H      -4.287054    -4.274912    -3.726299      34.76
 H      -5.139462    -2.257441    -4.793491      29.23
 H      -6.485394    -2.643382    -3.638467      27.53
55
name = lig-ACN-frame_515
 C       3.544433     1.687181    -0.415427      33.10
 H       2.997428     2.537854    -1.009769      20.78
 C       4.464468     0.665552     1.658790      48.79
 H       4.345108     0.374157     2.707257      22.16
 C       5.622261     0.244423     0.908365     -13.07
 O       6.562846    -0.761182     1.297272     243.88
 C       5.844857    -2.056301     1.344126      83.07
 H       4.838321    -1.976913     1.898699      27.29
 H       6.514861    -2.805846     1.913172      23.78
 H       5.761431    -2.682884     0.451448      26.70
 C       5.604993     0.455591    -0.543352      -5.14
 O       6.807676     0.093751    -1.280138     174.37
 H       7.459074    -0.508183    -0.801251      24.00
 C       4.775223     1.449429    -1.047629      40.32
 H       4.906280     1.782492    -2.189436      20.93
 C       3.400520     1.245309     1.001069      27.92
 C       2.341165     1.888638     1.796465      83.26
 H       2.580564     2.992775     2.200499      23.50
 O       2.073976     1.190354     2.968415     226.89
 H       1.742091     0.130093     2.827135      22.55
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 C       0.908180     2.093007     0.856735      64.54
 H       0.996919     2.672141    -0.145957      22.18
 C      -0.129387     2.920050     1.749161     117.34
 O       0.200064     4.267745     1.843560     329.98
 H       0.382254     4.363979     1.026844      35.74
 H      -0.297136     2.402489     2.730242      26.36
 H      -1.012955     2.656609     1.205442      27.77
 C      -1.628778    -1.961081    -0.900982      53.31
 H      -1.657153    -3.099167    -0.794668      22.45
 C      -1.356591    -0.127201    -2.438836      54.79
 H      -1.526241     0.104985    -3.525890      22.51
 C      -0.605892     0.649988    -1.594373      20.74
 O      -0.024120     1.958463    -1.837785     216.12
 C      -0.227403     2.667374    -3.101071     111.79
 H       0.639609     3.220055    -3.229831      27.06
 H      -0.362699     1.901396    -4.012464      24.77
 H      -1.200564     2.984576    -2.762974      25.48
 C      -0.447651     0.148896    -0.293969      18.78
 O       0.445632     0.707507     0.647635     147.12
 C      -0.899032    -1.162489    -0.031893      60.10
 H      -0.787762    -1.576457     0.866353      23.62
 C      -1.998863    -1.378677    -2.186122      49.38
 C      -2.880939    -1.952867    -3.126634      66.25
 H      -3.112631    -1.072552    -3.843389      28.00
 O      -2.355926    -3.329118    -3.675310     198.12
 H      -1.469334    -3.217907    -3.591608      30.34
 C      -4.426864    -2.111452    -2.702524      89.03
 H      -4.588489    -2.840404    -1.858441      29.56
 O      -4.960017    -0.816906    -2.557641     259.86
 H      -4.528641    -0.310144    -1.776108      27.89
 C      -5.361491    -2.768728    -3.835299     107.45
 O      -5.209025    -4.214383    -3.884929     152.10
 H      -4.171205    -4.463579    -3.783169      27.64
 H      -5.262913    -2.287412    -4.796275      29.29
 H      -6.383202    -2.508445    -3.367206      28.45
55
name = lig-ACN-frame_516
 C       3.552040     1.748071    -0.443584      61.66
 H       2.601322     2.343138    -0.879119      21.46
 C       4.484053     0.606686     1.692611      41.11
 H       4.353465     0.446625     2.724198      21.85
 C       5.561546     0.112287     0.906709      -5.99
 O       6.572535    -0.756766     1.360533     267.53
 C       5.930839    -2.106697     1.367293      79.02
 H       4.841273    -1.981710     1.639129      28.84
 H       6.485460    -2.573795     2.205245      23.01
 H       5.995248    -2.432860     0.291053      24.23
 C       5.703855     0.492058    -0.465343     -11.97
 O       6.810600     0.078038    -1.335301     167.09
 H       7.334139    -0.439223    -0.762295      28.41
 C       4.731314     1.395618    -1.119106      40.26
 H       5.126524     1.842875    -2.127199      20.18
 C       3.429168     1.349217     0.899683     -24.21
 C       2.251950     1.899310     1.770955      64.56
 H       2.533688     3.036253     2.129012      22.64
 O       2.083361     1.108230     3.036316     166.10
 H       2.227951     0.039808     2.544717      20.30
 C       0.974636     2.036643     1.002521      86.65
 H       1.228899     2.512180     0.060851      23.65
 C      -0.183977     2.785346     1.778731      99.14
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 O       0.179616     4.305453     1.816017     228.11
 H       0.488455     4.783820     0.937581      26.26
 H      -0.177960     2.433949     2.889220      24.79
 H      -1.123165     2.865262     1.349992      26.11
 C      -1.642964    -2.062758    -0.911230      48.78
 H      -2.086825    -3.016321    -0.682106      20.06
 C      -1.402817    -0.071157    -2.553705      59.38
 H      -1.712740     0.485820    -3.469013      23.12
 C      -0.618491     0.745769    -1.606168       5.80
 O       0.003109     1.949237    -1.832726     216.38
 C      -0.256346     2.619531    -3.109405     125.57
 H       0.566030     3.312755    -3.185366      26.53
 H      -0.340007     1.896993    -4.008396      25.50
 H      -0.940756     3.415537    -3.306600      27.59
 C      -0.407133     0.175742    -0.294285       5.87
 O       0.390976     0.695418     0.691888     161.68
 C      -0.910437    -1.160770     0.066424      36.85
 H      -0.495658    -1.322097     0.987407      23.61
 C      -1.864059    -1.378859    -2.102740      25.28
 C      -2.979323    -1.943974    -3.169833      66.35
 H      -2.842950    -1.418949    -4.159847      27.34
 O      -2.351899    -3.261581    -3.657130     182.63
 H      -1.267884    -3.247535    -3.481413      24.89
 C      -4.365526    -2.209087    -2.737604     103.37
 H      -4.304097    -2.663711    -1.707942      27.37
 O      -4.986064    -0.834548    -2.581146     258.43
 H      -4.870608    -0.508672    -1.787150      33.29
 C      -5.323452    -2.838555    -3.763109     108.21
 O      -5.265613    -4.230693    -3.948755     134.64
 H      -4.112354    -4.426941    -4.092731      26.32
 H      -5.147881    -2.343404    -4.717435      29.50
 H      -6.403040    -2.652875    -3.497879      28.79
55
name = lig-ACN-frame_517
 C       3.660961     1.746026    -0.403403      45.79
 H       2.765069     2.172560    -1.077424      21.19
 C       4.452134     0.616671     1.490093      61.66
 H       4.482859     0.442631     2.512135      25.30
 C       5.537136     0.065556     0.785330      -2.55
 O       6.499089    -0.739067     1.458207     280.92
 C       6.077803    -2.158821     1.424549      88.89
 H       4.975308    -2.134141     1.440240      30.35
 H       6.420719    -2.916558     2.081434      25.69
 H       6.376270    -2.720006     0.417754      24.77
 C       5.805520     0.614101    -0.512840       7.95
 O       6.719208     0.073855    -1.284010     156.62
 H       7.592805    -0.179192    -0.857678      22.10
 C       4.775637     1.270576    -1.145892      45.63
 H       4.855688     1.567687    -2.221154      20.24
 C       3.503913     1.469469     0.985404      31.49
 C       2.211300     1.810132     1.822392      80.85
 H       2.408389     2.984439     2.235563      23.37
 O       2.100310     1.061237     3.033308     220.25
 H       2.311649    -0.018906     2.843894      22.29
 C       0.830734     1.980822     1.067165      91.22
 H       1.009843     2.605684     0.232168      26.15
 C      -0.156425     2.853175     1.745925     110.15
 O       0.133093     4.258798     1.867056     175.18
 H       0.534514     4.815153     0.894696      23.30
 H      -0.224337     2.678119     2.902926      25.10
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 H      -1.044956     2.437186     1.371071      27.46
 C      -1.563690    -1.886368    -0.815189      52.48
 H      -2.057762    -2.674537    -0.455546      23.31
 C      -1.426175     0.001301    -2.495548      57.43
 H      -1.857078     0.331147    -3.440126      23.03
 C      -0.667396     0.720000    -1.582343      19.10
 O      -0.027683     1.958280    -1.851856     218.66
 C      -0.210971     2.648678    -3.179325     108.79
 H       0.804068     3.134307    -3.390071      24.49
 H      -0.217192     1.854658    -3.914509      26.97
 H      -1.152500     3.050680    -3.060967      27.76
 C      -0.385784     0.114196    -0.319371      17.15
 O       0.395201     0.644109     0.803623     145.07
 C      -0.885083    -1.156833     0.079473      52.73
 H      -0.726927    -1.721284     0.960366      23.65
 C      -1.943795    -1.294289    -2.229734      24.72
 C      -2.777506    -2.009796    -3.277699      59.31
 H      -3.071971    -1.213215    -4.057036      27.38
 O      -2.401185    -3.255234    -3.612634     186.90
 H      -1.231788    -3.400679    -3.502082      23.42
 C      -4.386175    -2.166283    -2.674888      80.06
 H      -4.490228    -2.822190    -1.733384      27.13
 O      -5.024150    -0.877686    -2.607908     231.61
 H      -4.763104    -0.455040    -1.713985      27.30
 C      -5.305776    -2.846118    -3.740769      97.48
 O      -5.254743    -4.337239    -4.005696     172.03
 H      -4.294471    -4.537643    -4.355507      30.04
 H      -5.130734    -2.259925    -4.650644      29.65
 H      -6.320676    -2.633561    -3.377251      29.30
55
name = lig-ACN-frame_518
 C       3.681860     1.751069    -0.410665      34.20
 H       2.956153     2.423675    -1.016710      23.14
 C       4.476659     0.611384     1.460154      29.32
 H       4.324975     0.100774     2.385474      21.94
 C       5.592111     0.136910     0.762467      11.22
 O       6.401663    -0.758651     1.539958     250.56
 C       6.178450    -2.249556     1.411826      91.68
 H       5.151019    -2.590824     1.438918      30.29
 H       6.660740    -2.332185     2.309842      24.09
 H       6.795992    -2.613919     0.448991      22.54
 C       5.799806     0.556639    -0.547362      -0.20
 O       6.822834     0.032161    -1.349337     144.91
 H       7.642615    -0.128073    -0.701482      21.48
 C       4.761719     1.287792    -1.170614      62.32
 H       4.722734     1.139905    -2.197436      22.72
 C       3.475011     1.529298     0.985847      22.60
 C       2.254377     1.831005     1.880281      72.08
 H       2.316741     2.971804     2.412181      22.73
 O       2.125782     1.021822     3.058619     252.15
 H       1.922036     0.107608     2.702136      25.75
 C       0.867852     1.956798     0.995492      75.35
 H       1.011312     2.228616     0.036432      25.86
 C      -0.256518     2.858219     1.870436     101.38
 O       0.083075     4.254705     1.900949     165.26
 H       0.373699     4.427040     0.800682      25.00
 H      -0.396924     2.349081     2.894812      26.03
 H      -1.156213     3.013217     1.300414      25.20
 C      -1.702914    -1.735395    -0.985390      65.78
 H      -1.822328    -2.701196    -0.899355      24.81
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 C      -1.514298     0.025397    -2.454487      54.56
 H      -1.461372     0.544016    -3.387473      19.54
 C      -0.630325     0.713444    -1.507610       6.67
 O      -0.053958     1.957345    -1.851699     210.51
 C      -0.187235     2.535887    -3.196640     116.62
 H       0.429454     3.589432    -3.045876      23.10
 H      -0.194027     1.979678    -4.060690      28.13
 H      -1.024469     3.138161    -3.289515      28.49
 C      -0.295004     0.152850    -0.179253      17.72
 O       0.369645     0.567788     0.873181     165.37
 C      -0.823623    -1.126578     0.028480      42.27
 H      -0.663460    -1.394630     1.132922      21.04
 C      -1.954323    -1.250837    -2.160210      49.38
 C      -2.849545    -1.944995    -3.178680      70.28
 H      -2.751977    -1.414505    -4.184041      25.16
 O      -2.390915    -3.397207    -3.615458     178.24
 H      -1.274692    -3.353450    -3.651778      24.55
 C      -4.340272    -2.160257    -2.711681      82.88
 H      -4.255262    -2.656284    -1.667873      27.16
 O      -5.045334    -0.902963    -2.577965     214.98
 H      -4.487757    -0.144358    -1.913860      24.02
 C      -5.302523    -2.921267    -3.780826     105.02
 O      -5.216723    -4.357893    -4.026041     244.46
 H      -4.429125    -4.462165    -4.336759      37.62
 H      -5.321734    -2.421623    -4.774963      29.24
 H      -6.297066    -2.838083    -3.379230      29.34
55
name = lig-ACN-frame_519
 C       3.605436     1.862723    -0.430025      59.18
 H       2.845145     2.518830    -0.860216      23.52
 C       4.445757     0.609314     1.557455      38.75
 H       4.204336     0.201289     2.576110      20.69
 C       5.605762     0.176552     0.865925      10.01
 O       6.291917    -0.779639     1.541202     226.41
 C       6.368210    -2.234918     1.465091      92.25
 H       5.389999    -2.648705     1.282575      31.35
 H       6.799217    -2.757977     2.244087      24.54
 H       7.069985    -2.646307     0.553869      24.14
 C       5.819155     0.405078    -0.643243     -12.34
 O       6.956302     0.014848    -1.402283     127.19
 H       7.603814    -0.485983    -0.867669      28.53
 C       4.763132     1.271055    -1.208485      35.98
 H       4.849941     1.612659    -2.170866      23.11
 C       3.515739     1.460571     0.925146      23.99
 C       2.235793     1.958808     1.848041      59.66
 H       2.566109     3.116745     2.257520      23.16
 O       2.119294     1.011968     3.051958     235.39
 H       2.064656     0.165208     2.776166      29.02
 C       0.904859     1.958211     1.089980      92.18
 H       1.059921     2.441974     0.237934      28.69
 C      -0.339728     2.746643     1.796377      91.14
 O       0.099847     4.269151     1.961337     220.01
 H       0.213530     4.663697     1.125991      29.80
 H      -0.417497     2.514861     2.905136      26.03
 H      -1.346560     2.470296     1.375871      26.75
 C      -1.716615    -1.857529    -0.891474      43.60
 H      -2.013762    -2.823325    -0.729327      22.50
 C      -1.428718     0.184307    -2.401738      66.42
 H      -1.658232     0.567830    -3.365131      23.17
 C      -0.585491     0.758954    -1.460677      28.50
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 O      -0.060025     1.936740    -1.837028     222.07
 C      -0.247295     2.560301    -3.153773     110.63
 H       0.734620     3.320584    -3.197316      23.19
 H       0.285393     1.931198    -3.735708      28.90
 H      -1.212860     2.701043    -3.418736      28.00
 C      -0.346156     0.162322    -0.221953      23.75
 O       0.420773     0.594635     1.010207     124.52
 C      -0.897665    -1.128386    -0.059320      49.84
 H      -0.578296    -1.817690     0.864496      20.90
 C      -2.048315    -1.144051    -2.228386      51.17
 C      -2.891278    -2.010682    -3.239746      68.09
 H      -2.946975    -1.409730    -4.197933      25.07
 O      -2.392453    -3.450459    -3.552531     213.71
 H      -1.459052    -3.397826    -3.691859      29.53
 C      -4.353281    -2.191874    -2.810998      91.05
 H      -4.341602    -2.821407    -1.836736      25.89
 O      -5.052430    -0.899966    -2.558810     235.06
 H      -4.380673    -0.290355    -1.917163      24.53
 C      -5.331926    -2.964782    -3.775688     106.78
 O      -5.134953    -4.357936    -4.012702     232.16
 H      -4.131390    -4.527708    -4.206652      30.07
 H      -5.217899    -2.334834    -4.700466      28.70
 H      -6.284316    -2.796055    -3.348895      28.76
55
name = lig-ACN-frame_520
 C       3.736286     1.809768    -0.451107      60.36
 H       3.121841     2.432254    -1.000625      26.87
 C       4.433900     0.661252     1.527110      26.54
 H       4.518392     0.538762     2.675969      21.16
 C       5.516523     0.037715     0.764395      -1.79
 O       6.348935    -0.807496     1.652144     235.99
 C       6.501558    -2.233176     1.396707     103.19
 H       5.565804    -2.698170     1.152460      31.48
 H       6.800536    -2.472173     2.391835      24.00
 H       7.323591    -2.364130     0.520577      22.51
 C       5.733690     0.380758    -0.580386      -7.83
 O       6.959247     0.019919    -1.391124     155.30
 H       7.529409    -0.560142    -0.910796      25.39
 C       4.781158     1.300864    -1.194042      45.42
 H       5.122032     1.780324    -2.039028      19.88
 C       3.412951     1.456800     0.944051      10.54
 C       2.288319     1.884758     1.837104      88.77
 H       2.448758     3.061452     2.337279      22.66
 O       2.130242     1.160243     3.009569     254.72
 H       2.201716     0.282195     2.685459      29.45
 C       0.841191     2.045274     1.193654      89.58
 H       0.954811     2.398396     0.256533      27.51
 C      -0.230313     2.783640     1.795096     121.53
 O       0.049725     4.171856     2.010565     278.24
 H       0.040725     4.691323     1.298487      32.16
 H      -0.435553     2.412650     2.819252      26.94
 H      -1.068692     2.533529     1.049810      26.74
 C      -1.748977    -1.848825    -1.027267      59.30
 H      -2.207215    -2.754533    -0.648577      22.15
 C      -1.488455     0.063839    -2.414035      60.40
 H      -1.731849     0.702648    -3.229935      23.94
 C      -0.616350     0.807524    -1.475380      -7.49
 O       0.012406     2.079000    -1.737916     206.47
 C      -0.142490     2.483052    -3.138018     119.28
 H      -0.113421     3.720366    -3.121931      23.95
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 H       0.159325     1.870435    -3.866188      30.21
 H      -1.175464     2.559054    -3.322155      29.08
 C      -0.362735     0.128580    -0.140241      -6.17
 O       0.424519     0.583271     0.963635     110.57
 C      -0.934346    -1.205007    -0.007407      34.25
 H      -0.412473    -1.801904     0.958500      22.21
 C      -2.084759    -1.202189    -2.162273      35.22
 C      -2.864839    -2.026706    -3.368905      57.79
 H      -2.953577    -1.546954    -4.369512      26.83
 O      -2.410611    -3.377873    -3.448509     278.14
 H      -1.541863    -3.481832    -3.510861      33.92
 C      -4.461312    -2.245109    -2.780060      89.67
 H      -4.444955    -2.897046    -1.830576      26.58
 O      -5.006806    -0.941713    -2.574485     272.24
 H      -4.697515    -0.591716    -1.763811      29.61
 C      -5.343015    -2.893961    -3.812995     106.71
 O      -5.034502    -4.372321    -3.983260     169.46
 H      -3.865663    -4.390748    -3.908725      25.44
 H      -5.432998    -2.480534    -4.851886      27.96
 H      -6.341592    -2.914570    -3.443954      28.82
55
name = lig-ACN-frame_521
 C       3.724358     1.767697    -0.438034      51.96
 H       3.167638     2.484171    -0.906366      24.75
 C       4.493135     0.654703     1.437994      39.72
 H       4.499436     0.518627     2.589720      21.97
 C       5.423914    -0.149996     0.796962       6.03
 O       6.366443    -0.726533     1.667235     264.10
 C       6.612229    -2.190116     1.338488     113.31
 H       5.746475    -2.757407     0.939861      29.08
 H       7.000237    -2.738270     2.232662      25.75
 H       7.526907    -2.425428     0.669570      24.98
 C       5.782836     0.334504    -0.556562      12.83
 O       6.791955     0.045382    -1.295844     136.07
 H       7.574838    -0.265631    -0.680396      21.07
 C       4.952015     1.315545    -1.117430      62.18
 H       5.067249     1.522649    -2.186899      23.43
 C       3.466127     1.425989     0.874548       8.91
 C       2.225037     1.962165     1.801644      82.93
 H       2.601683     3.156501     2.007472      22.57
 O       2.186464     1.231739     3.052552     210.40
 H       1.882883     0.201467     2.935847      24.06
 C       0.966479     1.973597     1.001084      67.74
 H       1.137359     2.502376     0.082673      26.48
 C      -0.264336     2.786054     1.860641     101.90
 O       0.020342     4.169220     2.115809     150.94
 H       0.013485     4.493919     1.031366      24.38
 H      -0.664745     2.293558     2.694943      28.28
 H      -1.182926     2.859088     1.182918      26.86
 C      -1.742894    -1.830404    -0.945120      20.80
 H      -2.006833    -2.942679    -1.002048      20.35
 C      -1.510329     0.060456    -2.388433      53.54
 H      -1.686793     0.380227    -3.420949      20.13
 C      -0.684977     0.703069    -1.382837       0.81
 O       0.059410     2.131567    -1.667738     137.56
 C      -0.208531     2.508422    -3.085360     110.36
 H       0.315021     3.613354    -3.228277      23.85
 H       0.528979     2.075810    -3.668202      28.59
 H      -1.234322     2.288502    -3.347058      26.40
 C      -0.403178     0.110444    -0.164348      23.87
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 O       0.388363     0.570316     0.860671     133.20
 C      -0.908575    -1.201709     0.001590      46.41
 H      -0.876775    -1.797008     1.142027      18.91
 C      -2.077393    -1.261063    -2.286451      21.43
 C      -2.972747    -2.000634    -3.241990      92.99
 H      -2.813361    -1.441521    -4.160566      26.21
 O      -2.416042    -3.355706    -3.356525     250.65
 H      -1.389699    -3.198739    -3.449591      27.62
 C      -4.417266    -2.205474    -2.842282      90.53
 H      -4.330754    -2.837613    -1.897627      27.62
 O      -5.004967    -0.948578    -2.566034     300.27
 H      -4.818510    -0.639879    -1.724851      32.05
 C      -5.408953    -2.998044    -3.893313      99.95
 O      -4.926868    -4.327541    -3.934602     230.04
 H      -3.850369    -4.280396    -3.778217      27.14
 H      -5.229932    -2.337091    -4.797729      28.62
 H      -6.441386    -2.962119    -3.562099      28.23
55
name = lig-ACN-frame_522
 C       3.744033     1.801894    -0.536970      72.79
 H       3.038440     2.375202    -1.075194      22.54
 C       4.412864     0.532905     1.531330      33.76
 H       4.216415     0.279617     2.604540      21.47
 C       5.480946    -0.128737     0.827534      11.73
 O       6.387713    -0.789712     1.603610     234.05
 C       6.739620    -2.143912     1.319120     109.64
 H       5.797557    -2.517062     0.846069      28.62
 H       6.878960    -2.685285     2.329723      23.95
 H       7.477951    -2.102508     0.583767      24.14
 C       5.677742     0.347828    -0.428582      17.20
 O       6.825922    -0.043119    -1.250422     146.80
 H       7.737026    -0.211945    -0.776298      22.40
 C       4.897291     1.333314    -1.050049      73.19
 H       5.268006     1.579446    -2.120936      23.84
 C       3.532706     1.405823     0.871966      -7.58
 C       2.334377     1.933719     1.684082      35.53
 H       2.272172     3.135643     2.091363      22.21
 O       2.231597     1.319045     3.105272     146.65
 H       1.803269     0.305576     2.735832      25.27
 C       0.864900     1.947764     0.925155      79.29
 H       0.980972     2.393094    -0.121857      24.37
 C      -0.299744     2.695994     1.739239      88.89
 O       0.040060     4.215025     2.213234      52.85
 H       0.273045     4.986850     1.335891      22.28
 H      -0.190582     2.324943     2.703831      28.38
 H      -1.188050     2.389802     1.066444      26.63
 C      -1.719172    -1.887195    -0.959925      56.61
 H      -1.912551    -2.961131    -0.506380      18.97
 C      -1.491938     0.083319    -2.421864      66.11
 H      -1.480888     0.648166    -3.370369      20.42
 C      -0.696614     0.779783    -1.478148       8.80
 O      -0.068068     1.969667    -1.637458     222.14
 C      -0.134657     2.544124    -2.982611     117.45
 H      -0.010280     3.741537    -3.003027      24.92
 H       0.385765     1.877476    -3.600553      29.30
 H      -1.182210     2.534275    -3.504894      26.69
 C      -0.432998     0.073693    -0.186552      12.45
 O       0.413086     0.601914     0.788038     164.23
 C      -0.995515    -1.212208     0.005296      29.55
 H      -0.697138    -1.743211     1.199195      22.88
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 C      -1.996824    -1.205442    -2.114693      50.89
 C      -2.939740    -1.957476    -3.179460      63.71
 H      -3.065219    -1.486925    -4.133119      28.40
 O      -2.429106    -3.358309    -3.287359     155.12
 H      -1.282894    -3.423892    -3.608038      22.84
 C      -4.487157    -2.189847    -2.836599      91.28
 H      -4.598047    -2.881039    -1.945138      26.69
 O      -5.087120    -0.886798    -2.559718     221.81
 H      -4.441263    -0.441342    -1.779676      24.04
 C      -5.275781    -2.967230    -3.891703     108.21
 O      -4.842297    -4.354664    -3.912269     279.85
 H      -3.956502    -4.260219    -3.969597      35.14
 H      -5.350933    -2.696718    -4.999969      27.37
 H      -6.336038    -2.957657    -3.531249      27.75
55
name = lig-ACN-frame_523
 C       3.705389     1.820142    -0.440575      55.10
 H       3.017958     2.473823    -1.046210      24.45
 C       4.279152     0.398961     1.592398      44.21
 H       4.071725     0.091007     2.596030      19.07
 C       5.495225     0.023033     0.966939      -1.04
 O       6.429583    -0.814365     1.615453     256.35
 C       6.733725    -2.180450     1.238360     112.79
 H       5.985060    -2.917792     0.817085      29.19
 H       7.067721    -2.573702     2.297649      24.17
 H       7.613537    -2.459974     0.807305      26.55
 C       5.790654     0.364800    -0.468246      -8.14
 O       6.855358    -0.136210    -1.201312     120.75
 H       7.471533    -0.435094    -0.550538      25.32
 C       4.884480     1.277494    -1.144383      26.55
 H       5.311873     1.839289    -2.120091      20.40
 C       3.484178     1.417482     0.889857      27.97
 C       2.278947     1.917716     1.677976      75.96
 H       2.743731     3.113280     1.760262      23.74
 O       2.233127     1.408462     2.994880     200.68
 H       2.108768     0.361703     3.028099      25.27
 C       0.874398     1.987102     0.923192      84.29
 H       1.074620     2.538733    -0.127951      25.89
 C      -0.132592     2.742408     1.699567     113.71
 O       0.017604     4.127393     2.218326     192.61
 H       0.249142     4.788475     1.485026      27.68
 H      -0.395112     2.162506     2.589550      28.35
 H      -1.192893     2.940658     1.287877      26.15
 C      -1.677354    -1.927491    -0.879317      31.42
 H      -2.399176    -2.886921    -0.975132      18.63
 C      -1.471317     0.066369    -2.455278      58.21
 H      -1.910703     0.412506    -3.394761      24.73
 C      -0.720159     0.661793    -1.456912      35.03
 O      -0.205681     1.920072    -1.672114     218.84
 C      -0.106285     2.579410    -2.919856     110.92
 H       0.502751     3.454638    -2.556884      26.14
 H       0.578440     2.279350    -3.752272      26.75
 H      -1.253916     2.834836    -3.180718      24.82
 C      -0.461906     0.119475    -0.252603      34.72
 O       0.439622     0.559926     0.745666     127.10
 C      -0.986562    -1.142279     0.093505      40.95
 H      -0.400408    -1.761251     1.149599      21.86
 C      -2.062462    -1.212113    -2.110708       8.07
 C      -2.872645    -1.974065    -3.130271      75.91
 H      -2.634788    -1.465112    -4.040227      26.37
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 O      -2.466276    -3.346911    -3.255192     166.01
 H      -1.269855    -3.405540    -3.458077      22.38
 C      -4.494829    -2.119066    -2.742143      81.28
 H      -4.582625    -2.704837    -1.797122      26.45
 O      -5.164683    -0.847509    -2.570675     198.53
 H      -4.492623    -0.161054    -1.924632      23.99
 C      -5.190807    -2.950185    -3.908517      92.71
 O      -4.780763    -4.407196    -3.895728     244.90
 H      -3.867496    -4.474908    -4.047881      32.85
 H      -5.061575    -2.324538    -4.867593      27.26
 H      -6.280277    -3.013473    -3.596580      26.75
55
name = lig-ACN-frame_524
 C       3.813967     1.737913    -0.366921      54.54
 H       3.203584     2.666089    -0.695505      27.85
 C       4.264857     0.390011     1.495463      29.34
 H       4.099819    -0.014812     2.443378      20.85
 C       5.538255     0.059042     0.898810       2.44
 O       6.428873    -0.775215     1.627436     186.92
 C       6.751761    -2.345583     1.270257      84.56
 H       5.751874    -2.589114     0.758125      28.28
 H       6.871532    -2.884602     2.270753      23.93
 H       7.487520    -2.223344     0.557936      25.05
 C       5.796881     0.435904    -0.448123       0.38
 O       6.864849    -0.209421    -1.100246      36.38
 H       7.536097    -0.700971    -0.607804      16.13
 C       4.897116     1.256629    -1.118898      82.46
 H       4.968561     1.509155    -2.291477      22.15
 C       3.383535     1.269853     0.911820      22.52
 C       2.246608     1.979266     1.637094      84.77
 H       2.344532     3.255913     1.909316      23.18
 O       2.183830     1.473545     2.953821     242.87
 H       2.170132     0.616231     2.799384      34.27
 C       1.015207     1.997106     0.887180      63.42
 H       1.176768     2.511851    -0.199765      27.50
 C      -0.226334     2.787991     1.764075     111.56
 O       0.092559     4.073565     2.219973     252.97
 H       0.140794     4.516664     1.502165      34.57
 H      -0.508370     2.110167     2.623641      27.68
 H      -0.859362     2.688455     0.815330      28.01
 C      -1.756179    -1.803853    -0.839389      62.06
 H      -1.818350    -2.916874    -0.406718      20.85
 C      -1.595716    -0.084590    -2.461159      62.12
 H      -1.692245     0.492360    -3.355504      22.72
 C      -0.765932     0.629806    -1.558798      -6.39
 O      -0.235244     1.939440    -1.646886     189.71
 C      -0.091073     2.730632    -2.873091     106.26
 H       0.587075     3.540507    -2.705614      27.19
 H       0.130813     1.799116    -3.552753      26.25
 H      -0.956163     3.350162    -3.431634      25.53
 C      -0.444171     0.069265    -0.142931      -2.75
 O       0.488588     0.599651     0.718984     131.39
 C      -0.947554    -1.212755     0.085212      33.77
 H      -0.665966    -1.688628     1.340756      20.88
 C      -2.053741    -1.319670    -2.096113      54.59
 C      -2.926305    -1.975804    -3.089518      84.00
 H      -2.986647    -1.477567    -4.044569      26.84
 O      -2.474476    -3.369892    -3.226587     208.00
 H      -1.362206    -3.333279    -3.191118      24.84
 C      -4.384216    -2.063817    -2.704670      87.74
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 H      -4.349905    -2.551558    -1.724797      27.96
 O      -5.201564    -0.832642    -2.621977     239.05
 H      -4.815427    -0.309662    -1.785624      27.38
 C      -5.109403    -2.980349    -3.824696      95.45
 O      -4.787937    -4.367362    -3.908227     207.09
 H      -3.640150    -4.320645    -3.958797      25.25
 H      -4.712873    -2.570987    -4.813732      27.97
 H      -6.243069    -2.873564    -3.968550      26.95
55
name = lig-ACN-frame_525
 C       3.820041     1.750155    -0.358671      42.58
 H       3.284309     2.566780    -1.002861      29.85
 C       4.378032     0.322735     1.480025      60.85
 H       4.194165    -0.087286     2.445938      26.19
 C       5.534283    -0.079657     0.875229      20.55
 O       6.435790    -0.798902     1.648178     263.97
 C       6.596882    -2.267630     1.265112      94.77
 H       5.667571    -2.775176     0.771363      28.60
 H       6.882443    -2.828669     2.164031      26.37
 H       7.520217    -2.578228     0.656519      24.95
 C       5.862351     0.364034    -0.419321      -2.34
 O       6.857642    -0.228091    -1.086513      87.85
 H       7.563948    -0.378319    -0.310236      20.09
 C       4.932458     1.228589    -1.058761      55.93
 H       5.122689     1.402747    -2.190966      18.59
 C       3.420427     1.255413     0.853694      -3.78
 C       2.334564     2.021090     1.640126      49.75
 H       2.749617     3.239209     1.656709      20.51
 O       2.091216     1.487755     3.003181     204.79
 H       1.799321     0.523036     2.939590      27.97
 C       0.858653     2.017548     0.907489      91.84
 H       1.004468     2.560060    -0.134149      26.61
 C      -0.262777     2.639216     1.595722      94.62
 O       0.191720     4.078962     2.214120     134.62
 H       0.055915     4.902962     1.563512      25.49
 H      -0.541315     2.151086     2.613934      27.58
 H      -1.306853     2.842333     1.174353      27.67
 C      -1.818441    -1.899344    -0.743718      16.93
 H      -2.185791    -3.011341    -0.610752      22.84
 C      -1.565768    -0.015607    -2.419848      49.55
 H      -1.814407     0.191896    -3.426120      21.38
 C      -0.738977     0.694171    -1.463512      21.34
 O      -0.309238     1.991629    -1.586910     185.04
 C      -0.077812     2.753116    -2.924721      88.96
 H       0.784503     3.224214    -2.762753      29.59
 H       0.204830     2.188314    -3.994093      25.66
 H      -1.118552     3.290357    -2.881597      24.86
 C      -0.385456     0.116228    -0.230341      23.49
 O       0.561954     0.646719     0.715443     142.59
 C      -0.888361    -1.156506     0.134725      25.63
 H      -0.765473    -1.888232     1.269887      19.59
 C      -2.057807    -1.370765    -2.071861      14.99
 C      -2.965090    -2.012637    -3.108819      71.12
 H      -2.868832    -1.463754    -4.061310      26.45
 O      -2.485389    -3.410458    -3.209296     256.80
 H      -1.546965    -3.472187    -3.370079      31.31
 C      -4.478807    -2.158789    -2.650273      96.65
 H      -4.635790    -2.658730    -1.716100      29.67
 O      -5.149946    -0.851957    -2.663818     253.25
 H      -4.988744    -0.503515    -1.883290      35.04
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 C      -5.011643    -2.916101    -3.845001      98.72
 O      -4.812470    -4.354059    -3.867560     181.43
 H      -3.645674    -4.470253    -3.740704      24.10
 H      -4.682891    -2.384996    -4.785560      28.50
 H      -6.131177    -2.730733    -3.598550      26.85
55
name = lig-ACN-frame_526
 C       3.814258     1.758368    -0.481369      53.81
 H       2.980678     2.362547    -0.979491      26.68
 C       4.316804     0.319078     1.547560      39.87
 H       4.083273     0.072933     2.610207      19.78
 C       5.533643    -0.197722     0.916032       0.89
 O       6.454761    -0.904612     1.628944     229.54
 C       6.484919    -2.232208     1.310351      98.37
 H       5.479533    -2.542449     0.812758      28.35
 H       6.533516    -2.721914     2.252120      25.11
 H       7.378007    -2.311809     0.541210      21.06
 C       5.810461     0.234726    -0.409665       6.43
 O       6.963130    -0.229611    -1.123064     140.87
 H       7.848626    -0.361461    -0.682489      23.56
 C       5.024354     1.204726    -1.060066      57.73
 H       5.456982     1.717303    -1.926967      22.02
 C       3.542075     1.285334     0.882254     -11.74
 C       2.271429     1.935468     1.696425      43.38
 H       2.802083     3.027645     2.043312      22.00
 O       2.034516     1.520413     3.029084     175.09
 H       1.513062     0.506903     2.855055      26.41
 C       0.862893     2.075788     0.821141      65.31
 H       1.020771     2.607772    -0.155476      25.57
 C      -0.310043     2.786034     1.680984     105.87
 O       0.250938     3.993051     2.162996     133.46
 H      -0.185295     4.694928     1.307787      23.11
 H      -0.397840     2.015417     2.542052      27.62
 H      -1.205621     2.845614     0.979144      27.73
 C      -1.760241    -1.917239    -0.750754      60.75
 H      -2.402046    -2.749670    -0.459193      24.56
 C      -1.492438    -0.039342    -2.307651      70.49
 H      -1.725812     0.548716    -3.161037      27.27
 C      -0.749307     0.758287    -1.432427      16.01
 O      -0.344116     2.088050    -1.638979     228.21
 C      -0.131769     2.708509    -2.867277     113.17
 H       0.722646     3.228479    -2.772713      28.96
 H      -0.308411     1.900011    -3.844214      24.20
 H      -0.792006     3.609579    -3.148097      25.87
 C      -0.307288     0.086250    -0.217157       9.48
 O       0.594595     0.593119     0.668206     126.61
 C      -0.973731    -1.207437     0.112507      39.80
 H      -0.222576    -1.345336     1.172335      23.31
 C      -2.041266    -1.253334    -1.974756      47.56
 C      -2.903696    -2.085042    -2.943389      74.27
 H      -2.959141    -1.564049    -3.933771      26.12
 O      -2.494611    -3.470467    -3.225381     253.50
 H      -1.622698    -3.491970    -3.487305      32.03
 C      -4.487892    -2.211299    -2.682419      99.29
 H      -4.676741    -2.807836    -1.814994      28.39
 O      -5.083055    -0.904303    -2.675310     254.90
 H      -4.641281    -0.402080    -1.946533      29.85
 C      -5.139231    -2.902954    -3.884048      99.08
 O      -4.850762    -4.341495    -3.811645     239.72
 H      -3.884475    -4.497393    -3.677902      29.44
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 H      -4.821255    -2.365713    -4.831023      28.03
 H      -6.300675    -2.938463    -4.016097      26.09
55
name = lig-ACN-frame_527
 C       3.864599     1.609125    -0.453442      45.53
 H       3.377925     2.417254    -1.026932      21.78
 C       4.304468     0.374191     1.569874      49.40
 H       4.102134     0.116395     2.669186      20.27
 C       5.451052    -0.166403     0.941434       4.53
 O       6.439153    -0.872279     1.676878     212.18
 C       6.402410    -2.406163     1.323994      78.51
 H       5.475510    -2.562500     0.727377      28.08
 H       6.526388    -3.102235     2.098541      26.92
 H       7.296374    -2.742884     0.576550      22.95
 C       5.836709     0.148390    -0.420245      -6.56
 O       7.035266    -0.207844    -1.188382     169.14
 H       7.703544    -0.488854    -0.595865      22.63
 C       5.073351     1.240461    -1.072369      27.64
 H       5.442617     1.584791    -1.975287      26.43
 C       3.480990     1.330176     0.912742      24.05
 C       2.250081     1.970918     1.664270      93.54
 H       2.291559     3.198711     1.744373      26.88
 O       1.958096     1.449441     3.033341     179.76
 H       1.614115     0.424906     3.011934      26.70
 C       1.012599     2.015514     0.852204      73.48
 H       1.172584     2.479656    -0.085648      29.47
 C      -0.232362     2.741251     1.707314     101.64
 O       0.254077     4.021339     2.105804     186.23
 H       0.116145     4.848184     1.447354      25.02
 H      -0.746602     2.283685     2.644659      27.89
 H      -1.091876     2.926634     1.035567      29.12
 C      -1.715354    -1.823309    -0.714345      36.72
 H      -1.949896    -2.783907    -0.410026      25.19
 C      -1.497624     0.043787    -2.299613      57.72
 H      -1.873214     0.400550    -3.265348      25.81
 C      -0.692814     0.785525    -1.371647      13.76
 O      -0.416628     2.144666    -1.574741     219.42
 C      -0.182075     2.684828    -2.945909      95.88
 H       0.814094     2.864414    -3.155224      28.06
 H      -0.242961     1.700199    -3.722753      24.55
 H      -0.993675     3.353143    -3.166423      26.07
 C      -0.332158     0.089311    -0.221269      24.98
 O       0.626699     0.575782     0.628639     128.05
 C      -0.833079    -1.152765     0.171583      61.91
 H      -0.874244    -1.918593     1.113178      22.29
 C      -2.075605    -1.332276    -1.925842      37.47
 C      -2.943223    -2.116371    -2.907218      68.29
 H      -2.771137    -1.495213    -3.845936      25.60
 O      -2.455772    -3.501448    -3.204568     219.84
 H      -1.379574    -3.581547    -3.253370      25.87
 C      -4.478263    -2.230496    -2.723812      94.48
 H      -4.715572    -2.739229    -1.814595      27.88
 O      -5.010021    -0.903428    -2.623547     205.65
 H      -4.331964    -0.281777    -1.953278      26.25
 C      -5.265223    -3.004746    -3.961485      94.27
 O      -4.944937    -4.349810    -3.787441     290.25
 H      -4.083470    -4.271590    -3.772622      34.46
 H      -4.802347    -2.723939    -4.932667      27.58
 H      -6.380048    -2.665430    -3.818412      26.25
55
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name = lig-ACN-frame_528
 C       3.886685     1.623345    -0.373004      67.25
 H       3.374970     2.400858    -0.874078      26.48
 C       4.345648     0.441636     1.568350      44.22
 H       4.223591     0.105497     2.663403      23.08
 C       5.506078    -0.139100     0.903069      -8.76
 O       6.369245    -0.972277     1.715763     190.04
 C       6.333834    -2.514394     1.290257      93.20
 H       5.483792    -2.813873     0.752951      29.82
 H       6.308786    -2.770035     2.325999      25.54
 H       7.371283    -2.645633     0.715793      21.64
 C       5.928506     0.213032    -0.481688      21.88
 O       6.996403    -0.188708    -1.141303      91.49
 H       7.601017    -0.753277    -0.542284      18.91
 C       5.074630     1.117846    -1.037960      81.71
 H       5.193223     1.406495    -1.993936      25.72
 C       3.428412     1.310591     0.914640      -2.31
 C       2.282298     1.994553     1.680585      71.21
 H       2.707793     3.031736     1.988845      24.23
 O       1.941352     1.371713     2.992296     257.18
 H       1.920504     0.514938     2.758266      33.84
 C       0.928985     1.907460     0.925114     105.70
 H       1.101909     2.431628     0.054856      29.53
 C      -0.133310     2.677164     1.565274     101.96
 O       0.284789     4.158676     2.114387     208.84
 H       0.262200     4.567610     1.361067      32.96
 H      -0.236646     2.116936     2.540161      27.10
 H      -0.969748     2.702783     0.902964      28.86
 C      -1.667526    -1.857246    -0.629297      52.17
 H      -1.896676    -2.831450    -0.562331      24.75
 C      -1.660235    -0.039519    -2.296855      47.84
 H      -1.836611     0.439477    -3.295374      21.29
 C      -0.755458     0.755504    -1.421102       1.42
 O      -0.468775     2.166199    -1.494753     173.72
 C      -0.235486     2.505639    -3.042234      96.22
 H       0.658051     3.127824    -2.787303      25.46
 H      -0.446419     1.692340    -3.908252      24.78
 H      -0.868383     3.288493    -3.218164      28.17
 C      -0.310716     0.180732    -0.148595       0.62
 O       0.737085     0.585063     0.672596     173.68
 C      -0.778616    -1.170581     0.224180      34.58
 H      -0.320997    -1.334880     1.256339      22.09
 C      -2.049145    -1.265603    -1.986227      29.99
 C      -2.912190    -2.131844    -3.054173      61.31
 H      -2.882114    -1.622342    -4.091132      25.91
 O      -2.429242    -3.510570    -3.133703     188.96
 H      -1.273840    -3.373503    -3.132610      24.10
 C      -4.512299    -2.228463    -2.775116      92.42
 H      -4.676876    -2.888987    -1.943532      28.87
 O      -4.954846    -0.843725    -2.580712     200.71
 H      -4.391455    -0.467843    -1.655003      24.59
 C      -5.238526    -2.950337    -3.919682     100.21
 O      -5.082967    -4.447998    -3.769019     226.56
 H      -4.144310    -4.685946    -3.859915      31.40
 H      -5.164069    -2.471171    -4.916629      28.20
 H      -6.379164    -2.915430    -3.706040      26.90
55
name = lig-ACN-frame_529
 C       3.853154     1.749815    -0.381282      56.33
 H       3.160780     2.263723    -0.954178      26.81
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 C       4.471459     0.405949     1.543393      59.31
 H       4.296150     0.124672     2.614321      24.63
 C       5.621854    -0.148933     0.943024      35.68
 O       6.222686    -1.114192     1.644991     275.24
 C       6.320129    -2.440684     1.374510     102.54
 H       5.666942    -2.676613     0.592755      32.35
 H       6.166941    -3.222342     2.154145      27.01
 H       7.336653    -2.773684     0.954953      23.75
 C       5.896509     0.259819    -0.321976       4.15
 O       7.024103    -0.231249    -1.101827     161.15
 H       7.753225    -0.818364    -0.652508      21.96
 C       4.895979     1.109673    -1.079020      17.25
 H       5.212207     1.418074    -2.042503      19.04
 C       3.545600     1.245490     0.964865      15.50
 C       2.347735     1.931917     1.769827     104.30
 H       2.560998     3.009628     2.050246      26.24
 O       2.015925     1.273050     2.944834     257.25
 H       1.893725     0.329273     2.884247      29.37
 C       1.111978     2.107734     0.806817      74.39
 H       1.197314     2.438441    -0.150699      27.98
 C      -0.118055     2.773742     1.661526     111.11
 O       0.260022     4.110962     2.016950     244.18
 H       0.389232     4.700818     1.280401      29.76
 H      -0.432205     2.232495     2.545309      28.23
 H      -1.015614     2.846715     1.097442      28.79
 C      -1.623909    -1.911815    -0.707122      41.50
 H      -1.966199    -2.771166    -0.249558      25.42
 C      -1.662592     0.067017    -2.246386      49.61
 H      -2.097773     0.526890    -3.185176      23.61
 C      -0.889142     0.745809    -1.338688      20.54
 O      -0.549470     2.044377    -1.642707     248.06
 C      -0.294797     2.490412    -2.935216     108.36
 H       0.804246     2.816605    -3.267369      25.25
 H      -0.082587     1.473824    -3.462480      26.96
 H      -1.068971     2.964981    -3.433600      27.54
 C      -0.346052     0.146603    -0.187300      11.56
 O       0.778434     0.526273     0.717848      59.69
 C      -0.777322    -1.114414     0.206160      52.88
 H      -0.309635    -1.623854     0.945760      26.94
 C      -2.076345    -1.394637    -1.956427      15.88
 C      -2.891660    -2.153039    -3.091695      71.09
 H      -2.747752    -1.578695    -4.095641      25.24
 O      -2.401756    -3.488909    -3.049308     211.14
 H      -1.383962    -3.695831    -3.418193      25.02
 C      -4.396528    -2.185517    -2.773827      96.21
 H      -4.513816    -2.688483    -1.813108      27.65
 O      -4.928769    -0.843970    -2.542978     230.43
 H      -4.767818    -0.602064    -1.604722      29.05
 C      -5.306576    -2.952385    -3.820631      91.04
 O      -5.217113    -4.475174    -3.795890     140.42
 H      -4.076902    -4.660259    -3.997963      27.14
 H      -4.941047    -2.722175    -4.826497      27.70
 H      -6.387365    -2.722674    -3.604285      27.56
55
name = lig-ACN-frame_530
 C       3.791037     1.700975    -0.381737      62.12
 H       3.155400     2.390602    -0.878569      23.56
 C       4.490881     0.388887     1.650038      50.50
 H       4.270923    -0.010580     2.622557      22.78
 C       5.586085    -0.180615     0.968533      -5.30
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 O       6.199040    -1.147145     1.759615     204.29
 C       6.310917    -2.571356     1.279720      95.80
 H       5.757853    -2.784973     0.420264      30.16
 H       5.833603    -2.972821     2.229670      25.75
 H       7.372913    -2.695963     1.218925      24.03
 C       5.888954     0.292844    -0.423309      16.43
 O       6.977609    -0.226318    -1.077125      84.78
 H       7.519329    -0.482608    -0.367145      23.88
 C       4.946441     1.109270    -1.034203      64.34
 H       5.095602     1.312472    -2.139463      20.55
 C       3.664039     1.387567     0.969532      21.55
 C       2.465038     1.879517     1.712579      67.34
 H       2.805609     2.842513     2.129860      26.74
 O       2.105153     1.152189     2.993750     190.91
 H       1.646522     0.216064     2.574672      25.43
 C       1.186277     2.079471     0.841780      59.17
 H       1.418966     2.720386     0.044393      28.06
 C      -0.106168     2.824593     1.631977     104.04
 O       0.260497     4.137601     1.979792     184.75
 H       0.095491     4.695985     0.981707      24.04
 H      -0.148737     2.360787     2.555912      28.86
 H      -0.942016     2.736317     0.982259      27.87
 C      -1.623967    -1.929534    -0.768790      55.51
 H      -1.841862    -3.016421    -0.650537      24.52
 C      -1.761126    -0.076249    -2.155902      66.48
 H      -2.209883     0.523971    -2.971588      26.39
 C      -0.961765     0.749372    -1.273818       8.58
 O      -0.602748     2.034798    -1.641984     223.27
 C      -0.243160     2.327875    -3.034552      84.74
 H       0.507642     3.263237    -2.655214      22.49
 H      -0.108868     1.492451    -3.744395      27.41
 H      -1.070640     3.030272    -3.336315      24.37
 C      -0.278488     0.120555    -0.124341      14.89
 O       0.707372     0.613517     0.629689     143.67
 C      -0.840712    -1.220997     0.103607      68.33
 H      -0.614080    -1.711114     0.889734      29.12
 C      -2.059822    -1.323146    -1.981173      51.26
 C      -2.799447    -2.110750    -2.950635      79.60
 H      -2.616623    -1.630381    -4.001809      26.54
 O      -2.416746    -3.558788    -3.036401     259.58
 H      -1.549700    -3.469343    -3.336741      31.89
 C      -4.337808    -2.209120    -2.653671      80.00
 H      -4.344368    -2.814489    -1.713107      28.14
 O      -4.928966    -0.872606    -2.550863     245.87
 H      -4.665958    -0.533233    -1.788521      34.58
 C      -5.317039    -2.993167    -3.765277      99.93
 O      -5.328143    -4.398440    -3.798122     180.84
 H      -4.203153    -4.598560    -3.949030      26.65
 H      -5.077820    -2.551589    -4.745435      27.96
 H      -6.295567    -2.563435    -3.592151      28.60
55
name = lig-ACN-frame_531
 C       3.902931     1.572033    -0.380841      20.69
 H       3.241236     2.300078    -0.911391      20.95
 C       4.454918     0.472677     1.654188      55.57
 H       4.150748     0.191946     2.604363      22.67
 C       5.479062    -0.180286     0.956465      14.84
 O       6.245105    -1.124264     1.809381     200.66
 C       6.298043    -2.660024     1.262829      85.58
 H       5.957954    -2.739878     0.224029      27.99
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 H       5.667031    -3.394987     1.899267      26.78
 H       7.221932    -3.020979     1.321089      25.28
 C       5.809673     0.204398    -0.353192      20.18
 O       6.945634    -0.214361    -1.057701     194.33
 H       7.776704    -0.385188    -0.540717      24.05
 C       5.006858     1.160233    -1.056422      46.48
 H       5.236395     1.385840    -2.218570      23.84
 C       3.710022     1.402203     1.045858      32.63
 C       2.460815     1.892948     1.823582     102.13
 H       2.580348     2.912451     2.175175      28.27
 O       2.218049     1.060621     2.953110     242.63
 H       1.609131     0.130450     2.721141      22.84
 C       1.098652     2.023020     0.965180     101.47
 H       1.324844     2.400467    -0.017132      26.11
 C       0.035377     2.709225     1.581897     113.90
 O       0.246293     4.246892     1.941286     136.19
 H       0.045645     5.013113     1.049356      22.41
 H      -0.265259     2.246640     2.449961      29.22
 H      -0.846499     2.631181     0.981544      27.87
 C      -1.625305    -2.028585    -0.816447      48.57
 H      -1.692673    -3.198855    -0.775634      20.73
 C      -1.836270     0.079468    -2.105899      45.99
 H      -2.125253     0.505844    -3.053309      20.66
 C      -0.949823     0.693166    -1.279670      15.90
 O      -0.645738     2.022037    -1.547196     179.76
 C      -0.223327     2.355496    -3.096934      70.16
 H       0.919412     2.947554    -3.102193      22.46
 H       0.183445     1.547625    -3.626430      28.21
 H      -1.099040     2.808628    -3.723866      23.34
 C      -0.407158     0.056895    -0.164295       6.18
 O       0.696773     0.732091     0.553127     157.12
 C      -0.765190    -1.292173     0.167812      51.35
 H      -0.460153    -1.529746     1.028008      25.30
 C      -2.039637    -1.387938    -1.927830      28.89
 C      -2.866150    -2.212746    -2.963051      76.33
 H      -2.837647    -1.707968    -4.019476      24.58
 O      -2.424057    -3.591971    -3.048016     290.89
 H      -1.535018    -3.762078    -3.030633      32.36
 C      -4.383200    -2.279175    -2.586563      92.85
 H      -4.640729    -2.789015    -1.608140      27.80
 O      -4.923368    -0.928982    -2.545577     227.32
 H      -4.421001    -0.341445    -1.868716      27.77
 C      -5.260271    -2.831050    -3.683126     105.69
 O      -5.376538    -4.333227    -3.782444     252.51
 H      -4.557387    -4.767795    -3.860467      34.03
 H      -5.061008    -2.391335    -4.656771      28.55
 H      -6.237219    -2.689076    -3.313211      27.85
55
name = lig-ACN-frame_532
 C       3.921296     1.669436    -0.352873      48.32
 H       3.152112     2.214842    -1.017300      26.27
 C       4.485050     0.469813     1.716340      39.55
 H       4.473521     0.290107     2.760619      23.87
 C       5.495536    -0.311469     1.061422       2.32
 O       6.270278    -1.196882     1.707753     246.44
 C       6.259639    -2.580323     1.281851      91.87
 H       6.149883    -2.463119     0.174106      26.00
 H       5.402070    -3.143792     1.729909      27.66
 H       7.213795    -2.899563     1.600386      23.94
 C       5.840667     0.128564    -0.313596       5.92
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 O       6.941973    -0.237348    -1.063543     128.08
 H       7.743304    -0.554664    -0.456570      23.13
 C       5.084795     1.060323    -1.017018      44.49
 H       5.529481     1.564979    -2.061080      19.11
 C       3.584711     1.419300     0.991061      -9.15
 C       2.341291     1.903151     1.869711      94.81
 H       2.451670     2.855746     2.333456      27.42
 O       2.304754     1.012205     2.978445     236.88
 H       1.995026     0.119831     2.676014      28.97
 C       1.191341     2.001727     0.870279      52.22
 H       1.483630     2.779764     0.127835      26.89
 C      -0.063202     2.855152     1.679366     105.76
 O       0.201820     4.183367     1.942928     216.56
 H       0.294471     4.622880     0.970465      26.24
 H      -0.263004     2.451221     2.613567      28.69
 H      -0.818323     2.805370     0.892000      27.11
 C      -1.440638    -2.064678    -0.704231      23.16
 H      -1.758852    -3.190199    -0.359986      21.60
 C      -1.927368    -0.003221    -2.172812      37.92
 H      -2.338817     0.540777    -3.012413      22.32
 C      -0.975138     0.741308    -1.349201      -1.03
 O      -0.598644     2.094595    -1.590930     213.48
 C      -0.139896     2.297520    -3.004095      87.30
 H       0.754798     3.208561    -3.004378      23.44
 H      -0.055682     1.337034    -3.275545      29.91
 H      -0.997652     2.831484    -3.605948      24.51
 C      -0.435075     0.100443    -0.117059       2.51
 O       0.662850     0.576819     0.525901     112.68
 C      -0.723131    -1.317705     0.212974      48.55
 H      -0.269209    -1.931815     0.875022      25.26
 C      -2.100818    -1.389029    -1.952826      14.51
 C      -2.946715    -2.311876    -2.972176      69.04
 H      -2.912585    -1.792426    -4.007687      26.11
 O      -2.456195    -3.673085    -3.051627     228.91
 H      -1.402551    -3.453693    -3.077600      25.81
 C      -4.422507    -2.280741    -2.535203      97.49
 H      -4.498805    -2.881527    -1.550691      28.48
 O      -4.898128    -0.935104    -2.513192     174.94
 H      -4.375695    -0.431278    -1.602399      24.33
 C      -5.338141    -2.826373    -3.623179     113.46
 O      -5.400205    -4.240746    -3.768185     280.10
 H      -4.525770    -4.394760    -3.849793      35.51
 H      -4.954432    -2.358438    -4.536521      29.01
 H      -6.276575    -2.361481    -3.542334      28.92
55
name = lig-ACN-frame_533
 C       3.932848     1.727524    -0.354111      70.85
 H       3.392531     2.515231    -1.017783      23.10
 C       4.516723     0.453203     1.711636      61.30
 H       4.340489     0.357220     2.795851      23.82
 C       5.498681    -0.274850     0.996138       8.94
 O       6.336124    -1.201747     1.705194     256.57
 C       6.241526    -2.523817     1.237363     103.32
 H       6.367461    -2.896868     0.178393      26.12
 H       5.290330    -2.930750     1.619549      29.66
 H       6.964505    -3.145670     1.766855      24.76
 C       5.869941     0.090644    -0.289788      15.35
 O       6.999108    -0.335459    -1.035461     161.46
 H       7.573443    -0.828432    -0.459504      25.01
 C       5.019327     1.056522    -0.842218      42.65
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 H       5.467928     1.356114    -1.954163      20.33
 C       3.612676     1.344249     1.006592      -9.30
 C       2.391709     1.817460     1.771280      82.89
 H       2.576096     2.794072     2.110235      26.45
 O       2.288458     1.006315     3.043166     247.19
 H       2.091680     0.174215     2.857972      32.47
 C       1.016840     2.035990     0.948282      73.22
 H       1.341479     2.293070    -0.104733      24.60
 C      -0.182828     2.793957     1.646620     111.52
 O       0.209404     4.190343     1.965715     283.17
 H       0.313439     4.675961     1.249211      33.41
 H      -0.299336     2.265772     2.583603      27.16
 H      -1.160737     2.723634     1.158726      27.02
 C      -1.471988    -1.966441    -0.772640      53.92
 H      -1.574413    -3.177820    -0.577244      22.39
 C      -1.888464    -0.124056    -2.174467      51.05
 H      -2.563815     0.251754    -2.941120      24.31
 C      -1.073837     0.709859    -1.299542      -1.69
 O      -0.565032     2.114186    -1.597678     211.17
 C      -0.116125     2.250477    -2.919731      99.58
 H       0.971457     2.896105    -2.788707      24.41
 H       0.328904     1.575195    -3.536020      28.84
 H      -0.895539     2.788756    -3.575066      24.91
 C      -0.415830     0.121535    -0.175345       0.48
 O       0.745490     0.524701     0.579551      92.52
 C      -0.680191    -1.227642     0.136747      48.90
 H      -0.116483    -1.509383     1.054962      22.60
 C      -2.091503    -1.517088    -1.881491      40.55
 C      -2.943242    -2.287681    -2.877938      72.21
 H      -2.848081    -1.847909    -3.912776      26.16
 O      -2.478429    -3.724281    -3.035046     176.14
 H      -1.428068    -3.914771    -3.420917      24.99
 C      -4.481227    -2.286904    -2.509373      87.13
 H      -4.666039    -2.851726    -1.503630      27.66
 O      -4.840634    -0.886303    -2.396421     202.77
 H      -4.719798    -0.448676    -1.365638      24.59
 C      -5.459601    -2.780195    -3.681817     105.02
 O      -5.407829    -4.196769    -3.741172     176.66
 H      -4.394702    -4.595663    -3.918869      28.35
 H      -5.072063    -2.351320    -4.605173      28.44
 H      -6.494254    -2.570328    -3.527643      28.82
55
name = lig-ACN-frame_534
 C       3.960576     1.680723    -0.227583      47.11
 H       3.448674     2.596911    -0.658934      22.06
 C       4.499099     0.395461     1.635203      55.42
 H       4.234558    -0.030177     2.661121      21.71
 C       5.601788    -0.235201     1.045026      16.11
 O       6.415496    -1.098205     1.701370     208.16
 C       6.197961    -2.677734     1.248207      80.52
 H       6.575808    -2.480525     0.219650      23.46
 H       5.181091    -2.931993     1.210267      30.16
 H       6.918827    -3.209219     1.987619      22.85
 C       5.875976     0.092129    -0.322089      12.90
 O       6.991579    -0.434531    -0.975093     188.72
 H       7.581501    -0.960251    -0.412863      24.08
 C       5.074919     1.121246    -0.939772      47.77
 H       5.158735     1.395524    -2.085576      23.54
 C       3.633883     1.277653     1.012238      33.15
 C       2.399266     1.790787     1.802299      81.23
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 H       2.659968     2.725320     2.107896      27.00
 O       2.217356     1.112698     3.046851     279.01
 H       1.691768     0.269584     2.915039      26.68
 C       0.947383     1.887882     0.946327      83.50
 H       0.964645     2.726964     0.092512      23.75
 C      -0.184085     2.667389     1.652817      91.69
 O       0.206135     4.165767     2.019886     244.71
 H      -0.002705     4.634234     1.264996      31.38
 H      -0.563952     2.333805     2.657117      25.56
 H      -0.931022     2.810596     0.835184      25.70
 C      -1.484739    -2.057719    -0.693600      39.84
 H      -1.388856    -3.239009    -0.534088      21.37
 C      -1.841900    -0.100687    -2.103549      57.59
 H      -2.123335     0.393733    -3.074898      23.09
 C      -1.064390     0.720087    -1.292621      21.07
 O      -0.638545     1.942831    -1.552405     194.58
 C       0.001498     2.304494    -2.974833      74.22
 H       0.882610     3.144162    -2.787126      23.08
 H       0.117471     1.294250    -3.157209      27.78
 H      -0.743294     2.791057    -3.652810      24.54
 C      -0.315549     0.137422    -0.215943      21.22
 O       0.720185     0.578370     0.631686     175.67
 C      -0.689851    -1.155097     0.030444      47.63
 H      -0.321623    -1.751891     1.051071      21.38
 C      -2.070267    -1.500853    -1.897840      27.16
 C      -2.903644    -2.375658    -2.822089      72.56
 H      -2.906649    -1.771560    -3.758660      27.16
 O      -2.563018    -3.757741    -3.002361     238.39
 H      -1.583526    -3.648259    -3.317672      26.95
 C      -4.580982    -2.221562    -2.534796      82.93
 H      -4.950702    -2.942830    -1.681885      26.97
 O      -4.804956    -0.834259    -2.241221     244.39
 H      -4.736743    -0.641336    -1.308256      29.21
 C      -5.458356    -2.725762    -3.692084     101.78
 O      -5.423446    -4.254583    -3.739833     117.40
 H      -4.242027    -4.414885    -3.925673      25.45
 H      -5.433903    -2.200033    -4.640863      28.33
 H      -6.434984    -2.499028    -3.244130      28.05
55
name = lig-ACN-frame_535
 C       4.052567     1.689054    -0.255415      37.70
 H       3.362139     2.368406    -0.767220      25.05
 C       4.456953     0.189076     1.693395      28.96
 H       4.233582    -0.247383     2.734950      20.43
 C       5.666664    -0.166027     1.007117      -2.03
 O       6.486553    -1.169440     1.719858     217.46
 C       6.232195    -2.572661     1.247613      81.87
 H       6.777267    -3.008420     0.336232      24.10
 H       5.205316    -2.816532     1.185923      31.38
 H       6.666192    -3.269458     2.153911      23.64
 C       5.909444     0.185961    -0.377549       1.64
 O       6.947566    -0.518667    -0.970235     120.40
 H       7.518440    -0.716294    -0.101839      21.25
 C       5.117985     1.134069    -1.050018      57.83
 H       5.474741     1.526080    -2.026352      20.88
 C       3.577339     1.197636     1.096881      -8.11
 C       2.322284     1.875533     1.828349      98.80
 H       2.459022     2.853396     2.017352      27.16
 O       2.101531     1.218386     3.071283     239.64
 H       1.484889     0.280794     2.857265      22.77
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 C       1.112779     1.960589     1.011092      63.11
 H       1.572587     2.376771    -0.033642      23.60
 C      -0.185389     2.714771     1.729471     103.71
 O       0.180481     3.993019     2.049892     210.85
 H      -0.089015     4.715164     1.201794      24.20
 H      -0.655006     2.036327     2.562765      25.16
 H      -0.989919     2.642080     0.960395      26.21
 C      -1.479535    -2.083041    -0.714671      56.04
 H      -1.758023    -3.096501    -0.292951      23.30
 C      -1.826077    -0.096416    -2.120713      35.50
 H      -2.115136     0.352092    -3.146822      21.93
 C      -0.900542     0.666830    -1.316579       7.83
 O      -0.697731     2.029407    -1.628838     236.02
 C       0.000642     2.248818    -2.924963     100.34
 H       0.922995     2.900746    -2.613186      25.70
 H       0.590596     1.526074    -3.574458      27.76
 H      -0.738963     2.729635    -3.552989      25.97
 C      -0.297547     0.031384    -0.159426      19.51
 O       0.613815     0.568286     0.624644     158.57
 C      -0.678501    -1.322575     0.129371      45.02
 H       0.038341    -1.781289     1.108724      21.21
 C      -2.065699    -1.520021    -1.859356      35.49
 C      -3.050825    -2.321389    -2.850601      80.90
 H      -2.862389    -2.022071    -3.870032      27.12
 O      -2.625480    -3.766890    -2.950283     236.48
 H      -1.750200    -3.879132    -2.966502      33.47
 C      -4.506841    -2.194335    -2.521595     100.87
 H      -4.696629    -2.866478    -1.578908      27.95
 O      -4.812365    -0.834891    -2.151956     267.14
 H      -4.546197    -0.602835    -1.339498      32.37
 C      -5.531486    -2.745424    -3.621571     102.13
 O      -5.393681    -4.173704    -3.786635     173.52
 H      -4.315294    -4.381712    -3.856371      28.30
 H      -5.237076    -2.361836    -4.608047      27.52
 H      -6.646561    -2.557581    -3.431164      27.14
55
name = lig-ACN-frame_536
 C       4.024617     1.640713    -0.259350      56.95
 H       3.493320     2.400989    -0.764871      25.02
 C       4.414144     0.119223     1.669164      51.91
 H       4.241236    -0.290138     2.699552      20.52
 C       5.593452    -0.210390     1.003035      -6.29
 O       6.539106    -1.189018     1.629089     244.24
 C       6.271025    -2.523667     1.314199      73.68
 H       6.920243    -2.840036     0.426786      22.45
 H       5.245295    -2.550555     0.968057      31.63
 H       6.390866    -3.128584     2.376617      21.40
 C       5.972663     0.191908    -0.302147       3.52
 O       6.936152    -0.553294    -0.973909     124.97
 H       7.752654    -0.762356    -0.472919      23.89
 C       5.136923     1.162690    -0.979249      58.32
 H       5.399173     1.564854    -1.890451      23.94
 C       3.660985     1.153099     1.058272      12.13
 C       2.390187     1.873368     1.875498      79.94
 H       2.719313     2.774246     2.094519      28.27
 O       1.965248     1.301789     3.146014     242.15
 H       1.654120     0.252701     2.911717      23.36
 C       1.046271     2.018051     0.935646      64.08
 H       1.202406     2.597900    -0.132109      24.47
 C      -0.104384     2.590386     1.606829     104.50
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 O       0.154623     3.947175     2.139189     144.89
 H       0.067927     4.659561     1.185952      25.63
 H      -0.053491     2.085378     2.663440      24.15
 H      -1.029694     2.600680     1.013850      27.08
 C      -1.552220    -2.094146    -0.711638      43.48
 H      -1.909616    -3.080165    -0.572267      25.00
 C      -1.722422    -0.178207    -2.161794      45.40
 H      -2.464427     0.348632    -2.878392      22.92
 C      -0.866135     0.568142    -1.407445      -5.54
 O      -0.715044     2.044777    -1.706557     188.58
 C       0.038538     2.297473    -2.908779      95.27
 H       0.832194     3.099084    -2.658490      25.67
 H       0.322061     1.165816    -3.227544      25.50
 H      -0.576263     2.772419    -3.630566      26.85
 C      -0.343943    -0.071785    -0.133014      -6.16
 O       0.641763     0.546170     0.737598      95.03
 C      -0.622058    -1.452184     0.180921      43.58
 H      -0.125342    -2.124171     1.246119      19.16
 C      -2.123334    -1.502184    -1.878191      30.56
 C      -2.985593    -2.260404    -2.919497      74.29
 H      -2.952680    -1.705596    -3.834216      27.83
 O      -2.736626    -3.770293    -2.854152     215.92
 H      -1.753992    -3.784305    -2.773074      29.19
 C      -4.533055    -2.229348    -2.402891      77.91
 H      -4.573719    -2.953593    -1.531053      27.78
 O      -4.863554    -0.862085    -2.176682     240.15
 H      -4.515467    -0.467232    -1.229943      25.16
 C      -5.489703    -2.717065    -3.585949     102.90
 O      -5.359777    -4.125146    -3.821787     251.83
 H      -4.503336    -4.244961    -3.722703      35.42
 H      -5.256561    -2.005372    -4.402777      27.83
 H      -6.620207    -2.475691    -3.303959      25.84
55
name = lig-ACN-frame_537
 C       3.953924     1.610788    -0.213743      38.52
 H       3.421282     2.457076    -0.526191      22.35
 C       4.423386     0.165266     1.614198      60.99
 H       4.080694    -0.213812     2.570211      23.54
 C       5.599869    -0.377142     1.018634       6.90
 O       6.573213    -1.050672     1.562068     256.12
 C       6.242600    -2.577341     1.344157      81.20
 H       7.156881    -2.987730     0.814960      23.54
 H       5.320984    -2.831618     0.763305      29.49
 H       6.289726    -3.176517     2.379694      23.79
 C       5.976087     0.136830    -0.240247      18.16
 O       6.941989    -0.522629    -1.040991     214.19
 H       7.716476    -0.651462    -0.525281      24.04
 C       5.207116     1.146144    -0.824798      61.22
 H       5.344425     1.371361    -1.777994      27.45
 C       3.590968     1.151789     1.062761      20.96
 C       2.478398     1.825594     1.835207      75.45
 H       2.784759     2.700200     2.113677      28.12
 O       1.903571     1.345852     3.148877     251.27
 H       1.707609     0.417318     3.116671      28.94
 C       1.040714     1.920327     0.765877      56.65
 H       1.188682     2.487868    -0.297115      23.40
 C      -0.075390     2.552481     1.681320      94.86
 O       0.139629     3.970679     2.166619     237.91
 H       0.285232     4.579030     1.365986      29.24
 H      -0.359926     1.808455     2.554897      24.52
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 H      -0.988276     2.438153     1.055603      26.75
 C      -1.627978    -2.165489    -0.698548      53.67
 H      -1.668985    -3.136024    -0.505800      25.72
 C      -1.729009    -0.203032    -2.230427      31.19
 H      -2.124342     0.445529    -3.104310      22.16
 C      -0.820743     0.548142    -1.317617       3.78
 O      -0.763021     1.890733    -1.657311     178.50
 C       0.086545     2.342718    -2.957066      76.62
 H       0.984734     2.869003    -2.711371      26.06
 H       0.647346     1.314855    -3.430649      25.72
 H      -0.570295     2.731937    -3.731870      25.12
 C      -0.254284    -0.042260    -0.134770      14.66
 O       0.657350     0.486588     0.786991     142.70
 C      -0.703783    -1.446214     0.049887      42.07
 H      -0.445471    -2.138336     1.157040      20.02
 C      -2.073651    -1.522695    -1.911105      29.26
 C      -3.027016    -2.295195    -2.784023      96.35
 H      -2.891212    -2.089569    -3.821125      27.19
 O      -2.786025    -3.676805    -2.786441     192.55
 H      -1.787865    -4.065286    -3.051971      25.67
 C      -4.521127    -2.223477    -2.408752      99.65
 H      -4.797978    -2.893083    -1.571801      28.15
 O      -4.954259    -0.870464    -2.204055     196.21
 H      -4.771790    -0.551667    -1.098524      23.62
 C      -5.426173    -2.615164    -3.494661     100.21
 O      -5.330597    -4.083373    -3.853180     212.21
 H      -4.476262    -4.384046    -3.802444      34.23
 H      -5.338312    -2.081430    -4.464864      27.41
 H      -6.515484    -2.514401    -3.014822      25.43
55
name = lig-ACN-frame_538
 C       3.993419     1.642616    -0.172720      63.72
 H       3.498513     2.293073    -0.864827      23.30
 C       4.415526     0.129975     1.696928      56.26
 H       4.336965    -0.233344     2.683407      21.71
 C       5.557877    -0.306099     0.965978      -5.35
 O       6.603041    -1.201862     1.609940     248.40
 C       6.353451    -2.615142     1.426453      83.58
 H       7.215083    -3.195129     1.041860      23.44
 H       5.471791    -2.633914     0.655602      28.92
 H       5.923797    -2.875815     2.448216      24.18
 C       5.906820     0.072267    -0.329873      11.64
 O       6.943802    -0.432873    -1.089908     136.67
 H       7.716260    -0.695996    -0.435423      23.30
 C       5.118308     1.167131    -0.785630      50.72
 H       5.538320     1.573855    -1.621729      22.95
 C       3.547992     1.094026     1.091151       9.56
 C       2.311897     1.816365     1.746882     102.01
 H       2.522620     2.757883     1.795359      27.79
 O       1.967463     1.361027     3.061664     315.47
 H       1.663579     0.539786     2.921679      31.89
 C       1.130576     1.791928     0.907725      76.18
 H       1.360529     2.026658    -0.209178      23.27
 C      -0.129665     2.624589     1.681923      99.02
 O       0.155337     3.914284     2.147041     301.53
 H       0.230967     4.350218     1.430754      36.23
 H      -0.187040     2.061595     2.684931      24.01
 H      -1.055424     2.719777     1.079582      26.05
 C      -1.591489    -2.140007    -0.765923      52.04
 H      -1.954308    -3.013974    -0.507971      24.48
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 C      -1.646262    -0.215942    -2.153129      56.50
 H      -1.800960     0.102530    -3.205842      23.65
 C      -0.851359     0.494568    -1.322560      25.68
 O      -0.690941     1.866455    -1.670528     223.86
 C       0.098066     2.237058    -2.908214      96.94
 H       0.678457     2.985058    -2.511761      27.11
 H       0.561749     1.416003    -3.721676      25.26
 H      -0.673886     2.854448    -3.421047      25.27
 C      -0.243351    -0.104186    -0.220663      23.56
 O       0.646502     0.405972     0.737386     168.46
 C      -0.749036    -1.342677     0.065856      52.27
 H      -0.126109    -1.719205     1.078926      21.23
 C      -2.065924    -1.573759    -1.930940      36.38
 C      -3.055652    -2.300518    -2.757594      82.10
 H      -3.048807    -1.798984    -3.712341      27.89
 O      -2.785884    -3.769527    -2.705477     192.74
 H      -1.828005    -3.645200    -3.143643      26.68
 C      -4.531213    -2.134891    -2.379402     100.84
 H      -4.630108    -2.756147    -1.548389      30.09
 O      -5.031182    -0.818910    -2.176102     250.09
 H      -4.932757    -0.531320    -1.179017      26.91
 C      -5.471437    -2.703969    -3.527934      99.99
 O      -5.341870    -4.023996    -3.870262     160.13
 H      -4.182875    -4.151702    -3.819090      25.89
 H      -5.291828    -1.925758    -4.342264      27.53
 H      -6.597369    -2.513465    -3.191955      26.16
55
name = lig-ACN-frame_539
 C       3.982093     1.636576    -0.122916      38.62
 H       3.290934     2.484907    -0.367802      24.07
 C       4.441711     0.108924     1.750388      29.03
 H       4.283153    -0.160569     2.766429      21.66
 C       5.647768    -0.401810     1.043428      -8.37
 O       6.561387    -1.231086     1.616186     254.98
 C       6.343173    -2.669164     1.518831      95.76
 H       7.387486    -3.042006     1.515824      22.66
 H       5.866107    -3.021083     0.488460      26.68
 H       5.878171    -3.214165     2.331274      27.41
 C       5.814556     0.064277    -0.380171       5.78
 O       6.952755    -0.315363    -1.103463     194.71
 H       7.521680    -0.902317    -0.505014      24.76
 C       5.116779     1.166287    -0.941087      60.96
 H       5.331581     1.846725    -1.751539      23.36
 C       3.553634     1.099308     1.094191      16.46
 C       2.286595     1.787636     1.723877      96.98
 H       2.441397     2.737054     1.807889      28.27
 O       2.078903     1.329813     3.015280     280.21
 H       1.619899     0.381241     3.064325      25.32
 C       0.914156     1.731609     0.918297      87.84
 H       1.176741     2.439453     0.069776      25.59
 C      -0.135218     2.551739     1.622752     104.90
 O       0.245976     3.937480     2.091090     235.76
 H       0.134381     4.694232     1.370638      27.90
 H      -0.500732     2.016992     2.527743      26.59
 H      -1.007238     2.458846     0.929183      26.83
 C      -1.538297    -2.099386    -0.667306      55.95
 H      -1.852607    -3.032392    -0.328366      23.95
 C      -1.635032    -0.327772    -2.272903      55.97
 H      -2.076844     0.274059    -3.044860      24.81
 C      -0.823749     0.577405    -1.432693      12.40
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 O      -0.559374     1.846025    -1.664857     256.77
 C       0.019008     2.272798    -2.827128     110.59
 H       0.933865     2.703531    -2.756628      28.43
 H       0.394227     1.184565    -3.274718      25.46
 H      -0.600593     2.801635    -3.680626      24.68
 C      -0.269604    -0.080728    -0.215973      14.80
 O       0.645150     0.305534     0.702841     180.77
 C      -0.710009    -1.416076     0.161518      38.08
 H      -0.468526    -2.028809     1.112248      21.37
 C      -2.059979    -1.549717    -1.909940      43.24
 C      -3.086548    -2.234222    -2.836396      59.69
 H      -2.918102    -2.099402    -3.886966      27.84
 O      -2.759481    -3.816313    -2.705532     176.64
 H      -1.871450    -4.067130    -2.687802      30.97
 C      -4.672511    -2.148634    -2.329423      91.40
 H      -4.844635    -2.753074    -1.510910      28.70
 O      -5.071741    -0.745369    -2.125511     286.26
 H      -4.865994    -0.442279    -1.339669      33.38
 C      -5.548511    -2.615191    -3.533596      93.59
 O      -5.309249    -4.055403    -3.903679     106.28
 H      -4.093723    -4.265125    -3.841724      24.42
 H      -5.352880    -2.053952    -4.503303      26.38
 H      -6.683792    -2.555979    -3.266630      26.40
55
name = lig-ACN-frame_540
 C       3.958209     1.630636    -0.160979      51.92
 H       3.622205     2.664712    -0.524381      22.71
 C       4.470277     0.134685     1.699269      72.73
 H       4.202170    -0.253407     2.684104      23.92
 C       5.524056    -0.385382     0.975119      13.25
 O       6.504150    -1.221568     1.619604     262.79
 C       6.407652    -2.801725     1.580798      87.08
 H       7.381820    -3.119806     1.933995      23.40
 H       6.160061    -3.179551     0.476693      25.26
 H       5.636816    -2.932071     2.245369      29.07
 C       5.822964     0.133030    -0.334645      -4.91
 O       6.950335    -0.237180    -1.091996     181.34
 H       7.409051    -0.908996    -0.653274      26.57
 C       4.990864     1.162458    -0.920051      42.77
 H       5.392921     1.284540    -1.976280      21.62
 C       3.642682     1.065719     1.108127      20.74
 C       2.360383     1.731528     1.728233      81.48
 H       2.605879     2.659347     1.864198      27.62
 O       2.165726     1.243694     3.121911     197.80
 H       1.790837     0.152363     2.993462      22.34
 C       0.916212     1.776185     0.832041      77.14
 H       0.849298     2.024665    -0.189588      22.63
 C      -0.282553     2.489516     1.632648      98.01
 O       0.342326     3.905653     1.986577     144.16
 H      -0.072982     4.439250     1.011374      24.93
 H      -0.584329     2.089748     2.547257      27.10
 H      -1.084232     2.865874     0.967148      25.95
 C      -1.656922    -2.169451    -0.643414      46.02
 H      -1.832462    -3.258218    -0.406925      23.67
 C      -1.637838    -0.180463    -2.383981      44.68
 H      -2.216611     0.153177    -3.174991      23.98
 C      -0.766821     0.400747    -1.432065      -6.87
 O      -0.500349     1.931135    -1.534432     139.81
 C       0.104176     2.218973    -2.978408      86.04
 H       0.878111     2.816358    -2.719597      26.97
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 H       0.263190     1.272761    -3.691698      25.17
 H      -0.842154     2.905775    -3.378858      23.00
 C      -0.352716    -0.171627    -0.180945      14.01
 O       0.662535     0.360947     0.679013     147.24
 C      -0.677775    -1.441480     0.194430      49.79
 H      -0.361466    -1.656988     1.133182      22.33
 C      -2.073457    -1.577644    -1.890893      12.53
 C      -3.087271    -2.405418    -2.751271      81.35
 H      -3.041054    -1.929963    -3.738790      28.15
 O      -2.810837    -3.795225    -2.725526     237.46
 H      -1.914935    -3.712963    -2.466284      30.33
 C      -4.722899    -2.118281    -2.412981      87.85
 H      -4.904104    -2.717749    -1.570442      29.69
 O      -5.081548    -0.731602    -2.098910     251.34
 H      -4.691651    -0.524851    -1.208996      28.97
 C      -5.605182    -2.621731    -3.569608     102.07
 O      -5.294170    -4.054590    -3.905378     114.57
 H      -4.155283    -4.225371    -3.606873      25.51
 H      -5.425447    -1.848755    -4.413104      26.64
 H      -6.710786    -2.563074    -3.269537      26.62
55
name = lig-ACN-frame_541
 C       3.939910     1.695722    -0.224600      43.74
 H       3.135658     2.386901    -0.734606      22.09
 C       4.396457     0.111182     1.640661      35.03
 H       4.303407    -0.354014     2.674914      21.11
 C       5.529785    -0.433547     0.905408       6.09
 O       6.456514    -1.264923     1.572143     282.92
 C       6.425983    -2.722314     1.651195      95.55
 H       7.241826    -3.045717     2.309891      22.66
 H       6.555742    -3.160118     0.560985      24.34
 H       5.592342    -3.167209     2.048740      32.34
 C       5.881221     0.167577    -0.310931      24.90
 O       6.916384    -0.183755    -1.067770     192.72
 H       7.544044    -0.748636    -0.483790      22.53
 C       4.993400     1.018553    -0.901377      53.24
 H       5.058982     1.536653    -1.955107      20.46
 C       3.571810     1.175902     1.048474      15.06
 C       2.389177     1.727283     1.816816      89.14
 H       2.547800     2.705148     1.981285      26.61
 O       2.212654     1.148326     3.149228     251.40
 H       1.881637     0.101980     3.027136      22.52
 C       1.022136     1.762570     0.860393      57.55
 H       1.448884     2.424586     0.189173      25.59
 C      -0.262597     2.602276     1.623138     109.22
 O       0.357847     3.805526     1.848072     239.66
 H       0.268067     4.504847     1.012265      26.46
 H      -0.393793     2.076543     2.495196      27.33
 H      -1.197020     2.449977     1.055874      26.54
 C      -1.677427    -2.152942    -0.683281      54.62
 H      -2.234948    -3.178921    -0.446336      20.33
 C      -1.691770    -0.287180    -2.226727      58.09
 H      -1.709499     0.239333    -3.108076      22.33
 C      -0.770061     0.464212    -1.414856      10.78
 O      -0.417188     1.825111    -1.558679     195.50
 C       0.072757     2.252891    -3.020952      84.26
 H       1.021045     2.769621    -2.919306      26.27
 H       0.321408     1.352912    -3.668096      26.57
 H      -0.844961     2.961703    -3.550704      22.58
 C      -0.303495    -0.171721    -0.182215      11.08
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 O       0.617007     0.362134     0.639184     165.23
 C      -0.812420    -1.529844     0.174677      39.97
 H      -0.447762    -1.995382     0.913923      24.74
 C      -2.137237    -1.577398    -1.891979      54.72
 C      -3.172709    -2.318280    -2.694942      73.84
 H      -2.975471    -2.105476    -3.755922      26.60
 O      -2.854272    -3.787707    -2.706262     165.97
 H      -1.865605    -4.142092    -2.934438      26.96
 C      -4.684362    -2.143067    -2.401598      99.06
 H      -4.978019    -2.757520    -1.573276      28.34
 O      -5.032557    -0.772747    -2.124648     220.17
 H      -4.737494    -0.509961    -1.032621      22.73
 C      -5.610204    -2.662410    -3.605945     106.56
 O      -5.314395    -3.988452    -3.882715     204.68
 H      -4.327574    -4.170389    -3.592353      29.40
 H      -5.548107    -2.082262    -4.621673      26.97
 H      -6.684796    -2.623378    -3.271353      27.05
55
name = lig-ACN-frame_542
 C       3.846160     1.612422    -0.239344      49.67
 H       3.175719     2.244821    -0.953819      22.95
 C       4.328042     0.112614     1.503338      57.61
 H       3.946705    -0.151198     2.559434      22.48
 C       5.502417    -0.451268     0.960111      12.56
 O       6.426662    -1.249049     1.536503     290.06
 C       6.437753    -2.665769     1.668478      99.51
 H       7.116547    -2.738052     2.531052      21.99
 H       6.960295    -3.190925     0.809939      24.36
 H       5.467745    -3.044514     1.893980      31.47
 C       5.829108     0.143290    -0.323725     -18.60
 O       7.022017    -0.200310    -1.075325     140.00
 H       7.801065    -0.486380    -0.461680      23.61
 C       4.938870     1.107470    -0.974074      34.34
 H       5.446233     1.385160    -2.000557      18.99
 C       3.552938     1.182693     1.067080      35.39
 C       2.296085     1.734046     1.925582     106.05
 H       2.419416     2.714037     2.199789      26.16
 O       2.243073     1.060656     3.138669     314.31
 H       1.807528     0.204677     3.013693      27.50
 C       1.076403     1.757988     1.037335      96.01
 H       1.204406     2.091529     0.086643      24.71
 C      -0.014406     2.461730     1.540668     121.89
 O       0.334005     3.905815     1.754522     282.85
 H       0.496750     4.256958     0.960502      33.72
 H      -0.314830     2.255588     2.509830      27.57
 H      -0.882165     2.498735     0.885182      26.63
 C      -1.799855    -2.160362    -0.726611      39.05
 H      -2.125200    -3.252956    -0.231825      20.71
 C      -1.634854    -0.263857    -2.132000      62.05
 H      -2.114351    -0.049665    -3.050428      25.74
 C      -0.833472     0.452074    -1.297428      27.55
 O      -0.291473     1.718107    -1.736688     225.92
 C       0.000332     2.226511    -2.957945     108.56
 H       0.961358     2.821998    -2.839065      24.57
 H       0.112473     1.368802    -3.610025      26.82
 H      -0.853241     2.997253    -3.566330      22.81
 C      -0.309817    -0.198425    -0.208822      16.75
 O       0.668873     0.365440     0.642669     197.84
 C      -0.836220    -1.494276     0.148062      36.77
 H      -0.547995    -2.018486     0.920714      24.59
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 C      -2.248405    -1.553763    -1.854568      41.86
 C      -3.170048    -2.232836    -2.826277      55.38
 H      -3.128627    -1.798283    -3.862307      28.02
 O      -2.936051    -3.837252    -2.657938     107.41
 H      -2.006158    -3.768870    -3.213831      26.29
 C      -4.710728    -2.187808    -2.388722      94.45
 H      -4.844554    -2.869743    -1.528908      28.59
 O      -4.966360    -0.801671    -2.154986     235.41
 H      -4.907238    -0.495101    -1.095183      24.63
 C      -5.584952    -2.603741    -3.568393     102.67
 O      -5.343051    -4.050536    -3.881171     216.63
 H      -4.480991    -4.103952    -3.706146      34.75
 H      -5.360178    -1.867015    -4.453214      27.77
 H      -6.623417    -2.483042    -3.239215      27.76
55
name = lig-ACN-frame_543
 C       3.769105     1.535797    -0.381496      47.45
 H       3.265294     2.516835    -0.610679      22.76
 C       4.262674     0.086432     1.582704      32.64
 H       4.109826    -0.472693     2.570775      20.05
 C       5.422607    -0.357301     0.832473      -8.19
 O       6.439020    -1.136002     1.546749     237.38
 C       6.470639    -2.676009     1.726431      84.16
 H       6.795724    -3.010343     2.731810      23.94
 H       6.974178    -3.114216     0.867765      24.40
 H       5.428289    -3.013189     1.595609      30.54
 C       5.821006     0.120505    -0.427554      22.46
 O       7.065148    -0.200282    -1.039304     228.20
 H       7.659746    -0.338183    -0.334387      25.13
 C       5.002975     1.124421    -0.949284      46.15
 H       5.157572     1.586082    -1.958475      23.32
 C       3.510229     1.171354     1.004052      -1.21
 C       2.411493     1.699137     1.900435      88.85
 H       2.564377     2.738173     2.100911      26.13
 O       2.206985     0.970208     3.193571     291.49
 H       1.828970     0.172134     3.076736      30.55
 C       1.154865     1.625780     0.938128      76.48
 H       1.534968     2.183449     0.171884      27.40
 C      -0.049715     2.525058     1.619131     101.05
 O       0.322274     4.027927     1.663089     259.14
 H       0.570715     4.267868     0.778284      30.72
 H      -0.405665     2.026877     2.492064      26.83
 H      -0.743411     2.368388     0.800380      26.68
 C      -1.846109    -2.150059    -0.581292      53.91
 H      -2.124294    -3.365620    -0.551636      21.86
 C      -1.796858    -0.257493    -2.248828      54.79
 H      -2.037627     0.559319    -2.955833      22.33
 C      -0.818810     0.455207    -1.376670      -0.79
 O      -0.195964     1.619224    -1.649800     173.73
 C      -0.063486     2.158555    -3.102711      96.36
 H       0.819407     2.953320    -2.973330      24.86
 H       0.159866     1.607799    -3.953005      27.68
 H      -1.099637     2.793986    -3.104511      23.40
 C      -0.308213    -0.151909    -0.089615      11.48
 O       0.767846     0.239060     0.731040     180.07
 C      -0.845249    -1.467346     0.130009      49.73
 H      -0.435678    -1.715567     1.079082      21.88
 C      -2.282912    -1.528257    -1.838101      28.39
 C      -3.228465    -2.326924    -2.820556      84.23
 H      -3.026721    -2.032254    -3.890425      27.89
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 O      -2.976551    -3.736544    -2.729758     215.51
 H      -2.063978    -4.057112    -2.729610      30.15
 C      -4.641842    -2.163512    -2.405837     101.82
 H      -4.802117    -2.771494    -1.447270      28.19
 O      -4.962512    -0.770794    -2.150498     281.47
 H      -4.826343    -0.653937    -1.285568      33.09
 C      -5.591633    -2.617764    -3.519304     102.46
 O      -5.403884    -4.052704    -3.895164     187.37
 H      -4.532472    -4.435802    -3.765069      33.81
 H      -5.307645    -1.958318    -4.436200      27.17
 H      -6.634251    -2.468901    -3.373257      28.18
55
name = lig-ACN-frame_544
 C       3.807025     1.539434    -0.312490      49.58
 H       3.370290     2.353123    -0.865587      22.85
 C       4.343189     0.040901     1.525083      52.40
 H       4.167979    -0.200448     2.595660      21.55
 C       5.456087    -0.418439     0.826673       3.99
 O       6.450036    -1.051424     1.571139     282.77
 C       6.383421    -2.587838     1.683694     101.18
 H       6.718156    -2.665170     2.740268      25.40
 H       7.196720    -2.935113     1.160540      24.95
 H       5.396003    -3.109980     1.420661      28.85
 C       5.803426     0.156741    -0.491741      -4.80
 O       7.053200    -0.178367    -0.974255     156.87
 H       7.563149    -0.569019    -0.225603      21.39
 C       4.981342     1.152545    -1.056211      48.08
 H       5.382200     1.726162    -1.856608      21.46
 C       3.535387     0.978892     0.972033      35.19
 C       2.425444     1.571004     1.853060      95.13
 H       2.683020     2.590872     2.161593      24.44
 O       2.202980     1.008914     3.182957     303.85
 H       1.857036     0.172943     2.976232      29.11
 C       1.154967     1.655366     0.973169      68.39
 H       1.283211     1.912969    -0.033525      23.18
 C      -0.089872     2.625952     1.524083     102.87
 O       0.284497     3.983054     1.615590     194.98
 H       0.454234     4.510681     0.597777      25.02
 H      -0.134922     2.604485     2.621025      24.07
 H      -1.115860     2.564839     1.163445      25.63
 C      -1.815487    -2.007357    -0.623886      42.02
 H      -2.094990    -3.121149    -0.169904      21.87
 C      -1.860955    -0.160194    -2.181722      49.40
 H      -2.292371     0.044683    -3.230640      21.21
 C      -0.763033     0.324141    -1.394616       9.23
 O      -0.053060     1.574620    -1.643199     124.16
 C      -0.187879     2.180193    -3.134480      89.53
 H       0.674279     3.036476    -3.320103      23.77
 H      -0.046766     1.301260    -3.630747      27.47
 H      -1.236186     2.622518    -3.592354      23.63
 C      -0.387514    -0.173198    -0.122165      21.58
 O       0.812336     0.141295     0.761813     106.92
 C      -0.858521    -1.418375     0.277692      36.13
 H      -0.541645    -2.230266     1.030147      19.95
 C      -2.271633    -1.517411    -1.850908      34.41
 C      -3.122877    -2.332074    -2.730655      82.78
 H      -3.003935    -1.872053    -3.765841      26.09
 O      -2.961494    -3.768129    -2.804356     269.83
 H      -2.211169    -3.804844    -2.298729      32.51
 C      -4.689473    -2.115075    -2.395748      82.94
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 H      -4.928023    -2.776211    -1.446652      27.38
 O      -4.988835    -0.726503    -2.138616     263.56
 H      -4.633764    -0.399637    -1.310424      29.18
 C      -5.587402    -2.686663    -3.561106     110.14
 O      -5.526188    -4.045767    -3.906419     161.39
 H      -4.447224    -4.349924    -3.616629      26.54
 H      -5.466640    -2.087621    -4.519559      27.37
 H      -6.548584    -2.572409    -3.125038      28.04
55
name = lig-ACN-frame_545
 C       3.905644     1.557434    -0.290002      50.19
 H       3.085137     2.123256    -0.513018      23.27
 C       4.445713    -0.032778     1.488037      41.87
 H       4.387802    -0.267191     2.531463      20.62
 C       5.532308    -0.426749     0.790993      13.14
 O       6.481429    -1.069018     1.558244     312.16
 C       6.401672    -2.430695     1.686834     103.21
 H       6.263688    -2.762113     2.737284      25.96
 H       7.117926    -2.932647     1.183710      25.38
 H       5.379504    -2.718973     1.167892      28.73
 C       5.802965     0.140424    -0.413417       7.77
 O       7.052539    -0.133205    -0.945141     189.93
 H       7.507403    -0.884033    -0.373936      21.43
 C       4.975638     1.140096    -1.091310      68.06
 H       5.311451     1.584393    -1.941107      22.54
 C       3.496960     0.881968     0.902491       9.39
 C       2.340455     1.570156     1.794067      88.56
 H       2.766755     2.591520     1.827102      24.26
 O       2.217543     1.052048     3.102810     292.50
 H       1.703801     0.168249     3.240716      24.75
 C       0.982494     1.679560     0.976726      70.65
 H       1.339040     2.154868     0.035774      23.30
 C      -0.044778     2.597172     1.563898     115.73
 O       0.286928     4.029768     1.523292     196.06
 H       0.262565     4.454352     0.415426      23.65
 H      -0.188523     2.168236     2.581913      25.81
 H      -0.911522     2.281903     0.964980      26.61
 C      -1.791541    -2.012494    -0.578696      66.75
 H      -2.385718    -2.988589    -0.336879      23.10
 C      -1.790804    -0.197224    -2.096544      53.04
 H      -1.987712     0.367945    -3.103311      20.56
 C      -0.701893     0.404905    -1.372497      -1.20
 O       0.019898     1.610668    -1.799191     195.00
 C      -0.312881     2.021994    -3.078760     105.76
 H       0.539689     2.983360    -3.254003      22.83
 H      -0.060226     1.373373    -3.913728      26.87
 H      -1.419769     2.369238    -3.041620      24.79
 C      -0.253031    -0.261241    -0.054594      16.05
 O       0.702214     0.179246     0.691685     151.82
 C      -0.982788    -1.440065     0.326335      45.32
 H      -0.475382    -1.811854     1.397292      19.59
 C      -2.201797    -1.460856    -1.758002      53.48
 C      -3.196468    -2.210971    -2.739188      51.34
 H      -3.031052    -1.834981    -3.795709      26.01
 O      -2.886252    -3.818877    -2.812357     138.33
 H      -1.966343    -4.244368    -2.428417      25.28
 C      -4.686243    -2.114893    -2.391815      88.55
 H      -4.921009    -2.760366    -1.419197      26.72
 O      -5.050323    -0.692867    -2.171474     178.95
 H      -4.456623    -0.438835    -1.227499      23.81
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 C      -5.682806    -2.589379    -3.540476      97.87
 O      -5.587280    -4.110573    -3.878147     130.02
 H      -4.517046    -4.370843    -3.661267      28.73
 H      -5.532332    -1.911345    -4.407723      28.12
 H      -6.716083    -2.394881    -3.270825      27.83
55
name = lig-ACN-frame_546
 C       3.822162     1.507807    -0.310964      50.01
 H       3.543462     2.353304    -0.800750      21.99
 C       4.322516    -0.041757     1.544496      44.62
 H       4.160635    -0.556744     2.440049      20.97
 C       5.570762    -0.362539     0.842721      -0.49
 O       6.642289    -1.008080     1.528663     325.26
 C       6.331002    -2.504862     1.666507      99.16
 H       6.251950    -2.771686     2.729902      27.81
 H       7.184937    -2.990648     1.378865      25.48
 H       5.435489    -2.849420     0.991265      27.31
 C       5.894282     0.166067    -0.459669      14.85
 O       7.112473    -0.101425    -1.025462     202.31
 H       7.565662    -0.758383    -0.496153      23.74
 C       5.027619     1.069775    -0.994511      51.45
 H       5.149753     1.416593    -1.955130      21.97
 C       3.468228     0.892204     0.935414      30.85
 C       2.337730     1.565093     1.646174      97.39
 H       2.474231     2.631882     1.918579      24.01
 O       2.222505     1.103635     3.061014     228.20
 H       1.651647     0.149896     2.842402      21.61
 C       1.063678     1.658455     0.891197      79.80
 H       1.179250     2.245862    -0.116905      21.08
 C      -0.108316     2.487352     1.601026      99.83
 O       0.272317     4.009416     1.463381     229.76
 H       0.286206     4.155206     0.481303      28.81
 H      -0.417538     2.495411     2.704209      24.49
 H      -1.050763     2.536608     1.060890      25.31
 C      -1.915310    -2.183093    -0.472735      22.90
 H      -2.256955    -3.207342    -0.252010      21.51
 C      -1.544055    -0.148238    -2.070409      56.60
 H      -2.096918     0.421692    -2.896863      23.92
 C      -0.621979     0.460518    -1.264912      33.89
 O       0.064995     1.490399    -1.822555     206.28
 C      -0.421790     1.980390    -3.138736     102.72
 H       0.030593     3.144933    -3.292284      22.54
 H      -0.378613     1.248959    -3.976093      25.95
 H      -1.545732     2.283097    -3.110649      24.81
 C      -0.297929    -0.224695    -0.188874      30.01
 O       0.662030     0.341401     0.742700     188.86
 C      -0.953105    -1.397399     0.360430      38.05
 H      -1.055435    -1.708494     1.573657      19.08
 C      -2.257785    -1.457066    -1.768759      14.69
 C      -3.171014    -2.256154    -2.737951      70.09
 H      -3.008329    -1.916212    -3.799104      27.06
 O      -2.871710    -3.747169    -2.799778     144.27
 H      -1.759980    -3.616954    -2.978250      24.49
 C      -4.751299    -2.107077    -2.412648      84.77
 H      -4.914364    -2.733935    -1.410141      26.01
 O      -5.070708    -0.721670    -2.191862     228.79
 H      -4.728257    -0.291019    -1.208656      23.32
 C      -5.717463    -2.576284    -3.509153     106.49
 O      -5.625008    -4.042942    -3.804435     209.31
 H      -4.731547    -4.260177    -3.768008      34.93
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 H      -5.436424    -2.140199    -4.439347      28.81
 H      -6.773448    -2.403632    -3.161661      26.93
55
name = lig-ACN-frame_547
 C       3.842656     1.421341    -0.373768      68.70
 H       3.211214     2.207237    -0.636926      23.98
 C       4.282235    -0.058026     1.492853      48.96
 H       3.885410    -0.404132     2.403640      21.83
 C       5.633144    -0.278574     0.971044     -12.14
 O       6.697709    -1.045627     1.455868     282.42
 C       6.352038    -2.574443     1.659595      81.43
 H       5.937051    -2.592628     2.665597      25.48
 H       7.244743    -3.129714     1.473905      24.50
 H       5.506374    -2.907701     0.946872      28.61
 C       5.961501     0.160808    -0.350743      -9.70
 O       7.201488    -0.091440    -1.153746     201.90
 H       7.865223    -0.381843    -0.524432      26.34
 C       4.988456     1.049461    -0.990216      52.67
 H       5.397043     1.558424    -1.870459      22.58
 C       3.499332     0.996210     0.918631      14.46
 C       2.367691     1.695521     1.716124      90.96
 H       2.849215     2.721576     1.726094      23.59
 O       2.162793     1.107781     2.960250     289.25
 H       1.745996     0.137396     3.015209      23.28
 C       0.995823     1.735548     0.855509      67.93
 H       1.247665     2.072537    -0.270331      21.09
 C      -0.146024     2.601892     1.543419     121.00
 O       0.229177     3.892264     1.448568     331.53
 H       0.483007     4.146532     0.678006      35.43
 H       0.047143     2.227127     2.637440      24.38
 H      -1.023391     2.112717     1.112643      26.94
 C      -1.912586    -2.056544    -0.491597      69.11
 H      -2.206218    -2.949810    -0.150809      26.25
 C      -1.665388    -0.375137    -2.117337      53.50
 H      -1.944390     0.021422    -3.118102      21.83
 C      -0.618822     0.378075    -1.378128       0.89
 O       0.150942     1.471116    -1.865372     152.70
 C      -0.591865     2.047001    -3.181173      88.94
 H       0.207142     2.940402    -3.499443      23.40
 H      -0.130706     1.227526    -3.846057      24.45
 H      -1.660681     2.100815    -3.036212      25.94
 C      -0.317438    -0.192148     0.030933      34.96
 O       0.604959     0.307746     0.809115     176.00
 C      -1.034149    -1.376820     0.288595      64.18
 H      -0.622577    -1.694293     1.401385      19.37
 C      -2.217056    -1.550059    -1.677372      38.55
 C      -3.195103    -2.242352    -2.741619      67.70
 H      -3.095869    -1.685570    -3.701754      27.45
 O      -2.827871    -3.591217    -2.789431     237.80
 H      -1.936609    -3.846984    -3.157461      27.87
 C      -4.729485    -2.108348    -2.385921      90.72
 H      -5.039152    -2.774195    -1.461198      26.89
 O      -5.082656    -0.723544    -2.206147     272.79
 H      -4.877239    -0.565046    -1.316169      30.72
 C      -5.693883    -2.602637    -3.516495     112.54
 O      -5.655131    -3.972711    -3.705913     229.31
 H      -4.769100    -4.288010    -3.779409      33.59
 H      -5.650686    -1.951392    -4.347985      29.61
 H      -6.737463    -2.332535    -3.125093      27.12
55
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name = lig-ACN-frame_548
 C       3.817888     1.458598    -0.404777      43.04
 H       3.145361     1.931485    -1.112224      21.19
 C       4.407339    -0.013994     1.476063      55.60
 H       4.262616    -0.413349     2.478680      21.21
 C       5.693319    -0.298732     0.953116     -11.80
 O       6.676190    -1.214235     1.435601     316.37
 C       6.352418    -2.513784     1.673007     109.93
 H       5.872974    -2.810044     2.604571      27.06
 H       7.338846    -3.096833     1.736381      22.95
 H       5.788892    -2.864171     0.766878      29.30
 C       6.040505     0.256277    -0.368717       8.91
 O       7.122125    -0.051773    -1.131098     157.16
 H       8.049800    -0.150541    -0.657811      21.00
 C       5.118224     1.020856    -1.049659      34.05
 H       5.344891     1.467972    -2.097928      21.58
 C       3.539275     0.990800     0.889391      34.85
 C       2.368483     1.760292     1.663036      86.61
 H       2.563433     2.797645     2.135572      22.88
 O       2.091986     1.129038     2.965141     302.82
 H       1.691532     0.391759     2.657363      29.01
 C       1.000475     1.748010     0.857889      78.85
 H       1.165804     2.188538    -0.272143      20.51
 C      -0.066953     2.456516     1.489697     107.59
 O       0.151777     3.967689     1.467973     197.12
 H       0.678046     4.149406     0.531912      27.11
 H      -0.211415     2.243511     2.624375      24.50
 H      -1.097215     2.494705     1.113966      24.39
 C      -1.905586    -2.027539    -0.394238      34.11
 H      -2.333669    -2.841085    -0.142177      23.91
 C      -1.642906    -0.413572    -2.217904      56.50
 H      -1.709164    -0.264392    -3.258053      22.66
 C      -0.638581     0.190148    -1.414070       7.12
 O       0.062663     1.467781    -1.978847     187.29
 C      -0.511102     1.988883    -3.134575     119.13
 H      -0.234595     3.153616    -3.310474      23.98
 H      -0.739294     1.494833    -4.184413      24.78
 H      -1.545681     2.225412    -2.965612      26.99
 C      -0.441262    -0.073261    -0.083323      28.49
 O       0.604412     0.261644     0.943673     118.34
 C      -0.970988    -1.329423     0.430084      33.29
 H      -0.605581    -2.063825     1.211833      19.44
 C      -2.313414    -1.599395    -1.776296      22.54
 C      -3.215917    -2.136683    -2.686907      85.59
 H      -3.067269    -1.626011    -3.651639      26.85
 O      -2.845116    -3.588390    -2.838280     225.16
 H      -1.942500    -3.565393    -2.751208      30.23
 C      -4.707918    -2.125844    -2.387032      96.98
 H      -4.851686    -2.721854    -1.419607      26.92
 O      -5.071814    -0.713707    -2.171882     278.11
 H      -4.807465    -0.374555    -1.379650      31.90
 C      -5.702262    -2.489791    -3.464899     102.45
 O      -5.675767    -4.030984    -3.648105     106.35
 H      -4.582270    -4.288815    -3.801572      28.18
 H      -5.464100    -2.070529    -4.379005      29.59
 H      -6.746782    -2.339668    -3.077305      27.47
55
name = lig-ACN-frame_549
 C       3.931245     1.404089    -0.518252      58.77
 H       3.208777     2.052384    -1.094114      22.54
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 C       4.601528     0.117017     1.532451      19.88
 H       4.294126    -0.322963     2.537594      18.90
 C       5.748937    -0.366303     0.781578      23.86
 O       6.658999    -1.176213     1.433999     306.70
 C       6.312421    -2.668830     1.667561      92.38
 H       5.598494    -2.621296     2.492894      28.87
 H       7.389178    -3.018800     2.010252      22.37
 H       5.954249    -3.236927     0.838823      27.46
 C       6.050670     0.349623    -0.366527       8.68
 O       7.123183    -0.024616    -1.112535     185.35
 H       7.831435    -0.370095    -0.497771      21.90
 C       5.084923     1.112446    -1.052017      61.33
 H       5.308391     1.097785    -2.205389      20.69
 C       3.575192     1.042027     0.872404       6.42
 C       2.373147     1.687096     1.659902      89.21
 H       2.649783     2.846284     1.572157      22.49
 O       2.025903     1.128946     2.957476     291.05
 H       1.563722     0.292109     3.005614      26.57
 C       1.116981     1.618187     0.853761      73.48
 H       1.182356     1.856887    -0.326511      19.86
 C      -0.162364     2.557689     1.525322      85.46
 O       0.101706     4.046441     1.502879     149.03
 H       0.685386     4.321575     0.494711      23.88
 H      -0.290479     2.277177     2.583378      25.12
 H      -0.908422     2.108813     0.799717      24.18
 C      -1.987389    -2.030964    -0.384477      81.11
 H      -2.220002    -2.923998    -0.066970      25.08
 C      -1.503666    -0.463565    -2.298895      54.04
 H      -1.738954    -0.008939    -3.203706      23.95
 C      -0.598187     0.318996    -1.502491      10.67
 O      -0.027243     1.281458    -2.031785     188.68
 C      -0.646174     2.094902    -3.135162      96.52
 H       0.164240     2.888210    -3.180090      23.99
 H      -0.277682     1.448314    -4.076746      23.25
 H      -1.663183     2.309636    -2.906533      26.72
 C      -0.394596    -0.189264    -0.007659      26.57
 O       0.546680     0.337957     0.874814     179.17
 C      -1.000331    -1.345925     0.407661      52.05
 H      -0.737774    -1.406086     1.390664      21.22
 C      -2.241563    -1.436990    -1.635875      27.06
 C      -3.285252    -2.249244    -2.790846      52.45
 H      -3.182930    -1.709230    -3.745515      27.08
 O      -2.882442    -3.610414    -2.909519     243.03
 H      -1.923191    -3.810327    -2.525590      25.64
 C      -4.741751    -2.027538    -2.292271      98.86
 H      -4.956764    -2.708675    -1.432785      27.48
 O      -5.068206    -0.659936    -2.112000     284.71
 H      -4.502979    -0.375733    -1.205028      22.81
 C      -5.681946    -2.604369    -3.440111     106.40
 O      -5.688063    -4.029349    -3.605083     200.06
 H      -4.609401    -4.217433    -3.669625      28.06
 H      -5.437722    -2.083662    -4.321387      30.21
 H      -6.682705    -2.203886    -3.247212      28.13
55
name = lig-ACN-frame_550
 C       3.832971     1.430239    -0.434016      44.17
 H       3.040338     2.118409    -0.894182      20.44
 C       4.656749     0.282734     1.499413      64.99
 H       4.508275    -0.001512     2.613408      21.60
 C       5.668764    -0.306519     0.830853      20.41
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 O       6.671431    -1.181858     1.381690     264.14
 C       6.294631    -2.719918     1.708788      82.35
 H       5.386609    -2.799273     2.320202      28.97
 H       7.180390    -3.248410     2.344489      23.03
 H       6.162372    -3.105089     0.749335      27.10
 C       6.071037     0.287089    -0.456956       2.14
 O       7.245730    -0.010210    -1.112897     185.31
 H       7.654060    -0.719417    -0.664971      20.19
 C       5.138579     1.129883    -1.143761      45.79
 H       5.389428     1.586765    -2.196441      20.52
 C       3.732860     1.030870     0.864628      43.77
 C       2.394539     1.513472     1.609811      85.39
 H       2.661257     2.617842     2.021099      21.88
 O       2.051251     1.173452     2.989740     240.67
 H       1.624818     0.169807     2.751741      23.02
 C       1.001192     1.687301     0.811995      80.65
 H       1.415932     2.136735    -0.164105      21.14
 C      -0.083297     2.677149     1.408708     108.45
 O       0.039189     4.047941     1.530099     245.42
 H       0.445767     4.451948     0.634655      27.04
 H      -0.248571     2.367192     2.410104      25.85
 H      -1.168238     2.590819     0.910671      23.30
 C      -1.999695    -1.985218    -0.409345      36.35
 H      -2.621792    -2.810104    -0.183066      23.53
 C      -1.466365    -0.482623    -2.205635      52.86
 H      -1.793740    -0.157868    -3.159064      24.15
 C      -0.658596     0.174544    -1.358773      32.01
 O       0.088185     1.347919    -2.084218     171.99
 C      -0.648869     2.163200    -3.137676     106.68
 H      -0.164030     3.133531    -3.150970      25.26
 H      -0.649604     1.623570    -4.244150      24.14
 H      -1.694780     2.465097    -3.175757      26.46
 C      -0.284461    -0.209351    -0.165138      27.90
 O       0.492625     0.312693     0.804783     205.75
 C      -1.101635    -1.335661     0.415252      34.32
 H      -1.159395    -1.642790     1.339429      22.25
 C      -2.304345    -1.550631    -1.769126      43.76
 C      -3.208974    -2.210632    -2.653122      70.80
 H      -3.169423    -1.766130    -3.653637      25.93
 O      -2.952560    -3.671384    -2.979573     166.13
 H      -1.910768    -4.037596    -2.726978      24.65
 C      -4.800614    -2.084681    -2.287375      89.97
 H      -5.002502    -2.527426    -1.352426      27.45
 O      -5.039482    -0.594285    -2.035766     239.17
 H      -4.487328    -0.280494    -1.045425      20.11
 C      -5.692453    -2.593920    -3.422686     112.67
 O      -5.668940    -4.042690    -3.555293     252.92
 H      -4.882015    -4.468710    -3.490264      35.65
 H      -5.367807    -2.176200    -4.340656      29.45
 H      -6.739984    -2.489988    -3.233632      27.37
55
name = lig-ACN-frame_551
 C       3.937239     1.480887    -0.477288      48.78
 H       3.178568     2.056486    -1.103883      20.66
 C       4.675533     0.286526     1.615996      11.29
 H       4.607792     0.148268     2.774862      19.02
 C       5.830732    -0.260105     0.793519      -7.51
 O       6.658455    -1.259632     1.366664     252.87
 C       6.250753    -2.584931     1.671937      94.12
 H       5.240612    -2.738575     2.095198      28.97
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 H       7.160553    -2.828954     2.437656      20.58
 H       6.388203    -3.271856     0.855372      25.39
 C       6.008037     0.182035    -0.589265     -11.66
 O       7.325380    -0.000185    -1.099380     167.28
 H       7.852141    -0.810864    -0.748195      29.98
 C       5.083708     1.140939    -1.122168      58.60
 H       5.389006     1.793347    -1.951382      21.46
 C       3.581526     1.075669     0.904974       7.08
 C       2.354917     1.634455     1.651143      79.96
 H       2.698865     2.803677     1.698256      21.04
 O       2.115632     1.071621     2.990892     244.92
 H       1.643635     0.121904     3.158518      22.21
 C       1.048236     1.823818     0.722740      66.95
 H       0.993585     1.963002    -0.363452      19.18
 C      -0.119329     2.624635     1.367610      95.34
 O       0.078367     4.162570     1.538934     267.60
 H       0.268771     4.537723     0.807860      34.08
 H      -0.228301     2.272468     2.337986      26.06
 H      -1.048497     2.318646     0.649286      23.49
 C      -2.099278    -1.995741    -0.499927      55.44
 H      -2.748473    -2.710400     0.119945      21.30
 C      -1.622148    -0.508487    -2.222226      50.77
 H      -1.523795    -0.211248    -3.263340      21.08
 C      -0.571166     0.260953    -1.525819     -15.32
 O       0.132388     1.444649    -2.098509     175.73
 C      -0.630321     2.202882    -3.121606      96.47
 H      -0.180852     3.114719    -3.166689      26.50
 H      -0.529893     1.760736    -4.259214      23.30
 H      -1.500681     2.102424    -2.536639      25.19
 C      -0.336825    -0.323253    -0.084146       2.47
 O       0.520616     0.335634     0.786406     125.40
 C      -1.178255    -1.328366     0.382109      57.26
 H      -0.875566    -1.591373     1.316323      20.69
 C      -2.184060    -1.703395    -1.773429      37.54
 C      -3.328577    -2.276806    -2.689164      68.51
 H      -3.227752    -1.615978    -3.564577      26.49
 O      -3.024662    -3.722866    -3.001955     240.59
 H      -2.018092    -3.700805    -3.028027      26.38
 C      -4.750507    -2.046360    -2.215258     105.85
 H      -5.027808    -2.722260    -1.471282      28.54
 O      -5.008561    -0.614084    -2.008417     284.78
 H      -4.708602    -0.421344    -0.990674      23.73
 C      -5.710355    -2.573513    -3.414251      97.38
 O      -5.678921    -4.115861    -3.496104     222.76
 H      -4.707932    -4.181515    -3.375016      30.59
 H      -5.466614    -2.082923    -4.350512      30.63
 H      -6.650297    -2.165768    -3.162040      29.38
55
name = lig-ACN-frame_552
 C       3.924800     1.485225    -0.391398      42.68
 H       3.315806     2.246994    -0.923160      21.30
 C       4.650786     0.291516     1.500370      52.25
 H       4.556107    -0.111747     2.553413      20.67
 C       5.748613    -0.250415     0.809613       7.07
 O       6.686169    -1.162683     1.301469     289.19
 C       6.232131    -2.514020     1.671392      74.43
 H       5.145504    -2.389515     1.871576      29.00
 H       6.670794    -2.883829     2.699057      22.71
 H       6.410477    -3.235512     0.841551      24.45
 C       6.073083     0.127266    -0.520213       4.05
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 O       7.270440     0.037649    -1.158883     184.03
 H       7.874115    -0.509880    -0.509854      24.57
 C       5.165807     1.091542    -1.094967      46.84
 H       5.327989     1.281954    -2.120589      20.98
 C       3.629162     1.049993     0.920278      29.08
 C       2.325088     1.811089     1.637542      71.70
 H       2.507943     2.888281     2.198853      21.37
 O       2.183030     1.021682     2.953065     266.15
 H       1.746043     0.323459     2.562388      28.26
 C       1.069982     1.754845     0.708272      86.97
 H       1.547439     2.133227    -0.144488      22.34
 C      -0.138655     2.665706     1.348189      91.84
 O       0.116031     4.148611     1.543916     235.36
 H       0.369496     4.476695     0.624878      27.98
 H      -0.381690     2.305019     2.310436      25.60
 H      -1.146242     2.501068     0.670090      22.57
 C      -2.122921    -2.081297    -0.337721      20.53
 H      -2.716467    -3.151792    -0.104427      19.61
 C      -1.488877    -0.408688    -2.371844      37.60
 H      -2.008569    -0.244840    -3.333842      18.59
 C      -0.536903     0.249478    -1.598068      11.65
 O       0.150633     1.387902    -2.048065     238.14
 C      -0.642345     2.212843    -2.991418     114.33
 H      -0.239976     3.113237    -3.089740      27.66
 H      -0.630917     1.592370    -4.021255      23.32
 H      -1.707824     2.416253    -3.064241      26.25
 C      -0.407109    -0.111080    -0.204127      15.22
 O       0.564409     0.348549     0.788211     153.38
 C      -1.140512    -1.323719     0.342827      33.66
 H      -1.124536    -1.560454     1.417695      21.74
 C      -2.219892    -1.719851    -1.853376      -6.76
 C      -3.308725    -2.317872    -2.810860      80.26
 H      -3.384238    -1.918618    -3.842183      24.00
 O      -3.097545    -3.710226    -2.993550     271.22
 H      -2.275817    -3.863013    -3.295634      32.23
 C      -4.796181    -2.093823    -2.230127      98.52
 H      -4.909587    -2.539283    -1.297420      30.47
 O      -4.982386    -0.699540    -1.977275     348.81
 H      -4.718225    -0.474224    -1.150945      31.95
 C      -5.743704    -2.584780    -3.339803     105.44
 O      -5.686371    -4.038349    -3.417925     206.51
 H      -4.690088    -4.480324    -3.555868      27.30
 H      -5.411880    -2.229829    -4.332213      29.10
 H      -6.779373    -2.422312    -3.176781      28.06
55
name = lig-ACN-frame_553
 C       4.010202     1.503499    -0.418602      63.26
 H       3.397723     2.247353    -0.905066      22.17
 C       4.526292     0.186127     1.486837      37.45
 H       4.304465    -0.200968     2.479989      21.37
 C       5.727707    -0.307544     0.760150      13.20
 O       6.759475    -1.053317     1.302989     249.62
 C       6.123936    -2.426807     1.704764      89.72
 H       5.008813    -2.487492     1.597505      28.71
 H       6.546894    -2.759519     2.683184      24.54
 H       6.585359    -3.100888     0.890217      23.67
 C       6.060336     0.331192    -0.435041      13.48
 O       7.201309     0.010718    -1.201804     209.82
 H       7.996529    -0.192665    -0.759427      22.25
 C       5.109671     0.996349    -1.081637      63.81
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 H       5.261137     1.308767    -2.046422      24.55
 C       3.682083     1.221198     0.906211      24.13
 C       2.446428     1.732432     1.730918      92.84
 H       2.619864     2.963787     1.796526      21.44
 O       2.190056     1.006795     2.831697     311.02
 H       1.820399     0.134690     2.748934      26.12
 C       1.058004     1.772498     0.860407      82.41
 H       1.152431     1.999253    -0.127593      22.64
 C      -0.119432     2.718290     1.298260     100.79
 O       0.173460     4.043802     1.513497     175.05
 H       0.686765     4.615021     0.612414      23.51
 H      -0.371664     2.338903     2.283355      25.18
 H      -1.125135     2.697525     0.605456      22.66
 C      -1.967273    -2.016046    -0.575154      59.44
 H      -2.310159    -3.051591     0.050867      19.66
 C      -1.501367    -0.612446    -2.411450      55.27
 H      -1.650804     0.106791    -3.219628      22.02
 C      -0.579566     0.225900    -1.582676       8.90
 O       0.078082     1.359781    -1.992577     223.51
 C      -0.613176     2.203844    -2.984807     104.42
 H      -0.045918     3.029320    -2.938802      27.35
 H      -0.451027     1.808362    -4.062220      23.94
 H      -1.563992     2.323253    -2.427782      25.10
 C      -0.461156    -0.082782    -0.200484      17.13
 O       0.572677     0.398666     0.664543     186.09
 C      -1.142068    -1.234256     0.285782      40.72
 H      -0.824305    -1.313969     1.410924      18.07
 C      -2.265169    -1.542353    -1.857983      62.89
 C      -3.237228    -2.267984    -2.811935      58.23
 H      -3.064795    -1.683645    -3.736024      26.52
 O      -3.149244    -3.783492    -2.981826     203.51
 H      -2.135978    -4.010928    -3.238370      26.80
 C      -4.765995    -2.142931    -2.246482      96.35
 H      -4.859998    -2.891334    -1.491029      27.18
 O      -4.990555    -0.731373    -1.979994     355.73
 H      -4.482705    -0.539449    -1.243240      29.71
 C      -5.802383    -2.646202    -3.278560     103.64
 O      -5.747835    -4.041131    -3.354771     250.91
 H      -4.706717    -4.152977    -3.587148      28.05
 H      -5.593010    -2.022869    -4.183091      29.61
 H      -6.803410    -2.274941    -2.995325      28.14
55
name = lig-ACN-frame_554
 C       3.959995     1.657097    -0.483358      46.81
 H       3.256749     2.199240    -1.097167      20.83
 C       4.439247     0.095138     1.471933      48.62
 H       4.183181    -0.276887     2.432317      21.14
 C       5.738451    -0.203034     0.811934      -6.03
 O       6.708181    -1.082582     1.396653     301.66
 C       6.156017    -2.327204     1.686453      91.44
 H       5.033938    -2.268429     1.542436      28.82
 H       6.270592    -2.444006     2.736648      24.74
 H       6.615977    -3.270119     1.132716      23.32
 C       6.120986     0.382670    -0.436094      -5.31
 O       7.144626    -0.002246    -1.247226     195.42
 H       7.875410    -0.316097    -0.648328      23.61
 C       5.003087     1.087991    -1.203142      40.75
 H       5.301312     1.447239    -2.160595      22.56
 C       3.753577     1.212686     0.940226      26.14
 C       2.453243     1.662382     1.567633      80.24
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 H       2.728167     2.671090     2.224749      20.86
 O       2.196539     0.980922     2.902932     193.51
 H       1.798662    -0.016569     2.580493      22.19
 C       1.064188     1.843223     0.765906      71.67
 H       1.396171     2.369581    -0.047380      23.78
 C      -0.128423     2.628012     1.337770      95.64
 O       0.294422     4.080787     1.502118     165.86
 H       0.956883     4.356179     0.603490      24.47
 H      -0.716401     2.384881     2.267172      24.33
 H      -0.783330     2.330269     0.410749      22.42
 C      -1.783687    -1.937504    -0.664315      52.45
 H      -2.433490    -2.951375    -0.308880      21.02
 C      -1.432463    -0.470332    -2.424827      46.81
 H      -1.525309    -0.580638    -3.476305      20.44
 C      -0.668231     0.203308    -1.537131      22.07
 O       0.047224     1.315645    -1.989760     253.06
 C      -0.531844     2.238482    -2.918758     119.77
 H      -0.025111     3.153892    -3.002454      26.55
 H      -0.827877     1.870330    -3.918900      25.28
 H      -1.647768     2.519320    -2.748689      25.19
 C      -0.391024    -0.077398    -0.185066      21.91
 O       0.562907     0.409470     0.597329     187.41
 C      -1.120518    -1.162212     0.264973      58.76
 H      -0.974740    -1.900029     1.208929      19.39
 C      -2.275900    -1.602678    -1.906136      33.69
 C      -3.297029    -2.285187    -2.756113      84.45
 H      -3.313523    -1.927096    -3.810144      22.55
 O      -3.100668    -3.778821    -2.974067     197.17
 H      -2.020672    -4.079064    -2.864248      25.71
 C      -4.670127    -2.142277    -2.295042     101.58
 H      -4.738261    -2.625911    -1.334577      24.95
 O      -5.015080    -0.785501    -1.966613     279.77
 H      -4.514507    -0.366000    -1.089407      22.38
 C      -5.871808    -2.551179    -3.228296      95.43
 O      -5.821535    -4.121698    -3.349779     262.47
 H      -4.948895    -4.352408    -3.393066      34.83
 H      -5.943912    -2.272866    -4.311186      26.95
 H      -6.778779    -2.341201    -2.600062      27.36
55
name = lig-ACN-frame_555
 C       3.904850     1.687445    -0.444308      58.09
 H       3.148833     2.432639    -0.733359      22.49
 C       4.522669     0.156070     1.379057      48.06
 H       4.237177    -0.372261     2.265921      20.62
 C       5.784433    -0.063866     0.853661      -7.42
 O       6.649519    -1.003612     1.414762     265.75
 C       6.108642    -2.364209     1.803707      81.41
 H       5.107424    -2.526782     1.300516      27.34
 H       6.101150    -2.586958     2.807045      23.98
 H       6.838041    -3.088324     1.183625      22.67
 C       5.924356     0.370009    -0.554652       8.11
 O       7.139898    -0.000442    -1.239355     174.29
 H       7.707313    -0.754451    -0.769493      24.78
 C       5.107287     1.254161    -1.193671      63.31
 H       5.148592     1.294775    -2.302093      21.47
 C       3.642102     1.108043     0.757143      27.03
 C       2.373818     1.665948     1.655782      80.48
 H       2.545857     2.890370     1.759188      22.05
 O       2.184901     0.916579     2.923348     250.76
 H       1.671671     0.016960     2.704750      22.93
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 C       1.154956     1.812044     0.703496      89.00
 H       1.307827     2.194498    -0.245706      22.78
 C      -0.072929     2.656045     1.296033      98.05
 O       0.369647     4.047703     1.483142     277.86
 H       0.894897     4.225761     0.759415      32.26
 H      -0.302750     2.142622     2.345923      24.04
 H      -0.988275     2.934513     0.729997      23.20
 C      -1.908739    -2.039027    -0.616205      69.08
 H      -2.274450    -3.080866    -0.127016      18.89
 C      -1.543507    -0.439513    -2.492651      45.89
 H      -1.346308     0.014032    -3.422947      18.90
 C      -0.666275     0.350127    -1.573673      14.41
 O       0.117483     1.363920    -2.018502     244.97
 C      -0.580454     2.295980    -2.935189     108.41
 H       0.233140     3.026896    -2.979421      25.66
 H      -0.442260     1.807894    -3.838775      25.59
 H      -1.558950     2.682046    -2.483097      25.40
 C      -0.389485    -0.094068    -0.220652      19.42
 O       0.682511     0.481976     0.596758     174.13
 C      -1.039338    -1.326770     0.272428      36.51
 H      -0.783480    -1.469013     1.491355      18.34
 C      -2.094697    -1.618614    -2.038606      30.50
 C      -3.235869    -2.374250    -2.887386      55.98
 H      -3.194464    -1.838917    -3.867114      26.60
 O      -3.003209    -3.757018    -2.919594     298.48
 H      -2.071918    -3.837518    -2.677490      29.28
 C      -4.779605    -2.118450    -2.215969      82.93
 H      -4.855329    -2.839074    -1.387907      27.72
 O      -5.041179    -0.731169    -1.976543     256.80
 H      -4.559126    -0.659224    -0.907407      18.44
 C      -5.881875    -2.704265    -3.135486      91.22
 O      -5.947719    -4.119541    -3.339517     284.00
 H      -5.026285    -4.473378    -3.235635      33.87
 H      -5.870438    -1.942517    -4.005380      28.37
 H      -6.895939    -2.463894    -2.626779      27.26
55
name = lig-ACN-frame_556
 C       3.928902     1.699133    -0.486347      49.94
 H       3.494075     2.587737    -1.042850      21.53
 C       4.528627     0.296569     1.341131      36.26
 H       4.302038    -0.130006     2.343837      18.11
 C       5.744552    -0.037723     0.730237      18.74
 O       6.624886    -0.916475     1.422848     245.41
 C       6.076900    -2.405859     1.824540      83.85
 H       5.126661    -2.734786     1.340835      27.05
 H       5.981751    -2.311714     2.847335      25.74
 H       7.035032    -3.028797     1.613283      23.60
 C       5.975174     0.316396    -0.600473       9.38
 O       7.077245    -0.004204    -1.230852     172.76
 H       7.383484    -0.794965    -0.758889      28.15
 C       5.064453     1.373587    -1.132354      57.09
 H       5.333158     1.888991    -2.156345      19.95
 C       3.438715     1.032317     0.777685      24.22
 C       2.369376     1.646737     1.649609      82.06
 H       2.845476     2.629334     2.243683      21.21
 O       2.154821     0.921667     2.858767     305.69
 H       1.578500     0.264784     2.700873      30.23
 C       1.060150     1.787809     0.666018      82.73
 H       1.558405     2.119061    -0.204888      22.17
 C       0.049413     2.724201     1.258366     114.41
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 O       0.461032     4.040782     1.523159     310.01
 H       0.729338     4.501837     0.806374      31.87
 H      -0.056046     2.350911     2.400355      23.56
 H      -0.859794     2.304735     0.796973      24.31
 C      -1.930461    -2.080240    -0.606324      32.89
 H      -2.532404    -2.998801    -0.335474      17.40
 C      -1.492959    -0.294654    -2.449088      59.61
 H      -2.109369     0.038853    -3.229207      19.31
 C      -0.652783     0.338602    -1.565684       4.23
 O       0.168199     1.480321    -2.051542     224.29
 C      -0.461156     2.360753    -2.991739     123.76
 H      -0.018052     3.397005    -3.124691      24.86
 H      -0.885031     2.132654    -3.881851      26.95
 H      -1.476492     2.643027    -2.519481      25.64
 C      -0.388143    -0.154145    -0.261882      31.46
 O       0.692673     0.346366     0.553294     168.39
 C      -0.932955    -1.356996     0.161634      37.03
 H      -0.805349    -1.675020     1.346510      19.69
 C      -2.105813    -1.711620    -1.997801      16.52
 C      -3.180079    -2.296483    -2.899264      78.39
 H      -3.238399    -2.040758    -3.975775      22.79
 O      -2.905742    -3.801253    -2.863197     269.75
 H      -2.021317    -3.961413    -2.981162      30.41
 C      -4.773960    -2.204484    -2.166876      63.52
 H      -4.608328    -2.545685    -1.131062      27.39
 O      -5.056189    -0.728980    -1.972923     263.00
 H      -4.667761    -0.284674    -1.007081      20.55
 C      -5.957982    -2.716028    -3.049751      98.11
 O      -6.032076    -4.137563    -3.336631     230.05
 H      -5.012791    -4.573282    -3.340858      30.25
 H      -5.836310    -2.388458    -4.141186      26.65
 H      -6.979478    -2.364870    -2.596559      26.86
55
name = lig-ACN-frame_557
 C       3.833179     1.711235    -0.471439      53.20
 H       3.072994     2.493759    -0.845777      22.49
 C       4.434807     0.355485     1.383068      44.44
 H       4.458352     0.206540     2.507613      21.01
 C       5.572820    -0.156711     0.681900      -9.43
 O       6.573455    -0.935480     1.392234     273.72
 C       6.146245    -2.257335     1.856606     103.59
 H       5.399343    -2.569101     1.118580      28.30
 H       5.644290    -2.228699     2.814202      28.67
 H       6.915815    -3.062489     1.848124      24.86
 C       5.960914     0.439612    -0.574128      10.79
 O       7.089462    -0.075466    -1.310435     155.80
 H       7.734322    -0.486723    -0.745225      23.33
 C       5.116477     1.342265    -1.104406      57.25
 H       5.550263     1.997333    -1.946849      19.11
 C       3.541140     1.122411     0.714834      38.33
 C       2.346269     1.600540     1.566931      95.76
 H       2.591115     2.821893     1.731993      22.10
 O       2.071145     0.908593     2.827463     262.25
 H       1.551449     0.060205     2.602326      24.71
 C       1.194413     1.761213     0.696129      70.21
 H       1.224543     2.205720    -0.321484      20.79
 C       0.051347     2.620787     1.339548      93.36
 O       0.538923     4.106576     1.542642     151.96
 H       0.541900     4.604595     0.551916      24.75
 H      -0.271240     2.270025     2.424596      24.32
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 H      -0.776465     2.953701     0.724186      24.07
 C      -1.809608    -2.079897    -0.717132      62.22
 H      -2.322841    -2.822244    -0.230340      22.89
 C      -1.623117    -0.395680    -2.326587      60.71
 H      -1.942008     0.117213    -3.220715      22.44
 C      -0.536428     0.409539    -1.653555      19.69
 O       0.180787     1.528800    -2.066696     243.57
 C      -0.525840     2.500226    -3.014277      98.89
 H       0.405174     3.225963    -3.196768      23.70
 H      -0.479391     1.938772    -3.830881      26.87
 H      -1.473836     2.878541    -2.564060      26.23
 C      -0.263809    -0.191313    -0.355696      22.56
 O       0.643093     0.215203     0.535652     118.51
 C      -0.983737    -1.415939     0.074405      49.74
 H      -0.549956    -1.978740     1.014239      19.87
 C      -2.186795    -1.494958    -1.946250      50.49
 C      -3.222219    -2.379452    -2.740999      64.01
 H      -3.215019    -1.848465    -3.715825      25.78
 O      -2.873237    -3.821812    -2.831246     238.69
 H      -1.923933    -3.811323    -3.289442      26.52
 C      -4.627682    -2.139627    -2.168896     100.61
 H      -4.725250    -2.796725    -1.240914      25.03
 O      -5.067734    -0.785817    -2.020158     295.08
 H      -4.565785    -0.543862    -1.206777      25.36
 C      -5.941952    -2.696255    -3.043318      74.39
 O      -6.090139    -4.215499    -3.274479     248.52
 H      -5.141666    -4.399572    -3.503408      34.01
 H      -5.930272    -1.946866    -3.935849      27.91
 H      -6.927321    -2.429926    -2.446760      27.33
55
name = lig-ACN-frame_558
 C       3.863127     1.700716    -0.584030      39.35
 H       3.119748     2.378629    -1.165416      21.36
 C       4.486727     0.271070     1.443932      51.69
 H       4.114423     0.015838     2.499287      19.95
 C       5.548607    -0.250255     0.739892      15.73
 O       6.526097    -0.923881     1.314562     300.42
 C       6.121943    -2.149703     1.850815     122.11
 H       5.631723    -2.816322     1.136260      27.87
 H       5.527604    -2.063879     2.798712      27.52
 H       7.087870    -2.514765     2.118062      24.41
 C       5.963570     0.365035    -0.507194       2.14
 O       7.045081    -0.089193    -1.340568     199.71
 H       7.893578    -0.144035    -0.739101      23.48
 C       5.068837     1.410019    -1.155021      47.01
 H       5.129430     1.437182    -2.266038      20.96
 C       3.620290     1.246000     0.823236      19.19
 C       2.368471     1.637892     1.501026      82.34
 H       2.479330     2.770308     2.027668      21.39
 O       1.992276     0.927598     2.754812     208.44
 H       1.755801    -0.145577     2.520555      21.92
 C       1.023941     1.627269     0.680906      80.97
 H       1.414065     1.925906    -0.375521      20.84
 C       0.013061     2.706641     1.380253     101.69
 O       0.598853     4.047303     1.595236     167.59
 H       0.598992     4.505820     0.480902      22.26
 H      -0.389307     2.206653     2.361728      24.33
 H      -0.830952     2.503061     0.686085      23.90
 C      -1.815593    -2.154953    -0.769066      18.66
 H      -1.971575    -3.136719    -0.622399      19.72
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 C      -1.614660    -0.140456    -2.402344     106.00
 H      -1.715908     0.079244    -3.473373      20.93
 C      -0.557266     0.324022    -1.673874       9.02
 O       0.119440     1.570393    -2.068559     212.27
 C      -0.464743     2.496853    -3.045370     111.56
 H       0.309215     3.484802    -3.110754      23.20
 H      -0.735234     2.216362    -3.958343      27.51
 H      -1.409028     3.025009    -2.850162      26.85
 C      -0.193580    -0.264614    -0.456641      15.00
 O       0.711266     0.252046     0.595812     162.64
 C      -0.779354    -1.359042     0.043298      29.95
 H      -0.433476    -1.651687     1.043313      19.63
 C      -2.346864    -1.530306    -1.857002      44.43
 C      -3.263101    -2.352345    -2.714061      63.15
 H      -3.289223    -2.043667    -3.767542      24.81
 O      -2.897280    -3.747747    -2.797518     200.83
 H      -1.781493    -3.860606    -3.055740      24.95
 C      -4.728001    -2.279794    -2.197187      93.53
 H      -4.756386    -2.720626    -1.128733      25.12
 O      -4.997184    -0.837744    -2.050294     298.14
 H      -4.654136    -0.505903    -1.324671      28.20
 C      -5.864734    -2.739413    -3.009490     108.21
 O      -6.061364    -4.147209    -3.198106     298.52
 H      -5.471620    -4.589327    -3.717338      37.71
 H      -6.090244    -2.268287    -4.051978      27.00
 H      -6.680232    -2.492106    -2.219764      27.39
55
name = lig-ACN-frame_559
 C       3.935872     1.695015    -0.523299      47.94
 H       3.174115     2.238279    -1.141866      22.82
 C       4.410641     0.290545     1.425598      52.46
 H       4.200969    -0.393608     2.273095      20.06
 C       5.612165    -0.063838     0.685189       8.31
 O       6.595347    -0.957098     1.257060     293.41
 C       6.164601    -2.220660     1.955483     103.22
 H       5.873601    -2.975712     1.258524      27.71
 H       5.241919    -1.914142     2.580888      26.83
 H       6.921476    -2.569987     2.552170      25.01
 C       5.875090     0.353300    -0.617825      29.63
 O       6.942850    -0.054560    -1.279389     140.93
 H       7.750045    -0.374561    -0.754933      22.19
 C       5.062954     1.202446    -1.251855      59.61
 H       5.323466     1.534238    -2.238958      21.43
 C       3.639083     1.288998     0.848456      11.92
 C       2.283244     1.715762     1.600130      76.54
 H       2.544499     2.845687     1.993642      21.63
 O       1.982461     0.921936     2.705293     267.44
 H       1.855204    -0.011097     2.381606      25.78
 C       1.003164     1.705910     0.668552      88.11
 H       1.028440     2.195796    -0.414676      20.99
 C      -0.042895     2.637554     1.310784     106.63
 O       0.585355     3.892718     1.611685     183.41
 H       0.956179     4.551567     0.792372      25.01
 H      -0.131289     2.422595     2.435956      24.61
 H      -1.009716     2.983436     0.897152      24.95
 C      -1.689253    -2.113821    -0.725957      58.08
 H      -1.938300    -3.116815    -0.526088      19.92
 C      -1.743245    -0.237367    -2.424786      44.25
 H      -2.173007     0.273384    -3.350905      20.55
 C      -0.598158     0.424856    -1.748576       7.11
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 O       0.041463     1.555250    -2.082985     215.99
 C      -0.457670     2.515031    -3.088718     103.18
 H       0.455941     3.406541    -3.154692      22.60
 H      -0.509809     2.105944    -3.983154      28.05
 H      -1.289628     2.783771    -2.514695      26.72
 C      -0.080906    -0.213439    -0.381286      10.87
 O       0.707255     0.273750     0.583252     166.01
 C      -0.683758    -1.508000    -0.011200      46.34
 H      -0.539732    -1.772185     0.974422      22.28
 C      -2.246010    -1.388802    -1.942317      19.78
 C      -3.333058    -2.316169    -2.839785      55.19
 H      -3.391584    -1.804367    -3.811303      26.15
 O      -2.920691    -3.716119    -2.747474     249.48
 H      -1.858577    -3.723505    -2.733724      25.79
 C      -4.723540    -2.305978    -2.145171      93.16
 H      -4.723038    -2.903681    -1.142394      26.07
 O      -4.955833    -0.865184    -2.092839     302.82
 H      -4.595822    -0.619508    -1.207146      25.71
 C      -5.945827    -2.798065    -2.994780      90.59
 O      -6.036881    -4.194964    -3.104800     246.36
 H      -5.359344    -4.327690    -3.929048      30.98
 H      -5.744107    -2.161360    -4.002388      28.16
 H      -6.934586    -2.394802    -2.646554      28.33
55
name = lig-ACN-frame_560
 C       3.930814     1.718433    -0.447399      46.18
 H       3.313451     2.546863    -0.790554      23.16
 C       4.439341     0.296210     1.327366      53.13
 H       4.170937     0.010174     2.321007      21.59
 C       5.666898    -0.031588     0.769572       5.10
 O       6.670650    -1.019063     1.212362     239.26
 C       6.172508    -2.219259     2.039663     102.17
 H       6.193989    -3.008197     1.321186      26.85
 H       5.109518    -2.148712     2.524578      26.15
 H       6.862416    -2.393282     2.765454      25.69
 C       5.840923     0.330792    -0.633046      -6.20
 O       7.013630    -0.099593    -1.294290     195.49
 H       7.228403    -0.813790    -0.709714      23.41
 C       4.889312     1.131897    -1.346167      61.21
 H       5.238431     1.671603    -2.178934      21.10
 C       3.520713     1.273324     0.803010      33.45
 C       2.286813     1.791878     1.556077      90.42
 H       2.308907     2.881148     2.044880      21.72
 O       2.007470     0.903589     2.740593     274.91
 H       1.649058     0.152420     2.414298      29.13
 C       1.048635     1.873778     0.642467      68.95
 H       1.417029     2.191714    -0.433327      21.93
 C      -0.125138     2.577915     1.366071     112.06
 O       0.601943     3.872843     1.645322     236.08
 H       0.814986     4.104256     0.798611      31.56
 H      -0.519333     1.882870     2.149828      25.36
 H      -0.980993     2.565406     0.643882      25.66
 C      -1.659851    -2.030246    -0.893240      38.23
 H      -2.305186    -2.747200    -0.326086      19.07
 C      -1.716892    -0.208001    -2.368829      71.00
 H      -2.430272     0.391490    -3.028910      21.23
 C      -0.674918     0.364906    -1.617856      16.93
 O       0.066792     1.550831    -2.113380     215.10
 C      -0.508038     2.487562    -3.070309     117.15
 H       0.405083     3.357109    -3.142514      23.20
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 H      -0.579217     2.048136    -3.970667      28.13
 H      -1.376490     3.054419    -3.181703      27.19
 C      -0.222941    -0.222831    -0.487710      14.21
 O       0.707669     0.354205     0.529205     103.25
 C      -0.578606    -1.494590    -0.015295      42.73
 H      -0.161098    -2.063466     0.672767      21.38
 C      -2.196248    -1.581615    -2.031465      55.83
 C      -3.298215    -2.298967    -2.769757      68.49
 H      -3.376792    -2.043701    -3.827795      25.34
 O      -2.923403    -3.686822    -2.748554     268.91
 H      -2.059620    -3.766424    -2.990960      32.43
 C      -4.725556    -2.208841    -2.154833      95.32
 H      -4.647661    -2.720276    -1.112223      26.35
 O      -4.972942    -0.840235    -2.047247     298.90
 H      -4.606589    -0.327477    -1.114790      21.23
 C      -5.979623    -2.729658    -3.016159      88.19
 O      -6.001312    -4.320166    -3.070708     196.88
 H      -5.299820    -4.695995    -3.724366      31.95
 H      -5.839784    -2.447447    -4.164971      27.30
 H      -6.916371    -2.365816    -2.602241      28.70
55
name = lig-ACN-frame_561
 C       3.777912     1.821516    -0.545817      61.51
 H       3.533688     2.752904    -0.930150      22.52
 C       4.451107     0.317710     1.422191      49.26
 H       4.302836     0.080878     2.421018      21.05
 C       5.692763    -0.154820     0.695789      -8.22
 O       6.628922    -1.033319     1.224210     270.47
 C       6.231257    -2.173516     2.031093     100.67
 H       6.379870    -3.141756     1.587854      26.67
 H       5.117746    -1.995445     2.312030      26.58
 H       6.799514    -2.057383     2.903281      25.54
 C       5.859132     0.274230    -0.651608       3.30
 O       7.043105    -0.178242    -1.280791     230.06
 H       7.464178    -1.008230    -0.999295      25.65
 C       4.828490     1.186281    -1.236465      44.57
 H       4.831665     1.314142    -2.301315      22.02
 C       3.532294     1.208931     0.761758      10.93
 C       2.342641     1.730910     1.580807      87.48
 H       2.783878     2.700783     1.996080      22.45
 O       2.040463     0.952156     2.759952     248.97
 H       1.366127     0.169485     2.492866      23.62
 C       1.054460     1.779800     0.643847      89.05
 H       1.224657     2.478634    -0.257605      23.02
 C      -0.087075     2.524394     1.297167     112.63
 O       0.461731     3.854814     1.698824     257.97
 H       0.644566     4.433140     0.997533      31.20
 H      -0.374385     2.248311     2.268199      27.09
 H      -0.905781     2.769104     0.588444      25.56
 C      -1.649397    -2.141288    -0.830986      49.94
 H      -2.004768    -3.258260    -0.538123      17.69
 C      -1.756846    -0.224478    -2.360010      55.74
 H      -1.960528     0.356543    -3.318515      18.36
 C      -0.737059     0.440753    -1.625508      12.03
 O      -0.009575     1.536238    -2.054810     212.64
 C      -0.516882     2.432635    -3.176762      99.15
 H       0.288926     3.356583    -3.249064      23.33
 H      -0.506950     1.969599    -4.094600      26.68
 H      -1.372824     2.662436    -2.631260      26.50
 C      -0.167520    -0.142482    -0.363198      17.72
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 O       0.701994     0.470489     0.370724     212.22
 C      -0.638201    -1.492419    -0.169866      57.57
 H      -0.131268    -1.840005     0.629484      23.42
 C      -2.141367    -1.506211    -2.104995      33.32
 C      -3.258408    -2.344938    -2.764393      90.21
 H      -3.337852    -1.859378    -3.744458      25.91
 O      -2.944791    -3.759602    -2.778608     282.59
 H      -2.110246    -3.862492    -3.221784      30.96
 C      -4.754138    -2.134482    -2.183432      77.23
 H      -4.929572    -2.676575    -1.174733      26.87
 O      -5.066121    -0.673833    -2.001740     230.63
 H      -4.534145    -0.623119    -0.955403      18.92
 C      -5.840337    -2.880927    -3.066292     110.95
 O      -5.987211    -4.305721    -3.010812     291.12
 H      -5.188451    -4.584298    -3.291932      37.03
 H      -6.097051    -2.353888    -4.057274      28.82
 H      -6.687065    -2.670048    -2.433861      29.08
55
name = lig-ACN-frame_562
 C       3.773210     1.725861    -0.532856      74.37
 H       2.939611     2.231099    -0.900764      22.23
 C       4.543195     0.330072     1.382826      88.08
 H       4.299407    -0.078169     2.309598      23.41
 C       5.522896    -0.245937     0.660265      14.12
 O       6.592626    -1.012978     1.191815     257.08
 C       6.248777    -2.087867     2.091648     103.88
 H       6.654376    -2.972655     1.574219      24.66
 H       5.133996    -2.241900     2.205748      28.85
 H       6.692653    -2.079905     3.098053      25.43
 C       5.836719     0.211172    -0.632997       7.83
 O       6.977932    -0.195219    -1.357298     140.53
 H       7.469247    -0.704763    -0.554966      18.94
 C       4.980812     1.166297    -1.199858      42.91
 H       5.229202     1.379167    -2.280555      20.55
 C       3.608308     1.197193     0.771736       8.66
 C       2.392835     1.642423     1.572443      98.14
 H       2.394079     2.721568     1.829875      25.03
 O       2.063662     1.006248     2.809916     243.45
 H       1.535443     0.056511     2.582826      24.01
 C       1.092990     1.833614     0.657317      81.03
 H       1.419332     2.265336    -0.310977      24.57
 C      -0.069633     2.635725     1.293061     122.41
 O       0.294235     3.888091     1.776279     196.45
 H       0.382095     4.682367     0.937499      24.10
 H      -0.401146     2.002321     2.049177      28.41
 H      -0.992848     2.537929     0.652773      26.71
 C      -1.607441    -2.201070    -0.902739      32.67
 H      -1.513265    -3.431574    -0.919707      18.39
 C      -1.717815    -0.200185    -2.435223      51.34
 H      -1.960918    -0.098798    -3.501299      20.13
 C      -0.752442     0.498884    -1.648691      17.57
 O      -0.037223     1.591484    -2.046012     237.09
 C      -0.571441     2.327424    -3.144652     115.16
 H       0.099951     3.261317    -3.248470      24.91
 H      -0.660076     1.773661    -4.094191      26.37
 H      -1.582492     2.756672    -3.188850      27.21
 C      -0.338929    -0.086832    -0.484687      17.27
 O       0.814795     0.432802     0.299779     139.53
 C      -0.622124    -1.441023    -0.115250      46.84
 H      -0.391225    -1.949181     0.781075      22.56
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 C      -2.196835    -1.549686    -1.935664      26.98
 C      -3.281828    -2.262233    -2.837435      64.00
 H      -3.301919    -2.077162    -3.908340      25.87
 O      -3.014590    -3.839276    -2.833083     165.78
 H      -1.932666    -3.919337    -3.089505      25.27
 C      -4.713741    -2.121921    -2.214849      78.40
 H      -4.605026    -2.571059    -1.171099      26.66
 O      -5.141604    -0.664093    -2.027783     181.26
 H      -4.766116    -0.110982    -1.112925      21.92
 C      -5.872194    -2.846549    -2.997526     104.74
 O      -5.879557    -4.305167    -2.972421     230.61
 H      -4.935321    -4.717856    -2.909272      30.68
 H      -5.687701    -2.629083    -4.089814      28.36
 H      -6.827036    -2.415316    -2.700354      29.26
55
name = lig-ACN-frame_563
 C       3.929570     1.455419    -0.530747      50.98
 H       3.240802     1.774256    -1.294987      23.05
 C       4.492179     0.278183     1.404103      42.83
 H       4.365752     0.051726     2.469143      21.72
 C       5.554304    -0.303484     0.622074      21.98
 O       6.555047    -0.996573     1.187200     268.93
 C       6.257996    -2.115940     2.134865      91.65
 H       6.895477    -2.996105     1.814922      23.79
 H       5.205876    -2.360087     2.157866      30.00
 H       6.619460    -1.644105     3.114485      24.77
 C       5.817702     0.205586    -0.676680      17.46
 O       6.883728    -0.225937    -1.359097     163.85
 H       7.734875    -0.442175    -0.858285      21.53
 C       5.031105     1.216363    -1.283594      52.47
 H       5.434962     1.916609    -2.119787      19.03
 C       3.603081     1.231398     0.831091      28.83
 C       2.322034     1.752098     1.546491      82.53
 H       2.693815     2.657545     1.941205      25.90
 O       2.089298     0.998782     2.871646     231.79
 H       1.964890     0.070137     2.715294      28.53
 C       1.175813     1.859802     0.585155      65.92
 H       1.468195     2.507633    -0.219405      24.79
 C      -0.116806     2.559091     1.303778      94.59
 O       0.136896     4.007156     1.872179     107.57
 H       0.138245     4.538861     0.794974      23.98
 H      -0.397474     2.109895     2.162443      27.62
 H      -0.823863     2.774821     0.462340      25.14
 C      -1.448943    -2.158971    -0.953809      50.89
 H      -1.847938    -3.276861    -0.547969      22.11
 C      -1.740313    -0.342202    -2.465503      62.79
 H      -2.163605     0.199874    -3.288367      23.58
 C      -0.814557     0.467676    -1.743357      -9.82
 O      -0.095988     1.692560    -2.048305     201.26
 C      -0.652342     2.319252    -3.253700     103.35
 H       0.073289     3.085305    -3.530926      25.49
 H      -0.400381     1.521091    -3.989107      25.45
 H      -1.687889     2.642104    -2.997666      26.00
 C      -0.327100    -0.106141    -0.399804      -2.42
 O       0.826225     0.317673     0.226784      86.07
 C      -0.715866    -1.426605    -0.034876      47.91
 H       0.038430    -1.677199     0.773354      20.96
 C      -2.272385    -1.536875    -1.998800      38.51
 C      -3.261495    -2.299736    -2.866415      75.00
 H      -3.157776    -1.803621    -3.837639      26.75
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 O      -3.097493    -3.786483    -2.881115     197.32
 H      -1.979436    -3.934252    -2.931493      24.94
 C      -4.705148    -2.073144    -2.166098      90.75
 H      -4.546761    -2.499279    -1.136393      28.09
 O      -5.173122    -0.753351    -2.144209     278.33
 H      -4.731628    -0.502107    -1.275338      26.89
 C      -5.826488    -2.757484    -3.020990      97.90
 O      -5.785236    -4.316430    -2.878868     177.26
 H      -4.700925    -4.314735    -2.720455      26.88
 H      -5.534473    -2.468885    -4.061123      28.88
 H      -6.849480    -2.480783    -2.837264      28.74
55
name = lig-ACN-frame_564
 C       3.800482     1.426515    -0.626160      24.81
 H       3.168536     2.306426    -0.834990      21.60
 C       4.455574     0.217670     1.462205      60.90
 H       4.573851     0.017956     2.575918      19.84
 C       5.520051    -0.222044     0.661992      -8.54
 O       6.579637    -1.087176     1.200423     254.16
 C       6.287604    -2.089804     2.158865      94.30
 H       7.052575    -2.958278     2.059653      23.99
 H       5.316693    -2.479765     2.013476      30.82
 H       6.277398    -1.829674     3.345353      24.68
 C       5.879452     0.223030    -0.699040      19.11
 O       6.952028    -0.294922    -1.449953     221.81
 H       7.488786    -0.734884    -0.808602      24.13
 C       5.135071     1.187654    -1.255815      45.66
 H       5.241931     1.602083    -2.367825      20.46
 C       3.600822     1.111702     0.792548       9.79
 C       2.411887     1.772185     1.630041      93.74
 H       2.424279     2.772350     1.867733      26.97
 O       2.108503     1.046570     2.841470     272.75
 H       2.114440     0.159207     2.581916      29.59
 C       1.077104     1.846848     0.637709      80.17
 H       1.244367     2.212356    -0.298874      25.14
 C      -0.111742     2.540128     1.286526     103.31
 O      -0.002686     4.019176     1.863189     194.82
 H       0.282173     4.822118     1.239821      26.27
 H      -0.492960     1.950770     2.064777      27.68
 H      -1.014555     2.516457     0.637079      26.04
 C      -1.552590    -2.139440    -0.884002      34.02
 H      -1.944406    -3.226758    -0.470025      21.79
 C      -1.788562    -0.265314    -2.484795      51.00
 H      -2.369897     0.130040    -3.270204      20.62
 C      -0.749256     0.421128    -1.640075      10.27
 O      -0.257630     1.684685    -2.026787     184.57
 C      -0.651857     2.295643    -3.412163     100.50
 H      -0.238464     3.197021    -3.583660      26.93
 H      -0.878551     1.674949    -4.375452      25.12
 H      -1.757833     2.578049    -3.297682      26.03
 C      -0.256930    -0.086405    -0.460257      36.92
 O       0.857268     0.389776     0.204942     167.91
 C      -0.699991    -1.347012    -0.047400      48.96
 H      -0.338822    -2.093742     0.801127      20.48
 C      -2.095562    -1.627408    -2.084880      35.66
 C      -3.295515    -2.300980    -2.784943      85.57
 H      -3.486301    -1.950725    -3.812980      26.55
 O      -3.125404    -3.679296    -2.929800     280.72
 H      -2.210716    -3.942776    -3.018749      31.33
 C      -4.740791    -2.156353    -2.198799      99.80
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 H      -4.928816    -2.613382    -1.228651      28.88
 O      -5.116604    -0.753745    -2.209855     275.63
 H      -4.906206    -0.261540    -1.486489      31.80
 C      -5.729392    -2.862734    -3.077194     118.53
 O      -5.685587    -4.194505    -2.787839     252.52
 H      -4.824196    -4.591024    -2.852090      30.79
 H      -5.791660    -2.538367    -4.149830      29.62
 H      -6.642918    -2.475736    -2.606948      29.21
55
name = lig-ACN-frame_565
 C       3.766618     1.575321    -0.556945      61.84
 H       3.212093     2.458594    -1.043130      23.40
 C       4.520237     0.203686     1.394859      62.50
 H       4.161512    -0.081459     2.468850      21.09
 C       5.710491    -0.257237     0.724805      12.27
 O       6.586121    -1.115755     1.169203     246.15
 C       6.244851    -2.141601     2.207273      93.51
 H       7.263366    -2.694451     2.176536      24.73
 H       5.477779    -2.769899     1.866046      29.59
 H       6.090600    -1.530935     3.253161      24.59
 C       5.945755     0.194046    -0.622615     -13.86
 O       7.050278    -0.380126    -1.451006     190.55
 H       7.392507    -1.233224    -1.058947      23.49
 C       4.938613     1.145328    -1.237086      36.71
 H       5.277008     1.234065    -2.354327      17.71
 C       3.525439     1.048349     0.734346      12.33
 C       2.392166     1.747771     1.537484      92.90
 H       2.826763     2.640682     1.810485      27.14
 O       2.145593     1.106082     2.788430     229.87
 H       1.778062     0.071370     2.691109      24.41
 C       1.083292     1.851459     0.673777      92.88
 H       1.361176     2.521639    -0.044013      28.16
 C      -0.236148     2.585560     1.328593     115.01
 O      -0.095162     3.901643     1.826615     303.26
 H       0.296476     4.247722     1.159873      36.27
 H      -0.345856     2.088726     2.271657      27.36
 H      -0.997883     2.497705     0.551608      27.54
 C      -1.712419    -2.081243    -0.828171      47.09
 H      -1.863034    -3.206249    -0.571468      22.73
 C      -1.759390    -0.258269    -2.368328      69.72
 H      -2.086451     0.229906    -3.250549      23.21
 C      -0.800419     0.484374    -1.766615       3.88
 O      -0.409222     1.709338    -2.143363     208.36
 C      -0.798580     2.261060    -3.441506     104.21
 H      -0.049503     2.885033    -3.484474      28.42
 H      -0.253259     1.471721    -4.145360      24.90
 H      -1.798549     2.781406    -3.481845      25.65
 C      -0.153748    -0.139415    -0.478553      -7.42
 O       0.885571     0.508066     0.282984     152.88
 C      -0.699420    -1.427644    -0.090952      45.34
 H      -0.427356    -1.471668     1.087029      21.83
 C      -2.033112    -1.609490    -2.105425      43.73
 C      -3.306516    -2.214753    -2.763162      82.49
 H      -3.336576    -1.641960    -3.707875      27.63
 O      -3.081107    -3.734476    -2.973748     222.42
 H      -2.243337    -3.722398    -3.279702      33.23
 C      -4.709411    -2.116459    -2.198326      98.46
 H      -4.735355    -2.539857    -1.220601      31.32
 O      -5.060305    -0.693309    -2.268386     258.31
 H      -4.575217    -0.464504    -1.379129      28.37
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 C      -5.763947    -2.858763    -3.103470     103.62
 O      -5.647846    -4.279944    -2.712429     220.17
 H      -4.867172    -4.429858    -3.159285      32.55
 H      -5.603474    -2.801813    -4.215943      28.97
 H      -6.774867    -2.529456    -2.830468      29.72
55
name = lig-ACN-frame_566
 C       3.925092     1.666241    -0.514514      47.04
 H       3.080423     2.082543    -1.195656      21.61
 C       4.496577     0.214975     1.257628      58.67
 H       4.263129    -0.383833     2.210744      19.34
 C       5.735535    -0.197864     0.692428      -8.28
 O       6.673643    -1.231739     1.203648     292.18
 C       6.270544    -2.142719     2.208602     101.25
 H       7.162141    -2.648677     2.719290      23.98
 H       5.567312    -2.889078     1.871710      29.16
 H       5.635789    -1.609421     3.111811      25.21
 C       5.946444     0.172446    -0.663724      12.29
 O       6.990611    -0.363333    -1.352612     186.53
 H       7.411959    -1.172998    -0.772897      18.53
 C       4.921664     0.939040    -1.228788      56.10
 H       4.939797     1.516109    -2.180496      21.72
 C       3.532784     1.065805     0.701117      21.25
 C       2.373534     1.700602     1.482645     102.48
 H       2.681739     2.666174     1.677950      26.60
 O       2.171739     1.119169     2.799359     230.67
 H       1.453859     0.313028     2.633143      23.63
 C       1.075051     2.036902     0.690568      70.15
 H       1.201864     2.545473    -0.177732      25.50
 C      -0.302110     2.424893     1.411591     111.45
 O      -0.119153     3.838295     1.749271     259.33
 H       0.207596     4.394765     1.031030      30.07
 H      -0.832966     1.777865     2.163440      25.79
 H      -1.111125     2.350585     0.687560      26.39
 C      -1.657297    -2.087933    -0.749088      39.91
 H      -2.248178    -2.939579    -0.364330      25.92
 C      -1.729705    -0.296085    -2.431621      50.87
 H      -2.240836     0.067387    -3.332008      23.54
 C      -0.734035     0.476899    -1.685515      20.00
 O      -0.540641     1.797061    -2.162053     248.01
 C      -0.729599     2.241902    -3.500474     114.58
 H      -0.284883     3.076031    -3.741595      27.86
 H      -0.875666     1.422340    -4.417663      24.37
 H      -1.820053     2.516040    -3.659325      25.90
 C      -0.133550    -0.072737    -0.579851      25.62
 O       0.808068     0.480186     0.309555     114.09
 C      -0.673841    -1.324006    -0.058734      42.54
 H      -0.334178    -1.857525     0.955230      21.49
 C      -2.260080    -1.534453    -1.980278      27.64
 C      -3.204774    -2.254653    -2.905400      66.41
 H      -3.252325    -1.844640    -3.933092      27.92
 O      -2.990913    -3.705713    -3.039559     189.17
 H      -2.031406    -3.975491    -3.399299      26.62
 C      -4.719650    -2.003654    -2.241551      92.50
 H      -4.745373    -2.344334    -1.253371      29.49
 O      -4.965056    -0.633316    -2.227284     238.63
 H      -4.650446     0.062280    -1.409043      23.33
 C      -5.766700    -2.899236    -3.065341      98.59
 O      -5.664142    -4.386378    -2.691531     139.64
 H      -4.706602    -4.768565    -3.014139      26.95
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 H      -5.431760    -2.666016    -4.081050      28.93
 H      -6.844102    -2.539579    -3.067313      28.43
55
name = lig-ACN-frame_567
 C       3.977958     1.529409    -0.584144      55.56
 H       3.341449     2.383910    -1.074705      23.22
 C       4.467678     0.101013     1.285892      45.78
 H       4.171067    -0.254918     2.289408      19.76
 C       5.676134    -0.259222     0.671752      -6.26
 O       6.694365    -1.214404     1.193786     293.47
 C       6.206777    -2.154172     2.281065      93.67
 H       7.160570    -2.409298     2.784481      23.49
 H       5.889690    -3.058691     1.720553      25.87
 H       5.419341    -1.627462     3.001943      25.23
 C       5.885193     0.127275    -0.649605      12.70
 O       6.986485    -0.349181    -1.285560     163.73
 H       7.666233    -0.636337    -0.569566      22.78
 C       5.024016     0.972646    -1.359484      59.29
 H       5.329031     0.936721    -2.380941      20.02
 C       3.625103     1.170871     0.728477      26.25
 C       2.386680     1.822819     1.541745      83.58
 H       2.657296     2.763098     1.843576      27.15
 O       2.138628     1.109721     2.788371     278.30
 H       1.683915     0.318035     2.669044      28.90
 C       0.941402     1.866325     0.677871      82.39
 H       1.051865     2.509403    -0.145012      26.71
 C      -0.295535     2.349451     1.336437     105.41
 O      -0.161287     3.804693     1.767099     154.36
 H      -0.056388     4.210300     0.678012      25.61
 H      -0.224279     1.909655     2.377347      25.83
 H      -1.066734     2.129337     0.603012      26.18
 C      -1.693254    -2.012043    -0.721540      66.21
 H      -1.949924    -2.788116    -0.062106      25.61
 C      -1.707371    -0.335819    -2.467115      55.76
 H      -2.099709     0.130150    -3.410000      23.18
 C      -0.809602     0.506757    -1.812720      -2.42
 O      -0.540643     1.869649    -2.065966     172.69
 C      -0.822747     2.238492    -3.655981      75.45
 H      -0.169132     2.946455    -3.820695      27.65
 H      -0.414804     1.289296    -4.381252      24.00
 H      -1.847667     2.559458    -3.494501      24.83
 C      -0.196967    -0.051901    -0.516941      14.10
 O       0.762245     0.488861     0.303264     175.06
 C      -0.670527    -1.265185    -0.080696      50.07
 H      -0.000309    -1.685879     0.723180      22.46
 C      -2.291753    -1.482283    -1.877977      31.32
 C      -3.238134    -2.297121    -2.937397      60.67
 H      -3.162281    -1.769287    -3.911595      27.16
 O      -2.912687    -3.689239    -3.100832     196.16
 H      -1.768821    -3.629961    -3.002100      22.49
 C      -4.651107    -2.064120    -2.276873      86.30
 H      -4.572522    -2.460890    -1.296168      29.64
 O      -4.926817    -0.523990    -2.235785     204.86
 H      -4.617074    -0.511155    -1.237789      25.15
 C      -5.672238    -2.964237    -3.058786     105.07
 O      -5.710414    -4.358680    -2.705838     189.60
 H      -4.658002    -4.584444    -2.663148      27.76
 H      -5.625882    -3.002205    -4.125550      28.62
 H      -6.721404    -2.702461    -2.626808      27.23
55
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name = lig-ACN-frame_568
 C       3.923517     1.486287    -0.727497      23.01
 H       3.547403     2.489944    -1.125542      21.58
 C       4.394042     0.099810     1.411729      63.93
 H       4.165279    -0.153693     2.406861      21.52
 C       5.558327    -0.433452     0.737975       5.99
 O       6.566977    -1.116345     1.233781     301.47
 C       6.222505    -2.132957     2.255284      97.52
 H       7.039101    -2.186940     2.947280      24.07
 H       5.892426    -3.166331     1.849712      25.82
 H       5.309273    -1.789665     2.845059      27.99
 C       5.897185     0.078428    -0.623412       8.68
 O       7.091967    -0.353175    -1.269624     211.84
 H       7.725715    -0.776803    -0.704510      25.17
 C       5.118349     0.992159    -1.419092      37.33
 H       5.221509     1.257590    -2.401610      19.61
 C       3.734927     1.197006     0.747267      -1.76
 C       2.353526     1.854932     1.539521      77.36
 H       2.489583     2.878527     1.759312      26.24
 O       2.099122     1.108374     2.787449     253.77
 H       2.194325     0.238302     2.450749      28.71
 C       1.048142     1.784817     0.604184      80.44
 H       1.313026     2.301810    -0.301625      25.37
 C      -0.260120     2.371497     1.426074     104.33
 O      -0.220761     3.719869     1.693464     175.38
 H      -0.166746     4.563413     0.880545      24.06
 H      -0.426379     1.750662     2.383466      24.91
 H      -1.292416     2.155065     1.119692      25.14
 C      -1.750505    -1.952577    -0.630017      44.95
 H      -1.991848    -2.945688    -0.568891      23.61
 C      -1.725945    -0.281539    -2.481313      34.41
 H      -2.129241    -0.066387    -3.515105      20.88
 C      -0.816987     0.588388    -1.754200      18.17
 O      -0.516964     1.876360    -2.137047     209.86
 C      -0.813938     2.241505    -3.578561      98.41
 H      -0.185900     3.039150    -3.795406      26.50
 H      -0.600918     1.166856    -4.120882      24.51
 H      -1.739500     2.543413    -4.006547      26.43
 C      -0.359707     0.042801    -0.562056      23.85
 O       0.784441     0.435349     0.276191     151.27
 C      -0.652445    -1.270602    -0.100699      45.17
 H      -0.300712    -1.540561     0.837744      22.06
 C      -2.190274    -1.543368    -2.014198      19.12
 C      -3.198934    -2.172050    -2.798773      90.43
 H      -3.232331    -1.628181    -3.769418      27.08
 O      -2.864366    -3.657838    -3.115881     152.81
 H      -1.777433    -3.868448    -3.051542      23.70
 C      -4.608951    -2.168439    -2.372579      94.72
 H      -4.689576    -2.479975    -1.334483      29.49
 O      -4.888279    -0.624214    -2.220290     215.76
 H      -4.797592    -0.256082    -1.407470      31.06
 C      -5.727732    -2.938503    -3.052902     121.43
 O      -5.679199    -4.353218    -2.667775     216.51
 H      -4.820675    -4.612968    -2.537727      33.10
 H      -5.700585    -2.646474    -4.098701      29.41
 H      -6.678702    -2.324367    -2.755119      28.09
55
name = lig-ACN-frame_569
 C       3.984085     1.509621    -0.640314      67.62
 H       3.219200     2.021479    -1.245305      22.24
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 C       4.385481     0.230699     1.392557      57.66
 H       4.256373    -0.015075     2.381042      21.06
 C       5.399613    -0.394477     0.614044      -0.02
 O       6.468374    -1.124097     1.357687     259.66
 C       6.216966    -2.116370     2.281189     107.68
 H       7.061020    -2.168202     2.921955      23.80
 H       6.267488    -3.123220     1.653435      23.17
 H       5.283629    -1.956543     2.840006      29.37
 C       5.947299     0.024935    -0.666507      -1.82
 O       7.153390    -0.355147    -1.216044     182.90
 H       7.465193    -1.098977    -0.644513      23.49
 C       5.088501     0.956306    -1.282229      64.51
 H       5.569729     1.438458    -2.014871      23.98
 C       3.605212     1.202831     0.669848      29.35
 C       2.370143     1.753789     1.430510      98.94
 H       2.493366     2.766348     1.771662      26.43
 O       2.117390     1.134732     2.727660     190.13
 H       2.134195     0.017064     2.780718      22.14
 C       1.102332     1.862055     0.603437      62.18
 H       1.168572     2.511892    -0.322287      24.72
 C      -0.215872     2.303314     1.416528     104.78
 O      -0.245380     3.772380     1.710934     244.11
 H      -0.151714     4.045527     0.751782      30.06
 H      -0.063634     1.885980     2.438797      25.22
 H      -0.870864     1.943116     0.639028      25.79
 C      -1.770699    -2.018698    -0.800768      58.95
 H      -2.087343    -2.838229    -0.267430      24.19
 C      -1.714206    -0.183954    -2.488801      62.63
 H      -2.112898     0.226427    -3.433578      22.74
 C      -0.927631     0.632281    -1.730130       6.16
 O      -0.504708     1.890339    -2.213188     225.13
 C      -0.704103     2.214447    -3.534138     105.65
 H      -0.003141     3.042145    -3.742402      25.28
 H      -0.469076     1.468796    -4.404967      26.01
 H      -1.744067     2.527877    -3.321583      24.68
 C      -0.323093     0.047882    -0.462273      17.87
 O       0.804604     0.338304     0.191033     133.67
 C      -0.803287    -1.236862    -0.035729      45.84
 H      -0.348588    -1.585264     0.781857      23.42
 C      -2.016300    -1.474564    -1.982474      42.74
 C      -3.093685    -2.247828    -2.899540      60.76
 H      -3.183653    -1.743629    -3.893041      28.53
 O      -2.880076    -3.602671    -3.097874     227.31
 H      -1.966333    -3.681875    -3.373181      28.96
 C      -4.651916    -2.098399    -2.169429      80.02
 H      -4.683865    -2.679527    -1.212267      30.43
 O      -4.914079    -0.801170    -2.266810     293.03
 H      -4.655902    -0.526901    -1.392404      31.09
 C      -5.763059    -2.834869    -3.095587      94.28
 O      -5.689851    -4.304118    -2.648589     194.79
 H      -4.741787    -4.428956    -2.817120      32.07
 H      -5.644808    -2.953815    -4.171027      27.93
 H      -6.816967    -2.666062    -2.691805      28.15
55
name = lig-ACN-frame_570
 C       3.935101     1.549842    -0.594633      50.32
 H       3.355862     2.113949    -1.295721      21.59
 C       4.432043     0.339574     1.222294      56.73
 H       4.316387     0.160534     2.258628      22.12
 C       5.499218    -0.386166     0.666901      29.79
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 O       6.363816    -1.020708     1.377658     274.91
 C       6.189525    -2.233569     2.354830      89.34
 H       6.996823    -2.061586     3.019159      25.73
 H       6.212672    -3.284039     1.800718      24.08
 H       5.293904    -2.248010     2.902786      31.34
 C       5.888136    -0.028110    -0.618689      13.15
 O       7.135111    -0.373621    -1.112406     174.32
 H       7.719347    -1.061369    -0.548589      22.91
 C       5.160784     1.032942    -1.216539      50.56
 H       5.340387     1.353638    -2.191751      20.79
 C       3.465534     1.097901     0.664317      33.69
 C       2.360878     1.741508     1.397133     102.87
 H       2.807252     2.693919     1.546620      24.71
 O       2.173299     1.132662     2.675470     234.43
 H       1.639927     0.149206     2.491416      22.40
 C       1.050784     1.795621     0.594338      97.68
 H       1.227065     2.508585    -0.322082      22.94
 C      -0.083520     2.266981     1.372598     116.50
 O      -0.253407     3.757085     1.651702     289.08
 H      -0.071866     4.280555     1.029990      35.48
 H      -0.283436     1.674753     2.266087      26.34
 H      -1.107840     2.102253     1.033682      25.57
 C      -1.641058    -2.028382    -0.797616      31.03
 H      -2.191597    -2.953118    -0.582425      22.74
 C      -1.724396    -0.131929    -2.471403      43.17
 H      -2.151188     0.256130    -3.385509      23.23
 C      -0.875993     0.657847    -1.617130      15.49
 O      -0.349820     1.826560    -2.068573     130.68
 C      -0.706649     2.326763    -3.613563      75.58
 H       0.031869     3.245151    -3.698615      23.23
 H      -0.478239     1.438290    -4.183966      26.37
 H      -1.667935     2.689283    -4.076656      24.47
 C      -0.374409    -0.036985    -0.493938      19.13
 O       0.910216     0.455829     0.139141     150.47
 C      -0.967240    -1.189496     0.046695      64.29
 H      -0.493275    -1.602720     0.851033      24.55
 C      -2.169944    -1.489428    -2.204056       5.97
 C      -3.175149    -2.229937    -2.928639      85.43
 H      -3.319912    -1.704973    -3.907251      27.87
 O      -2.855491    -3.674817    -3.097877     225.26
 H      -2.008919    -3.847014    -3.300585      31.74
 C      -4.585592    -2.212214    -2.262467      85.52
 H      -4.526556    -2.488917    -1.161870      27.78
 O      -5.014093    -0.760005    -2.194759     214.81
 H      -4.552181    -0.039740    -1.477287      24.74
 C      -5.719996    -2.918126    -3.009947     126.79
 O      -5.688651    -4.233559    -2.665459     165.66
 H      -4.812184    -4.755027    -3.064215      25.77
 H      -5.519696    -2.493740    -4.029606      28.62
 H      -6.667971    -2.330163    -2.915750      28.71
55
name = lig-ACN-frame_571
 C       3.896259     1.562077    -0.767822      55.29
 H       3.498074     2.486943    -1.039120      24.14
 C       4.396911     0.255067     1.337396      33.35
 H       4.221965     0.091671     2.428878      19.11
 C       5.526824    -0.311204     0.727104       1.43
 O       6.436464    -1.106393     1.559428     279.84
 C       6.134318    -2.242722     2.363493     103.23
 H       6.953639    -2.289810     3.096160      24.48
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 H       6.308555    -3.170794     1.683110      24.32
 H       5.211471    -2.176428     2.788639      32.69
 C       5.899555     0.044110    -0.593868       8.82
 O       7.105007    -0.401595    -1.072529     189.75
 H       7.563935    -0.789393    -0.215314      19.65
 C       5.129653     1.123073    -1.233089      64.71
 H       5.409559     1.355104    -2.287453      19.59
 C       3.504435     1.053431     0.490752      12.76
 C       2.366761     1.810928     1.412314      87.30
 H       2.384405     2.868959     1.699040      24.94
 O       2.175467     1.109800     2.663191     258.15
 H       1.792742     0.217242     2.434772      24.78
 C       1.079238     1.828692     0.518303      64.15
 H       1.291770     2.542500    -0.431032      22.24
 C      -0.241959     2.339357     1.390681     112.92
 O      -0.210088     3.705869     1.651495     259.80
 H       0.373385     4.067694     0.874772      28.04
 H      -0.009973     2.006932     2.343913      25.69
 H      -1.005427     1.886636     0.738157      25.00
 C      -1.745193    -1.987092    -0.972287      63.64
 H      -1.751741    -3.108502    -0.687418      20.68
 C      -1.814272    -0.141505    -2.454879      47.23
 H      -2.121368     0.389488    -3.302947      20.59
 C      -0.835318     0.541261    -1.664582      -0.33
 O      -0.250045     1.862759    -2.025625     143.78
 C      -0.606388     2.360308    -3.560453      84.28
 H       0.215371     3.298716    -3.670904      22.85
 H      -0.215563     1.659857    -4.186108      27.85
 H      -1.704675     2.651088    -3.588292      24.68
 C      -0.292811     0.052635    -0.435484      24.10
 O       0.859918     0.454461     0.047108     170.65
 C      -0.951516    -1.203618     0.064484      44.12
 H      -0.893317    -1.479402     1.118082      20.57
 C      -2.162085    -1.451202    -2.129998      35.64
 C      -3.267866    -2.234419    -3.030208      57.36
 H      -3.413829    -1.934183    -4.086921      26.91
 O      -2.858046    -3.773943    -3.117524     185.80
 H      -1.854116    -3.672148    -3.002067      26.91
 C      -4.547843    -2.090260    -2.244931      86.28
 H      -4.377234    -2.745774    -1.296934      27.54
 O      -5.118148    -0.691257    -2.157244     203.19
 H      -4.440558    -0.460250    -1.299982      23.10
 C      -5.595159    -2.826784    -3.001186      98.68
 O      -5.746405    -4.319028    -2.708359     162.53
 H      -4.924589    -4.683153    -3.133681      29.69
 H      -5.590020    -2.925141    -4.100426      27.82
 H      -6.499574    -2.547874    -2.493714      29.03
55
name = lig-ACN-frame_572
 C       3.911564     1.568433    -0.790181      42.42
 H       3.381303     2.297516    -1.364732      22.44
 C       4.293065     0.181034     1.345242      49.79
 H       3.877528     0.009744     2.409555      20.43
 C       5.540072    -0.317881     0.882283     -16.79
 O       6.562794    -1.061160     1.638241     296.97
 C       6.061589    -2.285544     2.339125      98.01
 H       6.708931    -2.441718     3.226680      24.71
 H       6.013689    -3.184846     1.661635      25.71
 H       5.112834    -2.174760     2.707145      31.83
 C       5.912640     0.203147    -0.486452      -5.02
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 O       7.057193    -0.403195    -1.066262     162.47
 H       7.626105    -0.895744    -0.475423      21.88
 C       5.157033     1.056018    -1.378981      49.40
 H       5.861567     1.620825    -2.119582      20.64
 C       3.564343     1.189216     0.599651      31.49
 C       2.366013     1.781487     1.301919      83.99
 H       2.857466     2.719422     1.658719      23.85
 O       2.129012     1.099654     2.650496     226.86
 H       2.239235     0.199386     2.566053      28.34
 C       1.014623     1.914522     0.559281      75.26
 H       1.061281     2.648548    -0.402456      22.46
 C      -0.230247     2.263183     1.341969     107.45
 O      -0.152161     3.763337     1.617419     133.70
 H       0.455080     4.292078     0.718223      24.09
 H      -0.386700     1.652979     2.152989      27.24
 H      -1.266385     2.185581     0.917022      25.42
 C      -1.724243    -1.961860    -0.858695      49.69
 H      -2.026489    -3.089278    -0.588651      22.61
 C      -1.826596    -0.030088    -2.470109      55.73
 H      -2.276542     0.337277    -3.357882      20.91
 C      -0.758774     0.575356    -1.783393       9.96
 O      -0.229282     1.815597    -2.104702     229.34
 C      -0.437387     2.337310    -3.314488     124.97
 H       0.023663     3.537429    -3.442696      22.87
 H      -0.400174     1.777549    -4.142734      28.83
 H      -1.559655     2.595053    -3.383679      25.62
 C      -0.403403    -0.021468    -0.482273      32.41
 O       0.859311     0.457578     0.061023     116.98
 C      -0.929514    -1.185113    -0.105670      56.28
 H      -0.619566    -1.666059     0.908833      21.66
 C      -2.222647    -1.441043    -2.209445       5.74
 C      -3.115128    -2.268885    -3.048984      83.85
 H      -3.160056    -1.769338    -4.044088      27.83
 O      -2.909921    -3.708086    -3.116776     170.40
 H      -1.803035    -4.011954    -3.046616      23.92
 C      -4.595868    -2.023553    -2.267750      68.04
 H      -4.465396    -2.326315    -1.166837      27.48
 O      -5.079078    -0.714866    -2.086861     280.29
 H      -5.037929    -0.205223    -1.278333      29.40
 C      -5.725905    -2.917367    -2.999941     105.81
 O      -5.761546    -4.381933    -2.755526     226.43
 H      -4.956942    -4.763374    -2.890282      32.61
 H      -5.665437    -2.452206    -4.052311      27.70
 H      -6.650627    -2.465836    -2.782367      30.00
55
name = lig-ACN-frame_573
 C       4.036015     1.535740    -0.715161      55.35
 H       3.238082     1.949732    -1.318274      22.36
 C       4.283723     0.190107     1.281174      54.75
 H       3.966198    -0.265374     2.301586      21.18
 C       5.596107    -0.234634     0.915114      -4.98
 O       6.553981    -0.962036     1.639047     332.28
 C       5.959596    -2.298423     2.299186      94.33
 H       6.718853    -2.561753     3.096284      25.17
 H       5.966749    -3.050687     1.565344      27.77
 H       5.006512    -2.015742     2.661455      28.89
 C       6.010677     0.155295    -0.347077      20.16
 O       7.013872    -0.355995    -1.076037     185.04
 H       7.477778    -0.987754    -0.527661      19.55
 C       5.184807     1.009120    -1.227037      56.48
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 H       5.406391     1.343634    -2.385380      21.33
 C       3.620213     1.201116     0.590016      45.92
 C       2.340642     1.771706     1.364990      89.52
 H       2.424452     2.916322     1.523870      23.82
 O       2.091880     1.157669     2.591007     259.63
 H       1.878912     0.128310     2.413596      21.49
 C       0.958268     1.801078     0.526455      74.68
 H       1.124631     2.585458    -0.395954      22.39
 C      -0.255505     2.345242     1.313950     105.44
 O      -0.086457     3.784770     1.631872     138.83
 H       0.274104     4.357468     0.627249      23.69
 H      -0.347923     1.932024     2.250962      26.42
 H      -0.984286     2.173460     0.477490      24.41
 C      -1.830976    -1.961721    -0.958259      54.04
 H      -2.372357    -2.894313    -0.509300      22.52
 C      -1.829271    -0.095717    -2.573311      70.18
 H      -2.200832     0.428431    -3.457604      22.59
 C      -0.839867     0.564815    -1.794881      17.54
 O      -0.099277     1.706661    -2.046531     197.96
 C      -0.497185     2.462723    -3.298013     101.61
 H       0.472000     3.336521    -3.150235      21.67
 H       0.016172     1.900213    -3.950532      27.64
 H      -1.574321     2.793849    -3.462080      25.08
 C      -0.307079     0.066802    -0.661601       5.49
 O       0.793347     0.485829     0.099837     171.03
 C      -0.841449    -1.239488    -0.115226      23.04
 H      -0.053692    -1.658290     0.696319      20.04
 C      -2.122067    -1.378137    -2.113957      41.58
 C      -3.124870    -2.173618    -2.972059      69.26
 H      -3.185184    -1.834699    -4.028132      27.69
 O      -2.949752    -3.616944    -3.095452     152.35
 H      -1.907118    -3.865636    -3.271500      25.03
 C      -4.655773    -2.138020    -2.256334      68.77
 H      -4.371564    -2.722375    -1.315318      29.38
 O      -5.050011    -0.678458    -2.129911     269.72
 H      -4.894832    -0.646740    -1.278400      32.94
 C      -5.854747    -2.930380    -3.000790     104.55
 O      -5.783328    -4.359802    -2.812533     177.60
 H      -4.720396    -4.445304    -2.731232      28.13
 H      -5.663701    -2.936238    -4.127675      26.09
 H      -6.798340    -2.724296    -2.693431      31.62
55
name = lig-ACN-frame_574
 C       3.996842     1.537902    -0.602739      58.15
 H       3.578982     2.278420    -1.349128      23.62
 C       4.405317     0.224203     1.354056      43.62
 H       3.935035    -0.044287     2.331330      18.71
 C       5.659538    -0.146422     0.900394      -4.83
 O       6.447118    -0.980410     1.698899     336.43
 C       5.933920    -2.150863     2.176326     113.40
 H       6.681998    -2.549818     2.917225      21.91
 H       5.767563    -2.825391     1.431863      28.46
 H       4.995425    -2.126166     2.791912      25.94
 C       6.057227     0.154067    -0.425077      19.10
 O       7.118979    -0.384994    -1.083911     164.97
 H       7.718788    -0.978274    -0.447711      25.35
 C       5.212825     0.993154    -1.070112      69.72
 H       5.400978     0.554838    -2.202928      20.71
 C       3.526492     1.146701     0.662822      29.23
 C       2.254531     1.834749     1.315341      91.17
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 H       2.433919     2.937828     1.704621      22.18
 O       2.063285     1.180828     2.602466     224.52
 H       1.426455     0.245607     2.475556      19.45
 C       1.057132     1.790277     0.498183      75.27
 H       1.278675     2.404092    -0.521068      19.83
 C      -0.261564     2.479419     1.247674     106.98
 O      -0.039137     3.807877     1.632185     243.56
 H       0.304324     4.342604     0.758084      26.18
 H      -0.445694     1.928086     2.157122      25.26
 H      -1.303628     2.346904     0.832585      24.70
 C      -1.748344    -1.883645    -0.848329      37.78
 H      -2.129062    -2.899626    -0.628260      22.54
 C      -1.715345    -0.122193    -2.656735      48.88
 H      -2.161136     0.155909    -3.667611      23.04
 C      -0.856024     0.593240    -1.788087       8.64
 O      -0.075117     1.728588    -2.094683     196.00
 C      -0.358244     2.564800    -3.294373     106.49
 H       0.064851     3.817957    -3.201800      22.01
 H      -0.433446     2.188378    -4.283357      27.16
 H      -1.500003     2.748617    -3.185748      26.03
 C      -0.262326    -0.132282    -0.606085      31.77
 O       0.709372     0.437642     0.092079     191.24
 C      -0.733151    -1.288378    -0.210955      58.03
 H      -0.510954    -1.769137     0.865045      19.32
 C      -2.262419    -1.390644    -2.179688      22.42
 C      -3.375555    -2.104753    -2.933069      82.56
 H      -3.488862    -1.518661    -3.883021      28.04
 O      -2.925588    -3.553784    -3.062381     179.72
 H      -2.057724    -3.569465    -3.248485      31.30
 C      -4.713770    -2.170748    -2.339784      97.53
 H      -4.834392    -2.605775    -1.329923      28.02
 O      -4.999500    -0.776295    -2.154925     303.02
 H      -4.811981    -0.155419    -1.345920      26.26
 C      -5.852016    -2.905999    -3.086751     111.93
 O      -5.758427    -4.371429    -2.810318     171.85
 H      -4.742866    -4.696057    -2.717744      26.43
 H      -6.065452    -2.512419    -4.146781      28.03
 H      -6.615485    -2.405629    -2.622651      30.99
55
name = lig-ACN-frame_575
 C       3.976276     1.552671    -0.559625      38.50
 H       3.387301     2.434955    -1.025880      20.00
 C       4.401127     0.388783     1.494533      40.86
 H       4.391026     0.098127     2.514565      19.93
 C       5.653780    -0.141871     0.943179      -8.05
 O       6.449143    -0.885174     1.740990     313.48
 C       5.855780    -2.192216     2.126659      97.75
 H       6.696588    -2.706334     2.617134      23.95
 H       5.553413    -2.737578     1.341351      29.91
 H       5.000521    -1.905097     2.822377      27.11
 C       6.123223     0.117530    -0.385094      -5.70
 O       7.273154    -0.443818    -1.080022     182.59
 H       7.927291    -0.903687    -0.380608      22.26
 C       5.171056     0.946677    -1.189065      47.87
 H       5.363411     1.631558    -2.231539      23.19
 C       3.504178     1.153813     0.735634      27.17
 C       2.295898     1.764364     1.380671      77.42
 H       2.729950     2.890448     1.397940      23.00
 O       1.978961     1.222180     2.686030     251.80
 H       1.762935     0.215530     2.385246      22.86
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 C       0.908349     1.907050     0.375786      75.67
 H       1.193167     2.486511    -0.592870      21.08
 C      -0.219232     2.466217     1.179372     105.19
 O       0.011246     3.905798     1.640729     271.31
 H       0.523713     4.329962     0.985254      31.44
 H      -0.289350     1.859004     2.113723      24.33
 H      -1.039503     2.478429     0.454205      25.56
 C      -1.841286    -1.956005    -0.992564      54.73
 H      -2.181021    -2.854862    -0.582099      24.08
 C      -1.673866    -0.227721    -2.646325      48.71
 H      -1.802984     0.355121    -3.623109      24.23
 C      -0.685122     0.557371    -1.857422      13.03
 O      -0.041592     1.783256    -2.220291     211.21
 C      -0.467651     2.651443    -3.231679      94.03
 H       0.466000     3.628722    -3.133612      21.05
 H      -0.147226     2.156488    -4.170497      24.77
 H      -1.531463     3.091516    -3.054459      24.86
 C      -0.287058    -0.028981    -0.663005       0.26
 O       0.787259     0.386287     0.190458     137.84
 C      -0.763856    -1.424478    -0.150445      15.28
 H      -0.352949    -1.796601     0.905777      17.30
 C      -2.368950    -1.328000    -2.137953      34.85
 C      -3.402253    -2.164017    -2.943377      74.73
 H      -3.593348    -1.774007    -3.968500      26.95
 O      -2.918224    -3.472064    -3.070329     185.45
 H      -1.944475    -3.460076    -3.138065      27.80
 C      -4.808531    -2.136702    -2.249687     101.69
 H      -4.671210    -2.685880    -1.318038      30.08
 O      -5.077398    -0.745346    -2.241776     272.84
 H      -4.505713    -0.638189    -1.252455      23.36
 C      -5.851869    -2.856968    -3.098244     107.17
 O      -5.773707    -4.326856    -2.838762     225.21
 H      -4.898949    -4.490559    -2.987865      32.94
 H      -5.792683    -2.691503    -4.218891      27.62
 H      -6.829358    -2.763285    -2.743511      29.67
55
name = lig-ACN-frame_576
 C       4.016055     1.454189    -0.544325      53.95
 H       3.363305     2.131170    -1.204161      20.93
 C       4.513710     0.482277     1.592151      44.91
 H       4.213008     0.471533     2.567412      19.49
 C       5.623035    -0.085677     0.898957      -0.02
 O       6.522675    -0.837460     1.809428     297.56
 C       5.810302    -2.218576     2.105738      89.45
 H       6.547021    -2.891913     2.470704      25.51
 H       5.346081    -2.518425     1.248619      28.58
 H       5.047105    -2.136882     2.993615      26.98
 C       6.022277     0.141761    -0.493184     -13.52
 O       7.288259    -0.415837    -0.996326     181.11
 H       7.781516    -0.969438    -0.317711      26.68
 C       5.155654     1.031162    -1.199229      62.73
 H       5.835892     1.689634    -1.952649      22.39
 C       3.590931     1.149831     0.761390      23.29
 C       2.291492     1.836233     1.391700      82.92
 H       2.348239     2.935907     1.912201      21.82
 O       1.874420     1.253539     2.696671     253.84
 H       2.213169     0.439781     2.818728      29.47
 C       1.051074     1.857007     0.437059      91.42
 H       1.090742     2.333284    -0.569007      21.06
 C      -0.223043     2.548058     1.116837     101.03
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 O       0.039803     3.895871     1.650880     281.57
 H       0.576083     4.377622     1.123980      33.35
 H      -0.525618     1.945152     2.068423      24.38
 H      -1.142029     2.435355     0.534088      26.32
 C      -1.911770    -2.043413    -0.989874      46.95
 H      -2.467251    -2.826744    -0.779245      22.84
 C      -1.620775    -0.134447    -2.623367      58.20
 H      -2.087245     0.108519    -3.621256      23.35
 C      -0.560770     0.438152    -1.942353       5.46
 O      -0.008342     1.702156    -2.238211     158.54
 C      -0.536298     2.751807    -3.255550      81.35
 H       0.362196     3.692972    -3.068565      21.38
 H      -0.609906     2.380097    -4.371378      23.74
 H      -1.614095     3.235684    -3.216690      24.43
 C      -0.227317    -0.116404    -0.545178      24.15
 O       0.777671     0.445458     0.217806     189.59
 C      -0.915886    -1.258499    -0.290748      47.76
 H      -0.345844    -1.880643     0.454319      22.42
 C      -2.339081    -1.320784    -2.116829       7.83
 C      -3.356327    -2.120941    -2.975074      61.50
 H      -3.450455    -1.628560    -3.964019      26.01
 O      -2.887602    -3.528794    -3.093536      90.39
 H      -1.756024    -3.588437    -3.004736      23.51
 C      -4.825934    -2.132222    -2.237599      86.42
 H      -4.862931    -2.450121    -1.224039      28.20
 O      -5.202852    -0.661156    -2.239254     255.10
 H      -4.882667     0.047530    -1.448847      23.35
 C      -5.926013    -2.910866    -3.069992     123.30
 O      -5.780899    -4.283117    -2.894262     224.55
 H      -4.893557    -4.580196    -3.185318      29.05
 H      -5.547312    -2.588121    -4.088540      27.84
 H      -6.848907    -2.400369    -3.118113      30.20
55
name = lig-ACN-frame_577
 C       3.955273     1.425475    -0.618619      39.09
 H       3.274093     2.031721    -1.280002      21.71
 C       4.604860     0.557783     1.564468      43.87
 H       4.721545     0.374777     2.570365      21.87
 C       5.717497    -0.093950     0.988949      -1.41
 O       6.497640    -0.892420     1.811294     314.53
 C       5.852713    -2.115576     2.065562     103.13
 H       6.635231    -2.806357     2.150407      24.21
 H       5.212973    -2.467238     1.257756      29.10
 H       5.171346    -1.986030     3.006968      25.71
 C       5.992878     0.100619    -0.421225      24.93
 O       7.123538    -0.306131    -0.900917     238.91
 H       7.527253    -0.825403    -0.219632      26.56
 C       5.320377     1.100441    -1.132515      46.56
 H       5.301513     1.161688    -2.306064      19.42
 C       3.611791     1.283480     0.807318      12.22
 C       2.283100     1.877779     1.456880      80.57
 H       2.644996     3.065729     1.371184      21.36
 O       1.825470     1.292912     2.714211     271.28
 H       1.991841     0.318972     2.526195      24.36
 C       1.109460     1.814661     0.506498      92.83
 H       1.594078     2.299830    -0.310086      22.44
 C      -0.217358     2.576553     1.127629      95.38
 O       0.023863     3.832780     1.691915     236.29
 H       0.282632     4.292731     0.749459      25.85
 H      -0.552362     1.878705     2.020275      22.91
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 H      -0.921511     2.681186     0.305885      24.17
 C      -1.927469    -1.888887    -0.936880      54.55
 H      -2.054030    -2.781950    -0.545983      23.66
 C      -1.690707    -0.176035    -2.626868      54.50
 H      -1.920799     0.488800    -3.466358      19.05
 C      -0.559938     0.445326    -1.903374      18.21
 O       0.019426     1.662578    -2.299714     197.32
 C      -0.589703     2.740970    -3.259435      76.43
 H       0.076841     3.816235    -3.284252      21.59
 H      -0.761652     2.368055    -4.398280      22.11
 H      -1.487831     2.790224    -2.536849      22.95
 C      -0.208199    -0.056715    -0.699670      19.46
 O       0.729768     0.408495     0.242925     178.56
 C      -0.924352    -1.307947    -0.211420      30.90
 H      -0.793581    -1.668711     0.789989      19.70
 C      -2.278081    -1.363496    -2.272829      42.47
 C      -3.365557    -2.042381    -2.912383      71.44
 H      -3.544386    -1.658097    -3.925443      28.25
 O      -2.869349    -3.586471    -3.116399      78.31
 H      -1.800653    -3.606053    -2.987044      25.43
 C      -4.815558    -1.941347    -2.249616      90.82
 H      -4.709911    -2.366635    -1.294904      30.65
 O      -5.348097    -0.622125    -2.283078     305.07
 H      -5.015213    -0.358652    -1.404685      29.39
 C      -5.817603    -2.780562    -3.163410      91.66
 O      -5.853406    -4.322013    -2.922929     128.86
 H      -4.785010    -4.545930    -3.141557      27.48
 H      -5.791609    -2.607272    -4.261389      27.73
 H      -6.774451    -2.688340    -2.665642      28.76
55
name = lig-ACN-frame_578
 C       3.952148     1.493551    -0.584888      61.55
 H       3.224676     1.861871    -1.293173      25.06
 C       4.619178     0.642989     1.583535      44.29
 H       4.281252     0.655575     2.592866      19.38
 C       5.699979    -0.003977     1.055944      11.81
 O       6.530065    -0.881368     1.736689     347.33
 C       5.876399    -2.146531     2.062335      96.17
 H       6.642763    -2.881911     2.165420      25.30
 H       5.129580    -2.384772     1.246369      27.88
 H       5.376379    -2.112941     3.108267      26.24
 C       5.996108     0.241432    -0.234127      21.61
 O       7.111210    -0.321193    -0.892282     221.95
 H       7.819130    -0.794943    -0.333562      25.29
 C       5.134434     1.042129    -1.083478      70.94
 H       5.451445     0.925655    -2.128772      17.35
 C       3.684246     1.344231     0.792349      31.39
 C       2.338085     1.845065     1.461085      76.49
 H       2.332425     3.011613     1.952464      19.57
 O       1.895378     1.320259     2.731670     222.96
 H       1.372312     0.364379     2.536334      20.94
 C       1.060002     1.853728     0.481738      94.65
 H       1.069282     2.277521    -0.448502      22.49
 C      -0.152161     2.441238     1.073067      91.69
 O      -0.020538     3.810739     1.736864     141.49
 H       0.460753     4.661007     1.031099      23.62
 H      -0.744313     1.775334     1.847619      23.75
 H      -0.862725     2.505536     0.237256      24.64
 C      -1.849194    -1.807174    -0.931573      42.38
 H      -2.511241    -2.553130    -0.715143      21.15
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 C      -1.661331    -0.106030    -2.704232      59.92
 H      -2.130682     0.251469    -3.591172      21.78
 C      -0.681568     0.549605    -1.951371      14.44
 O       0.118836     1.672446    -2.413703     230.42
 C      -0.722470     2.581993    -3.097493     106.89
 H       0.107215     3.438846    -3.183502      22.62
 H      -0.944560     2.092668    -4.230385      22.98
 H      -1.783041     3.070321    -2.888852      25.17
 C      -0.219768    -0.098693    -0.638574      21.42
 O       0.717111     0.368873     0.259520     162.52
 C      -0.823899    -1.176395    -0.084531      32.55
 H      -0.625483    -1.321612     0.914706      19.74
 C      -2.206230    -1.371914    -2.227160      39.37
 C      -3.384503    -2.096738    -3.021953      67.05
 H      -3.447471    -1.744575    -4.058845      27.52
 O      -2.946959    -3.514903    -3.101031     206.10
 H      -2.062712    -3.473379    -3.055803      30.99
 C      -4.788389    -1.951650    -2.383097      96.20
 H      -4.860744    -2.303978    -1.397961      27.30
 O      -5.419274    -0.584300    -2.289984     276.51
 H      -5.245604    -0.083732    -1.601631      32.75
 C      -5.808095    -2.786307    -3.123437     106.57
 O      -5.840473    -4.262942    -2.980776     220.53
 H      -4.966494    -4.717264    -2.852110      29.36
 H      -5.881346    -2.417731    -4.149894      28.47
 H      -6.777908    -2.270163    -2.753558      28.51
55
name = lig-ACN-frame_579
 C       3.878989     1.578517    -0.553238      50.10
 H       3.163430     2.064167    -1.172715      20.42
 C       4.488108     0.750345     1.763639      37.17
 H       4.137195     0.443939     2.782878      18.67
 C       5.690969     0.099129     1.175643     -28.83
 O       6.590397    -0.875488     1.715719     287.47
 C       5.905852    -2.208942     2.094658      92.99
 H       6.735381    -2.936557     2.006196      25.01
 H       5.073990    -2.524820     1.303711      25.13
 H       5.416945    -2.098472     3.084918      27.01
 C       6.098261     0.394553    -0.282586     -16.71
 O       7.120260    -0.329983    -0.919771     174.78
 H       7.523757    -0.784366    -0.043752      17.40
 C       5.055831     0.860790    -1.083031      65.76
 H       5.315543     1.279058    -1.995031      25.39
 C       3.609785     1.403791     0.826274      19.62
 C       2.303677     1.888504     1.394601      72.54
 H       2.595256     3.135621     1.537141      21.19
 O       1.986663     1.281262     2.755341     219.58
 H       1.539329     0.295701     2.533631      20.48
 C       1.099248     1.811009     0.417711      99.91
 H       1.460491     2.257697    -0.407496      23.15
 C      -0.234440     2.459782     1.083866      90.72
 O      -0.094633     3.729359     1.756529     180.34
 H       0.755915     4.195646     1.121005      24.93
 H      -0.436429     1.766773     1.978048      23.16
 H      -1.109222     2.546343     0.336782      23.32
 C      -1.800516    -1.820988    -0.876237      62.21
 H      -2.369165    -2.497127    -0.258956      22.17
 C      -1.660504    -0.111644    -2.753437      42.33
 H      -1.901267     0.229974    -3.711237      22.42
 C      -0.614007     0.554564    -1.872135      12.52
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 O       0.078153     1.602476    -2.397632     221.69
 C      -0.781056     2.543212    -3.140777      82.36
 H      -0.340277     3.532011    -3.443223      24.01
 H      -1.170121     2.020916    -4.206858      22.19
 H      -1.672470     2.575678    -2.276218      22.82
 C      -0.243633     0.052118    -0.632240      18.56
 O       0.797669     0.434063     0.258747     209.31
 C      -0.934464    -1.127123    -0.106126      49.53
 H      -0.549612    -1.636125     0.721741      23.32
 C      -2.193487    -1.228712    -2.199922      33.42
 C      -3.274521    -2.038547    -3.080362      55.96
 H      -3.291436    -1.540375    -4.050978      27.18
 O      -3.074024    -3.443466    -3.071254     210.43
 H      -2.137849    -3.703081    -3.110401      28.68
 C      -4.793200    -1.988691    -2.376043      78.07
 H      -4.512373    -2.356520    -1.409487      26.89
 O      -5.422683    -0.613240    -2.373106     272.91
 H      -4.770000    -0.329131    -1.699910      27.06
 C      -5.916180    -2.780982    -3.152251     103.65
 O      -5.844417    -4.171216    -3.005908     275.82
 H      -4.984012    -4.216756    -2.770555      33.26
 H      -5.725134    -2.606848    -4.176603      27.86
 H      -7.019838    -2.521489    -2.800619      26.69
55
name = lig-ACN-frame_580
 C       3.898874     1.507452    -0.472124      50.13
 H       3.407755     2.180477    -1.158387      22.84
 C       4.523986     0.693418     1.760078      32.43
 H       4.355483     0.393443     2.866140      20.14
 C       5.713175     0.217704     1.142638      -7.59
 O       6.541372    -0.876212     1.748661     279.29
 C       5.981819    -2.153320     2.082037      99.24
 H       6.843611    -2.922314     2.104778      23.25
 H       5.104109    -2.474405     1.295641      25.96
 H       5.611484    -2.190933     3.104098      25.01
 C       5.999033     0.339464    -0.231773      -0.08
 O       7.101727    -0.281753    -0.829850     239.56
 H       7.647957    -0.916489    -0.303619      25.65
 C       5.007569     0.984839    -1.139043      43.75
 H       5.088653     0.838363    -2.124281      22.62
 C       3.538270     1.391894     0.901057      28.24
 C       2.211791     1.956389     1.449607      85.23
 H       2.247951     3.230935     1.691262      21.93
 O       2.061237     1.291589     2.698896     251.39
 H       2.318490     0.364269     2.473372      24.06
 C       1.084272     1.890547     0.443552     105.71
 H       1.243189     2.384687    -0.441657      23.99
 C      -0.273844     2.418559     1.117939      99.64
 O      -0.101201     3.692665     1.745642     243.55
 H       0.557550     4.202633     1.236789      29.91
 H      -0.512827     1.609776     1.885311      23.84
 H      -1.154667     2.376698     0.353563      24.31
 C      -1.938076    -1.763703    -0.900290      37.29
 H      -2.082432    -2.889083    -0.756562      20.02
 C      -1.516332    -0.116110    -2.601777      56.09
 H      -1.588954     0.246582    -3.590370      19.79
 C      -0.567328     0.506091    -1.888062      10.69
 O       0.094702     1.609640    -2.411259     200.55
 C      -0.904367     2.521514    -3.153341      73.60
 H      -0.327843     3.366290    -3.236043      26.30
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 H      -1.392823     2.079820    -4.236629      20.93
 H      -1.914082     2.786468    -2.428513      23.77
 C      -0.280354     0.106037    -0.528829      34.94
 O       0.861768     0.471000     0.162990     196.42
 C      -0.902263    -1.069798    -0.149553      42.27
 H      -0.568100    -1.424390     0.850194      19.27
 C      -2.322983    -1.279652    -2.179420      40.06
 C      -3.310577    -1.890879    -3.008703      77.69
 H      -3.326742    -1.589432    -4.044170      28.39
 O      -3.153665    -3.444599    -3.068133      96.96
 H      -2.057012    -3.722976    -3.133548      25.22
 C      -4.829820    -1.939380    -2.435186      91.22
 H      -4.879697    -2.382259    -1.441807      28.09
 O      -5.286366    -0.700053    -2.412112     286.31
 H      -4.973263     0.173650    -1.795381      24.49
 C      -5.950769    -2.706055    -3.253334      91.00
 O      -5.837875    -4.179534    -2.971473     182.41
 H      -4.819655    -4.497548    -2.892997      26.43
 H      -6.025529    -2.350203    -4.233897      29.01
 H      -6.965035    -2.266384    -2.772950      28.03
55
name = lig-ACN-frame_581
 C       3.872064     1.517682    -0.449361      50.05
 H       2.970084     1.942565    -0.957351      22.91
 C       4.554847     0.641160     1.648648      57.10
 H       4.446677     0.658137     2.802869      21.90
 C       5.706846     0.088739     1.116947       5.49
 O       6.503907    -0.739002     1.785952     258.04
 C       6.018667    -2.090138     2.092871      87.89
 H       6.979318    -2.739657     1.921989      22.67
 H       5.193769    -2.501598     1.271042      25.69
 H       5.579782    -2.141900     3.055662      24.61
 C       5.890122     0.239716    -0.289542      37.50
 O       7.054517    -0.219095    -0.773108     236.90
 H       7.412014    -0.606595     0.004110      29.58
 C       5.092711     1.013564    -1.041303      47.22
 H       5.170258     0.925967    -2.019147      18.84
 C       3.636262     1.392797     0.926475      31.50
 C       2.275857     2.022456     1.508721      69.58
 H       2.346722     3.195350     1.981406      21.19
 O       2.049167     1.285311     2.703644     273.82
 H       2.351962     0.441102     2.610725      26.03
 C       0.951862     1.955649     0.496448     107.49
 H       1.107136     2.631840    -0.318288      23.95
 C      -0.272137     2.307338     1.144751      99.19
 O      -0.114563     3.711945     1.756619     247.19
 H       0.108446     4.215281     1.077175      34.11
 H      -0.617874     1.788141     2.016642      24.64
 H      -1.106949     2.406439     0.293143      23.32
 C      -1.933609    -1.742274    -0.826468      78.57
 H      -2.390290    -2.865901    -0.621951      20.87
 C      -1.529495    -0.206674    -2.584961      50.72
 H      -1.795847     0.064041    -3.611282      22.76
 C      -0.499238     0.527395    -1.827204      10.63
 O       0.032635     1.684514    -2.481832     225.97
 C      -0.928870     2.542387    -3.104652      90.38
 H      -0.455714     3.389593    -3.318601      26.45
 H      -1.061486     2.029857    -4.245973      21.02
 H      -2.013912     2.801749    -2.593838      24.59
 C      -0.254418     0.064597    -0.538623      34.35
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 O       0.914506     0.509697     0.066737     194.15
 C      -0.955010    -1.125068    -0.101742      27.64
 H      -0.610479    -1.550725     0.933519      18.24
 C      -2.309177    -1.192585    -2.143706      61.00
 C      -3.500659    -2.049723    -3.013725      73.51
 H      -3.504201    -1.440690    -3.916988      25.49
 O      -3.150538    -3.426857    -3.089184     197.85
 H      -2.078694    -3.427522    -3.169225      25.43
 C      -4.841403    -1.965614    -2.484959     104.63
 H      -4.810369    -2.472842    -1.499307      27.61
 O      -5.259652    -0.521223    -2.471686     247.68
 H      -4.830220    -0.281860    -1.383575      19.80
 C      -5.885082    -2.715188    -3.275600     103.88
 O      -5.876327    -4.144830    -2.974321     181.29
 H      -4.856693    -4.329850    -3.296587      26.99
 H      -5.931959    -2.589816    -4.299986      29.53
 H      -6.879818    -2.387113    -2.727294      28.11
55
name = lig-ACN-frame_582
 C       3.821278     1.553560    -0.508262      51.81
 H       3.132961     1.927250    -1.363225      18.38
 C       4.531317     0.687003     1.707393      37.83
 H       4.455673     0.536949     2.824350      18.92
 C       5.513410    -0.044949     1.046564       2.08
 O       6.569179    -0.653258     1.888935     335.20
 C       6.077394    -2.044781     2.081844      82.10
 H       6.998873    -2.785657     2.118773      23.12
 H       5.259621    -2.314144     1.212906      24.50
 H       5.624832    -2.110868     3.049675      28.28
 C       5.895164     0.208564    -0.273103      -7.02
 O       7.102315    -0.237916    -0.770067     180.54
 H       7.788626    -0.524172    -0.093041      22.71
 C       4.980290     1.043715    -1.068342      57.21
 H       5.401088     1.557449    -1.834664      24.92
 C       3.621049     1.473321     0.880700      27.99
 C       2.390033     1.961392     1.513788      75.00
 H       2.612691     3.162567     1.530414      20.77
 O       1.978505     1.275722     2.819633     221.93
 H       1.780437     0.338593     2.384387      21.14
 C       1.083869     1.902710     0.556503      78.73
 H       1.282704     2.567104    -0.301021      21.13
 C      -0.377623     2.394549     1.303835      93.44
 O      -0.180569     3.700157     1.743808     203.97
 H      -0.038366     4.306583     0.854699      25.70
 H      -0.484636     1.642998     2.038826      24.12
 H      -1.296272     2.238449     0.549862      22.80
 C      -1.972202    -1.798658    -0.774147      31.17
 H      -2.646451    -2.316215     0.125467      19.72
 C      -1.582094    -0.171613    -2.699209      29.30
 H      -1.753696     0.335837    -3.693436      20.38
 C      -0.640039     0.526630    -1.943270      -8.48
 O       0.002127     1.696357    -2.414192     207.66
 C      -0.923839     2.594326    -3.192587      91.44
 H      -0.570563     3.554608    -3.188435      26.16
 H      -1.347158     2.207433    -4.288731      22.27
 H      -1.820933     2.458797    -2.470298      24.47
 C      -0.167300    -0.015434    -0.631697      -4.28
 O       0.956256     0.570415     0.042863     197.04
 C      -0.915191    -1.116308     0.018492      31.87
 H      -0.541760    -1.764529     0.968870      19.76
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 C      -2.399207    -1.316635    -2.093492      22.30
 C      -3.393709    -2.010260    -3.019321      68.40
 H      -3.461803    -1.737065    -4.068006      25.85
 O      -3.066442    -3.449887    -3.144638     213.53
 H      -2.192524    -3.550354    -3.255184      31.39
 C      -4.940291    -1.893107    -2.425737      84.90
 H      -4.998321    -2.163789    -1.338197      25.45
 O      -5.244646    -0.456602    -2.474977     271.94
 H      -4.746966     0.129575    -1.586883      18.28
 C      -5.949740    -2.750479    -3.276795     109.73
 O      -5.881040    -4.137674    -3.007542     289.53
 H      -5.169806    -4.578134    -3.318648      33.99
 H      -5.627701    -2.487225    -4.259280      29.73
 H      -7.026113    -2.371331    -3.202970      28.27
55
name = lig-ACN-frame_583
 C       3.804661     1.562982    -0.569491      42.88
 H       3.244412     2.508121    -0.998454      21.51
 C       4.464171     0.728435     1.693628      43.41
 H       4.151648     0.687118     2.725402      18.72
 C       5.505371    -0.039929     1.108530      17.49
 O       6.531689    -0.643006     1.930673     347.29
 C       6.176383    -2.010878     2.138577      88.78
 H       7.114737    -2.710332     2.119367      23.80
 H       5.523597    -2.398283     1.190625      25.30
 H       5.520979    -2.154784     3.001185      28.49
 C       5.869695     0.233529    -0.296697      -0.19
 O       7.153000    -0.248822    -0.833159     155.06
 H       7.606179    -0.575833     0.063517      22.21
 C       5.053808     1.039690    -1.124269      29.63
 H       5.403196     1.294949    -2.138386      20.68
 C       3.554906     1.390291     0.858739      19.38
 C       2.257769     1.922605     1.560397      85.04
 H       2.290025     2.933997     2.121858      20.61
 O       1.949358     1.307253     2.834891     189.03
 H       1.502490     0.273990     2.769464      20.08
 C       1.077321     1.920123     0.609849      79.63
 H       1.213677     2.683595    -0.240286      20.00
 C      -0.236462     2.335934     1.376986      93.13
 O      -0.298366     3.767152     1.755792     121.84
 H       0.222679     4.438201     0.921968      24.06
 H      -0.414593     1.994806     2.332856      24.62
 H      -1.183122     2.099974     0.646120      22.08
 C      -2.010697    -1.639185    -0.702126      39.68
 H      -2.873753    -2.563057    -0.407759      19.02
 C      -1.737002    -0.242337    -2.677177      56.60
 H      -2.129483    -0.048557    -3.742560      16.85
 C      -0.681276     0.465267    -1.944802      -4.68
 O      -0.047075     1.672773    -2.372126     188.16
 C      -0.988558     2.604894    -3.158012      95.25
 H      -0.315615     3.465053    -3.073373      24.28
 H      -0.891359     2.342354    -4.345994      22.55
 H      -2.013895     2.821845    -2.881021      27.10
 C      -0.160884    -0.018768    -0.684455      16.79
 O       0.963415     0.500816     0.006206     171.80
 C      -0.839719    -1.075153    -0.118025      46.78
 H      -0.447405    -1.124157     1.020092      17.40
 C      -2.291006    -1.355956    -2.079456      36.78
 C      -3.375963    -2.019176    -2.929365      48.36
 H      -3.335538    -1.302015    -3.761468      26.51
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 O      -2.991832    -3.510882    -3.193401     191.42
 H      -2.021026    -3.505615    -3.196987      26.71
 C      -4.931630    -1.790048    -2.333588      82.37
 H      -5.055082    -2.270801    -1.300128      26.65
 O      -5.286841    -0.475291    -2.524011     329.37
 H      -4.782752     0.082233    -1.872551      29.08
 C      -5.929006    -2.668338    -3.355998      93.84
 O      -5.950196    -4.183126    -3.008593     219.24
 H      -5.002033    -4.336648    -3.271330      30.05
 H      -5.709718    -2.570100    -4.435720      29.49
 H      -6.970565    -2.391746    -3.202787      29.58
55
name = lig-ACN-frame_584
 C       3.917432     1.616724    -0.513760      53.40
 H       3.289682     2.333812    -1.226990      21.11
 C       4.393018     0.640996     1.622844      50.64
 H       4.347275     0.587558     2.673377      21.27
 C       5.642179     0.156538     1.114606       2.58
 O       6.441666    -0.618654     1.920600     271.32
 C       6.249219    -2.079348     2.175206      81.04
 H       7.308702    -2.343630     2.494656      21.10
 H       5.830936    -2.660105     1.236576      25.56
 H       5.616373    -2.229945     3.094926      25.35
 C       5.915091     0.219713    -0.294855      25.00
 O       7.059669    -0.230188    -0.814323     215.56
 H       7.624726    -0.744140    -0.190276      33.94
 C       5.066919     1.035412    -1.097630      53.58
 H       5.191155     0.946579    -2.258004      18.73
 C       3.446997     1.329082     0.805456      24.18
 C       2.157122     1.903158     1.586389      90.57
 H       2.405027     2.978012     1.592511      22.98
 O       1.902397     1.283618     2.885298     246.33
 H       2.066877     0.242387     2.602508      19.23
 C       0.966963     1.893964     0.622010      81.40
 H       1.199626     2.643460    -0.264304      20.56
 C      -0.191308     2.334296     1.442702     102.74
 O      -0.370763     3.849171     1.732784     182.05
 H       0.349940     4.244890     1.048310      26.41
 H      -0.087745     1.660882     2.278285      22.48
 H      -1.132406     1.951774     0.764138      22.78
 C      -1.995828    -1.588152    -0.708872      37.94
 H      -2.142255    -2.666748     0.021902      18.72
 C      -1.696285    -0.203549    -2.595098      78.45
 H      -2.019473     0.225020    -3.602929      17.72
 C      -0.673559     0.479949    -2.007891      20.09
 O      -0.236151     1.651172    -2.350537     241.81
 C      -0.870275     2.618784    -3.171424     101.88
 H      -0.451824     3.735782    -3.093176      22.55
 H      -0.873702     2.180312    -4.237239      22.66
 H      -1.850976     2.576987    -2.845267      27.20
 C      -0.190945     0.055361    -0.753363      23.68
 O       0.938731     0.464101    -0.022824     160.54
 C      -0.874010    -1.031084    -0.155705      35.48
 H      -0.703689    -1.420717     0.940095      18.12
 C      -2.293653    -1.388882    -2.011122      39.35
 C      -3.399525    -2.089172    -2.781107      92.41
 H      -3.530654    -1.788935    -3.835034      24.09
 O      -2.979802    -3.452661    -3.225581     194.78
 H      -1.863706    -3.498489    -3.099911      22.15
 C      -4.881967    -1.985631    -2.457566      84.68
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 H      -5.094786    -2.150172    -1.334367      25.78
 O      -5.341284    -0.447904    -2.572824     232.73
 H      -5.015497     0.046150    -1.858983      27.57
 C      -5.876765    -2.673257    -3.315737     107.93
 O      -5.970368    -4.092820    -3.060652     219.28
 H      -4.992505    -4.568140    -2.853332      27.57
 H      -5.626826    -2.462328    -4.399585      28.97
 H      -6.775029    -2.179772    -3.040638      29.74
55
name = lig-ACN-frame_585
 C       3.913422     1.656260    -0.499887      42.95
 H       3.174342     1.910390    -1.332508      17.96
 C       4.391581     0.553889     1.572342      54.50
 H       4.145699     0.222450     2.538203      21.14
 C       5.625162     0.229235     1.091041      10.18
 O       6.437840    -0.597250     1.947883     307.84
 C       6.345989    -2.073300     2.231447      84.22
 H       7.324452    -2.358468     2.633995      22.45
 H       6.179344    -2.768783     1.339253      25.97
 H       5.453454    -2.262230     2.954633      26.49
 C       5.950940     0.326236    -0.229252       8.38
 O       7.034881    -0.282968    -0.853808     202.85
 H       7.506186    -0.768326    -0.175716      24.55
 C       5.012793     0.985179    -1.013075      70.43
 H       5.375573     1.288489    -2.150530      23.87
 C       3.451612     1.315121     0.846212      35.28
 C       2.243132     1.891505     1.440510      88.48
 H       2.370114     2.841399     1.849943      24.44
 O       1.914149     1.228969     2.850510     204.67
 H       2.335099     0.423769     2.921633      26.56
 C       0.962416     1.841970     0.549698      73.21
 H       1.092494     2.624703    -0.369212      19.62
 C      -0.380198     2.345981     1.482044      89.16
 O      -0.365337     3.791951     1.666709     270.14
 H       0.260821     4.202923     1.256418      35.01
 H      -0.328103     2.045282     2.556161      23.45
 H      -1.494803     2.127995     1.121849      23.15
 C      -1.905103    -1.777018    -0.696513      27.36
 H      -2.670533    -2.659547    -0.059919      19.61
 C      -1.720574    -0.213889    -2.641957      40.12
 H      -2.171664     0.245016    -3.556797      21.18
 C      -0.697851     0.483395    -1.933150      -9.84
 O      -0.194885     1.794342    -2.326823     198.73
 C      -0.922588     2.588879    -3.287990      97.35
 H      -0.158332     3.560149    -2.976784      20.26
 H      -0.870301     2.439013    -4.373037      25.22
 H      -1.876185     2.778683    -3.003875      28.68
 C      -0.201742     0.036321    -0.666266      18.22
 O       0.886139     0.552870    -0.018420     207.19
 C      -0.899781    -0.964089    -0.027191      49.24
 H      -0.224606    -1.360539     0.776053      20.55
 C      -2.445989    -1.323811    -1.988822      18.34
 C      -3.388138    -2.103617    -2.927720      67.85
 H      -3.294191    -1.316125    -3.707467      25.68
 O      -2.987702    -3.462359    -3.172185     201.59
 H      -1.857182    -3.484806    -3.147783      23.91
 C      -4.864146    -1.982352    -2.383395      91.70
 H      -5.090198    -2.411050    -1.312954      25.05
 O      -5.331282    -0.555449    -2.630250     231.29
 H      -4.951846    -0.042959    -1.768986      23.10
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 C      -5.852034    -2.686003    -3.321994     107.18
 O      -5.994524    -4.063483    -3.111106     275.21
 H      -5.151290    -4.364744    -2.738569      32.94
 H      -5.663708    -2.418006    -4.435155      29.20
 H      -6.813678    -2.310337    -3.163112      29.29
55
name = lig-ACN-frame_586
 C       3.752622     1.554312    -0.524976      64.42
 H       3.131271     2.356079    -0.948932      22.41
 C       4.349603     0.529269     1.635175      41.89
 H       4.005522     0.136280     2.591795      21.47
 C       5.616944    -0.002871     1.172591      -0.46
 O       6.533368    -0.578173     2.005034     314.99
 C       6.397582    -1.993803     2.244879     102.41
 H       7.217505    -2.205874     2.874989      23.14
 H       6.425002    -2.473419     1.272596      27.91
 H       5.403756    -2.284945     2.829828      28.84
 C       6.003092     0.402648    -0.243231       0.86
 O       7.035015    -0.339759    -0.871309     122.90
 H       7.619122    -0.768977    -0.124282      21.71
 C       5.042443     1.085711    -1.034837      71.80
 H       5.401923     1.339848    -2.199406      21.46
 C       3.566573     1.352503     0.816288      33.41
 C       2.212857     1.840733     1.502738      96.42
 H       2.388461     2.840718     1.631765      24.35
 O       1.954922     1.244659     2.733638     279.92
 H       2.083117     0.249864     2.648744      23.76
 C       0.824081     1.917713     0.588456      77.57
 H       0.858107     2.809811    -0.233905      20.12
 C      -0.417511     2.354019     1.440224     105.27
 O      -0.362688     3.780488     1.609270     222.55
 H       0.348572     4.009627     0.965275      28.00
 H      -0.428604     1.651309     2.402605      22.45
 H      -1.223810     1.904790     0.650492      22.18
 C      -1.902354    -1.804393    -0.721834      56.20
 H      -2.573762    -2.822919    -0.266737      18.44
 C      -1.776775    -0.201387    -2.555886      24.20
 H      -2.093343     0.038452    -3.550990      21.66
 C      -0.768769     0.584795    -1.889217      -4.12
 O      -0.118382     1.808903    -2.288061     186.68
 C      -0.954386     2.678926    -3.388965      90.30
 H      -0.426930     3.834717    -3.632949      21.07
 H      -0.848022     1.979802    -4.111065      26.48
 H      -1.969963     2.752728    -3.172785      28.31
 C      -0.316735     0.063792    -0.615600      22.74
 O       0.863374     0.594263    -0.005044     175.15
 C      -0.913415    -1.135389     0.050736      34.46
 H      -0.651478    -1.359833     1.067788      18.84
 C      -2.358563    -1.273946    -1.958641      53.32
 C      -3.401670    -1.988240    -2.971327      22.94
 H      -3.519099    -1.755659    -4.069292      26.84
 O      -2.998430    -3.476021    -3.108613     213.65
 H      -2.020766    -3.444747    -3.262163      27.01
 C      -4.884581    -1.945637    -2.430328      93.96
 H      -4.765696    -2.217194    -1.306636      23.07
 O      -5.271754    -0.665953    -2.585080     263.63
 H      -4.688400     0.122879    -1.988911      19.58
 C      -5.927565    -2.650944    -3.391514      90.96
 O      -6.009291    -4.160846    -3.141177     258.74
 H      -5.146271    -4.437131    -2.994214      33.95
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 H      -5.412144    -2.528766    -4.448099      28.75
 H      -6.857605    -2.192720    -3.261849      28.25
55
name = lig-ACN-frame_587
 C       3.819626     1.526309    -0.564101      46.89
 H       3.300488     2.190224    -1.226534      24.45
 C       4.411386     0.465953     1.677553      34.99
 H       4.291982     0.540184     2.795583      20.03
 C       5.563515    -0.035896     1.090150      -0.46
 O       6.639239    -0.541716     2.060749     267.62
 C       6.456700    -1.960350     2.258466     100.97
 H       7.115147    -2.303164     3.004110      23.87
 H       6.636654    -2.563568     1.417698      27.26
 H       5.326176    -2.153033     2.577158      27.71
 C       5.917968     0.281255    -0.199420      10.87
 O       7.022597    -0.329321    -0.834919     182.94
 H       7.819847    -0.603172    -0.215159      25.96
 C       5.077508     1.191700    -1.048053      47.12
 H       5.335338     1.311295    -2.217230      17.93
 C       3.455371     1.290147     0.880078       6.56
 C       2.174359     1.970747     1.474648     106.22
 H       2.383664     2.884449     1.801904      25.17
 O       1.950922     1.208011     2.690866     244.74
 H       1.642249     0.203061     2.340839      19.56
 C       0.903141     1.964778     0.672826      86.39
 H       1.086529     2.630545    -0.278166      20.62
 C      -0.412665     2.253973     1.265631      96.09
 O      -0.362945     3.761430     1.582128     131.68
 H       0.250939     4.353552     0.802599      24.44
 H      -0.627748     1.716799     2.294416      23.36
 H      -1.376034     2.250884     0.678312      23.15
 C      -1.979440    -1.787645    -0.749473      28.39
 H      -2.151060    -2.944000    -0.325641      20.30
 C      -1.747937    -0.008953    -2.507946      74.05
 H      -1.934139     0.264219    -3.504799      20.71
 C      -0.815721     0.699449    -1.782401      -5.40
 O      -0.165381     1.836075    -2.297578     211.88
 C      -0.920866     2.524417    -3.415218      91.46
 H      -0.377578     3.619299    -3.609841      23.53
 H      -1.006706     2.109607    -4.341361      26.03
 H      -1.892772     2.723320    -2.911160      26.25
 C      -0.417270     0.052892    -0.496022      22.73
 O       0.738954     0.586451     0.005660     173.99
 C      -0.932699    -1.173084    -0.046430      57.15
 H      -0.831795    -1.501338     0.903537      20.68
 C      -2.322439    -1.366280    -2.060018      31.03
 C      -3.357989    -2.084295    -2.903312      82.76
 H      -3.220199    -1.406703    -3.832777      25.83
 O      -3.030286    -3.446979    -3.027406     286.60
 H      -2.171116    -3.462684    -3.195014      32.11
 C      -4.837379    -2.023897    -2.530973      84.59
 H      -5.131034    -2.524069    -1.533134      25.90
 O      -5.284105    -0.523501    -2.502985     250.51
 H      -4.468763     0.027260    -2.125930      24.28
 C      -5.867772    -2.792311    -3.405758     102.09
 O      -6.034858    -4.173543    -3.178629     208.83
 H      -5.063681    -4.587407    -3.436763      28.48
 H      -5.755932    -2.517341    -4.596203      27.49
 H      -6.842486    -2.362081    -3.238626      29.54
55
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name = lig-ACN-frame_588
 C       3.894944     1.570313    -0.441796      56.18
 H       3.136936     1.865781    -1.102487      20.15
 C       4.361420     0.585591     1.653965      37.60
 H       4.322253     0.508000     2.795221      20.44
 C       5.618158     0.025048     1.171549     -27.50
 O       6.625568    -0.478442     1.975574     275.16
 C       6.489880    -1.993793     2.291155      95.92
 H       7.052407    -2.160419     3.184369      24.01
 H       6.827036    -2.495847     1.486720      27.34
 H       5.358600    -2.183307     2.482306      29.23
 C       5.858558     0.147003    -0.312300      18.72
 O       7.025757    -0.274703    -0.808442     202.12
 H       7.482110    -0.517474     0.006081      21.33
 C       5.148924     1.045073    -0.971677      75.88
 H       5.588710     1.463138    -1.912291      20.50
 C       3.433874     1.220740     0.786769      30.31
 C       2.224249     1.954315     1.522948      90.14
 H       2.321126     2.886933     1.787281      26.88
 O       1.877221     1.167756     2.735261     230.65
 H       1.695467     0.073329     2.508585      18.37
 C       0.972963     1.900296     0.471521      84.98
 H       1.185105     2.676759    -0.377629      21.60
 C      -0.433199     2.427512     1.155972     100.09
 O      -0.391444     3.728301     1.611784     176.44
 H       0.188019     4.240236     0.736703      23.52
 H      -0.619970     1.811226     2.092334      23.91
 H      -1.073308     2.037333     0.329591      21.84
 C      -1.966165    -1.828852    -0.862037      49.58
 H      -2.577511    -2.805236    -0.595237      17.68
 C      -1.827568    -0.044821    -2.490439      30.12
 H      -2.179106     0.434078    -3.364662      18.91
 C      -0.896435     0.690760    -1.689337      11.25
 O      -0.228751     1.801616    -2.275233     243.21
 C      -0.904329     2.411663    -3.328427      97.58
 H      -0.241662     3.394169    -3.400295      21.95
 H      -0.789318     1.804251    -4.212225      25.08
 H      -2.042505     2.702751    -3.249594      26.15
 C      -0.449328     0.174329    -0.496530      20.48
 O       0.737961     0.541756     0.142568     198.42
 C      -0.997835    -1.101018    -0.077702      52.10
 H      -0.297050    -1.519344     0.500404      22.85
 C      -2.311030    -1.231041    -2.077315      42.45
 C      -3.305549    -2.051468    -2.924694      48.31
 H      -3.354316    -1.750555    -4.077728      24.94
 O      -3.038723    -3.517694    -2.979184     236.96
 H      -2.048720    -3.625046    -3.073026      28.97
 C      -4.890411    -1.963682    -2.527757      72.41
 H      -4.884448    -2.442377    -1.490068      25.07
 O      -5.274537    -0.510250    -2.456126     298.09
 H      -4.727479    -0.146245    -1.843411      28.14
 C      -5.852241    -2.787110    -3.511733      92.50
 O      -5.992122    -4.233303    -3.211698     199.62
 H      -5.297113    -4.840589    -3.691012      29.52
 H      -5.798076    -2.637482    -4.720180      26.55
 H      -6.771690    -2.402527    -3.032871      28.08
55
name = lig-ACN-frame_589
 C       3.891544     1.552328    -0.503831      54.71
 H       3.497571     2.408303    -1.053118      22.23
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 C       4.437998     0.635851     1.698498      58.06
 H       3.982476     0.452319     2.697290      19.50
 C       5.576323     0.091568     1.144197      22.73
 O       6.578735    -0.504797     1.903288     308.31
 C       6.495571    -1.908098     2.298079     105.41
 H       7.041401    -1.932923     3.274122      22.96
 H       6.935985    -2.564619     1.663777      27.35
 H       5.454617    -2.297046     2.434011      30.54
 C       5.868180     0.080012    -0.157876       2.37
 O       7.120243    -0.282028    -0.767847     220.90
 H       7.714188    -0.855391    -0.296175      31.58
 C       5.044829     1.007233    -1.008582      62.32
 H       5.439574     1.324097    -1.908709      20.40
 C       3.489299     1.268687     0.896871      13.33
 C       2.164888     1.726040     1.474584     108.36
 H       2.510780     2.608516     1.730538      24.86
 O       1.796777     1.181931     2.771208     268.97
 H       2.007673     0.196616     2.673300      24.39
 C       0.969433     1.939965     0.459507      94.46
 H       1.272079     2.254885    -0.561901      20.69
 C      -0.300928     2.434686     1.013393     108.02
 O      -0.417251     3.802471     1.624904     243.70
 H       0.146266     4.453835     1.146492      29.22
 H      -0.587119     1.667114     1.766753      23.84
 H      -1.164451     2.285970     0.430934      25.35
 C      -1.895258    -1.768779    -0.905852      57.21
 H      -2.243896    -2.742080    -0.488352      20.42
 C      -1.926786     0.031655    -2.514331     111.03
 H      -2.350119     0.391422    -3.459049      26.72
 C      -0.977690     0.667604    -1.753031       6.28
 O      -0.271130     1.746331    -2.112464     209.85
 C      -0.842396     2.433224    -3.372541      85.08
 H      -0.484081     3.401113    -3.717469      23.17
 H      -0.717545     1.632436    -4.132665      23.98
 H      -2.027173     2.405032    -3.045258      23.97
 C      -0.467177     0.120033    -0.488244      21.20
 O       0.763603     0.467155     0.258633     139.29
 C      -0.968943    -1.085395    -0.092014      40.20
 H      -0.657181    -1.655112     0.722531      21.11
 C      -2.479773    -1.258023    -2.083828      70.39
 C      -3.398812    -2.017153    -3.054831      34.98
 H      -3.205776    -1.750025    -4.165595      30.00
 O      -3.030620    -3.593521    -2.911380     137.11
 H      -1.893056    -3.490740    -3.041566      24.84
 C      -4.811389    -1.911263    -2.530407      93.31
 H      -4.975088    -2.402328    -1.535138      24.96
 O      -5.270031    -0.593222    -2.457063     262.83
 H      -5.136874    -0.140521    -1.570736      25.81
 C      -5.891811    -2.740625    -3.474201      79.08
 O      -5.931827    -4.269267    -3.249676     232.79
 H      -5.255247    -4.556243    -3.742715      35.08
 H      -5.443049    -2.430277    -4.549258      29.59
 H      -6.988142    -2.377351    -3.579162      28.52
55
name = lig-ACN-frame_590
 C       3.854450     1.564020    -0.486870      55.06
 H       3.397205     2.467898    -0.998822      21.75
 C       4.395123     0.614241     1.793204      38.10
 H       4.452730     0.405863     2.852313      20.63
 C       5.603206     0.019590     1.177682     -19.43
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 O       6.582246    -0.542443     1.931317     273.28
 C       6.482115    -1.858772     2.353816     107.85
 H       6.969648    -1.939923     3.377942      23.98
 H       7.003580    -2.466293     1.692685      25.75
 H       5.427542    -2.108039     2.432298      32.11
 C       5.953977     0.221081    -0.276026      -9.20
 O       7.133933    -0.302677    -0.744898     168.25
 H       7.526146    -0.812600     0.063233      17.30
 C       5.038732     0.892122    -1.040850      56.60
 H       5.275175     1.001358    -1.981016      24.53
 C       3.519818     1.312392     0.876808      23.01
 C       2.183357     1.796592     1.490148     104.00
 H       2.119891     2.751870     1.740806      27.44
 O       1.727691     1.158873     2.754432     267.68
 H       1.803914     0.255215     2.860959      28.60
 C       1.087979     1.796969     0.478725      87.61
 H       1.470268     2.451993    -0.294683      23.38
 C      -0.299588     2.463329     1.019361     102.67
 O      -0.393659     3.863903     1.646935     272.39
 H       0.261585     4.269579     1.294163      35.25
 H      -0.406051     1.963336     1.948810      24.90
 H      -0.893668     2.334362     0.154734      25.64
 C      -1.963609    -1.788765    -0.903093      52.73
 H      -2.061971    -2.819182    -0.719317      21.71
 C      -2.114849     0.011960    -2.524279      48.18
 H      -2.268644     0.523593    -3.508852      14.46
 C      -0.935716     0.599375    -1.685099       2.87
 O      -0.275961     1.884739    -2.078842     201.51
 C      -0.807408     2.353703    -3.341393      98.12
 H      -0.232452     3.192586    -3.286336      26.38
 H      -0.620567     1.858439    -4.405860      26.13
 H      -2.008641     2.737625    -3.270871      24.30
 C      -0.383195     0.013560    -0.504814      24.94
 O       0.630184     0.402279     0.234420     180.24
 C      -0.986906    -1.206016    -0.083309      51.41
 H      -0.869106    -1.331199     0.997959      19.87
 C      -2.530758    -1.254454    -2.137070      33.19
 C      -3.411690    -2.159831    -3.019887      58.36
 H      -3.422319    -1.617949    -4.013686      26.55
 O      -3.031924    -3.522212    -2.890906     216.02
 H      -1.891161    -3.541294    -3.066239      22.61
 C      -4.917741    -2.057395    -2.530881      87.03
 H      -4.739787    -2.529148    -1.541823      27.36
 O      -5.323106    -0.581895    -2.497398     159.38
 H      -4.952058    -0.307380    -1.449146      22.40
 C      -5.823873    -2.742489    -3.464586      97.54
 O      -5.872712    -4.152242    -3.308912     204.16
 H      -4.882229    -4.487668    -3.449072      30.13
 H      -5.459582    -2.688238    -4.590723      27.65
 H      -6.908120    -2.270059    -3.305946      27.18
55
name = lig-ACN-frame_591
 C       3.900667     1.495201    -0.403219      41.45
 H       3.053327     1.714586    -1.156110      19.00
 C       4.460623     0.534265     1.705563      51.55
 H       4.170453     0.624815     2.700807      20.66
 C       5.613954     0.053224     1.112296      16.36
 O       6.662975    -0.479184     1.983568     290.44
 C       6.421186    -1.956895     2.461490      80.38
 H       6.867914    -2.029838     3.514875      23.83
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 H       6.881591    -2.678243     1.788740      24.59
 H       5.425257    -2.226821     2.494051      32.46
 C       5.949092     0.295544    -0.220409      -0.77
 O       7.076719    -0.310341    -0.723431     136.51
 H       7.783267    -0.526513     0.039616      20.82
 C       4.988843     0.900065    -1.110705      51.58
 H       5.150809     1.043437    -2.125340      24.09
 C       3.548735     1.325973     0.984281      19.93
 C       2.194509     1.899633     1.600270      94.80
 H       2.363537     2.859991     1.846388      25.40
 O       1.710254     1.157765     2.744495     275.46
 H       1.659102     0.235298     2.267968      23.24
 C       1.017076     1.763415     0.504337      86.34
 H       1.235778     2.059554    -0.473948      21.43
 C      -0.257683     2.483810     1.168126     110.78
 O      -0.292656     3.853650     1.601519     271.45
 H       0.366036     4.393468     1.091996      28.28
 H      -0.778840     1.775574     1.737414      25.92
 H      -1.052818     2.352246     0.357952      24.56
 C      -2.087513    -1.934954    -0.922687      40.01
 H      -2.627033    -2.731210    -0.666861      20.81
 C      -1.993904     0.060411    -2.376579      38.82
 H      -2.580870     0.526188    -3.212526      20.60
 C      -0.940765     0.617920    -1.776665      21.91
 O      -0.386266     1.821474    -2.057168     242.48
 C      -0.699807     2.500840    -3.307205      87.75
 H      -0.171796     3.325996    -3.550607      26.62
 H      -0.463541     1.482597    -3.982598      23.32
 H      -1.913311     2.762752    -3.353799      23.25
 C      -0.455624    -0.102764    -0.642519      13.07
 O       0.640976     0.403436     0.236202     173.84
 C      -1.099904    -1.259819    -0.083878      48.24
 H      -0.616803    -1.903099     0.764334      21.25
 C      -2.450498    -1.269309    -2.096193      20.80
 C      -3.459322    -2.114859    -2.928665      69.68
 H      -3.464029    -1.999503    -3.999492      23.93
 O      -3.008968    -3.511806    -2.912893     227.20
 H      -2.025037    -3.511315    -3.174602      28.56
 C      -4.913484    -2.076238    -2.475699     102.57
 H      -5.423818    -2.455057    -1.597266      26.35
 O      -5.352677    -0.664017    -2.484037     248.43
 H      -4.733747    -0.013940    -1.936010      25.79
 C      -5.825828    -2.729980    -3.566657      93.71
 O      -5.812578    -4.144535    -3.341575     188.68
 H      -4.847840    -4.437136    -2.883741      27.44
 H      -5.743845    -2.139648    -4.563147      28.06
 H      -6.924494    -2.444205    -3.180562      26.76
55
name = lig-ACN-frame_592
 C       3.782178     1.361866    -0.422323      46.25
 H       2.889457     1.799934    -1.041455      22.71
 C       4.460094     0.556121     1.754468      27.56
 H       4.379120     0.089798     2.687132      20.82
 C       5.732975     0.079093     1.206206      -3.00
 O       6.675612    -0.527634     2.017104     290.32
 C       6.357587    -1.943471     2.519764      80.68
 H       6.844966    -1.958189     3.523836      24.20
 H       6.927742    -2.665981     1.827910      23.46
 H       5.356423    -2.032768     2.550073      32.04
 C       5.943690     0.253994    -0.206365       9.50
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 O       7.033850    -0.271994    -0.778361     182.81
 H       7.671489    -0.614248    -0.096893      23.22
 C       4.992841     0.963034    -0.985691      63.43
 H       5.232779     1.006086    -2.120304      21.83
 C       3.536859     1.339134     0.965564      34.58
 C       2.192662     1.867277     1.546669      90.61
 H       2.320617     2.828747     1.945705      25.50
 O       1.775696     1.141175     2.722993     219.27
 H       1.295307     0.138399     2.615476      22.04
 C       0.891051     1.898343     0.559433      68.96
 H       1.092312     2.544609    -0.232972      24.46
 C      -0.363315     2.425075     1.162030     109.12
 O      -0.162399     3.816209     1.605539     197.70
 H       0.585711     4.270824     0.881119      24.32
 H      -0.454764     2.024548     2.125656      25.75
 H      -1.124432     2.465733     0.335699      25.16
 C      -2.142778    -1.982579    -0.826997      74.80
 H      -2.588805    -2.747225    -0.436807      24.91
 C      -2.020712    -0.024872    -2.439511      83.73
 H      -2.552020     0.654022    -3.128627      20.59
 C      -0.899651     0.592346    -1.715050      11.75
 O      -0.422280     1.860476    -1.984906     195.78
 C      -0.631938     2.513235    -3.329716      95.88
 H       0.140944     3.234165    -3.186514      25.45
 H      -0.571118     1.944006    -4.483877      25.62
 H      -1.727193     3.004504    -3.274087      23.99
 C      -0.451946    -0.129518    -0.551696      15.84
 O       0.652423     0.291537     0.243114      98.75
 C      -1.136922    -1.345288    -0.208645      49.95
 H      -0.530991    -1.896365     0.688314      21.97
 C      -2.497696    -1.317954    -2.049978      30.16
 C      -3.468845    -2.038625    -2.902951      72.20
 H      -3.468643    -1.405295    -3.732848      30.70
 O      -2.986043    -3.565911    -2.914401     186.85
 H      -2.125962    -3.521246    -3.132376      30.99
 C      -5.003057    -1.989916    -2.462670     102.87
 H      -4.836438    -2.536731    -1.513283      27.89
 O      -5.379322    -0.668271    -2.474452     312.94
 H      -4.674705    -0.196593    -2.296327      35.93
 C      -5.927899    -2.658877    -3.532277      95.28
 O      -5.746583    -4.214596    -3.410211     202.41
 H      -4.910474    -4.268061    -2.998667      33.29
 H      -5.539733    -2.596412    -4.594722      27.47
 H      -7.083386    -2.377434    -3.451185      26.57
55
name = lig-ACN-frame_593
 C       3.654092     1.334759    -0.450813      38.85
 H       3.136743     2.037903    -1.192620      21.39
 C       4.501833     0.564878     1.840464      46.09
 H       4.081200     0.473910     2.842421      20.52
 C       5.720070     0.131856     1.300851       9.56
 O       6.673114    -0.619345     2.024613     291.33
 C       6.325298    -1.833255     2.548270      91.24
 H       6.706539    -1.986863     3.553080      23.56
 H       6.692153    -2.730961     1.855709      23.72
 H       5.313316    -2.031936     2.618954      31.82
 C       5.931740     0.253006    -0.130930      10.65
 O       7.056838    -0.258655    -0.874386     204.13
 H       7.581369    -0.822903    -0.306294      27.77
 C       5.005111     0.945012    -0.867421      41.39
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 H       5.281207     1.073846    -2.043717      20.84
 C       3.455923     1.217273     0.943923       5.87
 C       2.091398     1.733707     1.501876      99.53
 H       2.240105     2.793941     1.682040      24.41
 O       1.839415     1.129745     2.785697     267.18
 H       1.658938     0.176393     2.460509      24.36
 C       0.900679     1.881060     0.579294      69.02
 H       1.126121     2.301341    -0.351215      22.88
 C      -0.453733     2.430132     1.250380     108.17
 O      -0.115130     3.751171     1.638682     214.47
 H       0.718877     4.361444     1.102722      21.88
 H      -0.753956     1.777548     2.026469      25.31
 H      -1.455091     2.184794     0.708535      24.59
 C      -2.165802    -1.912732    -0.790100      33.72
 H      -2.373436    -2.906192    -0.661739      23.34
 C      -1.993540    -0.130806    -2.424780      31.59
 H      -2.172410     0.164135    -3.446614      21.06
 C      -0.999015     0.497632    -1.649005      -1.61
 O      -0.425603     1.876785    -1.977487     187.18
 C      -0.586236     2.586042    -3.248822      91.89
 H       0.306417     3.241684    -3.394200      25.58
 H      -0.387309     1.728733    -4.243106      23.36
 H      -1.466112     3.309291    -3.365574      25.19
 C      -0.424607    -0.093465    -0.472450      17.67
 O       0.662632     0.284008     0.235401     124.50
 C      -0.916503    -1.384658    -0.131033      38.57
 H      -0.762259    -1.767160     1.019534      18.88
 C      -2.635748    -1.305619    -1.979735      24.29
 C      -3.512328    -2.076647    -3.002624      88.29
 H      -3.382287    -1.963471    -4.002493      27.36
 O      -3.048779    -3.481485    -2.966563     238.93
 H      -2.047945    -3.496229    -3.057078      28.10
 C      -4.991957    -2.044485    -2.512772      89.18
 H      -5.298207    -2.329231    -1.514000      26.41
 O      -5.454576    -0.540764    -2.438786     215.68
 H      -4.677388     0.035549    -2.089818      27.31
 C      -5.887883    -2.827654    -3.486202     114.45
 O      -5.755528    -4.202535    -3.455082     267.46
 H      -4.844017    -4.348927    -3.456159      33.81
 H      -5.586659    -2.257031    -4.444467      28.60
 H      -6.996883    -2.452796    -3.395166      27.43
55
name = lig-ACN-frame_594
 C       3.778070     1.347275    -0.402677      64.53
 H       2.983275     1.769495    -1.018545      23.00
 C       4.324401     0.682486     1.821223      30.84
 H       4.409743     0.841659     2.937014      20.70
 C       5.701282     0.086946     1.287149     -14.42
 O       6.703699    -0.567793     1.998640     288.81
 C       6.217621    -1.902731     2.628869      77.98
 H       6.758578    -1.903324     3.538826      24.83
 H       6.654395    -2.772193     1.927681      23.91
 H       5.162301    -1.775453     2.694749      29.83
 C       5.971195     0.254630    -0.052356       4.75
 O       7.002313    -0.243459    -0.853136     199.69
 H       7.738343    -0.691029    -0.290590      22.84
 C       4.953325     0.914891    -0.904342      41.86
 H       5.344865     1.206671    -2.010763      20.01
 C       3.356059     1.035099     0.937670      26.80
 C       2.107033     1.716084     1.554142      90.40
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 H       2.438029     2.730237     1.826455      25.13
 O       1.846447     1.082214     2.843457     267.04
 H       2.044439     0.229695     2.893761      31.54
 C       0.807169     1.617385     0.565032      98.98
 H       1.015183     2.304124    -0.277251      24.05
 C      -0.382666     2.336615     1.298078      99.89
 O      -0.185939     3.720635     1.781683     176.23
 H       0.411043     4.014821     0.858404      25.17
 H      -0.596307     1.847767     2.209842      26.24
 H      -1.007400     2.614513     0.383466      23.34
 C      -2.010718    -1.857330    -0.763401      46.38
 H      -2.522798    -2.779464    -0.384202      22.75
 C      -1.924054    -0.164604    -2.438030      57.23
 H      -1.996396     0.106500    -3.458502      23.78
 C      -1.015902     0.614917    -1.645813      13.04
 O      -0.457223     1.781233    -1.929683     219.63
 C      -0.497267     2.578096    -3.188742      86.65
 H       0.460593     3.294597    -3.222798      23.19
 H      -0.724103     1.699653    -4.100028      20.84
 H      -1.462426     3.031137    -3.187546      25.24
 C      -0.461098    -0.130310    -0.471935      11.58
 O       0.683802     0.379007     0.243117     192.75
 C      -0.971426    -1.372444    -0.028112      52.43
 H      -0.364373    -1.992349     0.827643      22.44
 C      -2.637085    -1.291059    -1.951355      28.67
 C      -3.557181    -2.134863    -2.985042      72.56
 H      -3.564930    -1.497711    -3.780006      28.53
 O      -3.133161    -3.481575    -3.010368     203.78
 H      -2.015607    -3.359881    -3.182526      25.23
 C      -5.033067    -1.952816    -2.505006      89.90
 H      -4.975446    -2.533513    -1.584643      27.23
 O      -5.512388    -0.523952    -2.466079     173.31
 H      -4.778474    -0.044482    -1.720959      23.57
 C      -5.895927    -2.759327    -3.533685      97.78
 O      -5.743024    -4.267002    -3.487543     133.13
 H      -4.842972    -4.643300    -3.967695      27.92
 H      -5.989608    -2.518888    -4.610376      28.37
 H      -6.883067    -2.779266    -2.977014      27.32
55
name = lig-ACN-frame_595
 C       3.737918     1.291640    -0.366699      46.55
 H       3.078247     1.711121    -1.063183      23.76
 C       4.485907     0.611050     1.799875      61.12
 H       4.212971     0.716391     2.919032      23.52
 C       5.558991     0.100668     1.272425       9.80
 O       6.661561    -0.549976     2.040393     249.73
 C       6.184307    -1.842221     2.680587      81.29
 H       6.641694    -2.003722     3.616553      26.62
 H       6.312216    -2.785715     1.959371      24.57
 H       5.064020    -1.865451     2.918546      28.89
 C       5.878809     0.272583    -0.169922      16.25
 O       6.991114    -0.246861    -0.739403     119.66
 H       7.677115    -0.526386     0.017501      19.25
 C       5.040326     0.917844    -0.940780      62.07
 H       5.249218     1.069985    -2.063380      20.28
 C       3.332496     1.032752     0.955940      10.72
 C       2.109362     1.615011     1.613939     103.95
 H       2.174296     2.731490     1.756929      25.49
 O       1.815705     1.076050     2.940687     238.46
 H       2.103610     0.106167     2.858731      28.12
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 C       0.921359     1.755040     0.741915      76.25
 H       1.193493     2.341481    -0.181367      23.61
 C      -0.379225     2.274974     1.285196     104.44
 O      -0.197091     3.657981     1.891238     228.53
 H       0.115027     4.450598     1.406724      28.76
 H      -0.853730     1.606546     2.072008      25.81
 H      -1.324034     2.022112     0.663637      25.40
 C      -2.069135    -1.950196    -0.755146      27.81
 H      -2.613674    -2.845183    -0.183408      21.52
 C      -1.886737    -0.098996    -2.483329      64.33
 H      -2.359909     0.435206    -3.270305      24.36
 C      -1.004605     0.506594    -1.595855      16.86
 O      -0.390165     1.787521    -1.861213     204.12
 C      -0.568810     2.433453    -3.128065     106.45
 H       0.493238     3.096706    -2.976746      23.31
 H      -0.291844     2.058280    -4.274384      24.50
 H      -1.239559     3.194015    -3.092062      27.66
 C      -0.480633    -0.064692    -0.461801      30.83
 O       0.632099     0.229114     0.179652     135.50
 C      -1.013591    -1.258242    -0.021012      40.10
 H      -0.363466    -1.907722     0.692638      23.46
 C      -2.443177    -1.342142    -1.959315      48.19
 C      -3.520533    -1.893679    -2.826103      83.17
 H      -3.355799    -1.609321    -3.783885      30.96
 O      -3.188398    -3.497818    -3.094938      80.21
 H      -2.109707    -3.666317    -3.289249      25.74
 C      -5.048321    -1.963263    -2.547973     100.69
 H      -5.353361    -2.296167    -1.547994      27.24
 O      -5.506006    -0.626158    -2.494656     252.24
 H      -5.170304    -0.147253    -1.667470      29.60
 C      -6.067515    -2.774881    -3.494553      96.53
 O      -5.720357    -4.316493    -3.511625      95.32
 H      -4.856802    -4.305246    -4.165244      28.04
 H      -5.945993    -2.281456    -4.457429      29.72
 H      -7.119704    -2.525809    -3.241695      29.36
55
name = lig-ACN-frame_596
 C       3.643977     1.232206    -0.459943      55.45
 H       2.944325     1.776694    -0.993123      22.74
 C       4.410548     0.538783     1.838983      38.01
 H       4.344343     0.218899     2.928929      19.86
 C       5.686980     0.032110     1.205323       7.72
 O       6.514864    -0.552047     2.082765     291.50
 C       6.138770    -1.739902     2.703484      81.29
 H       6.928286    -1.884292     3.461190      22.58
 H       6.286042    -2.591789     1.924348      24.22
 H       5.043796    -1.582316     3.088701      26.29
 C       5.871072     0.191956    -0.120789      10.94
 O       7.074625    -0.282018    -0.612380     232.27
 H       7.613653    -0.731648     0.089268      24.66
 C       4.891214     1.012194    -0.999713      47.13
 H       5.150861     1.107932    -2.022584      22.20
 C       3.516964     1.135410     1.015507      23.04
 C       2.105833     1.615874     1.756239      92.88
 H       2.499732     2.565033     2.076145      25.11
 O       1.815948     1.039464     3.017680     240.63
 H       1.504288    -0.050148     2.956644      22.22
 C       0.949465     1.765353     0.742081      67.42
 H       1.392127     2.321187    -0.186309      22.49
 C      -0.421931     2.279948     1.380571     107.70
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 O      -0.265044     3.537195     2.008808     273.84
 H       0.046794     3.906666     1.283703      34.89
 H      -0.440866     1.599271     2.291805      23.96
 H      -1.114193     2.451508     0.501119      25.17
 C      -2.096510    -1.927596    -0.727942      46.83
 H      -2.503391    -3.099401    -0.671846      22.72
 C      -1.945134    -0.091187    -2.389588      61.61
 H      -2.453898     0.423584    -3.212450      20.47
 C      -0.908465     0.572017    -1.659579      14.19
 O      -0.346746     1.734891    -1.818075     223.32
 C      -0.495808     2.473755    -3.068571      93.61
 H       0.392004     3.368276    -3.351171      22.25
 H      -0.648942     1.479459    -3.682659      24.56
 H      -1.444613     2.788540    -3.201653      27.57
 C      -0.529284    -0.118421    -0.431238       9.94
 O       0.718562     0.237879     0.202511     102.76
 C      -1.112791    -1.345417    -0.010248      58.65
 H      -0.925722    -1.509786     1.052152      22.19
 C      -2.377375    -1.367966    -2.005155      36.70
 C      -3.463496    -1.996684    -2.898205      74.57
 H      -3.506188    -1.365322    -3.749360      27.01
 O      -3.240461    -3.434251    -3.155390     262.01
 H      -2.318991    -3.412462    -3.277954      30.56
 C      -5.109591    -2.042050    -2.428833      75.41
 H      -5.124389    -2.599807    -1.459328      28.19
 O      -5.554252    -0.627799    -2.562318     273.54
 H      -5.372001    -0.295833    -1.776531      33.87
 C      -6.055993    -2.840502    -3.487721     113.05
 O      -5.776958    -4.184956    -3.561685     225.65
 H      -4.816243    -4.214964    -3.650050      30.04
 H      -5.954207    -2.452256    -4.482121      29.39
 H      -7.041655    -2.772844    -3.097335      29.61
55
name = lig-ACN-frame_597
 C       3.592039     1.300514    -0.348765      38.04
 H       2.799130     1.623699    -0.993384      22.81
 C       4.403706     0.433704     1.786867      55.19
 H       4.141888     0.382585     2.825723      22.39
 C       5.544093     0.046607     1.263705      14.45
 O       6.539624    -0.499905     2.090402     268.23
 C       6.110650    -1.736060     2.749265      89.18
 H       6.917277    -1.998295     3.522367      24.57
 H       5.937723    -2.603097     2.049304      26.89
 H       5.137092    -1.711751     3.470607      25.93
 C       5.904959     0.215143    -0.183300      -0.36
 O       7.126590    -0.296129    -0.592387     150.76
 H       7.580085    -0.723044     0.111035      23.73
 C       4.932102     0.856633    -0.963472      58.58
 H       5.164181     1.221755    -1.869926      22.48
 C       3.422160     1.194112     1.050809      32.68
 C       2.266472     1.679443     1.821207      77.58
 H       2.210199     2.717258     2.156755      24.84
 O       1.792365     0.958201     3.094092     214.52
 H       1.440638     0.015735     2.694207      23.22
 C       0.904673     1.635720     0.751654      88.73
 H       0.985804     2.487646    -0.051877      22.58
 C      -0.338485     2.162801     1.453347     103.52
 O      -0.302698     3.500727     2.090149     219.09
 H       0.235586     4.298608     1.699476      27.42
 H      -0.992360     1.422629     2.049695      25.42
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 H      -1.193663     2.127901     0.710229      25.75
 C      -2.085335    -1.970642    -0.854919      22.08
 H      -2.504776    -3.074593    -0.386278      21.23
 C      -1.988813    -0.052187    -2.326735      42.02
 H      -2.217081     0.329168    -3.362605      20.73
 C      -0.896607     0.481491    -1.572111      -4.82
 O      -0.225849     1.836119    -1.773717     175.01
 C      -0.564343     2.357580    -3.108344     102.32
 H       0.336397     3.352396    -3.209085      22.88
 H      -0.235097     1.827072    -4.093194      26.04
 H      -1.454607     2.856633    -3.033276      28.13
 C      -0.428100    -0.179573    -0.398247       6.51
 O       0.752144     0.350862     0.275274     175.91
 C      -1.178558    -1.317921     0.141227      38.02
 H      -1.060452    -1.777596     1.049292      25.13
 C      -2.544996    -1.389099    -2.058015      26.75
 C      -3.611223    -2.074279    -2.990000      84.95
 H      -3.672812    -1.598006    -3.972685      28.07
 O      -3.201868    -3.407438    -3.227476     267.15
 H      -2.326529    -3.589858    -3.450881      32.08
 C      -5.053041    -2.040400    -2.462135      98.24
 H      -5.166731    -2.327354    -1.394375      27.66
 O      -5.612101    -0.684333    -2.569389     193.43
 H      -5.393260    -0.017814    -1.743316      27.52
 C      -5.987062    -2.736904    -3.407748     120.46
 O      -5.787527    -4.201195    -3.631151     201.37
 H      -5.150290    -4.487347    -2.981635      32.74
 H      -6.078613    -2.170404    -4.286900      30.42
 H      -6.944454    -2.572988    -3.001217      30.00
55
name = lig-ACN-frame_598
 C       3.778260     1.331042    -0.287532      67.88
 H       3.058211     1.849277    -0.992437      23.33
 C       4.261644     0.472361     1.831925      43.55
 H       4.193389     0.358633     2.847729      22.06
 C       5.561552     0.001235     1.218153       8.87
 O       6.584950    -0.504574     2.100110     288.98
 C       6.127175    -1.761714     2.847457      80.44
 H       7.084350    -2.219696     3.343240      23.58
 H       5.825712    -2.412499     2.052251      27.58
 H       5.190070    -1.333151     3.489519      25.02
 C       5.922719     0.195524    -0.068500       4.87
 O       7.090979    -0.248685    -0.648166     211.15
 H       7.706648    -0.537750     0.110070      23.00
 C       4.834495     0.782034    -0.878311      60.48
 H       5.003860     0.792556    -1.874837      23.34
 C       3.326318     1.144402     1.077909      33.52
 C       2.048080     1.718897     1.813889      96.26
 H       2.387478     2.796598     2.087079      24.27
 O       1.824898     0.921225     3.049266     263.65
 H       1.930589    -0.002344     2.885195      28.37
 C       0.934927     1.711448     0.942103      77.10
 H       1.263890     2.273338    -0.015197      23.20
 C      -0.442152     2.083493     1.499556     110.44
 O      -0.339433     3.445793     2.202034     141.01
 H       0.464811     3.924252     1.545797      27.22
 H      -0.484933     1.511551     2.463831      24.90
 H      -1.062208     2.216089     0.636449      26.31
 C      -2.070286    -1.954961    -0.842597      23.67
 H      -2.705462    -2.962059    -0.461179      21.86
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 C      -1.951525    -0.088945    -2.328351      50.35
 H      -2.206434     0.650421    -3.156164      22.67
 C      -0.903356     0.445715    -1.452870      -6.68
 O      -0.195638     1.744115    -1.831946     180.16
 C      -0.555755     2.383220    -3.117776      81.70
 H       0.135521     3.521637    -3.039770      22.13
 H      -0.360906     1.648705    -3.930429      26.18
 H      -1.627924     2.529006    -3.304396      25.79
 C      -0.374103    -0.172806    -0.280687      17.95
 O       0.726763     0.291595     0.334560     162.19
 C      -1.192697    -1.293586     0.060319      54.15
 H      -0.774824    -1.822652     0.775954      26.91
 C      -2.639222    -1.278174    -2.041255      30.53
 C      -3.580113    -1.981254    -3.059362      72.48
 H      -3.592790    -1.452649    -4.064531      28.60
 O      -3.166553    -3.536935    -3.297632     119.94
 H      -2.147998    -3.154061    -3.420747      27.04
 C      -5.029756    -1.961601    -2.478510      89.78
 H      -5.003552    -2.463964    -1.447205      28.45
 O      -5.646462    -0.690515    -2.555170     191.39
 H      -5.013079    -0.132105    -1.808493      27.06
 C      -6.052551    -2.705172    -3.365349     100.75
 O      -5.818611    -4.215394    -3.675669      64.12
 H      -5.412546    -4.575611    -2.723210      28.73
 H      -5.883611    -2.313371    -4.297668      30.40
 H      -6.986200    -2.585253    -2.932847      30.20
55
name = lig-ACN-frame_599
 C       3.698367     1.418387    -0.254020      32.73
 H       3.160292     2.157490    -0.981511      21.78
 C       4.345762     0.432783     1.901006      58.90
 H       4.172024     0.264221     2.911036      24.06
 C       5.554872    -0.016761     1.426780      15.50
 O       6.585373    -0.562000     2.127880     306.31
 C       6.167898    -1.678830     2.827930     104.97
 H       7.120757    -2.119745     3.330552      25.16
 H       5.684443    -2.387318     2.270478      30.83
 H       5.502792    -1.527573     3.883679      25.88
 C       5.846527     0.132856    -0.030199      18.93
 O       7.024272    -0.172483    -0.700384     161.40
 H       7.817674    -0.522700    -0.108305      21.15
 C       4.936354     0.700505    -0.838491      46.84
 H       4.992715     0.618332    -1.932705      21.18
 C       3.344999     1.126185     1.089869      20.50
 C       2.064035     1.599926     1.881951      90.40
 H       2.154988     2.733944     2.257972      24.16
 O       1.858960     0.937951     3.024582     295.13
 H       2.183440     0.092553     2.877817      29.85
 C       0.767068     1.749313     0.881694      65.64
 H       1.040290     2.556543     0.098254      25.28
 C      -0.494914     2.129046     1.650155     127.20
 O      -0.345436     3.375866     2.244428     246.12
 H       0.173173     3.984315     1.628508      30.20
 H      -0.792930     1.234644     2.238430      26.82
 H      -1.413154     2.026675     1.121424      28.70
 C      -2.195019    -1.836000    -0.815293      38.13
 H      -2.413573    -3.021438    -0.682294      23.89
 C      -1.864513    -0.018510    -2.276307      58.40
 H      -2.353966     0.486210    -3.152168      22.95
 C      -0.902403     0.571559    -1.517085      25.94
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 O      -0.234621     1.565175    -1.889974     220.64
 C      -0.562104     2.342107    -3.085407      92.03
 H      -0.013973     3.550296    -3.275886      23.15
 H      -0.045833     1.887093    -3.911902      26.78
 H      -1.704109     2.491835    -3.153041      25.07
 C      -0.504169    -0.106659    -0.284124       2.38
 O       0.735438     0.171310     0.468650      85.55
 C      -1.062207    -1.408876    -0.041500      45.40
 H      -0.871104    -1.905529     0.807496      23.73
 C      -2.533746    -1.242768    -1.989903      26.29
 C      -3.488298    -1.990872    -3.051897      65.88
 H      -3.394154    -1.324890    -4.003054      26.92
 O      -3.108480    -3.435186    -3.329142     157.40
 H      -2.055671    -3.859817    -3.309332      24.39
 C      -5.052605    -2.028763    -2.549665      76.01
 H      -4.946036    -2.380761    -1.455653      26.65
 O      -5.608203    -0.603104    -2.467899     233.16
 H      -5.014106     0.027637    -2.129830      32.65
 C      -6.105631    -2.835312    -3.448201     126.90
 O      -5.871912    -4.147031    -3.639087     191.69
 H      -5.587189    -4.722146    -2.905547      30.46
 H      -6.281392    -2.391169    -4.369401      30.08
 H      -7.047185    -2.605184    -3.039236      30.86
55
name = lig-ACN-frame_600
 C       3.715578     1.359359    -0.250046      66.94
 H       2.870378     1.956815    -0.800081      24.19
 C       4.351339     0.422441     1.962197      45.12
 H       4.084486     0.329067     3.023851      21.00
 C       5.608355     0.030100     1.394711      11.93
 O       6.614450    -0.574440     2.170373     311.60
 C       6.255305    -1.742489     2.967574      84.11
 H       7.230612    -2.275651     3.131251      24.20
 H       5.652079    -2.329164     2.366274      31.89
 H       5.593852    -1.292232     3.915131      23.33
 C       5.800621     0.083645     0.038354      -4.01
 O       6.988037    -0.148447    -0.692466     210.75
 H       7.568320    -0.646122    -0.099053      27.91
 C       4.773698     0.803640    -0.792399      49.30
 H       5.356610     1.051034    -1.753129      19.76
 C       3.457164     1.147043     1.151621      28.21
 C       2.161363     1.663486     1.771605      56.46
 H       2.320973     2.812904     2.114901      22.78
 O       1.867652     0.868429     3.125880     184.10
 H       1.626162    -0.151601     2.927383      22.22
 C       0.684538     1.556198     0.869673      85.09
 H       0.609953     2.078428    -0.121118      23.53
 C      -0.606574     2.022596     1.715131     105.40
 O      -0.341727     3.394505     2.352340     240.88
 H      -0.280594     3.986264     1.696865      34.08
 H      -0.636863     1.614793     2.683397      26.60
 H      -1.356288     2.139534     1.026531      28.72
 C      -2.161804    -1.888362    -0.763552      61.94
 H      -2.624916    -2.935211    -0.572213      25.93
 C      -2.009477     0.011718    -2.373737      71.06
 H      -1.909827     0.411294    -3.386772      20.65
 C      -0.931784     0.507343    -1.467579     -17.99
 O      -0.094066     1.653517    -1.954552     168.12
 C      -0.561518     2.310172    -3.137863      85.33
 H      -0.117576     3.363233    -2.555329      21.98
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 H      -0.294791     1.944700    -4.059242      28.38
 H      -1.764102     2.435862    -3.203692      26.00
 C      -0.489339    -0.173604    -0.283758      17.78
 O       0.567830     0.224539     0.512785     182.47
 C      -1.035030    -1.436155    -0.052507      48.34
 H      -0.552569    -1.981514     0.736368      22.93
 C      -2.500514    -1.276779    -2.029134      28.06
 C      -3.399381    -1.986897    -2.994348      91.14
 H      -3.393692    -1.458855    -4.057596      27.59
 O      -3.080147    -3.294228    -3.332393     243.17
 H      -2.137898    -3.331124    -3.064120      30.83
 C      -4.994809    -1.985563    -2.642727      80.49
 H      -5.226307    -2.585782    -1.693696      29.74
 O      -5.538639    -0.603354    -2.428234     225.45
 H      -4.751694    -0.179653    -2.200009      34.14
 C      -6.162892    -2.713824    -3.458620      99.33
 O      -5.914010    -4.249879    -3.650094     149.63
 H      -5.565132    -4.350553    -2.826401      34.54
 H      -6.175284    -2.322695    -4.429652      28.93
 H      -6.975080    -2.624566    -2.797834      28.42
55
name = lig-ACN-frame_601
 C       3.600375     1.310272    -0.139843      33.56
 H       2.867561     1.789558    -0.878497      21.79
 C       4.416157     0.465991     1.984448      46.43
 H       4.239314     0.271990     3.110153      23.25
 C       5.600202    -0.024948     1.422904       4.34
 O       6.688924    -0.552873     2.192561     299.12
 C       6.319760    -1.768623     3.053877     104.14
 H       7.211241    -2.297074     3.307585      26.44
 H       5.591238    -2.429159     2.598038      28.96
 H       5.894985    -1.451514     4.168680      27.37
 C       5.768427     0.192033    -0.059520      34.81
 O       6.931506    -0.188464    -0.609008     188.58
 H       7.534138    -0.620506    -0.017647      22.15
 C       4.884057     0.882197    -0.802052      57.62
 H       4.846530     1.269141    -1.894825      19.95
 C       3.425305     1.154836     1.201503      43.52
 C       2.053042     1.590588     1.770801      74.94
 H       2.100864     2.790136     2.097751      21.44
 O       1.872719     0.907612     3.128510     208.43
 H       1.483341    -0.055534     2.692986      20.97
 C       0.728385     1.533070     0.992649      87.27
 H       0.933965     2.261888     0.197879      23.51
 C      -0.550190     2.033089     1.837359     115.29
 O      -0.361801     3.389843     2.403887     194.05
 H      -0.484396     4.041660     1.552447      26.69
 H      -0.796258     1.224715     2.439415      27.61
 H      -1.418044     1.933137     1.310565      28.41
 C      -2.053603    -1.997780    -0.865278      43.68
 H      -2.592774    -2.855475    -0.562558      24.37
 C      -1.938119    -0.034190    -2.360052      48.71
 H      -2.203232     0.280145    -3.345537      22.59
 C      -0.896089     0.538366    -1.577844      11.53
 O      -0.045676     1.553147    -1.920866     193.60
 C      -0.574578     2.462093    -3.134175      84.34
 H      -0.238619     3.531802    -3.640684      22.27
 H      -0.189704     1.916812    -3.903463      27.40
 H      -1.775900     2.330385    -3.062540      24.41
 C      -0.490376    -0.227026    -0.392288      16.63
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 O       0.399394     0.150895     0.551351     177.49
 C      -1.085148    -1.461171     0.009439      46.83
 H      -0.605484    -2.131831     0.816573      23.28
 C      -2.562203    -1.271278    -2.000552      24.06
 C      -3.551500    -1.878265    -3.089818      70.13
 H      -3.385772    -1.054362    -3.913810      27.42
 O      -2.987216    -3.265606    -3.287905     210.82
 H      -2.102621    -3.370842    -3.298717      31.15
 C      -4.990968    -1.962617    -2.617867     104.88
 H      -4.781182    -2.474856    -1.665438      27.59
 O      -5.410924    -0.658003    -2.430877     202.69
 H      -4.670177     0.049366    -1.997556      26.39
 C      -6.090176    -2.644781    -3.520165     102.43
 O      -5.967589    -4.218736    -3.610222     111.51
 H      -5.234652    -4.633898    -2.950001      29.27
 H      -6.347429    -2.322170    -4.526859      27.54
 H      -7.041383    -2.348375    -3.079837      28.14
55
name = lig-ACN-frame_602
 C       3.607152     1.276057    -0.175032      55.77
 H       2.774824     1.736633    -0.703040      23.61
 C       4.438476     0.524984     2.024562      37.53
 H       4.338901     0.392979     3.191039      21.34
 C       5.582262    -0.033418     1.392867       0.33
 O       6.674822    -0.599089     2.179192     293.63
 C       6.418017    -1.671570     3.085017     106.02
 H       7.322722    -2.168310     3.133000      25.85
 H       5.599163    -2.358458     2.641302      27.27
 H       6.021595    -1.164181     4.079639      26.23
 C       5.831756     0.283626     0.027376     -19.73
 O       6.966063    -0.281203    -0.586464     156.17
 H       7.570361    -0.481593     0.241872      19.74
 C       4.799075     1.024880    -0.784030      53.25
 H       5.096946     0.779733    -1.850837      20.14
 C       3.295341     1.092745     1.257872      12.70
 C       1.965863     1.505875     1.938897     102.87
 H       2.058647     2.714187     2.189409      23.45
 O       1.827291     0.942503     3.113587     278.56
 H       2.004324    -0.052230     3.170658      26.49
 C       0.732876     1.621087     1.065364      80.57
 H       0.829890     2.227091     0.202849      26.12
 C      -0.458695     2.011096     1.898563     123.88
 O      -0.397320     3.321257     2.422634     168.86
 H      -0.435975     4.081055     1.627180      27.90
 H      -0.494434     1.575908     2.822220      28.22
 H      -1.186721     1.973809     1.187475      29.18
 C      -2.069749    -2.109349    -0.986052      40.14
 H      -2.211348    -3.089562    -0.973469      27.28
 C      -1.875659    -0.106567    -2.372182      84.90
 H      -2.343116     0.573862    -3.013893      26.61
 C      -0.792947     0.467934    -1.648754       6.49
 O      -0.039069     1.616309    -1.948890     188.71
 C      -0.574201     2.412046    -3.167183      80.11
 H       0.104156     3.320728    -2.738496      22.57
 H      -0.504015     1.862727    -4.081538      27.52
 H      -1.754256     2.730848    -3.017106      25.94
 C      -0.562988    -0.238451    -0.424233      -4.35
 O       0.386840     0.110112     0.638976      75.82
 C      -1.159240    -1.488719    -0.108713      43.37
 H      -0.965996    -1.810661     1.042441      21.41
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 C      -2.595868    -1.249900    -1.987719      34.14
 C      -3.455123    -1.848912    -3.126732      80.41
 H      -3.641086    -1.495975    -4.241790      27.98
 O      -2.987795    -3.237938    -3.293110     147.39
 H      -1.982981    -3.118298    -3.637718      27.72
 C      -4.940989    -2.027721    -2.594892      78.16
 H      -5.168854    -2.598778    -1.686776      29.35
 O      -5.374705    -0.589987    -2.430306     142.29
 H      -4.598192    -0.248483    -1.710470      28.99
 C      -5.998808    -2.709903    -3.538927     118.86
 O      -6.032855    -4.072859    -3.544391     143.99
 H      -4.966949    -4.250843    -3.454111      26.12
 H      -5.591620    -2.295328    -4.470592      27.24
 H      -6.997629    -2.433486    -3.142127      28.11
55
name = lig-ACN-frame_603
 C       3.520354     1.295710    -0.142395      53.96
 H       2.816457     1.573315    -0.838613      22.99
 C       4.362509     0.551575     2.034520      64.57
 H       4.282657     0.599354     3.178500      23.16
 C       5.572960     0.084868     1.457271       3.26
 O       6.620210    -0.567627     2.029556     267.06
 C       6.470381    -1.553793     3.082220     114.04
 H       7.379766    -2.041369     3.227619      26.67
 H       5.648357    -2.359382     2.825757      27.48
 H       6.212320    -1.131247     4.139528      27.69
 C       5.877424     0.315656     0.072093       6.93
 O       6.972156    -0.317256    -0.539258     121.47
 H       7.745803    -0.580699     0.077579      19.39
 C       4.870085     0.926715    -0.670435      40.82
 H       4.934666     1.206624    -1.724464      21.18
 C       3.333900     1.010660     1.229609      32.34
 C       2.084054     1.592773     1.898648      60.72
 H       2.362683     2.707259     2.256120      23.60
 O       1.742866     0.834180     3.357336     197.83
 H       2.210482     0.119981     3.165395      30.89
 C       0.700338     1.489972     1.036833      97.64
 H       0.797997     2.064588     0.180615      26.34
 C      -0.490005     1.974352     1.929492     120.42
 O      -0.408239     3.379812     2.444403     269.54
 H      -0.229226     3.907849     1.731663      33.64
 H      -0.432093     1.236637     2.671734      28.22
 H      -1.410029     1.693465     1.623654      30.50
 C      -2.078486    -2.152658    -1.096247      75.14
 H      -2.394927    -3.088802    -1.020585      27.09
 C      -1.882680    -0.002658    -2.399454      69.83
 H      -2.169441     0.538242    -3.279513      22.87
 C      -0.686006     0.362672    -1.616984       5.10
 O      -0.125159     1.605885    -2.002438     207.16
 C      -0.524797     2.401159    -3.065339     100.86
 H       0.298911     3.293668    -3.366539      23.98
 H      -0.457536     2.057586    -4.107600      25.84
 H      -1.537091     2.975486    -2.813349      24.84
 C      -0.497236    -0.206370    -0.271116      17.77
 O       0.380712     0.152082     0.671841     183.36
 C      -1.230730    -1.467455    -0.207689      42.06
 H      -0.959254    -2.118592     0.838759      23.49
 C      -2.502876    -1.300002    -2.177751       8.77
 C      -3.478738    -2.004065    -3.049825      92.97
 H      -3.337229    -1.135233    -3.876365      28.61
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 O      -2.993865    -3.271673    -3.371296     136.90
 H      -1.938739    -3.294494    -3.769200      25.81
 C      -4.957303    -1.994573    -2.542570     103.06
 H      -4.824005    -2.477838    -1.564249      30.03
 O      -5.339789    -0.575006    -2.402683     219.01
 H      -4.962969    -0.257553    -1.645030      34.71
 C      -5.875173    -2.528763    -3.608414     104.47
 O      -5.987144    -4.060136    -3.466605     131.06
 H      -5.383291    -4.462974    -4.025029      28.72
 H      -5.739973    -2.323011    -4.686784      27.59
 H      -6.894914    -2.004284    -3.574362      28.08
55
name = lig-ACN-frame_604
 C       3.620849     1.207368    -0.152153      73.20
 H       2.916060     1.632843    -0.735988      26.86
 C       4.360633     0.529699     2.085435      32.34
 H       4.156335     0.398867     3.150988      19.48
 C       5.600248     0.197000     1.479748      12.92
 O       6.637656    -0.553230     1.961873     304.11
 C       6.491395    -1.427847     3.104557      96.20
 H       7.487994    -1.880319     3.106810      25.69
 H       5.617565    -2.231755     2.899273      28.09
 H       6.287110    -0.808517     3.970713      26.56
 C       5.839052     0.277943     0.086717       3.88
 O       6.946039    -0.287146    -0.515366     149.03
 H       7.516151    -0.547257     0.186751      25.15
 C       4.849155     0.891263    -0.662055      76.45
 H       5.163113     1.201940    -1.598343      25.55
 C       3.279310     1.052496     1.244177      23.75
 C       2.051537     1.508985     1.980429      55.92
 H       2.054297     2.701821     2.259655      21.99
 O       1.748810     0.809088     3.431547     194.60
 H       1.727435    -0.209652     3.338041      22.81
 C       0.693573     1.514945     1.058172      83.91
 H       0.831726     2.102076     0.206679      25.54
 C      -0.544800     1.927062     2.031118     109.84
 O      -0.407738     3.361718     2.417862     244.19
 H       0.013500     3.815871     1.682351      32.32
 H      -0.408349     1.508146     2.998587      25.62
 H      -1.401855     1.911473     1.495232      28.39
 C      -2.002339    -1.986693    -1.146509      50.12
 H      -2.549436    -2.809500    -0.848137      25.93
 C      -1.834230    -0.072036    -2.402907      72.49
 H      -1.938912     0.469588    -3.356387      21.15
 C      -0.823770     0.439305    -1.617478      15.88
 O      -0.073751     1.521218    -1.935713     212.07
 C      -0.494050     2.490887    -3.091728      80.09
 H       0.431241     3.238538    -3.151191      23.82
 H      -0.842277     1.739949    -3.763544      25.71
 H      -1.511223     2.954944    -2.827587      26.87
 C      -0.539557    -0.269777    -0.349906      -1.99
 O       0.431380     0.093477     0.729658     120.42
 C      -1.149707    -1.499867    -0.105500      48.57
 H      -0.771924    -2.332181     0.747055      21.91
 C      -2.324849    -1.351150    -2.298292      51.89
 C      -3.454190    -1.918962    -3.134977      65.91
 H      -3.794960    -1.571653    -4.240998      28.45
 O      -3.044257    -3.424180    -3.517285     137.34
 H      -2.068351    -3.395509    -3.395024      29.11
 C      -4.878962    -1.885374    -2.527259      99.78
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 H      -5.344079    -2.587829    -1.803659      30.79
 O      -5.328192    -0.563665    -2.366098     227.66
 H      -5.075541    -0.178822    -1.504439      30.91
 C      -5.838661    -2.488284    -3.704725      68.32
 O      -5.966082    -3.988060    -3.408670     159.24
 H      -5.726162    -4.386218    -4.276894      28.59
 H      -5.239725    -2.240329    -4.618644      26.78
 H      -6.909473    -2.153549    -3.449651      26.58
55
name = lig-ACN-frame_605
 C       3.579595     1.209581    -0.114789      31.13
 H       2.904218     1.739839    -0.726479      23.45
 C       4.378692     0.507197     2.114653      61.05
 H       4.209102     0.169121     3.080105      22.50
 C       5.597406     0.173413     1.472615      13.96
 O       6.726802    -0.536755     1.994403     281.44
 C       6.519240    -1.284428     3.147030     113.62
 H       7.420833    -1.956720     3.385325      25.90
 H       5.591892    -2.011786     2.995243      27.85
 H       6.369506    -0.730006     4.047060      28.08
 C       5.783665     0.257700     0.065615      -1.29
 O       6.911123    -0.224131    -0.489436     195.82
 H       7.520390    -0.653245     0.165149      21.58
 C       4.852294     0.917140    -0.810262      51.42
 H       4.967276     0.768909    -1.822883      22.72
 C       3.322616     1.066591     1.360092      16.35
 C       1.860510     1.382861     2.097104      92.30
 H       2.129097     2.497955     2.500350      22.25
 O       1.803483     0.824728     3.336517     234.55
 H       1.344691    -0.168528     3.068362      24.29
 C       0.650839     1.460481     1.274026      82.72
 H       0.728507     2.137484     0.456688      26.12
 C      -0.520464     1.987864     2.048892     135.10
 O      -0.387215     3.348055     2.374386     193.37
 H       0.142953     3.868638     1.525325      26.81
 H      -0.786283     1.359994     2.902469      28.06
 H      -1.298837     1.664638     1.508468      30.22
 C      -1.974272    -2.008533    -1.005479      39.21
 H      -2.433759    -3.010689    -0.912833      25.63
 C      -1.731769    -0.083646    -2.607154      57.84
 H      -2.202138     0.544416    -3.432433      24.93
 C      -0.914811     0.512814    -1.467117      -2.45
 O       0.015998     1.566629    -1.862072     162.42
 C      -0.521018     2.400987    -3.007697     121.31
 H       0.432659     2.969699    -3.273510      26.53
 H      -0.556986     2.175612    -4.102465      27.28
 H      -1.198424     3.172610    -2.661175      28.75
 C      -0.471966    -0.263993    -0.341073      10.17
 O       0.434888     0.023265     0.655671     130.49
 C      -1.036120    -1.537096    -0.120812      55.47
 H      -0.831956    -1.907336     1.014738      22.86
 C      -2.290250    -1.374767    -2.361534       5.63
 C      -3.346848    -2.016186    -3.306941      68.16
 H      -3.165394    -1.231530    -4.249344      28.19
 O      -3.137341    -3.460569    -3.615167     195.18
 H      -2.436879    -3.789502    -3.169323      33.19
 C      -4.936994    -1.925986    -2.632526      76.87
 H      -4.683717    -2.392783    -1.633733      28.05
 O      -5.343742    -0.468990    -2.328637     104.15
 H      -4.787090    -0.342072    -1.341174      28.01
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 C      -5.791826    -2.530248    -3.657845     117.75
 O      -5.957975    -3.857170    -3.411187     146.49
 H      -5.830470    -4.503247    -4.263812      24.82
 H      -5.523541    -2.425943    -4.766690      25.33
 H      -6.748479    -1.870601    -3.812024      27.40
55
name = lig-ACN-frame_606
 C       3.526717     1.309320    -0.041057      64.93
 H       2.597473     1.535392    -0.603740      22.92
 C       4.421681     0.434885     2.151258      43.80
 H       4.309782     0.324677     3.188059      21.35
 C       5.621144     0.065107     1.442673      -8.98
 O       6.788863    -0.446238     2.021010     234.97
 C       6.508679    -1.225376     3.319917     108.25
 H       7.481387    -1.890440     3.408956      25.30
 H       5.523356    -1.825929     3.212169      27.82
 H       6.412252    -0.551027     4.056752      30.43
 C       5.742568     0.317191    -0.012363       6.87
 O       6.940862    -0.192584    -0.535511     134.32
 H       7.512070    -0.611082     0.258762      17.36
 C       4.691494     0.852484    -0.747145      64.61
 H       4.643983     0.892859    -1.817062      22.47
 C       3.322648     1.052364     1.292562      10.88
 C       2.045514     1.445238     2.087446      80.26
 H       1.918108     2.622001     2.270115      23.69
 O       1.786036     0.691134     3.334325     258.28
 H       1.734630    -0.358478     3.214926      24.14
 C       0.627845     1.318699     1.300162      90.42
 H       0.889659     2.036170     0.506709      26.77
 C      -0.656092     1.920463     2.029422     109.63
 O      -0.366832     3.382936     2.331934     196.01
 H       0.021480     3.840449     1.478635      29.80
 H      -0.701423     1.602155     3.100314      26.66
 H      -1.444375     2.032086     1.458324      29.45
 C      -1.995330    -2.124019    -1.078273      37.82
 H      -2.309345    -3.187882    -0.740185      26.85
 C      -1.641165    -0.128397    -2.522097      73.28
 H      -1.808957     0.449077    -3.481582      24.32
 C      -0.822217     0.510812    -1.575776       7.08
 O      -0.046849     1.600150    -1.821136     220.27
 C      -0.356660     2.447273    -2.905252     122.24
 H       0.427998     3.137305    -3.053784      25.24
 H      -0.837774     1.634315    -3.532894      24.76
 H      -1.282165     2.912028    -2.640372      30.98
 C      -0.489802    -0.216870    -0.333746     -13.30
 O       0.492597     0.092920     0.648728     157.10
 C      -1.061228    -1.501665    -0.147991      34.93
 H      -0.859845    -2.117760     0.811876      23.77
 C      -2.259442    -1.428654    -2.241851      27.15
 C      -3.235512    -2.045090    -3.322622      85.46
 H      -3.189628    -1.561662    -4.472749      27.20
 O      -3.232615    -3.417188    -3.717913     149.04
 H      -2.539998    -3.995985    -3.098706      27.36
 C      -4.716879    -1.777830    -2.769415      67.80
 H      -4.847259    -2.587270    -1.902867      29.50
 O      -5.302924    -0.502982    -2.310500     183.82
 H      -4.682474    -0.070233    -1.591554      30.10
 C      -5.840027    -2.436124    -3.752877      96.77
 O      -6.037757    -3.901170    -3.366173     149.95
 H      -5.723446    -4.328528    -4.108005      29.25
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 H      -5.261124    -2.298550    -4.713687      24.81
 H      -6.867679    -2.000837    -3.527961      26.06
55
name = lig-ACN-frame_607
 C       3.432028     1.307865    -0.002876      46.45
 H       2.564630     1.744659    -0.673737      22.31
 C       4.432090     0.419029     2.029506      68.55
 H       4.370807     0.415345     3.120142      23.76
 C       5.600920     0.042917     1.385247      13.92
 O       6.753358    -0.417191     2.119959     264.74
 C       6.535595    -1.081879     3.394137     114.54
 H       7.459715    -1.821482     3.544650      25.27
 H       5.625868    -1.714836     3.318062      28.93
 H       6.541487    -0.478687     4.186711      29.88
 C       5.760770     0.273089     0.031408      -0.06
 O       6.940715    -0.137954    -0.631671     186.47
 H       7.583634    -0.388371     0.110949      23.05
 C       4.536529     0.807993    -0.653117      40.70
 H       4.823424     1.065668    -1.721335      21.44
 C       3.364695     1.010002     1.420419      32.36
 C       2.033761     1.415787     2.066218      78.74
 H       2.317082     2.432087     2.650346      22.67
 O       1.836217     0.557886     3.376208     231.63
 H       2.283375    -0.171849     3.099515      30.07
 C       0.695065     1.438927     1.165089      71.75
 H       0.570842     2.188142     0.360852      24.81
 C      -0.676799     1.980833     2.037787     104.99
 O      -0.346884     3.383620     2.280839     281.47
 H      -0.160984     3.690489     1.489849      35.51
 H      -1.018328     1.390311     2.953986      27.00
 H      -1.429960     1.650930     1.467530      30.44
 C      -1.901102    -2.168597    -1.089965      49.72
 H      -2.474993    -3.220849    -0.980637      26.76
 C      -1.635502    -0.255486    -2.403694      64.51
 H      -1.696854     0.011240    -3.460415      24.43
 C      -0.619869     0.370921    -1.587619       7.27
 O      -0.048196     1.645319    -1.667487     199.70
 C      -0.367442     2.490685    -2.874107     123.99
 H       0.433782     3.063070    -3.041960      29.90
 H      -0.177786     2.101443    -3.989576      25.82
 H      -1.175750     3.105979    -2.739571      29.97
 C      -0.564070    -0.233153    -0.335084      -8.86
 O       0.529571     0.057231     0.629953     101.55
 C      -1.165455    -1.492274    -0.151116      66.01
 H      -0.641946    -2.028097     0.606282      25.57
 C      -2.230832    -1.481708    -2.281114      31.96
 C      -3.221552    -1.890380    -3.316216      78.60
 H      -2.942264    -1.170712    -4.286567      26.98
 O      -3.266150    -3.416005    -3.781560      74.55
 H      -2.533738    -3.904113    -3.107288      26.61
 C      -4.668425    -1.775403    -2.834329      96.53
 H      -4.662172    -2.524986    -1.875488      29.85
 O      -5.182482    -0.540140    -2.349312     225.35
 H      -4.566298    -0.018472    -2.047183      37.66
 C      -5.794354    -2.379651    -3.781942      87.91
 O      -6.132959    -3.876293    -3.372376      71.48
 H      -5.384703    -4.417937    -3.725768      25.91
 H      -5.961949    -2.372885    -4.898913      25.79
 H      -6.710574    -1.781458    -3.496302      27.23
55
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name = lig-ACN-frame_608
 C       3.405934     1.182318     0.041740      39.73
 H       2.668600     1.978827    -0.468177      22.65
 C       4.402723     0.437035     2.060377      50.69
 H       4.427949     0.140839     3.169807      22.23
 C       5.647419     0.032684     1.446322      15.23
 O       6.686278    -0.391256     2.161638     260.58
 C       6.559402    -0.972189     3.458584     122.31
 H       7.513222    -1.625495     3.564273      26.23
 H       5.652428    -1.554241     3.575163      30.35
 H       6.489370    -0.288718     4.206031      29.81
 C       5.716655     0.177769    -0.001323      26.67
 O       6.872063    -0.038426    -0.708487     205.79
 H       7.623060    -0.321401    -0.218194      25.76
 C       4.671378     0.806659    -0.641169      54.31
 H       4.629962     0.971931    -1.802837      22.86
 C       3.230326     1.040351     1.388772      21.48
 C       1.979360     1.328733     2.225380      86.94
 H       1.927144     2.513194     2.543284      23.07
 O       1.903063     0.499288     3.303316     294.10
 H       2.013297    -0.460894     3.118691      26.42
 C       0.676964     1.554500     1.214417      51.07
 H       1.103684     2.153347     0.346178      23.84
 C      -0.515596     1.959961     1.922189     124.57
 O      -0.406105     3.350719     2.248071     210.46
 H      -0.201466     3.930231     1.395538      29.22
 H      -0.435436     1.522258     2.972606      26.21
 H      -1.370758     1.989348     1.405398      28.96
 C      -1.930315    -2.230926    -1.075895      31.95
 H      -2.211097    -3.361624    -0.743131      25.10
 C      -1.489017    -0.223447    -2.537713      56.55
 H      -1.801083     0.504438    -3.250721      25.59
 C      -0.635578     0.312364    -1.530150      -9.78
 O      -0.065155     1.655356    -1.642202     158.69
 C      -0.271043     2.580369    -2.865494     111.60
 H       0.329421     3.264643    -2.596268      29.38
 H      -0.245267     1.939432    -3.871357      25.38
 H      -1.243520     2.907934    -2.835638      29.75
 C      -0.437244    -0.321528    -0.231994       1.26
 O       0.488633     0.021694     0.590299     111.09
 C      -1.127951    -1.573948    -0.033633      46.68
 H      -1.099851    -1.989608     0.893576      27.18
 C      -2.185312    -1.548743    -2.302130      10.15
 C      -3.257050    -1.867323    -3.401063      91.21
 H      -3.110016    -1.121048    -4.359301      26.37
 O      -3.209745    -3.303909    -3.793955     158.95
 H      -2.405294    -3.682423    -3.558449      31.22
 C      -4.708399    -1.890786    -2.870758      74.26
 H      -4.634289    -2.623684    -1.900636      29.79
 O      -5.068625    -0.495572    -2.430213     146.30
 H      -4.120477    -0.058911    -2.340392      31.18
 C      -5.858029    -2.452272    -3.707742     138.40
 O      -6.193432    -3.741692    -3.442932     125.50
 H      -5.244452    -4.105627    -3.011732      24.48
 H      -5.493518    -2.201744    -4.773779      26.08
 H      -6.731759    -1.867692    -3.349762      26.38
55
name = lig-ACN-frame_609
 C       3.505781     1.143072    -0.028402      54.22
 H       2.703418     1.510089    -0.833839      22.54
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 C       4.317727     0.437597     2.140720      50.05
 H       4.063768     0.320603     3.273144      20.15
 C       5.496064     0.088280     1.458403       6.79
 O       6.711629    -0.400913     2.148459     234.73
 C       6.551605    -0.884975     3.573906     121.55
 H       7.513961    -1.391257     3.783625      27.51
 H       5.752205    -1.575127     3.596869      30.98
 H       6.496401    -0.057627     4.202041      29.93
 C       5.699106     0.165593     0.046161       6.15
 O       6.838547     0.017184    -0.779155     178.22
 H       7.517816    -0.380450    -0.117423      23.00
 C       4.637085     0.830902    -0.644642      34.41
 H       4.887017     0.923399    -1.793398      21.54
 C       3.277270     0.958856     1.426196      23.53
 C       1.951665     1.356292     2.181444      90.05
 H       2.059800     2.321729     2.874487      23.39
 O       1.868824     0.408219     3.326566     239.31
 H       1.647751    -0.493415     2.759550      23.70
 C       0.871945     1.353977     1.211768      91.17
 H       1.140438     2.168037     0.391005      24.25
 C      -0.482160     1.995541     1.858966     104.69
 O      -0.445666     3.427627     2.254689     180.62
 H      -0.217122     4.001286     1.308123      26.77
 H      -0.614794     1.380844     2.801930      27.06
 H      -1.248891     1.476896     1.342874      28.53
 C      -1.910912    -2.168312    -1.045771      48.94
 H      -2.511145    -3.190024    -0.953086      26.03
 C      -1.415767    -0.239917    -2.571144      55.81
 H      -1.754327     0.326733    -3.402970      27.75
 C      -0.709144     0.404067    -1.510436      -1.18
 O      -0.102653     1.584208    -1.646213     200.77
 C      -0.242295     2.556107    -2.736184     119.94
 H       0.254545     3.372024    -2.707915      29.79
 H       0.359305     2.071857    -3.648199      26.22
 H      -1.217088     2.746454    -2.950014      29.99
 C      -0.402483    -0.460161    -0.319318      -9.22
 O       0.541057     0.107951     0.735473     135.62
 C      -1.132743    -1.679104     0.021471      63.21
 H      -1.116000    -2.057102     0.923583      28.46
 C      -2.100875    -1.451306    -2.365594      -4.35
 C      -3.283236    -1.976294    -3.402998      78.52
 H      -3.372738    -1.255087    -4.383710      29.17
 O      -3.066086    -3.248552    -3.849366     176.95
 H      -2.164650    -3.290053    -4.088671      31.97
 C      -4.717586    -1.839061    -2.735518      94.26
 H      -4.804109    -2.449800    -1.691615      29.39
 O      -4.944841    -0.485674    -2.541515     136.70
 H      -3.992467     0.088927    -2.266454      28.37
 C      -5.896797    -2.292000    -3.676971      97.28
 O      -6.211509    -3.768874    -3.486584     158.29
 H      -5.763279    -4.154874    -2.685686      29.17
 H      -5.590667    -2.275622    -4.803344      24.38
 H      -6.802174    -1.723287    -3.598386      27.98
55
name = lig-ACN-frame_610
 C       3.412872     1.161951    -0.026768      59.20
 H       2.435033     1.300640    -0.561417      23.79
 C       4.329270     0.408561     2.177794      63.39
 H       4.302120     0.363626     3.316249      23.34
 C       5.540231     0.032052     1.541801       5.53
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 O       6.669483    -0.425114     2.152355     227.60
 C       6.550235    -0.782629     3.583533     127.84
 H       7.470288    -1.144032     3.901364      28.50
 H       5.803686    -1.513076     3.694311      31.12
 H       6.101758    -0.037961     4.278421      29.08
 C       5.688017     0.296707     0.084766      18.78
 O       6.820488    -0.006520    -0.667753     146.70
 H       7.685915    -0.415415    -0.243812      22.12
 C       4.672921     0.769787    -0.703712      55.46
 H       4.841911     1.066323    -1.774920      21.91
 C       3.306957     0.968939     1.333849      33.68
 C       2.127257     1.263519     2.160193      78.65
 H       2.235054     2.464740     2.445650      23.83
 O       1.730832     0.353274     3.316778     188.61
 H       1.933729    -0.791087     3.154213      21.45
 C       0.828801     1.418617     1.180151      64.67
 H       1.114445     1.979250     0.188795      23.03
 C      -0.486174     1.979659     1.885154     111.68
 O      -0.485672     3.427995     2.186434     254.53
 H      -0.191007     3.923568     1.433959      32.80
 H      -0.766007     1.596421     2.874502      27.51
 H      -1.219171     2.108659     1.137829      27.40
 C      -1.959713    -2.075638    -1.145264      62.01
 H      -2.670335    -2.929852    -1.000907      26.85
 C      -1.468826    -0.205106    -2.586047      68.25
 H      -1.243757     0.116710    -3.589287      23.41
 C      -0.694973     0.314445    -1.493767       2.52
 O      -0.069720     1.592107    -1.546197     191.47
 C      -0.209801     2.446482    -2.696222     127.28
 H      -0.016719     3.158412    -2.114756      31.09
 H       0.431733     2.220978    -3.595540      27.97
 H      -1.210165     2.572043    -3.044570      30.63
 C      -0.367727    -0.349779    -0.276075     -12.39
 O       0.531489    -0.053923     0.790449     114.64
 C      -1.077424    -1.608738    -0.090963      47.40
 H      -0.747838    -2.200316     0.658316      29.05
 C      -2.126255    -1.475951    -2.330483      29.62
 C      -3.238415    -1.945302    -3.279381      81.95
 H      -3.228036    -1.056375    -4.038543      29.03
 O      -2.886005    -3.339681    -3.927585      24.52
 H      -1.898159    -3.226243    -4.454478      28.34
 C      -4.701664    -1.803331    -2.679907      90.71
 H      -4.791961    -2.315462    -1.578205      30.20
 O      -4.859121    -0.343793    -2.613961     146.76
 H      -4.133965    -0.032531    -2.000789      33.22
 C      -5.860118    -2.264027    -3.637588      98.38
 O      -6.246838    -3.775821    -3.529773     172.58
 H      -6.244966    -3.882133    -2.631437      32.83
 H      -5.687259    -2.101140    -4.757696      23.87
 H      -6.643572    -1.628122    -3.235971      28.09
55
name = lig-ACN-frame_611
 C       3.392147     1.085331    -0.067968      58.93
 H       2.671295     1.567554    -0.658082      24.14
 C       4.442753     0.405508     2.098686      75.15
 H       4.216471     0.277610     3.145396      24.49
 C       5.605326     0.045558     1.483826      23.67
 O       6.674719    -0.480175     2.216204     268.33
 C       6.494545    -0.732688     3.590179     127.42
 H       7.449506    -0.749869     3.905301      28.10
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 H       6.029850    -1.666443     3.690689      29.07
 H       6.080017     0.239744     4.014021      27.52
 C       5.727732     0.346488     0.134973       7.22
 O       6.869738    -0.057946    -0.513249     131.85
 H       7.402798    -0.362800     0.232257      22.35
 C       4.578330     0.817945    -0.671132      44.48
 H       4.759012     0.817554    -1.710917      22.72
 C       3.364881     0.881674     1.374778      24.01
 C       1.977500     1.195751     2.102967      90.15
 H       2.254436     2.125799     2.858577      22.41
 O       1.651625     0.407076     3.255341     246.07
 H       2.193871    -0.512388     3.026930      25.63
 C       0.748756     1.432325     1.284150      65.87
 H       0.896774     2.025610     0.336274      24.16
 C      -0.544222     2.036531     1.805967     126.65
 O      -0.456270     3.438575     2.147515     290.49
 H      -0.012850     3.851218     1.460786      33.64
 H      -0.731194     1.387604     2.648867      28.26
 H      -1.313473     1.551307     1.166132      29.17
 C      -1.982406    -2.066561    -1.068843      53.09
 H      -2.176236    -3.080419    -0.806688      27.85
 C      -1.417661    -0.212756    -2.524559      67.12
 H      -1.486984     0.387588    -3.474800      23.68
 C      -0.581325     0.317637    -1.492299      13.20
 O      -0.035875     1.520758    -1.472914     216.88
 C      -0.205074     2.470310    -2.615716     126.88
 H      -0.100757     3.428262    -2.620091      30.18
 H       0.585202     2.238967    -3.314858      28.85
 H      -1.151719     2.150393    -3.074017      27.54
 C      -0.444050    -0.334057    -0.190120      13.24
 O       0.483043    -0.174730     0.769028      78.42
 C      -0.995974    -1.572603    -0.259685      49.62
 H      -0.791395    -2.210803     0.602628      24.09
 C      -2.178542    -1.381318    -2.323068      33.62
 C      -3.153749    -1.972370    -3.331014      95.94
 H      -3.216161    -1.451337    -4.287576      29.40
 O      -2.791029    -3.323772    -3.945433     110.58
 H      -1.781449    -3.105835    -4.162541      29.72
 C      -4.593924    -1.810252    -2.752445      72.55
 H      -4.779460    -2.182239    -1.621242      27.58
 O      -4.815560    -0.224795    -2.626463     130.09
 H      -4.421568     0.044441    -1.890166      34.75
 C      -5.851501    -2.324687    -3.521411     102.67
 O      -6.237533    -3.647964    -3.564027     148.71
 H      -6.777308    -3.914957    -2.683034      26.55
 H      -5.644142    -1.956954    -4.556617      26.95
 H      -6.764048    -1.809912    -3.182680      28.34
55
name = lig-ACN-frame_612
 C       3.396894     1.045957    -0.006293      64.01
 H       2.626722     1.417160    -0.539416      24.57
 C       4.383133     0.408292     2.093060      52.05
 H       4.288152     0.123094     3.072353      24.05
 C       5.626246     0.120320     1.497088       0.12
 O       6.729582    -0.528047     2.152704     221.88
 C       6.513425    -0.682345     3.664682     124.60
 H       7.389294    -0.698148     4.161847      29.99
 H       5.995753    -1.595892     3.876933      29.85
 H       5.740975    -0.023122     4.225379      26.44
 C       5.760170     0.295002     0.063735      10.53
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 O       6.975328    -0.107443    -0.382896     115.84
 H       7.632638    -0.432201     0.224514      23.31
 C       4.688746     0.799811    -0.642077      83.20
 H       4.758927     0.859506    -1.645248      25.73
 C       3.176262     0.841734     1.353762       4.72
 C       1.898864     1.275067     2.177897      83.98
 H       1.959578     2.507021     2.319216      23.30
 O       1.628797     0.373614     3.233707     308.33
 H       1.585389    -0.550982     3.012079      28.01
 C       0.698683     1.298055     1.199248      86.10
 H       1.098440     1.891988     0.402673      26.14
 C      -0.629126     1.925568     1.835412     103.45
 O      -0.427350     3.418925     2.090783     173.10
 H       0.207021     3.911955     1.330429      27.48
 H      -0.911282     1.738335     2.824715      28.07
 H      -1.482597     1.961458     1.062351      26.89
 C      -1.947150    -2.139669    -1.123400      40.88
 H      -2.424678    -3.071552    -1.210241      26.59
 C      -1.367312    -0.183941    -2.461645      78.06
 H      -1.873495     0.455254    -3.263226      24.16
 C      -0.557493     0.364454    -1.446999      10.82
 O       0.069420     1.653320    -1.446083     209.19
 C      -0.180715     2.400614    -2.639168     120.25
 H      -0.256241     3.262342    -2.046879      28.21
 H       0.599021     2.218721    -3.283589      29.49
 H      -1.141947     2.239831    -3.244265      27.59
 C      -0.453790    -0.399385    -0.274578      -3.86
 O       0.456990    -0.047663     0.810764     129.41
 C      -1.014036    -1.714153    -0.131402      77.94
 H      -0.684022    -2.275457     0.847818      23.61
 C      -2.169299    -1.357582    -2.271675     -14.83
 C      -3.166453    -1.940842    -3.543377      93.74
 H      -3.076996    -1.147837    -4.218985      29.97
 O      -2.729744    -3.259509    -3.877907     215.99
 H      -1.921798    -3.509326    -3.571317      31.34
 C      -4.553071    -1.736615    -2.735902      67.49
 H      -4.273696    -2.230311    -1.712921      25.30
 O      -4.786418    -0.289998    -2.665853     145.09
 H      -4.488909     0.099223    -1.689416      28.36
 C      -5.863868    -2.165715    -3.492381      98.43
 O      -6.201467    -3.650734    -3.569402     154.96
 H      -6.947142    -3.895442    -2.877942      26.90
 H      -5.806625    -1.949853    -4.554904      27.23
 H      -6.583213    -1.438680    -3.033583      27.94
55
name = lig-ACN-frame_613
 C       3.442962     1.031983    -0.008905      45.01
 H       2.728465     1.194379    -0.742285      25.05
 C       4.230178     0.366793     2.136158      58.43
 H       4.063257     0.249848     3.145104      22.22
 C       5.566735     0.136716     1.567780       5.71
 O       6.683329    -0.490778     2.190774     254.33
 C       6.529563    -0.701485     3.689192     115.17
 H       7.503823    -0.617337     4.072663      27.72
 H       6.123407    -1.718814     3.718294      27.42
 H       5.959909     0.255347     3.947410      26.60
 C       5.857672     0.202503     0.179371      -8.10
 O       7.112512    -0.140085    -0.417996     123.85
 H       7.643362    -0.479347     0.408984      22.74
 C       4.739851     0.757166    -0.651401      26.01
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 H       4.906675     1.073159    -1.618267      22.23
 C       3.167334     0.852727     1.407294      35.48
 C       1.854735     1.267600     2.107357      80.47
 H       1.976951     2.234475     2.844066      23.40
 O       1.593396     0.376358     3.315633     260.18
 H       1.387958    -0.418934     2.835883      28.27
 C       0.579482     1.324120     1.174376      94.92
 H       0.697679     1.917142     0.355237      25.42
 C      -0.649883     1.982652     1.837847     117.96
 O      -0.379598     3.377582     2.034365     222.98
 H       0.188432     3.647653     1.139967      27.18
 H      -0.892021     1.330915     2.632862      28.51
 H      -1.579421     1.815005     1.095160      26.88
 C      -1.882463    -2.271069    -1.193768      28.11
 H      -2.499672    -3.075210    -0.896786      24.62
 C      -1.465546    -0.075413    -2.416936      34.77
 H      -1.379196     0.490483    -3.400192      22.51
 C      -0.577161     0.396375    -1.390706      -1.51
 O       0.101654     1.612430    -1.456052     204.81
 C      -0.125765     2.493851    -2.678029     112.06
 H      -0.174972     3.616172    -2.591783      26.46
 H       0.565728     2.539554    -3.366025      29.89
 H      -1.174523     2.177220    -3.023432      25.72
 C      -0.322838    -0.522997    -0.220027      19.29
 O       0.366841    -0.044529     0.783709     172.84
 C      -1.086473    -1.744076    -0.030374      30.86
 H      -0.897359    -2.512348     0.933313      23.31
 C      -2.075113    -1.381825    -2.363356      30.64
 C      -3.030259    -1.753472    -3.432586     102.15
 H      -3.062484    -1.367967    -4.356444      30.92
 O      -2.729493    -3.197375    -3.827576     122.86
 H      -2.321610    -3.517584    -3.007524      31.81
 C      -4.514621    -1.728773    -2.844298      84.82
 H      -4.679662    -2.294104    -1.864269      29.64
 O      -4.751257    -0.356494    -2.657325     147.85
 H      -4.338182     0.019362    -1.698193      28.53
 C      -5.874020    -2.083700    -3.514679      92.47
 O      -6.153593    -3.588742    -3.543125     193.50
 H      -6.738008    -3.655476    -2.885684      31.54
 H      -5.820250    -1.573981    -4.462806      28.16
 H      -6.806167    -1.784432    -2.917752      27.86
55
name = lig-ACN-frame_614
 C       3.534796     0.987871    -0.073369      70.01
 H       2.759303     1.490277    -0.678618      23.55
 C       4.253037     0.316672     2.225355      50.52
 H       4.023688     0.197463     3.279990      21.71
 C       5.499015     0.006932     1.618978      17.87
 O       6.588483    -0.407234     2.304064     243.30
 C       6.584468    -0.683818     3.619978     136.21
 H       7.630996    -0.818237     3.961402      27.83
 H       6.015299    -1.579802     3.986853      28.59
 H       6.055632    -0.003149     4.390038      27.39
 C       5.840696     0.217673     0.207720       7.10
 O       7.098746    -0.123015    -0.397994     135.25
 H       7.888414    -0.608073     0.113075      21.74
 C       4.807651     0.703398    -0.529103      64.49
 H       5.044823     0.797467    -1.591253      24.37
 C       3.224936     0.893997     1.307278     -10.67
 C       1.779974     1.200047     2.121945      72.20
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 H       2.052042     2.348341     2.442798      23.65
 O       1.532777     0.401948     3.298812     240.58
 H       1.607957    -0.678329     3.391009      23.03
 C       0.574127     1.465354     1.205306      78.56
 H       0.883158     1.922515     0.357047      26.17
 C      -0.701919     1.950414     1.812882     117.19
 O      -0.336855     3.347490     2.011011     266.96
 H       0.029782     3.744814     1.295113      33.74
 H      -0.826920     1.778570     2.842392      27.67
 H      -1.648806     1.683761     1.111007      26.66
 C      -1.815491    -2.183009    -1.171952      71.67
 H      -2.270161    -3.178655    -1.202842      25.87
 C      -1.472528    -0.064261    -2.367227     110.71
 H      -1.548441     0.395999    -3.357620      20.38
 C      -0.626271     0.304034    -1.361125      22.32
 O       0.126169     1.555778    -1.534259     172.59
 C      -0.127248     2.564608    -2.704928      94.28
 H       0.026477     3.615381    -2.034280      24.50
 H       0.530248     2.198531    -3.270988      30.45
 H      -1.101379     2.432885    -3.272527      26.10
 C      -0.415217    -0.521303    -0.267431      23.53
 O       0.365200    -0.164310     0.875594      54.44
 C      -1.123292    -1.718918    -0.192434      63.33
 H      -1.151326    -2.178345     0.978726      23.65
 C      -1.941891    -1.370443    -2.321934      28.50
 C      -3.010631    -1.842577    -3.369267     107.69
 H      -2.851582    -1.089295    -4.009763      31.83
 O      -2.754900    -3.108531    -3.780527     171.48
 H      -2.477365    -3.885144    -3.030467      26.03
 C      -4.515690    -1.718125    -2.870984      83.58
 H      -4.428028    -2.351386    -1.940038      31.10
 O      -4.751729    -0.271818    -2.564210     202.27
 H      -4.103087    -0.040706    -1.986157      36.92
 C      -5.870290    -2.129499    -3.598579     110.67
 O      -6.070092    -3.467288    -3.565179     187.80
 H      -6.540311    -3.830341    -2.706639      27.17
 H      -6.216522    -1.858715    -4.586799      27.33
 H      -6.428666    -1.384016    -2.862951      26.02
55
name = lig-ACN-frame_615
 C       3.537025     1.030924    -0.023267      32.69
 H       2.846009     1.510862    -0.839273      23.75
 C       4.227990     0.336573     2.137898      65.55
 H       4.152545     0.101828     3.254340      23.18
 C       5.478211    -0.093628     1.637304      27.68
 O       6.605035    -0.341878     2.370692     238.93
 C       6.612402    -0.733988     3.831282     113.31
 H       7.729233    -1.058451     3.879046      25.94
 H       5.967563    -1.649556     3.786525      26.48
 H       6.412565     0.207507     4.370277      26.67
 C       5.833644     0.152316     0.312789      25.90
 O       6.980212    -0.071350    -0.362334     147.18
 H       7.565943    -0.508323     0.301980      21.68
 C       4.876748     0.668318    -0.582118      26.67
 H       5.056280     0.667830    -1.730392      21.74
 C       3.205438     0.799337     1.375652      39.33
 C       1.891468     1.210997     2.088365      90.22
 H       1.974213     2.262446     2.599203      24.59
 O       1.489206     0.456289     3.301985     226.04
 H       1.973685    -0.409075     2.829648      25.23
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 C       0.650070     1.179031     1.215399      97.37
 H       0.817557     1.802900     0.391489      26.83
 C      -0.659671     1.984430     1.850748      98.60
 O      -0.369720     3.418016     2.018844     254.61
 H      -0.135620     3.814086     1.166704      30.15
 H      -0.964998     1.442492     2.733935      27.74
 H      -1.631221     1.958259     1.097330      25.82
 C      -1.847624    -2.213386    -1.257174      35.69
 H      -2.192061    -3.313249    -1.271338      24.99
 C      -1.447517    -0.136795    -2.425700      69.76
 H      -1.871063     0.620421    -3.004986      25.42
 C      -0.567874     0.405510    -1.448385      21.71
 O       0.094727     1.500410    -1.599435     215.23
 C      -0.079251     2.467436    -2.652845     123.83
 H       0.372210     3.528142    -2.072553      24.94
 H       0.495096     2.570253    -3.407941      31.30
 H      -1.092678     2.801697    -2.904097      29.30
 C      -0.451520    -0.343512    -0.159452       2.45
 O       0.344537    -0.177244     0.917013     173.94
 C      -1.044205    -1.666122    -0.109674      17.29
 H      -0.925391    -2.342320     0.940809      21.56
 C      -2.086076    -1.391110    -2.333616      54.76
 C      -3.016112    -1.797298    -3.358660     110.98
 H      -2.964673    -1.404553    -4.282464      32.12
 O      -2.781427    -3.180028    -3.874191     161.72
 H      -2.451600    -3.708159    -3.111441      32.41
 C      -4.479620    -1.579746    -2.830919      89.86
 H      -4.678587    -2.192536    -1.928828      30.95
 O      -4.745181    -0.226167    -2.439002     218.97
 H      -3.957977     0.255198    -2.211799      32.88
 C      -5.790142    -1.994349    -3.630264      84.81
 O      -6.045691    -3.527638    -3.587480      90.23
 H      -5.990892    -3.772960    -2.533406      29.37
 H      -5.545353    -1.760720    -4.694179      27.76
 H      -6.825148    -1.606813    -3.190064      25.55
55
name = lig-ACN-frame_616
 C       3.550483     1.055523     0.009607      71.49
 H       2.638470     1.379440    -0.678240      25.09
 C       4.262372     0.230582     2.181951      42.95
 H       3.960473     0.302875     3.307809      20.58
 C       5.530008    -0.067266     1.676647      10.13
 O       6.722452    -0.331567     2.504021     226.86
 C       6.636177    -0.782413     3.890218     119.11
 H       7.699129    -1.232754     4.275657      25.80
 H       5.818513    -1.455604     4.257229      28.01
 H       6.442936    -0.015268     4.630183      27.82
 C       5.716841     0.101170     0.246105       8.17
 O       6.972467    -0.085543    -0.274316     166.63
 H       7.681868    -0.371157     0.286218      25.64
 C       4.682316     0.673021    -0.550103      57.62
 H       5.119769     0.981514    -1.615782      20.67
 C       3.179697     0.767766     1.332667      13.81
 C       1.923452     1.272194     2.081204      89.13
 H       2.050391     2.389658     2.261616      24.83
 O       1.577237     0.442546     3.269963     280.04
 H       1.536823    -0.503040     3.400662      27.32
 C       0.677776     1.203013     1.229023      92.39
 H       0.937077     1.517606     0.212247      23.50
 C      -0.534910     2.007076     1.828355     101.78
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 O      -0.413752     3.439896     2.081338     186.12
 H      -0.105766     3.854734     1.063899      25.62
 H      -0.843881     1.676685     2.835385      26.39
 H      -1.316760     1.723520     0.934733      25.37
 C      -1.770444    -2.231027    -1.125457      31.98
 H      -2.184460    -3.277726    -0.816310      23.07
 C      -1.494915    -0.116792    -2.467674      53.33
 H      -1.532943     0.424501    -3.384123      23.64
 C      -0.592640     0.301516    -1.421321      16.11
 O       0.188981     1.526739    -1.639876     211.21
 C      -0.040522     2.554405    -2.606360     101.39
 H       0.539783     3.614813    -2.209332      23.70
 H       0.168428     2.092707    -3.445116      28.68
 H      -1.103352     2.639911    -2.634984      27.90
 C      -0.532159    -0.368350    -0.199776      26.09
 O       0.317103    -0.185077     0.938727     132.05
 C      -1.080875    -1.657878    -0.157464      48.04
 H      -0.535845    -2.335651     0.639472      23.54
 C      -2.147614    -1.348675    -2.358237       9.42
 C      -3.160360    -1.810103    -3.549501      77.90
 H      -3.055153    -1.050137    -4.258308      31.77
 O      -2.842062    -3.259836    -3.948056     167.90
 H      -2.261976    -3.609624    -3.362258      32.73
 C      -4.584231    -1.529577    -2.687165      97.43
 H      -4.405659    -2.111929    -1.807691      30.35
 O      -4.757105    -0.139908    -2.327178     137.24
 H      -3.733379     0.365955    -2.246783      26.18
 C      -5.647938    -2.001069    -3.710193      98.66
 O      -5.983650    -3.501017    -3.588195     200.47
 H      -5.488899    -3.717680    -2.850369      33.87
 H      -5.402504    -1.804712    -4.825054      26.46
 H      -6.633823    -1.311432    -3.564047      26.33
55
name = lig-ACN-frame_617
 C       3.335697     1.046295     0.015789      31.31
 H       2.601455     1.720664    -0.593066      20.81
 C       4.254629     0.173511     2.248630      64.22
 H       4.122795     0.058254     3.382079      21.74
 C       5.590713    -0.023850     1.796915       1.25
 O       6.761016    -0.343656     2.556499     235.64
 C       6.602744    -0.765080     3.979125     105.70
 H       7.616341    -1.449582     4.074616      24.67
 H       5.735604    -1.453362     3.855631      26.35
 H       6.547978     0.111682     4.539950      27.93
 C       5.731389     0.062304     0.312162      -0.93
 O       6.991186    -0.108444    -0.258351     125.75
 H       7.551204    -0.441103     0.539502      20.35
 C       4.690778     0.656580    -0.531129      25.50
 H       4.826448     1.046496    -1.634199      22.82
 C       3.267500     0.735512     1.425712      37.00
 C       1.933957     1.123090     2.070191      97.53
 H       2.137007     2.092767     2.498067      26.43
 O       1.692287     0.508665     3.329244     303.83
 H       1.563026    -0.263143     2.902513      32.34
 C       0.749574     1.444557     1.171729      59.41
 H       0.975696     2.159612     0.299429      22.35
 C      -0.484105     2.000146     1.795447     102.29
 O      -0.422608     3.421495     2.079350     244.03
 H       0.134649     4.149338     1.508666      25.60
 H      -0.657352     1.437778     2.810336      25.50
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 H      -1.526118     1.842880     1.217951      25.37
 C      -1.911090    -2.162614    -1.236636      50.17
 H      -2.326245    -3.255597    -1.293525      24.91
 C      -1.487656    -0.135954    -2.470861      92.41
 H      -1.268338     0.159849    -3.495575      22.64
 C      -0.626326     0.405349    -1.465175      14.15
 O       0.319362     1.446998    -1.533561     174.43
 C      -0.154254     2.553912    -2.660552     105.83
 H       0.713772     3.380379    -2.519402      26.20
 H       0.099912     2.330899    -3.623446      28.88
 H      -1.042491     3.112188    -2.545002      29.49
 C      -0.468861    -0.390254    -0.222672      -0.49
 O       0.241819    -0.194862     0.921516      41.99
 C      -1.038207    -1.732430    -0.148875      44.47
 H      -0.891413    -2.258907     0.807107      21.82
 C      -2.112212    -1.478252    -2.358839      43.85
 C      -3.174571    -1.829710    -3.419284      86.47
 H      -3.198883    -1.304698    -4.367632      30.05
 O      -2.981662    -3.196279    -3.988788     159.73
 H      -1.920603    -3.279321    -3.788370      27.54
 C      -4.564120    -1.578237    -2.726330      91.38
 H      -4.811183    -2.165794    -1.901220      31.50
 O      -4.779633    -0.102721    -2.278119     147.49
 H      -3.784343     0.213483    -1.920917      27.07
 C      -5.600934    -2.056873    -3.757663     108.61
 O      -5.909392    -3.366390    -3.567238     214.55
 H      -5.087765    -3.909763    -3.398083      27.66
 H      -5.055953    -1.950007    -4.793594      26.81
 H      -6.615901    -1.446465    -3.606013      25.90
55
name = lig-ACN-frame_618
 C       3.470205     0.915752     0.108868      74.14
 H       2.747589     1.466593    -0.501604      22.58
 C       4.314227     0.165922     2.318855      47.89
 H       3.962051    -0.105433     3.311497      20.71
 C       5.601740    -0.012799     1.775763      17.85
 O       6.729263    -0.328141     2.519532     233.74
 C       6.540017    -0.761401     3.914845     116.19
 H       7.516454    -1.383903     4.274459      25.73
 H       5.645388    -1.359702     4.201010      27.98
 H       6.508667    -0.004098     4.651731      27.91
 C       5.744755     0.167451     0.411572      10.44
 O       6.969310    -0.143213    -0.224078     122.77
 H       7.750330    -0.623814     0.282763      22.85
 C       4.687590     0.650959    -0.403906      60.23
 H       5.113150     0.605102    -1.434157      22.93
 C       3.232394     0.678117     1.459709      22.34
 C       2.030011     1.260714     2.167398      83.62
 H       2.290195     2.265159     2.388804      26.32
 O       1.742717     0.467171     3.359946     277.05
 H       1.479897    -0.505817     3.527230      24.61
 C       0.745793     1.422872     1.152840      75.04
 H       1.100046     1.876686     0.128986      20.35
 C      -0.508373     2.050182     1.849861     104.50
 O      -0.424416     3.447004     2.126171     306.47
 H       0.283002     3.672092     1.645627      32.62
 H      -0.564369     1.450384     2.868369      24.79
 H      -1.349056     1.705545     1.031991      24.62
 C      -1.972478    -2.234904    -1.220045      28.69
 H      -2.546158    -3.232707    -1.124161      24.85
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 C      -1.344283    -0.196514    -2.515483      72.40
 H      -1.712817     0.548997    -3.297154      22.97
 C      -0.603111     0.357666    -1.401658      32.61
 O       0.265695     1.468512    -1.624303     211.99
 C      -0.116793     2.506333    -2.626261     117.55
 H       0.630112     3.308747    -2.422996      25.82
 H      -0.376833     2.101887    -3.583931      28.26
 H      -1.056810     2.681508    -2.201268      29.67
 C      -0.445033    -0.478043    -0.286039      10.77
 O       0.252871     0.049703     0.847541     132.77
 C      -1.136222    -1.798812    -0.229446      50.64
 H      -1.202570    -2.295520     0.655350      24.20
 C      -2.012535    -1.369365    -2.427787      43.67
 C      -3.142021    -1.783622    -3.273088      87.48
 H      -3.043042    -0.879814    -3.955700      29.82
 O      -3.102549    -3.125871    -3.947497     107.35
 H      -2.147795    -3.348816    -4.483607      27.02
 C      -4.565543    -1.561663    -2.729449     104.26
 H      -4.681510    -2.196331    -1.936816      32.37
 O      -4.767545    -0.215447    -2.322299     276.53
 H      -4.291587     0.047618    -1.607749      33.60
 C      -5.569946    -1.940535    -3.833056      93.61
 O      -5.858404    -3.417070    -3.526101     126.83
 H      -5.107512    -3.847413    -4.207364      25.44
 H      -5.323418    -1.703374    -4.973440      27.21
 H      -6.590528    -1.394088    -3.757553      28.25
55
name = lig-ACN-frame_619
 C       3.589032     0.835734     0.169763      59.42
 H       2.790341     0.913360    -0.483737      26.03
 C       4.282318     0.175434     2.351681      64.51
 H       4.211460     0.107356     3.373469      22.78
 C       5.551806    -0.004723     1.851192      25.38
 O       6.688967    -0.360668     2.525320     244.34
 C       6.499705    -0.732119     3.885335     123.73
 H       7.475978    -1.350311     4.073208      26.24
 H       5.609941    -1.379866     3.894123      29.64
 H       6.389006     0.204207     4.399524      29.27
 C       5.904946     0.233271     0.447678      24.05
 O       6.946387    -0.172909    -0.229823     120.39
 H       7.494673    -0.603561     0.446161      20.14
 C       4.861454     0.565383    -0.371029      51.03
 H       4.844664     0.658281    -1.389355      22.30
 C       3.256206     0.633474     1.564687      37.47
 C       1.983883     1.236849     2.174069      88.64
 H       2.168780     2.203040     2.538605      26.69
 O       1.745449     0.509474     3.474958     217.92
 H       1.642872    -0.410654     2.860036      24.47
 C       0.744700     1.355368     1.238090      89.46
 H       1.046523     2.137745     0.380622      22.45
 C      -0.475921     2.037848     1.885114      95.93
 O      -0.412868     3.467433     2.178209     276.05
 H       0.090207     4.113114     1.667625      28.66
 H      -0.927654     1.575419     2.881940      24.75
 H      -1.476565     2.008837     1.172359      24.06
 C      -1.899101    -2.232308    -1.255361      59.81
 H      -2.633212    -3.025504    -1.085878      25.17
 C      -1.260361    -0.167665    -2.525126      60.19
 H      -1.690537     0.611966    -3.284038      22.02
 C      -0.472615     0.235006    -1.536160      14.19
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 O       0.227977     1.419516    -1.678446     248.80
 C      -0.251471     2.428582    -2.522230     135.85
 H       0.410829     3.210010    -2.638717      29.16
 H      -0.102968     2.095590    -3.609756      25.90
 H      -1.107450     3.035088    -2.358823      29.30
 C      -0.431290    -0.488061    -0.274198      11.35
 O       0.278123     0.101074     0.784869     187.03
 C      -1.165176    -1.702136    -0.120583      64.58
 H      -0.916377    -2.233489     0.650684      27.39
 C      -2.004945    -1.441870    -2.341878      41.77
 C      -3.118569    -1.622207    -3.417020      85.67
 H      -3.167507    -1.016392    -4.415486      30.07
 O      -3.198816    -3.036409    -3.887177     200.27
 H      -2.492149    -3.021945    -4.492814      34.18
 C      -4.533096    -1.606574    -2.724766      91.89
 H      -4.742196    -2.267384    -1.976432      33.46
 O      -4.799250    -0.246304    -2.356690     226.12
 H      -4.627798    -0.121921    -1.412502      30.55
 C      -5.647333    -1.924524    -3.831158      86.56
 O      -5.787845    -3.428187    -3.592143     168.18
 H      -5.642570    -3.980939    -4.403622      28.18
 H      -5.217380    -1.770681    -4.911246      27.66
 H      -6.520638    -1.295386    -3.461526      28.82
55
name = lig-ACN-frame_620
 C       3.524712     0.737043     0.190028      63.30
 H       2.809702     0.964081    -0.515793      23.78
 C       4.307808     0.218319     2.484234      57.76
 H       4.125764     0.214119     3.506506      21.81
 C       5.625470     0.039648     1.820635      10.26
 O       6.704059    -0.424845     2.522131     241.02
 C       6.481121    -0.726586     3.892842     116.62
 H       7.381072    -1.192537     4.334869      26.77
 H       5.658430    -1.453165     4.044580      29.05
 H       6.296377     0.083910     4.631751      27.25
 C       5.885973     0.220318     0.476040      -5.65
 O       7.117965    -0.255227    -0.199057     187.16
 H       7.885641    -0.527140     0.293754      26.11
 C       4.848987     0.573501    -0.409603      46.37
 H       5.195260     0.580109    -1.344990      23.06
 C       3.274805     0.685475     1.566538      11.31
 C       1.922883     1.148713     2.224645      91.70
 H       2.177851     2.186515     2.367524      26.76
 O       1.695343     0.530067     3.478446     266.43
 H       1.596216    -0.503326     3.575841      24.87
 C       0.712804     1.439469     1.323645      62.52
 H       1.126783     2.110870     0.430399      22.77
 C      -0.549795     2.121820     1.906951      99.80
 O      -0.391786     3.501028     2.293616     225.31
 H      -0.062889     3.916516     1.320782      25.06
 H      -0.697111     1.488620     2.894235      24.38
 H      -1.275597     1.795980     0.958699      23.26
 C      -1.827759    -2.155369    -1.159052      36.89
 H      -2.190768    -3.157045    -1.145784      25.50
 C      -1.368156    -0.273666    -2.578318     120.70
 H      -1.225250     0.153034    -3.648049      22.68
 C      -0.329239     0.139336    -1.601666      26.51
 O       0.267370     1.388885    -1.591939     190.56
 C      -0.349497     2.475405    -2.610865      86.26
 H       0.305288     3.113024    -2.303148      29.46
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 H      -0.484130     2.131427    -3.741490      22.89
 H      -1.354509     2.604364    -2.223172      27.29
 C      -0.400039    -0.363291    -0.317488      18.46
 O       0.352754    -0.077639     0.813077      91.06
 C      -1.074887    -1.613825    -0.030169      26.49
 H      -1.014507    -2.061212     0.859132      22.43
 C      -2.086035    -1.383846    -2.482472      31.45
 C      -3.179455    -1.648544    -3.464331      95.47
 H      -2.978573    -0.776342    -4.256575      30.00
 O      -3.193501    -2.969894    -3.901552     239.61
 H      -2.422993    -3.273055    -4.322925      33.31
 C      -4.553293    -1.543475    -2.844323     103.75
 H      -4.360301    -2.242577    -2.087902      31.29
 O      -4.876457    -0.186505    -2.333728     162.19
 H      -4.535678    -0.017978    -1.244945      24.85
 C      -5.639769    -2.065792    -3.720594     113.03
 O      -5.819997    -3.415370    -3.686315     281.99
 H      -6.079442    -3.597413    -4.537266      33.57
 H      -5.480224    -1.621079    -4.804712      29.30
 H      -6.655805    -1.636048    -3.551054      29.72
55
name = lig-ACN-frame_621
 C       3.471081     0.706518     0.122146      44.13
 H       2.644925     1.128883    -0.421499      20.52
 C       4.404716     0.350293     2.389551      47.19
 H       4.179554     0.004633     3.421152      18.38
 C       5.648048     0.055129     1.897802       4.84
 O       6.769638    -0.486828     2.574684     250.26
 C       6.498539    -0.787213     4.017419     122.34
 H       7.436815    -1.098128     4.320982      26.82
 H       5.732194    -1.559648     4.087797      30.27
 H       6.122352     0.230955     4.373355      28.47
 C       5.946575     0.089883     0.391728      -0.01
 O       7.174056    -0.256750    -0.140916     163.51
 H       7.692945    -0.501440     0.717315      20.81
 C       4.818372     0.545318    -0.379634      56.78
 H       4.812941     0.617426    -1.401835      24.86
 C       3.287272     0.660628     1.563336      27.76
 C       1.966525     1.164598     2.255802      93.43
 H       2.195112     2.096736     2.738511      24.49
 O       1.592635     0.543787     3.554763     289.21
 H       1.538568    -0.363603     3.467406      30.22
 C       0.725822     1.338302     1.305868      84.03
 H       0.995760     1.794047     0.303665      20.54
 C      -0.563900     2.074969     1.936030      89.09
 O      -0.415870     3.458395     2.353308     221.43
 H       0.151465     4.226487     1.695751      22.37
 H      -1.042643     1.581323     2.907768      23.62
 H      -1.578937     2.185562     1.257412      22.86
 C      -1.863438    -2.089153    -1.162069      66.69
 H      -2.084556    -3.077074    -0.914985      25.03
 C      -1.210689    -0.271981    -2.666560      84.69
 H      -1.231664     0.238264    -3.659194      19.93
 C      -0.386726     0.177349    -1.627840       0.12
 O       0.317135     1.465183    -1.696139     217.51
 C      -0.397470     2.434610    -2.513813     103.05
 H      -0.247650     3.378631    -2.574968      28.71
 H      -0.214836     2.163913    -3.698161      22.85
 H      -1.459866     2.350604    -2.260167      26.71
 C      -0.348951    -0.418165    -0.235137      18.98
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 O       0.473341    -0.073855     0.901662     140.52
 C      -1.067922    -1.560229    -0.170950      50.71
 H      -1.073214    -2.035601     0.798251      21.65
 C      -2.090417    -1.437468    -2.326490      43.37
 C      -3.160084    -1.638424    -3.466812      69.97
 H      -3.076488    -0.913255    -4.413492      27.38
 O      -3.149490    -3.042236    -4.035517     127.62
 H      -2.083755    -3.233253    -3.738447      26.17
 C      -4.574999    -1.456360    -2.761180      89.24
 H      -4.719674    -2.046556    -1.864339      29.77
 O      -4.960675    -0.150080    -2.325893     217.38
 H      -4.164306     0.069098    -1.622951      26.22
 C      -5.766556    -1.972396    -3.717355      82.82
 O      -5.880820    -3.547444    -3.786929     149.65
 H      -6.475663    -3.778393    -4.660545      26.25
 H      -5.591519    -1.682863    -4.810638      27.25
 H      -6.571154    -1.494820    -3.151340      27.96
55
name = lig-ACN-frame_622
 C       3.509691     0.760128     0.192947      49.25
 H       2.803900     0.907000    -0.682542      23.97
 C       4.458615     0.378550     2.291092      43.96
 H       4.287872     0.351463     3.439295      19.04
 C       5.776888    -0.016727     1.783210      11.64
 O       6.775310    -0.536231     2.648948     253.83
 C       6.561391    -0.803782     4.045608     124.02
 H       7.411290    -1.007813     4.508314      29.13
 H       5.867187    -1.635783     4.160054      29.29
 H       6.190212     0.073848     4.756294      26.66
 C       5.856715     0.031106     0.436044      16.89
 O       7.121514    -0.211537    -0.049931     113.79
 H       7.805162    -0.760973     0.521803      24.41
 C       4.769856     0.428454    -0.391598      55.67
 H       5.054107     0.593962    -1.454026      20.95
 C       3.261811     0.664905     1.549269      28.85
 C       2.003376     1.257914     2.317535      79.25
 H       2.207111     2.330369     2.360580      24.39
 O       1.510908     0.518385     3.596671     230.99
 H       1.212601    -0.406972     3.194350      24.88
 C       0.735957     1.261771     1.309951      88.93
 H       0.984412     1.990616     0.540952      23.95
 C      -0.573244     2.034804     1.955214      95.11
 O      -0.432224     3.403621     2.443470     249.27
 H       0.395690     3.813118     1.924585      26.16
 H      -0.836035     1.341276     2.855989      24.20
 H      -1.207492     1.841791     0.918335      23.07
 C      -1.971663    -2.162096    -1.177873      18.34
 H      -2.865687    -2.739759    -1.067780      23.85
 C      -1.076092    -0.327898    -2.587052      38.39
 H      -1.359189     0.256370    -3.413010      22.39
 C      -0.359174     0.391419    -1.499132      20.55
 O       0.364402     1.496156    -1.803801     239.78
 C      -0.509413     2.418601    -2.527585      94.45
 H      -0.120786     3.203273    -2.057977      27.24
 H      -0.187617     2.249573    -3.680040      24.20
 H      -1.604912     2.204538    -2.472361      27.04
 C      -0.217731    -0.356721    -0.277267      11.81
 O       0.486762    -0.079173     0.901949     185.20
 C      -1.056707    -1.600264    -0.126870      20.54
 H      -0.839337    -2.299495     0.778418      22.28
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 C      -2.012286    -1.332989    -2.436330      22.49
 C      -3.182511    -1.714524    -3.355027      79.60
 H      -3.088021    -0.913426    -4.211014      27.65
 O      -3.017410    -3.065038    -4.117754      89.62
 H      -2.311480    -3.680578    -3.539669      28.49
 C      -4.673698    -1.570640    -2.751855      83.75
 H      -4.631581    -2.274905    -1.874738      28.08
 O      -4.985651    -0.090707    -2.334708     199.42
 H      -4.343873     0.465957    -2.123456      32.71
 C      -5.868808    -1.945328    -3.694394      96.20
 O      -5.942544    -3.546255    -3.843506     181.29
 H      -6.578742    -3.640075    -4.672241      26.71
 H      -5.835536    -1.398175    -4.664439      28.43
 H      -6.866042    -1.755983    -3.369072      28.56
55
name = lig-ACN-frame_623
 C       3.539454     0.761294     0.126904      41.91
 H       2.571497     1.032282    -0.462347      21.15
 C       4.462573     0.329356     2.355930      45.55
 H       4.477115     0.482648     3.460683      19.17
 C       5.645271    -0.116226     1.913725      25.97
 O       6.784322    -0.524726     2.641315     251.28
 C       6.610686    -0.835630     4.094416     136.78
 H       7.542625    -1.066642     4.268610      28.41
 H       5.961295    -1.697013     4.232334      30.07
 H       6.174633     0.119783     4.617145      28.38
 C       5.887691    -0.030131     0.469243      18.63
 O       7.102304    -0.184814    -0.100072     142.11
 H       7.581000    -0.756435     0.521997      23.79
 C       4.799673     0.326477    -0.368910      51.06
 H       5.017681     0.324015    -1.530008      20.65
 C       3.339321     0.740197     1.596989      18.71
 C       1.930077     1.236279     2.311414      93.97
 H       2.111989     2.111506     2.949575      22.48
 O       1.528109     0.564674     3.505547     236.39
 H       1.056023    -0.464446     3.477678      22.02
 C       0.815499     1.417472     1.384571      78.86
 H       1.142590     1.792520     0.478538      22.92
 C      -0.504195     1.877572     1.933949     107.09
 O      -0.419151     3.247959     2.500821     278.83
 H      -0.006216     3.828476     1.939810      32.01
 H      -1.004792     1.262579     2.755526      24.52
 H      -1.417004     2.034592     1.162656      23.75
 C      -1.970343    -1.964928    -1.130043      66.16
 H      -2.662038    -2.733463    -0.730897      25.79
 C      -1.087393    -0.229563    -2.494130      86.34
 H      -0.814696     0.199713    -3.391074      23.23
 C      -0.300643     0.316896    -1.469780       2.56
 O       0.385638     1.490962    -1.844471     196.74
 C      -0.537258     2.548629    -2.602723      68.89
 H      -0.585387     3.498361    -2.207144      27.07
 H      -0.381634     2.906703    -3.724603      23.01
 H      -1.563543     2.137891    -2.353719      26.39
 C      -0.264170    -0.495353    -0.268281      27.49
 O       0.473380    -0.106181     0.865199     105.42
 C      -1.040771    -1.669085    -0.205797      30.93
 H      -0.907101    -2.121390     0.922986      18.43
 C      -1.992007    -1.416698    -2.371070      54.84
 C      -3.200726    -1.781196    -3.388067      67.10
 H      -3.290697    -1.031116    -4.250374      29.48
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 O      -2.868633    -2.996318    -4.109786     224.18
 H      -2.820516    -3.668812    -3.516382      33.75
 C      -4.731640    -1.624957    -2.725402      81.20
 H      -4.923889    -2.192310    -1.720676      28.72
 O      -5.025172    -0.164236    -2.417203     226.57
 H      -4.083263     0.034503    -2.226459      31.37
 C      -5.945898    -2.053201    -3.664540     113.37
 O      -5.996263    -3.383633    -3.907227     284.91
 H      -6.318640    -3.550597    -4.720317      33.89
 H      -5.755702    -1.556077    -4.597583      29.57
 H      -6.708157    -1.596729    -3.074798      28.65
55
name = lig-ACN-frame_624
 C       3.557472     0.703317     0.208200      57.26
 H       2.860799     1.080483    -0.629861      21.77
 C       4.337849     0.307566     2.543377      43.02
 H       4.001628     0.028913     3.507583      18.79
 C       5.621376    -0.213854     1.910762      13.27
 O       6.757811    -0.505677     2.640998     242.29
 C       6.693051    -0.854242     4.039913     129.27
 H       7.600824    -1.069842     4.475003      27.31
 H       5.959252    -1.637189     4.189557      30.66
 H       6.396917     0.054227     4.675206      29.66
 C       5.844212    -0.077406     0.506726      13.22
 O       7.119952    -0.230561    -0.147285     195.73
 H       7.870677    -0.480791     0.382082      26.93
 C       4.783961     0.282290    -0.325630      45.32
 H       4.908629     0.122730    -1.517836      21.69
 C       3.354249     0.826696     1.594008      22.85
 C       2.043916     1.218207     2.325084      84.74
 H       2.248799     2.309481     2.396243      24.11
 O       1.547494     0.523535     3.503097     270.09
 H       1.448415    -0.436241     3.130333      25.35
 C       0.795052     1.394892     1.232393      73.63
 H       0.968720     2.176756     0.577122      24.02
 C      -0.524513     1.849012     1.911781     104.08
 O      -0.387793     3.081509     2.583265     281.43
 H      -0.486270     3.739486     1.875315      30.11
 H      -0.681849     1.084096     2.673596      25.31
 H      -1.231477     1.700821     0.947933      23.44
 C      -2.021070    -1.938683    -1.038285      40.94
 H      -2.534807    -2.954716    -0.962206      24.58
 C      -1.210006    -0.263723    -2.586175      56.00
 H      -1.121357     0.026677    -3.588230      22.89
 C      -0.289348     0.181418    -1.567536      -9.03
 O       0.378346     1.562115    -1.875609     167.56
 C      -0.583034     2.653501    -2.541193      77.66
 H      -0.424970     3.542084    -1.982350      26.24
 H       0.004496     2.457050    -3.515747      21.16
 H      -1.611304     2.245344    -2.826765      24.38
 C      -0.213627    -0.421228    -0.195121      17.81
 O       0.505582    -0.122654     0.895928     144.51
 C      -0.946648    -1.640574    -0.100782      31.84
 H      -1.236273    -2.316520     0.901305      19.55
 C      -2.084358    -1.311206    -2.353857      23.40
 C      -3.179707    -1.727571    -3.411267      71.41
 H      -3.189480    -0.910210    -4.163105      29.43
 O      -2.793970    -2.950937    -4.071620     213.35
 H      -3.029380    -3.722213    -3.494228      30.67
 C      -4.742936    -1.677087    -2.721523      93.31
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 H      -4.740497    -2.301543    -1.703740      27.60
 O      -4.963823    -0.334805    -2.534498     191.87
 H      -4.342656     0.245344    -1.766209      24.09
 C      -5.909630    -1.924399    -3.632004     109.22
 O      -6.076352    -3.396968    -3.951296     264.31
 H      -5.984471    -3.368706    -4.981912      27.65
 H      -5.899080    -1.265388    -4.452197      30.33
 H      -6.849592    -1.700598    -3.213080      29.80
55
name = lig-ACN-frame_625
 C       3.571287     0.711544     0.281410      49.34
 H       2.723619     0.992260    -0.361451      24.39
 C       4.323015     0.146837     2.497573      63.03
 H       4.074141    -0.084013     3.478836      22.58
 C       5.561055    -0.161376     1.970257      13.17
 O       6.776641    -0.519789     2.632654     255.85
 C       6.721306    -0.834398     4.028847     126.53
 H       7.721959    -1.237478     4.092735      26.22
 H       6.029531    -1.667564     4.217437      29.74
 H       6.400316     0.014276     4.644269      29.03
 C       5.865807    -0.119248     0.547348       8.43
 O       7.066051    -0.304544    -0.137720     141.77
 H       7.727632    -0.410829     0.657407      23.52
 C       4.766820     0.217693    -0.271130      36.58
 H       4.991515     0.305874    -1.447375      19.96
 C       3.345361     0.741130     1.693062      34.61
 C       2.025201     1.384189     2.130192      76.89
 H       2.077834     2.302869     2.770420      23.94
 O       1.633588     0.493127     3.457227     218.09
 H       1.557576    -0.383111     3.374924      29.24
 C       0.850692     1.276928     1.208220     109.15
 H       1.093333     1.564506     0.246222      24.05
 C      -0.495650     1.700618     1.892269     102.76
 O      -0.409457     2.972357     2.656171     181.14
 H      -0.407927     3.878797     1.978997      25.76
 H      -0.757118     0.973210     2.612067      26.79
 H      -1.415992     1.887646     1.266347      25.02
 C      -1.954854    -2.007604    -1.043263      55.72
 H      -2.689786    -2.866343    -0.812747      24.86
 C      -1.263608    -0.320936    -2.676096      27.99
 H      -1.497177     0.396385    -3.444823      23.18
 C      -0.272960     0.286553    -1.623682       0.22
 O       0.247452     1.508209    -1.828179     222.62
 C      -0.450954     2.567284    -2.531392      97.57
 H      -0.371167     3.432373    -1.780859      25.85
 H      -0.060947     3.098972    -3.480060      24.50
 H      -1.576744     2.485202    -2.539656      26.93
 C      -0.215600    -0.364886    -0.325817      -4.82
 O       0.610003    -0.020309     0.892614     151.41
 C      -1.086803    -1.600133    -0.040779      29.99
 H      -0.495423    -2.107833     0.908614      20.30
 C      -2.246510    -1.234802    -2.241243      35.99
 C      -3.209810    -1.674179    -3.339196      98.06
 H      -3.189877    -0.977595    -4.150600      30.72
 O      -2.769130    -2.934531    -4.036608     116.13
 H      -3.113161    -3.860997    -3.488828      28.21
 C      -4.567695    -1.738215    -2.801601      82.19
 H      -4.632004    -2.534270    -1.893172      28.06
 O      -4.896507    -0.288390    -2.530040     132.62
 H      -4.696831    -0.129152    -1.468375      25.95
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 C      -5.947558    -1.936742    -3.657043      95.97
 O      -6.117337    -3.379475    -4.029463     225.04
 H      -5.853643    -3.540199    -5.073325      26.10
 H      -5.814656    -1.325183    -4.479683      30.05
 H      -6.695122    -1.633322    -2.985106      29.11
55
name = lig-ACN-frame_626
 C       3.566403     0.717852     0.294679      60.71
 H       2.870494     1.099297    -0.382821      23.18
 C       4.347230     0.002138     2.526939      69.49
 H       4.411992     0.244296     3.557465      22.39
 C       5.662348    -0.152219     1.941842       9.39
 O       6.761382    -0.521804     2.610668     273.74
 C       6.746845    -0.867686     4.032908     108.53
 H       7.826306    -1.123716     4.427711      24.29
 H       5.995073    -1.642819     4.221545      29.06
 H       6.609746    -0.005508     4.628921      28.52
 C       5.792330    -0.109229     0.537018      16.79
 O       7.005147    -0.392451    -0.002186     189.63
 H       7.750472    -0.777956     0.587705      22.42
 C       4.741291     0.229027    -0.251909      71.15
 H       4.904354     0.324234    -1.371452      21.98
 C       3.290590     0.678676     1.666353      11.16
 C       1.998336     1.273430     2.240630      89.23
 H       2.084169     2.425652     2.440845      24.25
 O       1.732065     0.600852     3.389653     282.64
 H       1.411659    -0.288101     3.069269      25.88
 C       0.837038     1.324558     1.136957      79.47
 H       0.958006     2.203902     0.543277      23.32
 C      -0.464001     1.706211     1.921154     112.04
 O      -0.447673     2.883824     2.730321     249.40
 H       0.084379     3.569551     2.116986      28.06
 H      -0.686381     0.898381     2.553634      26.42
 H      -1.113561     1.651010     1.033793      25.03
 C      -1.979317    -2.025697    -1.012304      48.33
 H      -2.534720    -2.928637    -0.595884      23.73
 C      -1.295754    -0.185388    -2.519785      30.23
 H      -1.489912     0.263207    -3.546624      22.08
 C      -0.476015     0.249639    -1.657785      25.50
 O       0.239760     1.475320    -1.812494     239.60
 C      -0.390540     2.604502    -2.422407      93.70
 H      -0.178887     3.525320    -1.722282      23.53
 H       0.047417     2.713115    -3.505201      23.87
 H      -1.439678     2.273585    -2.557506      26.14
 C      -0.246333    -0.390225    -0.385284      27.79
 O       0.637994    -0.176369     0.690963     163.74
 C      -1.029103    -1.423527    -0.133802      59.12
 H      -0.970110    -2.136076     0.817213      22.05
 C      -2.192246    -1.286258    -2.173955      50.90
 C      -3.154188    -1.715666    -3.361089      84.01
 H      -3.117237    -0.943990    -4.084397      32.01
 O      -2.784316    -2.930619    -3.983080     214.46
 H      -3.062073    -3.639407    -3.347597      32.03
 C      -4.673143    -1.694658    -2.891286      82.35
 H      -4.737949    -2.254463    -1.818527      27.05
 O      -4.827765    -0.238038    -2.393252     190.04
 H      -4.608674    -0.181999    -1.550296      30.21
 C      -5.822949    -2.070534    -3.725785     125.85
 O      -6.156965    -3.349706    -4.076572     329.68
 H      -6.061785    -3.405392    -4.985593      31.81
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 H      -6.027002    -1.405920    -4.499748      30.07
 H      -6.632931    -1.780975    -3.090958      29.35
55
name = lig-ACN-frame_627
 C       3.492467     0.732571     0.242697      33.51
 H       2.813158     1.208295    -0.363949      22.13
 C       4.348584     0.129294     2.517423      68.34
 H       4.075360    -0.026803     3.601176      20.43
 C       5.591891    -0.211825     1.953489      10.52
 O       6.856679    -0.558467     2.645701     244.42
 C       6.742948    -0.832791     4.049664     124.61
 H       7.826361    -1.338628     4.266325      24.66
 H       5.989372    -1.636170     4.254789      28.13
 H       6.394922    -0.042730     4.604789      29.72
 C       5.792781    -0.144342     0.565618       5.95
 O       7.033868    -0.503876     0.061218     155.36
 H       7.405029    -1.011301     0.775183      22.90
 C       4.740051     0.304111    -0.333878      29.68
 H       4.886061     0.188547    -1.381311      23.04
 C       3.371172     0.562724     1.667282      41.12
 C       2.095348     1.189449     2.147619      80.83
 H       2.472943     2.275827     2.417079      23.63
 O       1.715728     0.679491     3.477269     216.30
 H       1.199423    -0.331935     3.467277      22.67
 C       0.837355     1.343264     1.232675      76.82
 H       1.130844     1.854391     0.312891      22.03
 C      -0.513038     1.606547     1.896858     116.97
 O      -0.442659     2.837629     2.750298     291.09
 H       0.137977     3.435946     2.506121      35.36
 H      -0.703066     0.831158     2.601921      26.13
 H      -1.319522     1.853503     1.283030      27.18
 C      -2.051976    -1.962117    -0.999801      67.58
 H      -2.589205    -2.916574    -0.864418      25.09
 C      -1.579154    -0.181468    -2.493661      92.15
 H      -1.389890     0.237981    -3.568567      22.38
 C      -0.460825     0.417880    -1.505007       7.04
 O       0.345327     1.436865    -1.747394     226.02
 C      -0.393149     2.605288    -2.403955      98.77
 H      -0.034349     3.660224    -1.871843      24.85
 H       0.106477     2.687508    -3.379988      24.84
 H      -1.456433     2.707906    -2.520572      28.38
 C      -0.258884    -0.403156    -0.382441      23.14
 O       0.738759    -0.149563     0.462852     132.10
 C      -1.061867    -1.560616    -0.110163      37.71
 H      -1.047873    -1.677725     0.988966      21.14
 C      -2.140836    -1.392752    -2.330111      42.89
 C      -3.135527    -1.695006    -3.337364      95.84
 H      -2.984631    -1.015517    -4.150995      31.39
 O      -2.817251    -2.999147    -3.960456     258.34
 H      -2.723070    -3.617609    -3.314068      34.92
 C      -4.621591    -1.561184    -2.753745      84.09
 H      -4.753125    -2.490325    -1.976171      28.07
 O      -4.829308    -0.248655    -2.313362     257.50
 H      -4.111191    -0.084779    -1.645519      28.85
 C      -5.893585    -1.919278    -3.786031      89.16
 O      -6.138459    -3.480929    -4.125438     228.66
 H      -6.517729    -3.530802    -5.012345      29.39
 H      -5.688882    -1.386962    -4.686059      29.33
 H      -6.743994    -1.626449    -3.217240      29.07
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name = lig-ACN-frame_628
 C       3.587327     0.704373     0.162867      71.94
 H       2.710586     0.943262    -0.417666      22.56
 C       4.391022     0.201827     2.534298      50.56
 H       3.994289    -0.101286     3.597546      19.93
 C       5.638670    -0.260288     2.018443       5.61
 O       6.823042    -0.565086     2.628263     227.53
 C       6.689061    -0.851366     4.078940     113.14
 H       7.788497    -1.093290     4.532621      24.28
 H       5.955222    -1.701214     4.169099      26.54
 H       6.502542     0.014555     4.596957      28.60
 C       5.790846    -0.177383     0.527537      -1.46
 O       7.030078    -0.630198     0.088446     139.82
 H       7.682176    -0.938599     0.756332      21.67
 C       4.809733     0.328719    -0.354293      79.07
 H       5.020587     0.396380    -1.338943      23.49
 C       3.330061     0.527590     1.530589      14.98
 C       2.104825     1.169871     2.156775      64.87
 H       2.314668     2.259220     2.520289      23.38
 O       1.653320     0.743906     3.639321     144.10
 H       1.369311    -0.314626     3.612140      23.97
 C       0.897838     1.177773     1.189371      86.39
 H       0.909650     2.179702     0.543487      22.13
 C      -0.526144     1.595048     1.938013     104.23
 O      -0.444606     2.772044     2.792627     253.81
 H       0.098450     3.360033     2.147800      29.00
 H      -0.916225     0.730301     2.520699      26.09
 H      -1.138979     1.579813     1.112960      27.23
 C      -2.099781    -2.041238    -1.062570      49.70
 H      -2.801326    -2.791332    -0.751685      22.63
 C      -1.478907     0.006683    -2.435570      77.51
 H      -1.875303     0.630042    -3.316252      21.86
 C      -0.649218     0.350577    -1.531077      17.37
 O       0.359416     1.510716    -1.723421     181.22
 C      -0.272402     2.651648    -2.445056      96.60
 H       0.120022     3.549303    -1.660308      22.17
 H      -0.253943     2.785523    -3.492329      26.08
 H      -1.226292     2.378456    -2.095342      27.22
 C      -0.333709    -0.428445    -0.369834      11.34
 O       0.920831    -0.031320     0.422963     151.50
 C      -1.138154    -1.587789    -0.019557      49.95
 H      -0.959342    -2.227700     0.793979      21.85
 C      -2.129468    -1.360433    -2.308460      42.35
 C      -3.220490    -1.796668    -3.416758      66.03
 H      -3.263458    -1.077327    -4.253597      28.21
 O      -2.887647    -3.090644    -3.969176     167.73
 H      -2.350939    -3.644170    -3.190405      28.73
 C      -4.615305    -1.636062    -2.756513      76.28
 H      -4.679780    -2.267339    -1.739805      26.79
 O      -4.861869    -0.258441    -2.205079     146.59
 H      -3.948694     0.349000    -1.924893      23.44
 C      -5.900473    -1.835394    -3.811224      83.86
 O      -6.046233    -3.462477    -4.093094     160.10
 H      -6.701271    -3.402618    -4.957946      26.86
 H      -5.677907    -1.542329    -4.848506      27.79
 H      -6.786920    -1.257970    -3.578890      28.89
55
name = lig-ACN-frame_629
 C       3.632787     0.635229     0.116136       0.66
 H       3.049747     0.924405    -0.809586      21.59
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 C       4.371847     0.144998     2.432789      63.04
 H       4.381596     0.532296     3.557502      18.61
 C       5.640037    -0.196512     1.914141      25.93
 O       6.761742    -0.595726     2.683969     274.49
 C       6.644639    -0.833835     4.089906     107.43
 H       7.687054    -1.154008     4.432555      24.91
 H       5.909735    -1.681895     4.353476      27.62
 H       6.137312    -0.056590     4.602161      27.68
 C       5.892984    -0.230183     0.598159      22.80
 O       7.012898    -0.744924     0.029057     149.58
 H       7.741248    -0.716442     0.780444      19.22
 C       4.986376     0.303242    -0.347447      37.95
 H       5.284726     0.458307    -1.314678      24.27
 C       3.350330     0.575094     1.635711      -0.20
 C       1.986736     1.152465     2.329051      82.23
 H       2.235162     2.269417     2.275364      25.54
 O       1.650003     0.790278     3.651974     281.61
 H       1.408752    -0.105538     3.600092      30.33
 C       0.835373     1.176746     1.252035      87.10
 H       1.245012     2.010201     0.481449      22.90
 C      -0.484116     1.454847     1.929912     111.18
 O      -0.421639     2.690825     2.734801     184.15
 H      -0.330281     3.671620     2.164725      26.63
 H      -0.867172     0.728529     2.726073      24.93
 H      -1.152340     1.807989     1.231368      26.26
 C      -2.009968    -2.011203    -1.088700      67.47
 H      -2.574403    -2.905432    -1.022338      25.13
 C      -1.569570    -0.048169    -2.517777      30.46
 H      -1.794563     0.742922    -3.198755      22.00
 C      -0.476111     0.409616    -1.435731       0.81
 O       0.287854     1.476158    -1.721745     229.65
 C      -0.281656     2.654701    -2.325065     118.06
 H       0.250560     3.732579    -2.107691      24.64
 H      -0.023893     2.486690    -3.306833      27.05
 H      -1.296682     3.027859    -2.290202      28.51
 C      -0.303094    -0.409815    -0.243324      20.97
 O       0.897620    -0.030408     0.365197     192.58
 C      -1.166314    -1.581630    -0.079750      37.14
 H      -0.868501    -2.242507     0.584759      24.07
 C      -2.270767    -1.201314    -2.288837      35.18
 C      -3.231467    -1.819433    -3.417168      60.35
 H      -3.124564    -1.135951    -4.325721      28.96
 O      -2.981272    -3.191275    -3.942583     187.06
 H      -2.052288    -3.517245    -3.467529      27.44
 C      -4.771986    -1.664274    -2.795433      72.63
 H      -4.968127    -2.581362    -2.033759      26.80
 O      -4.926082    -0.301007    -2.181557     179.03
 H      -3.896525     0.018578    -1.915013      22.52
 C      -5.742201    -1.940287    -3.854927     112.18
 O      -5.984823    -3.253487    -3.964742     248.98
 H      -6.304695    -3.448432    -4.990297      26.67
 H      -5.334951    -1.299347    -4.668081      28.46
 H      -6.698946    -1.581758    -3.439652      27.00
55
name = lig-ACN-frame_630
 C       3.727955     0.575340     0.220789      56.55
 H       2.837690     1.045594    -0.342867      21.79
 C       4.401829     0.205116     2.425663      57.15
 H       4.319125     0.371994     3.596580      19.79
 C       5.676535    -0.203011     1.963587      13.87
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 O       6.707845    -0.621771     2.727501     234.79
 C       6.516943    -0.832059     4.145410     120.81
 H       7.532616    -0.902491     4.502629      26.43
 H       5.974250    -1.830943     4.204188      25.93
 H       6.223716     0.051458     4.719269      26.16
 C       5.995171    -0.261076     0.507577       6.58
 O       7.108972    -0.847638    -0.031550     161.53
 H       7.844751    -1.143467     0.606537      21.89
 C       4.989762     0.298959    -0.272090      70.01
 H       5.184869     0.216652    -1.333386      25.02
 C       3.312529     0.645402     1.535138      25.18
 C       2.006109     1.217427     2.274633      93.93
 H       2.177321     2.264704     2.630609      25.15
 O       1.676838     0.783370     3.646830     248.47
 H       1.272876    -0.037721     3.703280      30.83
 C       0.854792     1.185831     1.331346      83.20
 H       0.956526     2.075706     0.491835      22.04
 C      -0.551888     1.441017     1.890048     111.08
 O      -0.371286     2.649851     2.712376     251.38
 H      -0.635922     3.356486     1.993323      28.19
 H      -0.710902     0.463391     2.509339      25.47
 H      -1.329547     1.217282     1.177621      26.90
 C      -1.991008    -1.934767    -1.184101      43.10
 H      -2.138027    -2.980331    -1.124888      24.13
 C      -1.500126    -0.000192    -2.384716      99.68
 H      -1.423699     0.281627    -3.355951      21.72
 C      -0.610916     0.312990    -1.519602      25.44
 O       0.236653     1.484330    -1.624997     206.70
 C      -0.303232     2.692520    -2.346897      92.53
 H       0.363510     3.336341    -1.612514      23.05
 H      -0.085382     2.790295    -3.372513      26.55
 H      -1.379874     2.655772    -2.132473      27.27
 C      -0.314111    -0.339851    -0.350918      31.54
 O       0.805607    -0.131692     0.461177     148.78
 C      -0.984813    -1.540947    -0.143827      31.58
 H      -0.978617    -1.997225     0.718010      21.28
 C      -2.366245    -1.215998    -2.294531      46.89
 C      -3.297989    -1.755633    -3.297729      63.32
 H      -3.222769    -1.135637    -4.283123      25.29
 O      -3.038698    -3.233462    -3.839872     193.58
 H      -2.135356    -3.279519    -3.939115      31.92
 C      -4.687223    -1.675105    -2.770955      93.43
 H      -4.835291    -2.512658    -1.925401      27.27
 O      -4.998526    -0.445885    -2.232911     272.63
 H      -4.425139    -0.280397    -1.481957      29.91
 C      -5.737677    -1.754304    -3.888619      95.43
 O      -5.939837    -3.259000    -3.927952     297.02
 H      -5.908142    -3.530704    -4.790479      34.12
 H      -5.519828    -1.532916    -4.983579      27.40
 H      -6.591619    -1.081402    -3.676890      28.65
55
name = lig-ACN-frame_631
 C       3.648057     0.688299     0.233195      19.90
 H       3.016008     0.828334    -0.727819      21.52
 C       4.460881     0.311326     2.480357      83.28
 H       4.059626    -0.095961     3.447257      21.82
 C       5.679620    -0.234324     1.937684       7.86
 O       6.717835    -0.642346     2.794525     234.03
 C       6.464514    -0.840809     4.224414     118.82
 H       7.350742    -1.005446     4.678616      27.72
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 H       5.765880    -1.678049     4.447873      27.38
 H       5.747043    -0.039342     4.572642      24.12
 C       6.019310    -0.283163     0.554930       9.14
 O       7.186772    -0.915514    -0.083998     132.95
 H       7.713088    -1.357092     0.572995      23.49
 C       4.961675     0.210971    -0.297979       8.87
 H       4.920993     0.211274    -1.441495      20.03
 C       3.421058     0.647099     1.684168      -1.31
 C       2.109797     1.264728     2.179073      52.32
 H       2.317322     2.319820     2.177228      25.98
 O       1.736639     0.732496     3.641317     177.23
 H       1.271653    -0.160997     3.278361      25.78
 C       0.775467     1.164809     1.179199      85.28
 H       1.009131     2.104546     0.431906      22.68
 C      -0.529029     1.323950     1.956518     107.97
 O      -0.442941     2.616606     2.646817     294.57
 H      -0.455989     3.336986     2.159417      35.75
 H      -0.785306     0.708526     2.912615      23.77
 H      -1.306543     1.569473     1.191284      24.43
 C      -1.896534    -2.042427    -1.085169      68.18
 H      -2.531384    -2.918552    -0.962222      25.66
 C      -1.625692    -0.042972    -2.581359      70.15
 H      -1.588598     0.508281    -3.424651      20.44
 C      -0.571469     0.453655    -1.523404      32.52
 O       0.208500     1.499085    -1.607467     233.48
 C      -0.309205     2.685788    -2.250631     122.17
 H      -0.098008     3.744961    -1.827311      25.52
 H      -0.081961     2.703462    -3.322547      26.82
 H      -1.424093     2.718766    -2.228282      29.83
 C      -0.260843    -0.382430    -0.361855      23.76
 O       0.728151    -0.166229     0.656107     183.92
 C      -0.987223    -1.586966    -0.255092      45.16
 H      -0.650814    -2.132763     0.582509      23.83
 C      -2.214723    -1.229617    -2.246229      25.09
 C      -3.248656    -1.753049    -3.341463      65.94
 H      -3.258289    -0.910664    -4.177961      28.56
 O      -3.075644    -3.147469    -3.663063     236.62
 H      -2.315974    -3.147634    -4.250850      31.06
 C      -4.710478    -1.706377    -2.788983      76.76
 H      -4.869010    -2.665147    -2.125780      25.96
 O      -5.060818    -0.420292    -2.173385     208.96
 H      -4.920647    -0.329108    -1.271494      28.15
 C      -5.769758    -1.749104    -3.973300      79.02
 O      -5.968541    -3.288024    -3.902624     263.73
 H      -5.998721    -3.530470    -4.868648      30.59
 H      -5.138095    -1.376581    -4.877237      27.72
 H      -6.728547    -1.213842    -3.739562      28.52
55
name = lig-ACN-frame_632
 C       3.739783     0.721085     0.205709      84.81
 H       2.770775     0.989650    -0.278322      23.95
 C       4.529684     0.229369     2.538897      55.90
 H       4.472852     0.249503     3.606876      21.71
 C       5.775914    -0.249527     1.984738       6.00
 O       6.759770    -0.698202     2.864643     198.85
 C       6.337480    -0.827962     4.268502     123.05
 H       7.204318    -0.881254     4.763720      28.07
 H       5.799371    -1.737003     4.246573      26.89
 H       5.974845     0.155924     4.756227      23.72
 C       5.959977    -0.321779     0.525888      12.58
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 O       7.067327    -0.886166    -0.051782     120.22
 H       7.807529    -1.049024     0.577625      25.54
 C       4.877191     0.119206    -0.274555      43.62
 H       5.282913     0.016806    -1.369013      18.74
 C       3.457582     0.739630     1.590430     -19.14
 C       2.077949     1.234330     2.172034      92.41
 H       2.142924     2.238849     2.525999      27.10
 O       1.840678     0.734610     3.445845     198.29
 H       1.276296    -0.234314     3.583086      24.58
 C       0.818243     1.114089     1.212243      94.44
 H       0.741940     1.706611     0.194641      20.38
 C      -0.496111     1.414768     2.004268     100.79
 O      -0.553528     2.674650     2.675296     265.03
 H      -0.009509     3.146710     1.914683      27.56
 H      -0.595351     0.408340     2.592152      25.67
 H      -1.428094     1.076270     1.316413      25.19
 C      -1.955792    -2.142292    -1.154040      17.37
 H      -2.570299    -3.007691    -0.775346      22.34
 C      -1.469160    -0.018743    -2.514713      43.46
 H      -2.153352     0.517679    -3.236307      19.51
 C      -0.590459     0.409496    -1.516503      15.87
 O       0.257140     1.642512    -1.619302     224.23
 C      -0.425829     2.741059    -2.256296     102.57
 H       0.102833     3.537192    -1.685461      25.84
 H       0.083862     2.752053    -3.265714      26.10
 H      -1.542931     2.682736    -2.305632      28.08
 C      -0.236401    -0.434232    -0.410249      10.32
 O       0.635816    -0.224465     0.707434     172.70
 C      -0.877722    -1.701757    -0.160829      38.12
 H      -0.539011    -2.465274     0.611668      22.19
 C      -2.152232    -1.323602    -2.336283      32.87
 C      -3.205553    -1.678858    -3.261934      73.93
 H      -2.956019    -1.266328    -4.326097      26.36
 O      -3.076127    -3.061973    -3.547467     124.79
 H      -2.300796    -3.332513    -4.301401      27.24
 C      -4.842964    -1.600597    -2.798212      71.87
 H      -5.018069    -2.479141    -2.061174      27.66
 O      -5.150602    -0.358272    -2.093164     198.40
 H      -4.423925    -0.482472    -1.244934      22.94
 C      -5.697133    -1.966320    -3.955361     108.67
 O      -6.037459    -3.269901    -3.979973     229.95
 H      -6.575489    -3.623106    -4.870857      27.16
 H      -5.434797    -1.543927    -5.026937      25.73
 H      -6.673227    -1.350421    -3.788884      26.44
55
name = lig-ACN-frame_633
 C       3.737608     0.699067     0.204377      17.15
 H       3.208998     1.186067    -0.595017      24.10
 C       4.516659     0.226575     2.433127      48.06
 H       4.343135     0.638483     3.347351      20.72
 C       5.764200    -0.249825     2.051833      30.96
 O       6.802863    -0.720329     2.890429     249.46
 C       6.349135    -0.826286     4.295950     111.84
 H       7.151624    -1.163444     4.833082      27.59
 H       5.529251    -1.454205     4.411437      28.12
 H       5.777015     0.119251     4.657181      23.50
 C       5.856958    -0.369133     0.652843      19.45
 O       6.959828    -0.832506    -0.012641     157.74
 H       7.797296    -0.882256     0.611564      19.78
 C       4.917784     0.058760    -0.305085      46.57
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 H       4.887339    -0.048527    -1.469451      24.94
 C       3.567262     0.780484     1.623042      21.87
 C       2.079133     1.241460     2.099137      75.84
 H       2.103073     2.292867     2.111222      28.17
 O       1.926957     0.674363     3.403831     220.50
 H       1.379126    -0.178241     3.219292      28.18
 C       0.816882     1.130937     1.246047      78.25
 H       1.152525     1.978557     0.569319      24.16
 C      -0.486321     1.374737     2.026459      92.12
 O      -0.623744     2.745095     2.670301     166.25
 H      -0.044798     3.659239     2.250527      26.00
 H      -0.475805     0.895226     3.063769      23.59
 H      -1.403841     1.300981     1.233730      24.33
 C      -1.830393    -2.120234    -1.152173      66.05
 H      -2.283833    -3.127787    -1.363295      24.27
 C      -1.425076    -0.134056    -2.329904      82.31
 H      -1.469006     0.771965    -3.126400      18.79
 C      -0.409766     0.378312    -1.446127       7.57
 O       0.188478     1.618779    -1.590179     209.77
 C      -0.434223     2.849989    -2.323573      91.10
 H      -0.309577     3.734825    -1.745856      27.16
 H      -0.404465     3.083784    -3.456072      23.78
 H      -1.529523     2.692372    -2.104839      25.23
 C      -0.256988    -0.580094    -0.351522      31.75
 O       0.606871    -0.321465     0.677268     132.89
 C      -0.915902    -1.821160    -0.301588      49.61
 H      -0.745216    -2.261472     0.801118      20.71
 C      -2.085016    -1.301379    -2.236868      44.98
 C      -3.288940    -1.638824    -3.260477      77.18
 H      -3.330692    -0.790316    -4.071541      27.74
 O      -3.104155    -3.144828    -3.481739     160.78
 H      -2.200054    -3.129236    -3.949012      29.29
 C      -4.716990    -1.524757    -2.755521      81.00
 H      -4.767956    -2.377268    -2.009296      27.67
 O      -5.219888    -0.352971    -2.050626     232.16
 H      -4.419148     0.356881    -1.611364      23.42
 C      -5.781463    -1.908517    -4.002851      66.76
 O      -6.140293    -3.447081    -4.054596     218.65
 H      -6.747782    -3.287968    -4.838835      29.83
 H      -5.129959    -1.767969    -4.966702      26.20
 H      -6.706113    -1.222847    -3.878344      26.46
55
name = lig-ACN-frame_634
 C       3.722750     0.724431     0.118318      97.14
 H       2.999106     1.100384    -0.528430      24.55
 C       4.463030     0.388371     2.529280      44.49
 H       4.226334     0.114447     3.494939      21.93
 C       5.697418    -0.288697     2.055101      -2.38
 O       6.767767    -0.711024     2.900941     192.66
 C       6.349612    -0.822308     4.303562     118.04
 H       7.145327    -1.297098     4.880870      26.09
 H       5.481014    -1.391220     4.287678      26.28
 H       6.384131     0.229608     4.733950      22.94
 C       5.853324    -0.432563     0.643481      15.40
 O       6.999549    -0.832260     0.028619     155.61
 H       7.667692    -1.218301     0.675069      22.65
 C       4.889759     0.033168    -0.256056      48.93
 H       5.283619    -0.185054    -1.284442      21.52
 C       3.465215     0.795756     1.469814       4.65
 C       2.215975     1.251198     2.087153      85.53
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 H       2.253667     2.228492     2.493273      25.77
 O       1.976446     0.603952     3.440848     194.10
 H       1.464565    -0.121528     3.389743      31.73
 C       0.825834     1.073788     1.204330      88.79
 H       0.597911     1.540163     0.257410      20.81
 C      -0.440300     1.491828     2.115913      93.51
 O      -0.664365     2.827470     2.656191     242.68
 H      -0.321623     3.547297     1.923245      26.55
 H      -0.685976     0.622956     2.804990      25.63
 H      -1.415214     1.226273     1.364294      24.08
 C      -1.824247    -2.295615    -1.328981      21.37
 H      -2.233377    -3.327922    -1.131497      22.99
 C      -1.336381    -0.011197    -2.297715     110.80
 H      -1.463449     0.298949    -3.430801      22.95
 C      -0.358947     0.275262    -1.400226      17.71
 O       0.176489     1.627512    -1.582523     193.34
 C      -0.584014     2.809385    -2.250054      70.19
 H      -0.007989     3.556990    -1.861193      27.95
 H      -0.070546     2.541576    -3.268872      21.97
 H      -1.715531     2.821339    -2.241535      25.82
 C      -0.168556    -0.542664    -0.261045      21.26
 O       0.714776    -0.311715     0.760645     190.35
 C      -0.860715    -1.812910    -0.232083      27.01
 H      -0.764041    -2.676373     0.667286      21.80
 C      -2.210859    -1.218444    -2.237306      40.85
 C      -3.236284    -1.611520    -3.182577      81.48
 H      -2.998563    -1.287083    -4.261538      23.51
 O      -3.136980    -3.115103    -3.507247     175.75
 H      -2.283822    -3.313317    -3.452441      33.29
 C      -4.757164    -1.618341    -2.668871      73.20
 H      -4.886344    -2.465286    -1.979861      25.90
 O      -5.272009    -0.323497    -2.099427     227.17
 H      -4.510341     0.266724    -1.842056      28.03
 C      -5.724091    -1.912505    -3.946641      73.25
 O      -6.236480    -3.455607    -4.074162     262.76
 H      -6.457713    -3.649201    -4.931965      32.63
 H      -5.218693    -1.552737    -4.933000      26.07
 H      -6.758637    -1.350534    -3.983445      25.93
55
name = lig-ACN-frame_635
 C       3.667370     0.732658     0.060635      44.76
 H       2.886469     0.818099    -0.652719      23.67
 C       4.464542     0.397983     2.461214      95.55
 H       3.986379     0.467940     3.444068      23.04
 C       5.587738    -0.243880     2.082411      19.18
 O       6.647626    -0.692876     2.865809     208.34
 C       6.403788    -0.808455     4.310045     115.17
 H       7.185237    -1.593263     4.547256      25.75
 H       5.431816    -1.179709     4.566880      26.70
 H       6.345727     0.109876     4.927315      24.90
 C       5.894635    -0.438518     0.660459       9.84
 O       7.118445    -0.896287     0.087754     181.59
 H       7.644322    -1.410306     0.672525      24.19
 C       4.926395     0.004868    -0.314340      22.15
 H       5.163832     0.011597    -1.352288      22.05
 C       3.470693     0.760742     1.526138      -2.88
 C       2.098678     1.252166     2.157912      95.05
 H       2.230110     2.308129     2.324246      28.43
 O       2.027319     0.569593     3.463229     193.97
 H       1.334308    -0.143717     3.307056      29.32
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 C       0.867988     1.149055     1.289203      90.65
 H       1.130108     1.833964     0.538723      26.79
 C      -0.482183     1.484450     2.121732      95.89
 O      -0.626861     2.881218     2.600406     270.55
 H      -0.559050     3.405417     1.859855      32.87
 H      -0.492096     0.924067     3.067095      26.62
 H      -1.363271     1.347319     1.259971      23.88
 C      -1.687437    -2.197778    -1.259696      76.50
 H      -2.362303    -3.047973    -1.223513      25.45
 C      -1.434904    -0.101022    -2.425605      47.80
 H      -1.569983     0.798957    -3.097198      21.46
 C      -0.444250     0.363761    -1.420161     -13.17
 O       0.178382     1.579394    -1.494574     201.44
 C      -0.542677     2.608706    -2.221836     105.93
 H      -0.262241     3.501754    -1.852701      29.19
 H      -0.583118     2.732070    -3.424010      24.92
 H      -1.651113     2.645469    -1.914214      27.89
 C      -0.139194    -0.612675    -0.196434      -6.40
 O       0.845113    -0.305559     0.908584     120.15
 C      -0.852525    -1.835549    -0.271473      52.54
 H      -0.327088    -2.599018     0.532816      22.92
 C      -2.163290    -1.267795    -2.163572      25.06
 C      -3.247599    -1.728670    -3.223361      69.73
 H      -3.296934    -0.881249    -4.034271      26.24
 O      -3.148458    -3.063998    -3.546361     185.50
 H      -2.353886    -3.518859    -3.029933      27.24
 C      -4.910879    -1.654902    -2.700446      81.87
 H      -4.940766    -2.304063    -1.862131      27.85
 O      -5.280603    -0.366194    -2.225713     259.52
 H      -4.751316    -0.242946    -1.532374      32.27
 C      -5.749537    -2.060675    -3.879072      96.35
 O      -6.210477    -3.319056    -4.017219     296.93
 H      -6.072522    -3.442850    -5.019472      27.02
 H      -5.242531    -1.744407    -4.849491      24.92
 H      -6.592658    -1.277376    -3.561052      24.54
55
name = lig-ACN-frame_636
 C       3.728176     0.548558     0.158064      49.46
 H       3.042280     0.899504    -0.633086      24.18
 C       4.364516     0.385847     2.398108      23.36
 H       4.628978     0.792991     3.428403      18.43
 C       5.637153    -0.219873     1.945807      11.55
 O       6.528251    -0.675960     2.893930     230.64
 C       6.424958    -0.841237     4.312524     108.43
 H       7.257106    -1.601884     4.690631      24.26
 H       5.398576    -1.187092     4.567667      25.57
 H       6.797447     0.037184     4.753235      25.20
 C       5.918203    -0.383440     0.589324      14.89
 O       7.130600    -0.948850     0.174824     178.00
 H       7.795315    -1.127733     0.921113      21.68
 C       4.933755     0.084850    -0.348685      65.49
 H       5.030789    -0.136936    -1.347775      25.25
 C       3.374519     0.797092     1.476348      33.57
 C       2.134750     1.253144     2.292057     102.25
 H       2.165291     2.307378     2.656082      26.42
 O       2.000730     0.568147     3.502962     164.59
 H       1.284748    -0.312055     3.413940      24.31
 C       0.876258     1.199989     1.442658      92.48
 H       0.954831     1.742686     0.584768      26.01
 C      -0.470807     1.514108     2.060717     107.44
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 O      -0.566615     2.889907     2.528264     271.35
 H      -0.483097     3.668002     1.865379      27.72
 H      -0.566552     0.933387     2.938038      27.27
 H      -1.461565     0.980274     1.512957      24.94
 C      -1.715714    -2.111212    -1.140541      38.46
 H      -1.957722    -3.143857    -0.973267      24.82
 C      -1.468595    -0.068017    -2.345836      58.63
 H      -2.030824     0.475263    -3.014605      21.95
 C      -0.545993     0.267857    -1.317534      14.38
 O       0.195358     1.494185    -1.433845     219.41
 C      -0.576141     2.533227    -2.154124      94.13
 H      -0.179681     3.427779    -1.930046      27.63
 H      -0.579477     2.224472    -3.310921      23.68
 H      -1.592641     2.276205    -1.784474      26.42
 C      -0.105704    -0.501775    -0.269373      19.01
 O       0.804289    -0.270273     0.855008     115.53
 C      -0.605468    -1.823195    -0.181892      30.22
 H      -0.551129    -2.638949     0.652037      20.44
 C      -2.118930    -1.333191    -2.303949      21.17
 C      -3.401561    -1.703593    -3.101906      84.52
 H      -3.276416    -1.103220    -4.094135      25.94
 O      -3.122475    -3.113408    -3.662755     107.85
 H      -2.347869    -3.440652    -2.927595      27.34
 C      -4.796493    -1.739093    -2.655772     102.43
 H      -5.012857    -2.520063    -2.007857      29.56
 O      -5.257631    -0.377740    -2.329448     221.83
 H      -5.328958    -0.182632    -1.320023      27.52
 C      -5.840110    -1.909109    -3.837528      80.59
 O      -6.178087    -3.358824    -3.957474     237.03
 H      -6.366713    -3.734895    -4.980160      27.00
 H      -5.278516    -1.533658    -4.741302      26.86
 H      -6.848887    -1.356836    -3.920627      25.73
55
name = lig-ACN-frame_637
 C       3.618656     0.496497     0.147656       5.20
 H       2.852182     0.800810    -0.663047      21.81
 C       4.484870     0.421098     2.367955      89.25
 H       4.198406     0.561876     3.494562      21.78
 C       5.569002    -0.178425     1.934894      18.11
 O       6.562543    -0.708563     2.847048     208.15
 C       6.414994    -0.828166     4.320181     105.65
 H       7.116523    -1.797249     4.453922      24.57
 H       5.372304    -1.082406     4.725908      26.42
 H       6.655579     0.007349     4.881217      26.92
 C       5.980256    -0.337289     0.538115      16.22
 O       7.083365    -0.978167     0.213721      81.86
 H       7.744255    -0.827937     1.006213      19.99
 C       4.992313     0.063065    -0.350450      48.02
 H       5.141064    -0.085086    -1.387730      23.37
 C       3.391169     0.772176     1.574287      12.17
 C       2.144576     1.291550     2.317780      73.61
 H       2.426944     2.353797     2.651443      25.71
 O       1.938914     0.526153     3.638938     137.84
 H       1.379900    -0.403477     3.401392      25.35
 C       0.808193     1.165146     1.347147      93.05
 H       0.961401     1.890202     0.626058      26.35
 C      -0.479016     1.502265     2.137678     102.63
 O      -0.557545     2.888437     2.491519     243.43
 H       0.054997     3.234362     1.639033      25.40
 H      -0.666159     0.936610     2.965155      27.35
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 H      -1.263071     1.430627     1.114831      22.61
 C      -1.638007    -2.197735    -1.051292      65.07
 H      -2.140113    -3.120311    -0.940891      25.93
 C      -1.587857    -0.081230    -2.216971      86.50
 H      -1.579921     0.597553    -2.908991      17.56
 C      -0.504114     0.292417    -1.308736      11.02
 O       0.181418     1.428063    -1.379211     228.77
 C      -0.633342     2.432399    -2.094283     117.24
 H      -0.076611     3.307100    -1.985416      28.81
 H      -0.456985     2.224839    -3.208193      24.96
 H      -1.628064     2.809161    -1.959511      28.59
 C      -0.070132    -0.542971    -0.213754      29.23
 O       0.743966    -0.116898     0.763817     199.31
 C      -0.614475    -1.783597    -0.224141      57.31
 H      -0.268536    -2.291389     0.672592      22.49
 C      -2.132099    -1.407892    -2.163975      26.29
 C      -3.297097    -1.787993    -3.142168      66.86
 H      -3.416937    -1.021067    -3.993635      27.60
 O      -3.086517    -3.147942    -3.746657     213.14
 H      -2.388242    -3.590527    -3.328743      33.06
 C      -4.902126    -1.719197    -2.613753      82.64
 H      -5.035013    -2.313632    -1.780705      28.96
 O      -5.221268    -0.350685    -2.322072     160.37
 H      -5.104926    -0.161849    -1.189867      23.98
 C      -5.866692    -1.894627    -3.925203      79.86
 O      -6.158108    -3.435567    -3.902422     269.79
 H      -6.586179    -3.438333    -4.782372      30.01
 H      -5.518703    -1.524518    -4.901517      26.72
 H      -6.681713    -1.305202    -3.408174      26.42
55
name = lig-ACN-frame_638
 C       3.627701     0.526663     0.126894      74.90
 H       2.686265     0.495748    -0.551094      22.99
 C       4.488811     0.499217     2.509009      54.74
 H       4.199234     0.224007     3.575866      20.96
 C       5.716060    -0.192725     2.024430       6.14
 O       6.647290    -0.747708     2.789404     199.01
 C       6.373664    -0.828520     4.267000      98.80
 H       7.058715    -1.723583     4.707301      24.28
 H       5.229988    -1.034425     4.359462      24.48
 H       6.765196     0.029702     4.676169      26.02
 C       5.882339    -0.272240     0.643386       1.83
 O       7.106180    -0.996659     0.187540     169.05
 H       7.811444    -1.190307     0.820298      22.79
 C       4.808960     0.071721    -0.335033      49.35
 H       5.076219     0.033640    -1.415922      20.86
 C       3.428898     0.691478     1.526937      -2.67
 C       2.057158     1.164659     2.260846      75.94
 H       2.072079     2.308001     2.542683      25.09
 O       1.883301     0.536459     3.681894     199.71
 H       1.378740    -0.207542     3.447175      30.98
 C       0.840757     1.261776     1.373038      89.91
 H       0.985174     2.017229     0.627144      25.43
 C      -0.540436     1.483933     2.087677      90.07
 O      -0.517394     2.905847     2.471795     245.83
 H       0.027017     3.721553     2.055415      26.18
 H      -0.715601     0.830066     2.900122      27.14
 H      -1.629357     1.245075     1.443755      24.67
 C      -1.638585    -2.370288    -1.104294      49.25
 H      -2.024583    -3.333375    -0.863454      23.04
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 C      -1.572431    -0.137816    -2.097452      81.57
 H      -1.945458     0.279868    -2.916546      27.15
 C      -0.531491     0.250047    -1.340985      17.89
 O       0.078860     1.501300    -1.366708     226.57
 C      -0.521001     2.526944    -2.161404     107.36
 H       0.027170     3.478400    -1.954314      26.12
 H      -0.805131     2.340871    -3.176865      27.04
 H      -1.391256     2.384094    -1.539920      26.58
 C      -0.143833    -0.535688    -0.230778      12.15
 O       0.813723    -0.061848     0.747313     146.24
 C      -0.668156    -1.879116    -0.121525      40.78
 H      -0.332404    -2.588753     0.496741      27.34
 C      -2.207372    -1.413312    -1.950295      25.80
 C      -3.213861    -1.900744    -3.134604      66.66
 H      -2.952498    -1.089211    -3.861056      27.59
 O      -3.070458    -3.147032    -3.808164     223.68
 H      -2.195772    -3.415407    -3.599661      32.50
 C      -4.895919    -1.640122    -2.727040      89.22
 H      -5.209471    -2.358665    -2.034187      28.93
 O      -5.167165    -0.291302    -2.209914     218.79
 H      -4.331735    -0.032938    -1.583129      26.53
 C      -5.895753    -2.085662    -3.779169     118.12
 O      -6.153768    -3.393254    -3.909357     308.74
 H      -6.655144    -3.648761    -4.626039      33.07
 H      -5.504703    -1.710231    -4.724327      26.76
 H      -6.905084    -1.574436    -3.758794      26.48
55
name = lig-ACN-frame_639
 C       3.550289     0.556650     0.233707      16.04
 H       2.729184     0.742789    -0.542277      22.71
 C       4.483468     0.394696     2.540764      72.08
 H       4.338902     0.794959     3.549986      20.50
 C       5.691787    -0.079460     2.072385      -1.88
 O       6.795403    -0.825237     2.840159     221.90
 C       6.382925    -0.812403     4.156176     107.39
 H       6.966728    -1.679793     4.708887      24.40
 H       5.223783    -1.052857     4.373479      24.70
 H       6.507668     0.095490     4.677906      25.12
 C       5.894368    -0.325763     0.604298      12.74
 O       6.983869    -0.930393     0.098578     122.02
 H       7.453818    -1.215161     0.881722      23.98
 C       4.884825     0.032822    -0.239696      53.74
 H       4.908716    -0.276123    -1.356287      23.61
 C       3.371643     0.679051     1.633132      20.09
 C       2.058854     1.115075     2.293648      82.08
 H       2.425013     2.181297     2.680703      24.77
 O       1.813777     0.571148     3.577696     261.21
 H       1.279738    -0.177902     3.710397      30.61
 C       0.775061     1.214070     1.371303      84.70
 H       1.019370     1.960813     0.553098      24.31
 C      -0.511207     1.592922     2.031467     109.41
 O      -0.561028     2.927641     2.563084     296.19
 H      -0.264144     3.299002     1.740756      31.53
 H      -0.490353     1.063149     2.972159      26.63
 H      -1.308953     1.126648     1.173177      25.72
 C      -1.644595    -2.466668    -0.992023      53.56
 H      -1.782662    -3.525966    -1.226387      23.59
 C      -1.690162    -0.255480    -2.139958      58.96
 H      -2.111756     0.509866    -2.750004      24.04
 C      -0.577763     0.305635    -1.295213     -14.49
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 O       0.108573     1.532484    -1.414795     185.60
 C      -0.600556     2.667545    -2.144037     113.28
 H       0.228447     3.524625    -2.128889      25.15
 H      -0.514255     2.371274    -3.124255      27.54
 H      -1.546836     3.154394    -1.984727      28.34
 C      -0.178334    -0.618674    -0.102804      10.70
 O       0.852894    -0.179599     0.655008     135.04
 C      -0.679534    -1.981183    -0.060215      47.82
 H      -0.332351    -2.524411     0.670289      24.48
 C      -2.289034    -1.573367    -1.922868      25.09
 C      -3.291296    -1.765619    -3.062965      79.42
 H      -3.140108    -1.051621    -3.856475      27.80
 O      -3.031431    -3.172091    -3.763852      71.57
 H      -1.927102    -3.218623    -3.940942      26.25
 C      -4.764915    -1.696496    -2.691255      98.28
 H      -4.726404    -2.321143    -1.864636      29.03
 O      -5.056554    -0.311264    -2.150295     247.82
 H      -4.334430     0.106729    -1.938772      35.09
 C      -5.928828    -1.965830    -3.850639      88.94
 O      -6.146869    -3.559845    -3.842019     210.41
 H      -6.433778    -3.540631    -4.893256      25.27
 H      -5.546510    -1.700595    -4.816615      26.41
 H      -6.794936    -1.360880    -3.529157      26.73
55
name = lig-ACN-frame_640
 C       3.637416     0.509202     0.348422      58.92
 H       2.906042     0.914747    -0.338182      25.88
 C       4.459285     0.359197     2.548667      27.72
 H       4.464087     0.684441     3.544002      19.70
 C       5.812059    -0.161493     2.003344      17.65
 O       6.774275    -0.748951     2.759101     245.92
 C       6.400321    -0.839330     4.257375      83.02
 H       7.190383    -1.498115     4.730967      23.87
 H       5.340069    -1.324004     4.174846      24.68
 H       6.447534     0.182465     4.671025      22.74
 C       5.826751    -0.331483     0.680465      21.82
 O       6.922868    -0.900350     0.027101     146.80
 H       7.710227    -1.250696     0.603870      25.62
 C       4.757394     0.049089    -0.179083      67.73
 H       4.987155    -0.256585    -1.273404      21.84
 C       3.358103     0.626637     1.731959      40.42
 C       2.066508     1.219970     2.310916      85.37
 H       2.061616     2.389552     2.436408      25.48
 O       1.731638     0.561766     3.580358     182.68
 H       1.265174    -0.253540     3.035851      25.72
 C       0.915211     1.098421     1.289818      75.56
 H       1.056112     1.866772     0.398302      23.36
 C      -0.483082     1.530463     2.084364      98.61
 O      -0.584973     2.968181     2.553892     276.27
 H      -0.675500     3.683653     1.987961      31.51
 H      -0.933182     0.779278     2.793185      26.33
 H      -1.418362     1.678652     1.389017      24.87
 C      -1.680079    -2.485835    -0.964790      41.68
 H      -1.872070    -3.610322    -0.906469      26.85
 C      -1.704334    -0.239931    -2.002603      62.77
 H      -2.054714     0.403022    -2.872404      19.68
 C      -0.750959     0.169197    -1.180986      14.75
 O       0.015631     1.543264    -1.447897     145.15
 C      -0.550958     2.750352    -2.242213      97.09
 H       0.262480     3.623316    -1.905872      23.78
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 H      -0.625967     2.567210    -3.239974      27.23
 H      -1.515830     2.958748    -1.835072      28.26
 C      -0.262536    -0.628699    -0.197952      27.85
 O       0.847419    -0.279591     0.676506     139.86
 C      -0.682941    -1.966180    -0.050428      43.64
 H      -0.253804    -2.579421     0.664779      21.30
 C      -2.208369    -1.573265    -1.990901      29.14
 C      -3.294144    -1.814055    -3.123095      75.53
 H      -3.211539    -0.941036    -3.728618      28.46
 O      -3.007349    -3.105009    -3.622106     142.73
 H      -1.986435    -2.976784    -3.968123      26.11
 C      -4.742068    -1.735858    -2.589627     104.53
 H      -5.147275    -2.479562    -1.963717      29.08
 O      -4.987577    -0.405181    -2.197547     249.06
 H      -4.302524    -0.075372    -1.512009      27.64
 C      -5.782136    -1.984847    -3.779436      87.74
 O      -6.167278    -3.539113    -3.826379     246.47
 H      -6.081163    -4.064287    -4.748941      26.63
 H      -5.707549    -1.615961    -4.768237      26.71
 H      -6.691408    -1.575117    -3.380624      27.54
55
name = lig-ACN-frame_641
 C       3.518564     0.552045     0.408339      40.30
 H       2.746570     0.743230    -0.250848      23.80
 C       4.591923     0.320217     2.641856      81.90
 H       4.360400     0.095538     3.615764      21.70
 C       5.650828    -0.229277     2.080291      12.86
 O       6.764528    -0.649365     2.809708     233.78
 C       6.477432    -0.864225     4.229804     110.74
 H       7.347340    -1.302782     4.608382      25.81
 H       5.560048    -1.487330     4.559699      28.01
 H       6.307117     0.147658     4.778741      26.11
 C       5.852812    -0.373529     0.589373      11.28
 O       6.934602    -0.919150    -0.073095     144.71
 H       7.669944    -0.977213     0.632581      22.88
 C       4.763323    -0.004524    -0.188012      48.63
 H       4.777360     0.218987    -1.288140      21.19
 C       3.460368     0.663590     1.799210      17.69
 C       2.064361     1.262147     2.261337      76.94
 H       2.047273     2.337431     2.704094      24.83
 O       1.634253     0.547301     3.544619     168.16
 H       1.275209    -0.507505     3.542822      24.88
 C       0.904118     1.053466     1.271283      78.22
 H       1.001519     1.789060     0.318037      22.22
 C      -0.546004     1.567149     1.941179      93.02
 O      -0.548522     2.931094     2.638904     240.42
 H      -0.564400     3.377066     1.639730      26.40
 H      -0.604942     0.962011     2.918788      24.35
 H      -1.129580     1.271037     1.046442      24.86
 C      -1.701496    -2.412231    -1.027421      62.09
 H      -2.299659    -3.366012    -0.780633      22.01
 C      -1.786141    -0.206820    -1.986543      54.58
 H      -2.069496     0.451104    -2.963951      20.42
 C      -0.742556     0.383162    -1.146321      24.57
 O      -0.123556     1.445576    -1.457176     215.06
 C      -0.541050     2.672756    -2.242979     102.86
 H       0.226063     3.594660    -1.926280      23.90
 H      -0.592094     2.654446    -3.286417      27.11
 H      -1.492892     2.932333    -1.870979      29.39
 C      -0.186228    -0.622090    -0.125907      19.72
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 O       0.795294    -0.338579     0.762539     165.10
 C      -0.756014    -1.954075    -0.131953      54.60
 H      -0.293167    -2.682848     0.599886      25.76
 C      -2.169464    -1.567713    -1.995229      44.11
 C      -3.210659    -1.862373    -2.990980      90.34
 H      -3.212623    -1.241424    -3.822978      30.43
 O      -2.972008    -3.133435    -3.568247     220.88
 H      -2.101006    -3.279771    -3.677715      34.36
 C      -4.777751    -1.847897    -2.621240     102.06
 H      -4.778569    -2.451844    -1.730617      29.85
 O      -4.950114    -0.442133    -2.209036     155.89
 H      -4.816298    -0.475194    -1.067682      24.45
 C      -5.766754    -2.164098    -3.675294     121.71
 O      -6.149230    -3.428286    -3.794052     355.73
 H      -5.692796    -3.679029    -4.508950      33.55
 H      -5.279702    -1.721366    -4.516569      27.55
 H      -6.627019    -1.561202    -3.445592      28.11
55
name = lig-ACN-frame_642
 C       3.572594     0.532093     0.410795      62.83
 H       2.719089     0.728676    -0.123902      26.06
 C       4.422448     0.281033     2.715988      21.68
 H       4.343873     0.258254     3.794508      19.28
 C       5.699675    -0.354741     1.990154      -5.77
 O       6.755575    -0.594054     2.873510     210.04
 C       6.614265    -0.848976     4.250498     104.14
 H       7.493702    -1.206619     4.601464      24.80
 H       5.881709    -1.668287     4.239030      27.40
 H       6.244682     0.118105     4.885263      23.53
 C       5.800991    -0.403063     0.561030      11.59
 O       6.983353    -0.915047    -0.090670     185.93
 H       7.730206    -0.985710     0.476415      26.96
 C       4.684595     0.066586    -0.222841      57.97
 H       4.882608    -0.156189    -1.267992      20.77
 C       3.437210     0.790566     1.841908      27.72
 C       2.033538     1.060736     2.357947      95.70
 H       2.238651     2.189514     2.531229      25.06
 O       1.575406     0.568146     3.557509     267.66
 H       1.343592    -0.318771     3.290837      30.06
 C       0.809124     1.160463     1.278310      79.86
 H       1.193376     1.733218     0.320016      23.79
 C      -0.478163     1.528108     1.894618     110.55
 O      -0.501967     2.808310     2.524564     269.65
 H      -0.175905     3.768359     2.207027      27.21
 H      -0.770037     0.638231     2.646228      25.54
 H      -1.389450     1.623613     1.417905      27.23
 C      -1.751803    -2.367225    -1.026456      43.49
 H      -2.072508    -3.477846    -1.096296      26.56
 C      -1.747724    -0.098706    -2.024395      49.55
 H      -2.297696     0.757752    -2.727545      21.82
 C      -0.813916     0.252347    -1.134096      27.01
 O      -0.078380     1.517075    -1.450961     206.90
 C      -0.632619     2.571892    -2.195836     110.46
 H       0.274068     3.339196    -1.984642      23.89
 H      -0.397407     2.147239    -3.155434      26.12
 H      -1.568724     3.039290    -2.155249      29.09
 C      -0.258202    -0.582201    -0.167697      21.00
 O       0.764203    -0.327803     0.912789     103.33
 C      -0.710682    -1.886766    -0.153255      41.26
 H      -0.409908    -2.596964     0.774111      19.14
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 C      -2.252557    -1.397283    -1.964742      32.35
 C      -3.247351    -1.884732    -3.018767      84.58
 H      -3.182377    -1.076568    -3.640139      30.77
 O      -2.928014    -3.361059    -3.552941     145.00
 H      -2.035440    -3.493833    -3.213031      31.24
 C      -4.615733    -1.893928    -2.422516      86.03
 H      -4.861845    -2.625169    -1.617336      27.68
 O      -4.957502    -0.484546    -2.166909     164.53
 H      -5.236965    -0.226648    -1.168100      27.11
 C      -5.737250    -2.048943    -3.628392      86.01
 O      -6.174995    -3.525502    -3.793851     265.82
 H      -5.574054    -4.043715    -4.463720      27.87
 H      -5.307413    -1.878018    -4.583275      26.58
 H      -6.566457    -1.399085    -3.523020      28.43
55
name = lig-ACN-frame_643
 C       3.574798     0.596452     0.426207      34.40
 H       2.840240     0.829693    -0.342087      23.72
 C       4.435880     0.150558     2.564594      69.17
 H       4.401720     0.521458     3.619147      20.05
 C       5.588935    -0.290822     2.108259      15.42
 O       6.829065    -0.542141     2.764153     234.58
 C       6.638530    -0.878960     4.288784     102.66
 H       7.631421    -1.137274     4.693588      24.95
 H       5.946249    -1.625059     4.450632      30.38
 H       6.219816     0.106426     4.891257      24.94
 C       5.806076    -0.434310     0.647840       4.75
 O       6.959951    -0.868885    -0.063843     183.20
 H       7.621256    -1.148660     0.640494      23.02
 C       4.770536     0.027179    -0.221194      48.77
 H       4.539022    -0.194249    -1.212712      22.78
 C       3.350321     0.639935     1.791356      37.58
 C       1.957873     1.220296     2.366015      86.61
 H       1.885086     2.284367     2.761359      25.13
 O       1.541973     0.494247     3.635847     259.24
 H       1.112619    -0.295379     3.596228      30.33
 C       0.906441     1.092331     1.314031      90.70
 H       1.039379     1.885964     0.487025      23.49
 C      -0.525175     1.533397     1.847988     106.97
 O      -0.439986     2.772410     2.540405     299.70
 H       0.162422     3.096870     1.926686      33.59
 H      -0.855183     0.824986     2.747648      24.78
 H      -1.001510     1.414556     0.945516      27.38
 C      -1.713256    -2.239805    -1.030075      70.90
 H      -1.798775    -3.349252    -1.121096      25.22
 C      -1.805848    -0.039926    -2.043747      89.81
 H      -2.263458     0.794010    -2.796945      21.07
 C      -0.671816     0.340177    -1.186617      12.43
 O      -0.043668     1.498087    -1.242905     193.44
 C      -0.614406     2.505415    -2.326998      95.43
 H      -0.226454     3.567842    -2.217471      25.00
 H      -0.762004     2.330413    -3.410438      25.79
 H      -1.562128     2.387538    -1.879424      26.32
 C      -0.246413    -0.584619    -0.083329      23.33
 O       0.603734    -0.244218     0.896286     172.31
 C      -0.756223    -1.907805    -0.111708      53.97
 H      -0.216270    -2.666188     0.711130      20.76
 C      -2.330469    -1.403496    -1.974170      36.10
 C      -3.223772    -2.005334    -3.062010      68.45
 H      -3.321942    -1.745059    -4.015919      29.80
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 O      -2.894729    -3.416988    -3.452869     132.18
 H      -1.854183    -3.664645    -3.085802      24.83
 C      -4.713509    -1.854299    -2.418726      83.79
 H      -4.805286    -2.643237    -1.579778      28.11
 O      -4.960253    -0.482759    -2.070757     243.73
 H      -4.844676    -0.321855    -1.226346      32.80
 C      -5.637425    -2.153957    -3.618406      94.94
 O      -6.228002    -3.574594    -3.751667     252.55
 H      -5.559005    -4.104468    -4.407127      26.79
 H      -5.297957    -1.532703    -4.453125      26.91
 H      -6.546998    -1.757543    -3.283625      27.60
55
name = lig-ACN-frame_644
 C       3.567043     0.603971     0.304970      68.25
 H       2.821419     1.118327    -0.382911      24.73
 C       4.350847     0.165681     2.595648      21.85
 H       4.251461     0.102920     3.756577      19.42
 C       5.729020    -0.274892     2.013354       6.42
 O       6.839772    -0.534987     2.801106     237.95
 C       6.608416    -0.830216     4.186502      96.42
 H       7.603503    -1.260108     4.679932      23.42
 H       5.870928    -1.544080     4.194790      29.60
 H       6.256692     0.216728     4.743146      22.86
 C       5.790519    -0.423940     0.653680      26.37
 O       6.921822    -0.841504     0.068106     180.36
 H       7.612594    -1.280800     0.716019      21.79
 C       4.725104    -0.017844    -0.111503      64.24
 H       5.177486     0.025849    -1.055364      21.83
 C       3.231537     0.522768     1.735523      -2.38
 C       1.962986     1.178074     2.436977      84.14
 H       2.208239     2.216921     2.694141      24.16
 O       1.561925     0.460429     3.728436     211.98
 H       1.012964    -0.344609     3.275037      25.08
 C       0.787483     1.110770     1.390592      98.30
 H       1.231300     1.628928     0.533882      24.66
 C      -0.545013     1.499302     1.846926     113.88
 O      -0.369338     2.824047     2.512871     286.07
 H      -0.094156     3.585526     2.012247      31.22
 H      -1.085991     0.646212     2.456651      25.73
 H      -1.265369     1.713964     1.170256      28.40
 C      -1.696000    -2.263650    -1.077964      37.65
 H      -2.134436    -3.250628    -1.010527      21.16
 C      -1.780342    -0.045426    -1.997474      77.89
 H      -2.056680     0.502028    -2.947346      21.00
 C      -0.654154     0.286030    -1.220825      12.57
 O       0.040757     1.620203    -1.201150     187.12
 C      -0.708843     2.420563    -2.300710      91.04
 H      -0.197981     3.314224    -2.149126      27.97
 H      -0.326362     1.877824    -3.252076      25.94
 H      -1.813840     2.640699    -2.228251      27.15
 C      -0.316220    -0.530387    -0.136257      27.63
 O       0.590609    -0.229303     0.880928     148.90
 C      -0.765784    -1.835015    -0.047385      44.95
 H      -0.344086    -2.824790     0.511040      23.01
 C      -2.222349    -1.406475    -2.046740      22.87
 C      -3.233595    -2.102869    -3.033777      97.10
 H      -3.094238    -1.327443    -3.681904      28.51
 O      -2.878353    -3.462145    -3.256163     177.08
 H      -1.767546    -3.465123    -3.308503      26.94
 C      -4.702190    -1.926894    -2.558211      82.21
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 H      -4.894464    -2.513830    -1.568492      26.61
 O      -4.972487    -0.486751    -1.978155     174.23
 H      -4.138943    -0.362616    -1.464926      30.32
 C      -5.825643    -2.285346    -3.539284     116.36
 O      -6.177201    -3.562989    -3.735814     329.54
 H      -5.672405    -4.037886    -4.285309      33.18
 H      -5.470937    -2.060737    -4.587359      24.93
 H      -6.640513    -1.638555    -3.316549      26.94
55
name = lig-ACN-frame_645
 C       3.475937     0.551089     0.324693      25.39
 H       2.867643     1.079148    -0.516083      22.53
 C       4.356417     0.114563     2.560881      75.28
 H       3.957418    -0.111242     3.622238      21.42
 C       5.619393    -0.204348     2.147282      18.76
 O       6.842459    -0.525792     2.777358     252.16
 C       6.530204    -0.789293     4.131816     106.38
 H       7.502494    -1.292858     4.546109      25.04
 H       5.715394    -1.435128     4.255529      29.22
 H       6.287854     0.209258     4.841851      24.12
 C       5.776446    -0.411079     0.727779      -1.72
 O       6.979057    -0.874514     0.134774     130.77
 H       7.600731    -1.110925     0.852300      23.71
 C       4.729460     0.032852    -0.207844      28.97
 H       4.833302     0.214705    -1.261648      22.54
 C       3.288458     0.484820     1.746798      34.20
 C       1.969012     0.947829     2.472297      91.47
 H       2.185628     1.963344     2.730012      26.42
 O       1.614634     0.469226     3.718767     217.54
 H       1.134409    -0.591741     3.701828      22.82
 C       0.745656     1.143130     1.371973      77.40
 H       0.964754     1.924071     0.692170      25.78
 C      -0.661288     1.702430     1.887791     119.41
 O      -0.327898     2.893574     2.564599     277.34
 H      -0.779810     3.492204     1.778091      26.72
 H      -0.945531     1.063193     2.795647      25.89
 H      -1.277264     1.678567     1.098089      29.15
 C      -1.705517    -2.374561    -1.000814      65.34
 H      -2.068668    -3.349834    -0.926290      23.45
 C      -1.647710    -0.103720    -2.111291      72.43
 H      -2.026946     0.567830    -2.800292      21.87
 C      -0.664094     0.375034    -1.149851      17.35
 O      -0.090354     1.636256    -1.273821     230.63
 C      -0.607440     2.415359    -2.264117     113.11
 H      -0.226435     3.318133    -2.396071      28.32
 H      -0.491033     1.911874    -3.363819      26.03
 H      -1.784087     2.434242    -2.207368      26.32
 C      -0.290113    -0.530437    -0.115055      20.38
 O       0.675912    -0.299648     0.878461     136.13
 C      -0.829081    -1.846915    -0.121232      52.23
 H      -0.507806    -2.211205     0.915173      21.72
 C      -2.128157    -1.478438    -2.011739      47.37
 C      -3.204574    -1.949191    -2.987494      70.49
 H      -3.259170    -1.738426    -4.011762      30.13
 O      -2.854566    -3.488077    -3.105446     129.58
 H      -2.015217    -3.466326    -3.505616      31.59
 C      -4.705815    -1.942187    -2.476604      72.21
 H      -4.779852    -2.916248    -1.824463      27.01
 O      -4.938015    -0.619895    -1.991139     151.19
 H      -4.046894     0.084361    -1.812067      24.60
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 C      -5.935474    -2.159805    -3.632988      76.20
 O      -6.213236    -3.735790    -3.651332     252.70
 H      -5.594313    -3.931679    -4.435444      27.45
 H      -5.670646    -1.579514    -4.606390      25.95
 H      -6.890350    -1.773299    -3.271143      26.44
55
name = lig-ACN-frame_646
 C       3.520596     0.462187     0.362188      63.26
 H       2.525948     0.661600    -0.157144      22.56
 C       4.281567     0.019746     2.662025      43.15
 H       4.223272     0.185660     3.773465      19.65
 C       5.603105    -0.211909     2.033475      -0.85
 O       6.730862    -0.498277     2.760448     208.98
 C       6.521341    -0.800479     4.249698      87.86
 H       7.418424    -1.304257     4.686254      24.91
 H       5.580795    -1.411104     4.312107      27.20
 H       6.361193     0.305835     4.698850      24.12
 C       5.762547    -0.326139     0.614313       9.34
 O       6.969466    -0.883755     0.213966     198.10
 H       7.611445    -0.978740     0.905221      22.39
 C       4.745860     0.126651    -0.218066      77.03
 H       4.847107    -0.235434    -1.253681      22.42
 C       3.264467     0.453271     1.727398      26.37
 C       1.931478     0.967646     2.340830      87.59
 H       2.117962     1.958019     2.644511      26.57
 O       1.640714     0.379165     3.761764     201.49
 H       1.421839    -0.641989     3.846022      25.26
 C       0.784508     1.059019     1.444462      96.97
 H       1.132239     1.608660     0.661849      25.33
 C      -0.635174     1.691100     2.034685     106.60
 O      -0.361654     3.099028     2.560313     264.66
 H      -0.802420     3.931106     2.241938      28.86
 H      -1.236158     1.018103     2.688156      26.51
 H      -1.265391     1.877590     1.285311      27.42
 C      -1.746085    -2.396556    -0.963531      34.60
 H      -2.025738    -3.419420    -0.930678      19.59
 C      -1.506706    -0.211736    -2.151163      69.40
 H      -1.902035     0.368454    -2.880262      25.68
 C      -0.723308     0.363042    -1.150221      23.40
 O      -0.171402     1.600160    -1.245689     189.93
 C      -0.605053     2.513123    -2.440356      89.08
 H      -0.055601     3.290816    -2.189000      27.38
 H      -0.542138     2.064082    -3.557618      24.43
 H      -1.680666     2.814210    -2.077899      25.60
 C      -0.221761    -0.526713    -0.117637      25.24
 O       0.699311    -0.262550     0.834545     170.32
 C      -0.810026    -1.830172     0.026545      35.75
 H      -0.696508    -2.482204     0.855319      23.35
 C      -2.118103    -1.489662    -2.024986      45.34
 C      -3.184516    -2.064353    -3.027007      80.27
 H      -3.049977    -1.427858    -3.929649      30.75
 O      -2.896860    -3.463009    -3.022311     210.69
 H      -2.015224    -3.555744    -3.319516      33.37
 C      -4.729258    -1.939972    -2.550257      86.19
 H      -4.884527    -2.606798    -1.595173      25.84
 O      -4.982686    -0.696143    -1.973793     209.64
 H      -4.001219    -0.206515    -1.843346      27.42
 C      -5.901512    -2.190745    -3.560278      86.08
 O      -6.193731    -3.716488    -3.653556     222.68
 H      -5.906918    -4.313013    -4.523783      25.56
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 H      -5.885664    -1.729771    -4.631102      26.01
 H      -6.807394    -1.800876    -2.997321      25.82
55
name = lig-ACN-frame_647
 C       3.472925     0.378645     0.367470      29.72
 H       2.771416     0.371283    -0.480784      23.39
 C       4.316654     0.039711     2.623847      82.45
 H       4.224603     0.205481     3.675048      23.79
 C       5.489468    -0.253424     2.026721      16.77
 O       6.633489    -0.531716     2.849395     214.98
 C       6.506099    -0.739889     4.244448     107.23
 H       7.432729    -1.201009     4.472896      26.71
 H       5.646265    -1.479592     4.541756      26.80
 H       6.368294     0.197684     5.001305      24.65
 C       5.828404    -0.220799     0.628924      15.07
 O       6.914260    -0.857095     0.181318      87.63
 H       7.528149    -1.065422     0.992184      18.65
 C       4.750510     0.066856    -0.249910      18.28
 H       4.847581    -0.014223    -1.394765      18.96
 C       3.228382     0.383097     1.843239      16.37
 C       1.980377     1.037883     2.477892      86.60
 H       2.146322     2.066763     2.644088      28.42
 O       1.689862     0.319201     3.733322     279.06
 H       1.474050    -0.446234     3.370332      34.27
 C       0.724419     1.072946     1.467569      99.00
 H       0.923631     1.830780     0.832748      27.80
 C      -0.548975     1.751842     2.060458     112.99
 O      -0.347862     3.209708     2.622364     277.08
 H      -0.964627     3.511612     2.029572      31.55
 H      -0.883215     1.165334     2.869483      28.57
 H      -1.196147     1.728581     1.242383      28.29
 C      -1.710700    -2.258047    -0.874910      71.48
 H      -2.243311    -3.213968    -0.743578      21.00
 C      -1.531420    -0.294762    -2.206047      48.68
 H      -1.556862     0.203219    -3.137048      22.15
 C      -0.682088     0.227207    -1.189669       4.44
 O      -0.210761     1.640283    -1.300786     171.85
 C      -0.621567     2.615344    -2.415191      92.56
 H       0.130663     3.289832    -2.491643      27.69
 H      -0.338035     2.013325    -3.397521      24.43
 H      -1.649996     3.150381    -2.702337      25.25
 C      -0.319862    -0.600339    -0.103332      21.97
 O       0.686786    -0.229125     0.842661     174.41
 C      -0.852093    -1.867557     0.099965      71.28
 H      -0.339427    -2.440317     0.724457      28.80
 C      -2.170630    -1.570587    -1.983594      39.30
 C      -3.199209    -2.121970    -3.011425      77.01
 H      -2.986230    -1.717548    -4.053997      28.00
 O      -2.961112    -3.543936    -3.078813     157.92
 H      -1.881079    -3.610219    -2.957107      27.20
 C      -4.664592    -2.019367    -2.615174      72.18
 H      -4.704969    -2.956738    -1.877969      25.83
 O      -5.033628    -0.611617    -1.960551     186.84
 H      -4.340998    -0.390958    -1.435449      31.79
 C      -5.851178    -2.375632    -3.479035     105.79
 O      -6.174171    -3.640653    -3.671024     295.88
 H      -6.191327    -3.654465    -4.610095      28.60
 H      -5.652495    -1.818675    -4.508254      25.55
 H      -6.725296    -1.747578    -3.014822      25.97
55
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name = lig-ACN-frame_648
 C       3.412218     0.272699     0.361842      70.30
 H       2.575500     0.668655    -0.124792      25.10
 C       4.270228     0.153400     2.614967      55.18
 H       4.117857    -0.032190     3.619359      24.84
 C       5.569382    -0.280644     2.117559      14.93
 O       6.576051    -0.579615     2.883056     210.90
 C       6.519912    -0.721396     4.295757     106.42
 H       7.426257    -1.114100     4.585980      27.03
 H       5.609806    -1.501887     4.572172      25.32
 H       6.358109     0.344738     4.745243      24.63
 C       5.764368    -0.236405     0.710509      13.33
 O       6.928805    -0.805452     0.086352     181.58
 H       7.635549    -1.236599     0.706678      20.77
 C       4.678413     0.006050    -0.165260      54.04
 H       4.873164     0.276135    -1.272994      20.65
 C       3.179400     0.406372     1.707560      12.46
 C       1.987228     1.064506     2.539394     100.34
 H       2.299871     1.948742     3.052089      26.03
 O       1.729846     0.304136     3.675142     269.17
 H       1.183740    -0.541161     3.714215      26.66
 C       0.827292     1.305913     1.497100      77.58
 H       1.164035     1.772799     0.666401      26.35
 C      -0.492798     1.772802     2.148255     124.78
 O      -0.350787     3.147932     2.590620     242.33
 H      -0.760531     3.935550     1.979528      27.45
 H      -0.763503     1.171013     2.890891      29.75
 H      -1.362872     1.729199     1.533998      28.14
 C      -1.898783    -2.346454    -0.780386      41.93
 H      -2.308696    -3.388843    -0.521045      23.73
 C      -1.550286    -0.333050    -2.251302      43.22
 H      -1.834310     0.181134    -3.223856      21.72
 C      -0.652488     0.271162    -1.334970      10.53
 O      -0.306729     1.630924    -1.334333     219.94
 C      -0.494526     2.552524    -2.467366      89.27
 H       0.068392     3.444850    -2.235602      26.15
 H      -0.498178     2.061933    -3.495000      25.67
 H      -1.615715     2.784197    -2.073328      23.82
 C      -0.335623    -0.464703    -0.013443       6.26
 O       0.609170    -0.195744     0.891257     107.79
 C      -0.812416    -1.869499     0.105696      32.18
 H      -0.633037    -2.462068     0.966008      22.20
 C      -2.206014    -1.531994    -1.981558      27.06
 C      -3.172104    -2.143539    -3.000414      62.41
 H      -3.117047    -1.665302    -4.093806      26.73
 O      -2.992179    -3.717344    -3.187950      70.61
 H      -1.904886    -3.938386    -3.004469      25.63
 C      -4.636785    -2.024008    -2.400950      82.95
 H      -4.684643    -2.672102    -1.435035      27.29
 O      -5.019312    -0.656119    -2.025131     203.63
 H      -4.872613    -0.489732    -1.108855      30.77
 C      -5.774409    -2.185283    -3.493148      72.35
 O      -6.179677    -3.743280    -3.768803     216.64
 H      -6.712885    -3.897903    -4.530253      29.32
 H      -5.511866    -1.686782    -4.532135      25.73
 H      -6.740959    -1.722743    -3.014552      25.97
55
name = lig-ACN-frame_649
 C       3.287689     0.318985     0.317646      42.76
 H       2.721912     0.536749    -0.517726      23.56
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 C       4.259890     0.160023     2.616360      75.36
 H       3.992752     0.299686     3.609181      22.63
 C       5.506467    -0.211226     2.125802       9.35
 O       6.696267    -0.688823     2.908347     196.15
 C       6.510285    -0.673521     4.369042     104.70
 H       7.418344    -0.963377     4.833267      26.92
 H       5.555022    -1.387353     4.681417      25.48
 H       6.233583     0.339211     4.811759      25.52
 C       5.729619    -0.431408     0.701920      11.67
 O       6.892379    -0.696268     0.000928     192.75
 H       7.574276    -0.991190     0.600437      23.99
 C       4.639852    -0.002061    -0.079523      32.78
 H       4.905107    -0.216923    -1.187579      22.15
 C       3.217994     0.482742     1.769972      34.72
 C       2.025824     1.026159     2.404814      92.67
 H       2.353593     2.038925     2.663003      26.57
 O       1.697656     0.277700     3.754896     151.73
 H       1.084095    -0.550292     3.292132      23.63
 C       0.878710     1.377826     1.498800      80.09
 H       1.166780     2.164617     0.818543      26.60
 C      -0.472303     1.794104     2.153352     115.67
 O      -0.358736     3.121919     2.614539     221.16
 H      -0.192671     3.765741     1.753602      27.69
 H      -0.523705     1.255174     2.952282      29.82
 H      -1.268744     1.559122     1.389828      26.56
 C      -1.957855    -2.303257    -0.736571      53.97
 H      -2.410503    -3.365546    -0.680135      25.03
 C      -1.560702    -0.349963    -2.248127      62.69
 H      -2.024735     0.333158    -3.127272      20.62
 C      -0.697429     0.279413    -1.302510      16.15
 O      -0.260391     1.568136    -1.335963     228.55
 C      -0.550668     2.459999    -2.423661     104.83
 H       0.279614     3.233709    -2.246727      24.88
 H      -0.255176     2.134464    -3.418914      27.08
 H      -1.645526     3.004715    -2.601769      24.71
 C      -0.379240    -0.432916    -0.126922       3.60
 O       0.549573    -0.024107     1.028479      89.94
 C      -0.969489    -1.770692     0.042465      50.16
 H      -0.754046    -2.131552     1.064395      23.02
 C      -2.185908    -1.667031    -1.921583      35.41
 C      -3.206002    -2.313220    -2.910747      59.02
 H      -3.188632    -1.519684    -3.789764      27.82
 O      -3.031316    -3.755491    -3.268704     215.81
 H      -2.063600    -3.750509    -3.368538      28.90
 C      -4.691898    -2.030193    -2.310693      85.02
 H      -4.946477    -2.713895    -1.460602      28.63
 O      -4.955982    -0.653626    -2.067741     159.05
 H      -5.022492    -0.492044    -0.933668      25.65
 C      -5.782344    -2.257269    -3.510600      70.04
 O      -6.115743    -3.710415    -3.830562     192.05
 H      -6.844234    -3.682927    -4.650045      25.99
 H      -5.282318    -1.697189    -4.421324      26.77
 H      -6.767375    -1.623959    -3.246890      26.27
55
name = lig-ACN-frame_650
 C       3.406311     0.390867     0.332712      73.86
 H       2.473059     0.411414    -0.152585      24.78
 C       4.347119     0.162595     2.631196      36.60
 H       4.364346     0.447596     3.679994      21.37
 C       5.638036    -0.329094     2.151878      11.55
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 O       6.713814    -0.728832     2.930770     177.48
 C       6.480094    -0.586881     4.400188     103.06
 H       7.394907    -1.023447     4.835333      25.76
 H       5.544834    -1.346109     4.660196      24.39
 H       6.271934     0.445074     4.648259      24.65
 C       5.644341    -0.472953     0.723819      13.71
 O       6.836959    -0.604105    -0.021095     155.98
 H       7.610338    -0.873132     0.505132      21.52
 C       4.573299    -0.124719    -0.150542      63.33
 H       4.599713    -0.337379    -1.248361      24.08
 C       3.218481     0.495278     1.705303       5.01
 C       2.016623     1.118588     2.484972      88.71
 H       2.221973     2.076248     3.021545      26.01
 O       1.645614     0.352370     3.675941     204.74
 H       1.305284    -0.666778     3.542547      25.37
 C       0.781743     1.298450     1.457347     100.66
 H       1.122858     1.908005     0.612667      26.16
 C      -0.422186     1.775420     2.160502     118.32
 O      -0.354903     3.208515     2.630515     262.51
 H       0.092242     3.674129     1.946574      32.47
 H      -0.667823     1.041432     2.876488      28.86
 H      -1.325083     1.719830     1.423614      26.34
 C      -1.897221    -2.280092    -0.742696      44.65
 H      -2.367638    -3.214368    -0.293633      20.53
 C      -1.651737    -0.438335    -2.166581      41.38
 H      -1.931551     0.157841    -3.215953      21.73
 C      -0.816123     0.254574    -1.274092      12.30
 O      -0.202754     1.533614    -1.321899     218.89
 C      -0.517853     2.425311    -2.466880      91.19
 H       0.082643     3.490662    -2.386791      23.36
 H      -0.292932     1.803807    -3.267959      27.32
 H      -1.703311     2.689715    -2.557984      25.22
 C      -0.346481    -0.466353    -0.094386      19.91
 O       0.409883     0.051603     0.968856     180.28
 C      -1.082086    -1.594525     0.229902      44.15
 H      -0.695489    -2.213928     1.157528      24.76
 C      -2.209952    -1.712703    -2.011122      36.32
 C      -3.332932    -2.336558    -2.809682      75.68
 H      -3.268178    -1.882102    -3.881462      25.50
 O      -3.048487    -3.681311    -3.303034     227.14
 H      -2.271143    -3.625112    -3.734045      33.04
 C      -4.818943    -2.174072    -2.418095      92.78
 H      -4.981775    -2.760956    -1.524615      28.60
 O      -4.863666    -0.602718    -2.058675     111.45
 H      -4.730986    -0.390249    -1.007589      25.86
 C      -5.757081    -2.371974    -3.515846      94.53
 O      -6.051290    -3.620637    -3.868293     255.80
 H      -6.293489    -3.606862    -4.918748      25.74
 H      -5.261099    -1.877404    -4.469771      24.81
 H      -6.766398    -1.760770    -3.273974      25.07
55
name = lig-ACN-frame_651
 C       3.389367     0.391693     0.429348      24.89
 H       2.642678     0.726982    -0.352628      21.98
 C       4.468719     0.191517     2.593971      71.05
 H       4.214777     0.290554     3.695687      22.58
 C       5.578204    -0.451993     2.094151      23.12
 O       6.691894    -0.725025     2.954606     234.78
 C       6.477171    -0.534884     4.343374     105.38
 H       7.447041    -0.836196     4.927736      24.97
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 H       5.495566    -1.064671     4.785051      25.42
 H       6.406395     0.500337     4.611700      26.72
 C       5.684322    -0.421015     0.648913       3.63
 O       6.820166    -0.562968    -0.019544     169.21
 H       7.532187    -1.113557     0.519948      21.92
 C       4.537493    -0.299484    -0.215598      38.68
 H       4.858829    -0.306766    -1.256016      22.07
 C       3.362698     0.556080     1.877847      36.90
 C       1.947987     1.127852     2.469906      94.05
 H       2.156876     2.236151     2.729717      26.00
 O       1.586943     0.437435     3.629491     271.14
 H       1.587222    -0.429340     3.434315      32.75
 C       0.782051     1.306082     1.434660      77.80
 H       1.037948     2.030860     0.570831      24.39
 C      -0.523147     1.892761     2.164537     105.22
 O      -0.343060     3.240950     2.654647     242.26
 H       0.232315     3.867330     2.120094      29.86
 H      -0.709401     1.350935     3.106692      26.99
 H      -1.469310     1.916286     1.431467      24.91
 C      -1.839575    -2.289569    -0.640061      43.75
 H      -2.208152    -3.326925    -0.524687      21.01
 C      -1.726665    -0.408693    -2.198898      52.08
 H      -1.981254     0.110851    -3.278307      20.58
 C      -0.822754     0.253021    -1.228899      19.36
 O      -0.181470     1.511193    -1.332687     221.47
 C      -0.524078     2.289302    -2.547206     100.72
 H       0.026837     3.412435    -2.297439      22.97
 H      -0.321009     2.053226    -3.544105      27.12
 H      -1.645662     2.401528    -2.363136      25.90
 C      -0.533584    -0.388563    -0.062523      25.54
 O       0.397839    -0.052152     0.950131     144.88
 C      -1.139468    -1.634015     0.346292      46.92
 H      -1.037879    -2.137966     1.454592      23.58
 C      -2.271958    -1.729526    -1.875740      43.92
 C      -3.364923    -2.275568    -2.972469      50.02
 H      -3.461037    -1.351231    -3.627391      28.37
 O      -3.083820    -3.675105    -3.289322     176.84
 H      -2.072774    -3.592537    -3.667600      25.47
 C      -4.777066    -2.120984    -2.339142      99.80
 H      -5.131939    -2.688181    -1.549206      29.39
 O      -4.813023    -0.682566    -2.076446     235.63
 H      -4.288533    -0.649861    -1.388968      34.83
 C      -5.772598    -2.207184    -3.619591      65.98
 O      -6.047535    -3.738916    -3.948436     298.70
 H      -5.869777    -4.011960    -4.796024      31.03
 H      -5.393726    -1.487866    -4.456084      25.91
 H      -6.780407    -1.741284    -3.205608      25.23
55
name = lig-ACN-frame_652
 C       3.427071     0.297084     0.469255      50.02
 H       2.644759     0.888893    -0.158437      23.67
 C       4.418300     0.185706     2.700782      33.19
 H       4.522443     0.151168     3.853655      21.64
 C       5.542920    -0.440068     2.045755       2.94
 O       6.661239    -0.756398     2.869896     164.65
 C       6.506633    -0.419444     4.341124      99.49
 H       7.447979    -1.015999     4.762548      24.23
 H       5.573468    -0.980513     4.749659      25.38
 H       6.395675     0.628628     4.514882      26.27
 C       5.690068    -0.483885     0.616388      15.73
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 O       6.942504    -0.597617    -0.051065     143.29
 H       7.637004    -1.074016     0.545848      22.27
 C       4.511369    -0.268857    -0.092930      73.16
 H       4.456971    -0.308091    -1.140886      24.62
 C       3.310639     0.670626     1.800189      30.38
 C       2.015629     1.199916     2.327907      78.18
 H       2.145297     2.287399     2.729707      25.90
 O       1.534689     0.510869     3.653910     158.88
 H       1.398063    -0.476195     3.462828      27.73
 C       0.678783     1.305933     1.450226      84.06
 H       1.048232     1.993971     0.556450      25.48
 C      -0.558240     2.025660     2.099425      95.23
 O      -0.308455     3.325737     2.718371     207.15
 H       0.177380     3.765794     1.847374      27.80
 H      -0.983655     1.252362     2.946039      25.71
 H      -1.401512     1.881322     1.233910      25.32
 C      -1.968487    -2.434430    -0.627659      58.16
 H      -2.140819    -3.466254    -0.482669      23.61
 C      -1.720928    -0.356484    -2.124399      57.90
 H      -2.046891     0.158443    -3.099608      21.70
 C      -0.849186     0.246138    -1.272478       9.40
 O      -0.160202     1.422486    -1.443432     214.13
 C      -0.621288     2.233741    -2.543245      93.59
 H       0.070882     3.322048    -2.432521      23.55
 H      -0.115466     1.618947    -3.259847      26.10
 H      -1.633008     2.491860    -2.810273      27.14
 C      -0.780458    -0.385028     0.100580       3.21
 O       0.487422    -0.071116     1.020924      58.66
 C      -1.184019    -1.712625     0.331054      26.05
 H      -0.873268    -1.937457     1.527938      19.97
 C      -2.293181    -1.625115    -1.808595      26.15
 C      -3.244054    -2.230564    -2.887419      76.92
 H      -2.957580    -1.909394    -3.922437      24.92
 O      -3.087211    -3.598474    -3.338435     151.41
 H      -1.994444    -3.901939    -3.228505      25.37
 C      -4.755832    -2.035816    -2.509613     104.47
 H      -4.815495    -2.749671    -1.758419      29.39
 O      -4.832843    -0.725849    -2.013038     238.25
 H      -3.965424    -0.332615    -1.821621      31.10
 C      -5.850981    -2.243009    -3.636068      91.52
 O      -6.012545    -3.702915    -3.930468     311.52
 H      -5.873500    -3.718024    -4.924541      27.80
 H      -5.483291    -1.722096    -4.592337      25.97
 H      -6.931075    -1.891612    -3.433954      25.68
55
name = lig-ACN-frame_653
 C       3.348221     0.345857     0.484389      36.01
 H       2.448753     0.199630    -0.267895      22.69
 C       4.286184     0.163375     2.630306      71.14
 H       4.057942     0.536270     3.694568      21.56
 C       5.547214    -0.304429     2.104739      11.68
 O       6.614531    -0.778492     2.813257     212.26
 C       6.576064    -0.396072     4.233370     105.84
 H       7.608471    -0.680364     4.768645      24.98
 H       5.696715    -0.843429     4.766005      25.59
 H       6.640710     0.694689     4.336908      25.78
 C       5.752225    -0.568564     0.658740       6.77
 O       6.977106    -0.670883    -0.044402     173.52
 H       7.715612    -0.942087     0.512280      23.38
 C       4.596749    -0.217454    -0.125887      35.49
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 H       4.611135    -0.490895    -1.144917      22.99
 C       3.265282     0.628086     1.863075      32.41
 C       1.915630     1.301820     2.422050      95.24
 H       2.193291     2.365357     2.810146      25.87
 O       1.561018     0.620704     3.622356     189.33
 H       1.028928    -0.376862     3.492426      24.08
 C       0.722557     1.338589     1.438326      85.80
 H       0.818786     1.877788     0.385969      22.43
 C      -0.577589     2.001184     2.051133      92.13
 O      -0.239003     3.378346     2.677026     207.43
 H      -0.198250     4.162581     2.069225      29.98
 H      -1.166463     1.340740     2.933052      24.93
 H      -1.264085     2.539086     1.273298      23.99
 C      -2.043709    -2.401043    -0.651515      53.99
 H      -2.458334    -3.357104    -0.624638      21.88
 C      -1.784286    -0.386613    -2.031317      59.25
 H      -1.902660     0.043010    -2.996299      22.97
 C      -0.896192     0.229442    -1.049791       9.00
 O      -0.189510     1.342208    -1.478583     204.02
 C      -0.574019     2.165941    -2.673910      83.88
 H      -0.060971     3.358514    -2.545254      22.71
 H      -0.493855     1.884397    -3.767154      24.82
 H      -1.581753     2.197761    -2.477700      28.22
 C      -0.664881    -0.333009     0.223687      24.45
 O       0.370958    -0.061134     1.004542     166.99
 C      -1.285866    -1.771537     0.333990      21.05
 H      -0.798203    -2.659899     1.085843      23.55
 C      -2.319782    -1.697556    -1.806527      21.41
 C      -3.110984    -2.190516    -2.989529      75.34
 H      -2.851859    -1.328836    -3.681981      26.66
 O      -3.048136    -3.622155    -3.298634     233.19
 H      -2.111469    -3.874025    -3.082772      29.99
 C      -4.677528    -2.033609    -2.683241      76.22
 H      -4.936642    -2.729867    -1.962878      29.71
 O      -4.951768    -0.643257    -1.920397      51.93
 H      -3.974036    -0.103982    -2.222117      27.22
 C      -5.843644    -2.305436    -3.671502      98.48
 O      -5.951459    -3.637451    -3.890383     230.20
 H      -6.542241    -3.937742    -4.787344      24.67
 H      -5.665137    -1.732708    -4.659116      25.88
 H      -6.662729    -1.727735    -3.111766      25.91
55
name = lig-ACN-frame_654
 C       3.371982     0.278195     0.353551      45.39
 H       2.419433     0.267446    -0.292253      24.65
 C       4.285924     0.227192     2.625898      55.54
 H       4.356142     0.225806     3.740336      22.92
 C       5.515878    -0.253090     2.064152      11.42
 O       6.601346    -0.782111     2.850113     208.30
 C       6.705876    -0.338798     4.154704     113.97
 H       7.723162    -0.791053     4.522834      25.47
 H       5.894509    -0.724756     4.784297      27.04
 H       6.501598     0.784174     4.233347      24.84
 C       5.707250    -0.422878     0.698920      22.61
 O       6.874745    -0.749364     0.012095     173.77
 H       7.552147    -1.205209     0.516822      23.61
 C       4.612629    -0.191950    -0.123670      56.90
 H       4.816872    -0.320006    -1.173198      22.93
 C       3.084672     0.567346     1.754425     -26.79
 C       1.886133     1.291418     2.438224      83.08
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 H       2.018062     2.429469     2.530892      25.19
 O       1.535763     0.709984     3.696629     233.54
 H       1.053880    -0.136406     3.287616      26.55
 C       0.660991     1.413721     1.389438      73.01
 H       1.276582     2.052571     0.567798      24.13
 C      -0.538781     2.178246     1.961174     110.24
 O      -0.166176     3.367584     2.675663     288.41
 H      -0.489252     3.953331     2.022370      31.28
 H      -1.072365     1.458210     2.867355      25.77
 H      -1.317563     1.952837     1.112612      24.59
 C      -2.105093    -2.316898    -0.663591      59.59
 H      -2.281526    -3.370958    -0.450240      22.83
 C      -1.786890    -0.432814    -1.881585      60.95
 H      -1.715031     0.015599    -2.766911      25.66
 C      -1.036904     0.223043    -0.973576      20.61
 O      -0.124145     1.319532    -1.503816     169.53
 C      -0.668405     2.089182    -2.691786      84.37
 H       0.075526     3.108713    -2.513920      23.01
 H      -0.394833     1.468844    -3.675537      24.77
 H      -1.631009     2.465895    -2.653675      29.39
 C      -0.644206    -0.581697     0.189208      19.00
 O       0.314004    -0.040071     1.121885     126.67
 C      -1.244378    -1.747216     0.358347      54.95
 H      -0.879263    -2.425761     1.301575      24.82
 C      -2.334191    -1.676517    -1.907191      39.02
 C      -3.184340    -2.148431    -3.111896      85.67
 H      -2.947819    -1.837062    -4.177608      26.47
 O      -2.965216    -3.617629    -3.244966     233.38
 H      -2.102390    -3.700559    -3.448230      32.86
 C      -4.635287    -1.923353    -2.647796      91.95
 H      -4.708831    -2.685048    -1.893972      28.63
 O      -5.030682    -0.682345    -1.961219     151.62
 H      -4.461430     0.243057    -2.121880      28.06
 C      -5.749447    -2.109949    -3.733468      96.73
 O      -5.941006    -3.730409    -3.855871     226.31
 H      -6.729848    -3.767553    -4.474748      28.28
 H      -5.840494    -1.504477    -4.663898      27.16
 H      -6.676455    -1.957839    -3.166898      26.54
55
name = lig-ACN-frame_655
 C       3.274256     0.232043     0.313149      52.53
 H       2.736405     0.691679    -0.517203      24.88
 C       4.273793     0.282637     2.571550      73.83
 H       3.985572     0.272783     3.609307      25.49
 C       5.480017    -0.268271     2.104347      14.63
 O       6.553955    -0.771049     2.780486     198.44
 C       6.802725    -0.264094     4.221824      99.38
 H       7.861378    -0.499779     4.475314      26.05
 H       6.155436    -0.748230     4.920235      26.99
 H       6.893645     0.908680     4.245958      24.35
 C       5.660234    -0.265923     0.658939      16.51
 O       6.745901    -0.836706     0.071337     165.87
 H       7.408957    -1.168124     0.792169      21.25
 C       4.560676    -0.127217    -0.182849      41.31
 H       4.664416    -0.158975    -1.296532      22.24
 C       3.157703     0.484963     1.684679      22.64
 C       1.876350     1.265783     2.280070      77.39
 H       2.396272     2.150036     2.672351      26.05
 O       1.464690     0.758948     3.757284     191.55
 H       1.235507    -0.085533     3.875051      31.82
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 C       0.696746     1.404579     1.395500      98.45
 H       0.832689     1.692591     0.246191      23.20
 C      -0.539406     2.155820     1.929510      98.22
 O      -0.142562     3.394246     2.580688     214.63
 H      -0.299384     4.388156     2.288098      28.39
 H      -0.906365     1.332941     2.824802      25.00
 H      -1.319252     2.667341     1.278248      24.83
 C      -2.093673    -2.375728    -0.646435      48.19
 H      -2.537777    -3.455329    -0.630026      24.61
 C      -1.807020    -0.309814    -2.027009      63.10
 H      -2.052119     0.200994    -2.836349      24.29
 C      -0.912560     0.249209    -0.981885      25.42
 O      -0.187989     1.263950    -1.443725     233.82
 C      -0.644728     2.015129    -2.599000      92.10
 H       0.108062     2.858300    -2.964628      24.57
 H      -0.644896     1.214896    -3.542284      24.56
 H      -1.673525     2.293853    -2.573719      28.46
 C      -0.566273    -0.444758     0.158794      11.83
 O       0.261531    -0.033755     1.243818     119.03
 C      -1.246658    -1.841838     0.360551      30.28
 H      -1.254615    -2.173346     1.461217      21.05
 C      -2.335275    -1.644757    -1.915203      16.87
 C      -3.200668    -2.184872    -3.101576      83.90
 H      -2.921546    -1.511908    -4.000532      27.44
 O      -2.913294    -3.598579    -3.210240     199.77
 H      -2.074719    -3.594204    -3.853811      26.77
 C      -4.698882    -1.874687    -2.677283     101.10
 H      -4.884032    -2.664521    -1.915431      29.46
 O      -5.082094    -0.689547    -2.000188     243.08
 H      -4.507602    -0.076733    -2.197695      37.79
 C      -5.778176    -2.181610    -3.679316     108.98
 O      -5.905217    -3.629229    -3.832912     289.44
 H      -6.258034    -3.862210    -4.639268      30.94
 H      -5.317954    -1.843822    -4.613269      27.48
 H      -6.662834    -1.572601    -3.458841      27.67
55
name = lig-ACN-frame_656
 C       3.230254     0.318124     0.246681      66.86
 H       2.312948     0.488668    -0.223309      24.35
 C       4.182209     0.246429     2.574864      62.66
 H       4.078632     0.576445     3.562521      23.37
 C       5.425430    -0.204244     2.053992       5.81
 O       6.546603    -0.717521     2.835278     199.95
 C       6.934824    -0.208846     4.179374     106.77
 H       7.917144    -0.569675     4.297394      26.90
 H       6.231972    -0.540213     4.910328      27.69
 H       6.644559     0.968538     4.229630      24.95
 C       5.558456    -0.300255     0.639752       9.57
 O       6.698372    -0.925783     0.125503     100.07
 H       7.449678    -0.916365     0.832815      20.68
 C       4.474891    -0.006293    -0.278816      53.31
 H       4.767585    -0.231445    -1.361335      21.89
 C       3.124038     0.473567     1.664906      30.35
 C       1.980191     1.166063     2.312345      87.24
 H       2.117723     2.240719     2.344977      27.27
 O       1.433445     0.829600     3.707176     211.00
 H       1.442572    -0.150128     3.586838      28.91
 C       0.642998     1.293965     1.309566      78.37
 H       1.019858     1.852647     0.345299      22.37
 C      -0.542252     2.226509     1.942386      89.77
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 O      -0.056896     3.452915     2.598660     285.70
 H      -0.292665     3.920409     1.726235      27.87
 H      -1.334170     1.725714     2.763210      25.40
 H      -1.174755     2.143710     0.980858      24.87
 C      -1.996431    -2.346469    -0.741750      50.40
 H      -2.614517    -3.356435    -0.605573      19.70
 C      -1.835482    -0.313017    -2.073437      66.21
 H      -2.231015     0.264826    -2.868370      23.20
 C      -0.838187     0.128279    -1.162299       0.32
 O      -0.166028     1.387555    -1.346839     192.26
 C      -0.600027     1.919427    -2.579030      98.62
 H       0.025014     2.806044    -2.612565      26.42
 H      -0.700341     1.260107    -3.653340      23.70
 H      -1.516376     2.412712    -2.273843      26.95
 C      -0.634422    -0.493919     0.237648      15.29
 O       0.152127    -0.071939     1.288289     155.74
 C      -1.264877    -1.700984     0.308757      55.06
 H      -1.141795    -2.342834     1.161185      25.72
 C      -2.290371    -1.577738    -1.822522      42.93
 C      -3.190320    -2.110794    -2.898941      69.76
 H      -3.057277    -1.532009    -3.879255      26.17
 O      -2.898691    -3.552414    -3.247783     131.14
 H      -1.937332    -3.764488    -3.853228      23.94
 C      -4.806350    -2.071321    -2.592045      76.06
 H      -5.013662    -2.816229    -1.749744      27.06
 O      -5.078227    -0.617212    -2.038890     152.73
 H      -4.205518    -0.121090    -2.018909      31.71
 C      -5.728066    -2.203581    -3.837153     104.49
 O      -5.931097    -3.582019    -3.805376     321.44
 H      -5.753111    -3.863878    -4.779053      27.13
 H      -5.307604    -1.845364    -4.770117      26.48
 H      -6.686437    -1.710802    -3.725011      26.24
55
name = lig-ACN-frame_657
 C       3.180954     0.410911     0.265574      41.39
 H       2.461155     0.212035    -0.433941      24.92
 C       4.190280     0.221957     2.589083      66.90
 H       4.174778     0.380999     3.633567      23.32
 C       5.405086    -0.167365     2.056020       9.16
 O       6.504125    -0.637079     2.822762     218.01
 C       6.932584    -0.132174     4.082018     116.71
 H       7.918777    -0.354925     4.217639      27.83
 H       6.444929    -0.613600     4.898936      26.75
 H       7.074275     1.081362     4.137680      24.69
 C       5.487441    -0.430066     0.616132       4.40
 O       6.651357    -0.973344     0.142834     174.25
 H       7.340912    -1.009970     0.788431      22.81
 C       4.481359     0.038549    -0.293008      44.47
 H       4.504469    -0.110847    -1.427128      23.07
 C       3.049347     0.506211     1.708165      20.99
 C       1.773396     1.260155     2.295613     113.40
 H       2.192275     2.232426     2.455759      28.02
 O       1.507216     0.825023     3.554786     212.82
 H       1.179342    -0.233370     3.723125      25.13
 C       0.621200     1.229900     1.495909     108.59
 H       0.931576     1.507222     0.473363      24.79
 C      -0.486903     2.187080     1.914216     103.93
 O      -0.028009     3.502795     2.481609     265.70
 H       0.404809     4.113773     1.971290      33.13
 H      -1.057426     1.522947     2.777185      25.74
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 H      -1.151199     2.689122     1.197763      25.56
 C      -1.921165    -2.299557    -0.716480      41.33
 H      -2.058376    -3.475002    -0.600340      21.34
 C      -1.741919    -0.311140    -1.992801      56.86
 H      -1.930299     0.305116    -2.972136      21.34
 C      -0.734298     0.150929    -1.104344      35.19
 O      -0.134184     1.376683    -1.284155     243.33
 C      -0.562656     2.121825    -2.545257      86.44
 H       0.122606     2.791598    -2.854677      27.85
 H      -0.352746     1.156005    -3.302936      23.84
 H      -1.641982     2.351465    -2.795064      25.94
 C      -0.735465    -0.481191     0.068580      20.54
 O       0.021660    -0.115443     1.222412     130.14
 C      -1.287420    -1.757613     0.362154      65.41
 H      -0.899006    -2.225549     1.161691      28.03
 C      -2.373813    -1.578121    -1.886632      42.42
 C      -3.329500    -2.181240    -2.838964      89.82
 H      -3.218849    -1.446260    -3.722261      26.85
 O      -2.916483    -3.492064    -3.277950     217.76
 H      -1.941662    -3.213492    -3.451812      27.68
 C      -4.781639    -1.978394    -2.482581      95.31
 H      -5.293990    -2.771831    -1.798858      26.97
 O      -5.029977    -0.640124    -2.124490     134.49
 H      -4.164058    -0.355916    -1.376696      25.87
 C      -5.622788    -2.138777    -3.890507      73.06
 O      -5.993799    -3.716031    -3.867843     243.81
 H      -5.993925    -4.299232    -4.789803      24.70
 H      -5.140655    -1.724404    -4.725486      27.29
 H      -6.529877    -1.607637    -3.733205      26.94
55
name = lig-ACN-frame_658
 C       3.241788     0.401523     0.339054      66.88
 H       2.514272     0.914488    -0.216036      24.08
 C       4.105453     0.280804     2.556990      67.51
 H       3.825645     0.194404     3.612065      23.15
 C       5.346737    -0.220251     2.017992      14.86
 O       6.475728    -0.579359     2.709179     199.81
 C       6.958726    -0.043288     4.036438      99.57
 H       7.920777    -0.350197     3.979512      26.95
 H       6.350395    -0.411342     4.866546      26.99
 H       6.628292     1.128459     4.141995      24.84
 C       5.487398    -0.442175     0.627119      19.35
 O       6.626155    -1.031298     0.092903     150.87
 H       7.151733    -1.301964     0.872770      23.36
 C       4.442761    -0.020874    -0.173513      63.46
 H       4.656801    -0.088539    -1.253437      24.61
 C       3.022181     0.590888     1.706953      27.17
 C       1.810914     1.249952     2.294597      98.15
 H       1.872887     2.310969     2.360829      27.01
 O       1.548494     0.736415     3.656420     235.14
 H       1.040947    -0.125399     3.389918      27.40
 C       0.475857     1.262068     1.312567      98.87
 H       0.829589     1.663560     0.419213      24.62
 C      -0.505936     2.293225     1.909405     111.91
 O       0.022633     3.518616     2.423768     276.00
 H       0.745143     3.609189     1.738316      30.32
 H      -1.035455     1.915148     2.909850      26.17
 H      -1.231906     2.131949     1.117443      27.29
 C      -2.002636    -2.439696    -0.678118      46.43
 H      -2.338615    -3.515827    -0.863488      22.12
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 C      -1.677440    -0.350884    -2.043593      49.95
 H      -1.948479     0.244251    -3.079645      23.64
 C      -0.814116     0.269192    -1.117541      15.26
 O      -0.122567     1.480597    -1.304001     200.46
 C      -0.415724     2.195248    -2.553580      93.68
 H       0.041798     3.032413    -2.374114      28.78
 H      -0.192091     1.635136    -3.667541      24.31
 H      -1.508486     2.548096    -2.320043      25.60
 C      -0.678631    -0.465610     0.189944      14.47
 O      -0.039737    -0.108184     1.268239     174.55
 C      -1.219599    -1.802065     0.335725      62.03
 H      -1.091908    -2.248421     1.245787      24.62
 C      -2.327736    -1.591272    -1.787833       9.47
 C      -3.363098    -2.124068    -2.920859      73.09
 H      -3.297113    -1.436154    -3.840266      26.82
 O      -2.937176    -3.445232    -3.295786     247.52
 H      -2.089914    -3.514820    -3.438525      33.34
 C      -4.878279    -1.985896    -2.587641      99.91
 H      -5.111894    -2.621249    -1.626813      26.62
 O      -4.953689    -0.590982    -2.144329     120.05
 H      -4.712028    -0.591319    -1.070326      27.44
 C      -5.611092    -2.311044    -3.794725     117.58
 O      -6.008211    -3.680108    -3.935771     280.09
 H      -6.425306    -3.589659    -4.854523      26.26
 H      -4.921768    -2.231011    -4.566550      24.71
 H      -6.403052    -1.633320    -3.957258      27.79
55
name = lig-ACN-frame_659
 C       3.222391     0.537027     0.328492      47.46
 H       2.669048     1.059507    -0.482813      23.38
 C       4.076025     0.245612     2.580825      68.93
 H       4.093798     0.445463     3.706056      21.77
 C       5.252461    -0.246603     2.053225      16.69
 O       6.512689    -0.553168     2.674998     238.03
 C       6.856394     0.016858     3.928020     120.14
 H       7.912911     0.046217     4.124581      27.30
 H       6.442817    -0.587165     4.746842      28.36
 H       6.659310     1.169090     3.994649      27.50
 C       5.494999    -0.453795     0.660399      12.67
 O       6.597813    -1.083725     0.058591     150.86
 H       7.326797    -1.409264     0.732068      21.30
 C       4.422716    -0.127164    -0.190274      48.77
 H       4.539454    -0.117513    -1.247316      23.09
 C       3.057957     0.658662     1.720326      34.44
 C       1.783471     1.247241     2.298774      91.56
 H       2.131756     2.205494     2.628850      24.42
 O       1.528530     0.635764     3.711247     236.32
 H       1.177189    -0.170974     3.706043      30.87
 C       0.539307     1.339419     1.330953      83.57
 H       0.709661     1.550023     0.370704      23.36
 C      -0.674126     2.301484     1.933567     105.40
 O       0.101279     3.527226     2.293472     256.68
 H       0.584951     4.090881     1.493714      26.25
 H      -1.125220     1.766242     2.756558      27.70
 H      -1.447930     2.782876     1.383217      25.87
 C      -2.101983    -2.439237    -0.680605      54.10
 H      -2.644976    -3.251723    -0.273734      23.98
 C      -1.655913    -0.399984    -2.065575      42.70
 H      -1.982593     0.142440    -3.097337      24.36
 C      -0.928123     0.256062    -1.055458       1.42
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 O      -0.106317     1.509876    -1.368303     186.81
 C      -0.348706     2.386794    -2.466399     105.06
 H       0.236318     3.167566    -2.346219      28.07
 H       0.073312     1.996667    -3.541585      25.62
 H      -1.509508     2.649979    -2.761032      25.17
 C      -0.721708    -0.558769     0.143410      -0.41
 O      -0.003958     0.018579     1.420972      87.27
 C      -1.206166    -1.859090     0.249340      54.45
 H      -1.022445    -2.329464     1.207317      24.91
 C      -2.322828    -1.622938    -1.841372      31.73
 C      -3.163099    -2.007832    -2.925182      74.27
 H      -2.962256    -1.342780    -3.818486      27.01
 O      -3.028080    -3.475076    -3.323014     150.16
 H      -2.044716    -3.508430    -3.696061      26.77
 C      -4.781544    -2.055030    -2.524193      57.81
 H      -5.089002    -2.840839    -1.702368      26.59
 O      -4.960620    -0.515530    -2.152615     181.86
 H      -5.079685    -0.523916    -1.298707      33.14
 C      -5.624701    -2.358947    -3.894724     102.87
 O      -6.110429    -3.687040    -3.977545     317.13
 H      -6.592289    -3.910877    -4.698655      31.95
 H      -4.977709    -2.053245    -4.655950      27.51
 H      -6.420304    -1.652158    -3.972286      27.69
55
name = lig-ACN-frame_660
 C       3.310971     0.635788     0.247865      55.23
 H       2.361537     0.720629    -0.412097      23.45
 C       4.138867     0.212234     2.631238      43.33
 H       3.975371     0.527919     3.740168      19.88
 C       5.375985    -0.307290     2.040973       5.72
 O       6.537392    -0.541364     2.658405     217.38
 C       6.770908     0.085709     3.929579     104.53
 H       7.885439     0.103913     3.876967      24.52
 H       6.346180    -0.509912     4.770887      26.80
 H       6.167040     1.036375     4.035782      26.80
 C       5.398398    -0.556146     0.607734      14.79
 O       6.561484    -1.117849     0.056699     181.27
 H       7.240234    -1.043616     0.768256      23.53
 C       4.371592    -0.114445    -0.246989      61.14
 H       4.475521    -0.417798    -1.246753      23.35
 C       3.028703     0.676216     1.696127     -15.81
 C       1.749828     1.299234     2.469215      93.02
 H       1.888638     2.339724     2.745470      25.14
 O       1.479145     0.588979     3.681667     250.19
 H       1.417442    -0.373321     3.424218      27.03
 C       0.481440     1.422783     1.512722      83.00
 H       0.979047     1.778314     0.673966      24.80
 C      -0.589379     2.396303     1.879668     130.69
 O       0.122084     3.573304     2.252837     325.66
 H      -0.001833     4.033438     1.396526      29.98
 H      -0.975342     2.031777     2.772876      28.04
 H      -1.299417     2.389409     1.083781      27.42
 C      -2.158287    -2.302814    -0.644754      61.42
 H      -2.657729    -3.214015    -0.648888      27.78
 C      -1.656855    -0.389425    -2.025890      57.18
 H      -1.619483     0.187532    -3.026223      21.30
 C      -0.876827     0.266052    -1.041439      23.62
 O      -0.176318     1.369931    -1.324133     195.84
 C      -0.318989     2.573040    -2.485784      71.34
 H       0.152081     3.405972    -2.037177      26.36
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 H       0.202186     1.938230    -3.226357      24.28
 H      -1.457180     2.860525    -2.752352      24.52
 C      -0.622539    -0.428889     0.209114       7.57
 O      -0.086258    -0.047030     1.349456     138.01
 C      -1.214727    -1.837752     0.300422      32.82
 H      -0.872790    -2.545726     1.151115      21.52
 C      -2.253578    -1.652492    -1.873123      35.74
 C      -3.232436    -2.157430    -2.996563      95.86
 H      -3.160319    -1.416210    -3.847280      26.47
 O      -3.065306    -3.465319    -3.366500     205.20
 H      -2.145696    -3.719185    -3.985652      24.43
 C      -4.600130    -1.913086    -2.626366      86.98
 H      -4.818900    -2.636267    -1.755999      26.04
 O      -5.014076    -0.597438    -2.209428     185.45
 H      -5.229503    -0.453649    -1.226810      27.88
 C      -5.596696    -2.217611    -3.962606      71.50
 O      -6.232498    -3.774956    -3.938409     249.34
 H      -6.070360    -3.894714    -4.916586      25.87
 H      -5.182531    -2.055772    -4.892621      26.07
 H      -6.435648    -1.630035    -3.673392      25.66
55
name = lig-ACN-frame_661
 C       3.224709     0.593845     0.335572      42.34
 H       2.353557     0.987120    -0.384301      20.74
 C       4.159370     0.248798     2.474923      63.80
 H       4.056583     0.054225     3.580626      21.00
 C       5.294521    -0.305004     1.941644       4.15
 O       6.583958    -0.569647     2.650539     202.48
 C       6.700861     0.138024     3.982623     107.24
 H       7.783245     0.516826     4.254903      25.29
 H       6.402540    -0.534296     4.829200      27.83
 H       6.200347     1.053179     3.927823      30.67
 C       5.353201    -0.627384     0.582752      19.73
 O       6.519351    -1.149031     0.071171     196.84
 H       7.220274    -1.025037     0.688653      24.59
 C       4.353726    -0.113284    -0.283225      51.54
 H       4.370396    -0.313372    -1.340481      23.04
 C       3.127412     0.705880     1.738212      28.06
 C       1.747248     1.309096     2.529999      96.25
 H       1.977114     2.345833     2.847793      24.03
 O       1.435388     0.531811     3.689940     234.93
 H       1.322550    -0.550587     3.349286      22.01
 C       0.579687     1.311991     1.600967      98.12
 H       0.811565     1.702106     0.612442      21.91
 C      -0.539533     2.383317     1.941085     114.40
 O       0.039851     3.707989     2.221317     328.61
 H       0.435097     4.292155     1.606251      31.73
 H      -1.274542     2.233756     2.628935      28.03
 H      -1.138715     2.518759     1.068133      26.34
 C      -2.118218    -2.238686    -0.626960      45.09
 H      -2.277272    -3.262346    -0.501704      27.47
 C      -1.617937    -0.360166    -2.061569      57.81
 H      -1.718525     0.108998    -3.014996      22.49
 C      -0.830238     0.183019    -1.057034      13.94
 O      -0.176617     1.441940    -1.262107     172.25
 C      -0.307574     2.512315    -2.394502      93.00
 H       0.164339     3.269473    -1.685449      24.76
 H       0.147146     2.676711    -3.301178      26.94
 H      -1.439601     2.723286    -2.489740      25.53
 C      -0.718064    -0.502515     0.172550      27.28
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 O      -0.042367     0.033123     1.367004     162.18
 C      -1.244149    -1.680140     0.347524      45.79
 H      -0.967102    -2.235179     1.388084      19.70
 C      -2.244187    -1.587146    -1.944966      24.06
 C      -3.127898    -2.083581    -3.120991      73.30
 H      -2.755268    -1.620608    -4.051481      25.41
 O      -3.094079    -3.589656    -3.446194     223.28
 H      -2.188052    -3.539225    -3.893817      27.37
 C      -4.747408    -1.925000    -2.797403      76.50
 H      -5.009835    -2.730654    -2.028431      24.46
 O      -5.046559    -0.611884    -2.294903     137.03
 H      -4.838665    -0.907378    -1.190897      24.14
 C      -5.688548    -2.273826    -3.840884     114.57
 O      -6.221364    -3.639550    -3.894231     267.88
 H      -5.937371    -4.194733    -4.807723      25.12
 H      -5.244562    -2.091294    -4.760729      26.70
 H      -6.541069    -1.582032    -3.926121      26.02
55
name = lig-ACN-frame_662
 C       3.152200     0.498875     0.363585      48.52
 H       2.580358     1.197028    -0.395180      21.61
 C       4.185040     0.233145     2.528117      37.28
 H       4.106142     0.303725     3.597582      20.08
 C       5.385326    -0.338524     1.906064      -0.12
 O       6.540180    -0.554935     2.674418     217.47
 C       6.637569     0.172691     3.965697      87.01
 H       7.828439     0.270335     4.044108      23.75
 H       6.188666    -0.483891     4.758982      27.07
 H       6.099465     0.972580     3.929601      32.50
 C       5.378203    -0.583303     0.504532      14.43
 O       6.510252    -1.218330     0.021389     159.02
 H       7.156661    -1.307744     0.816231      21.44
 C       4.236706    -0.113687    -0.231168      60.82
 H       4.372235     0.025623    -1.324339      22.74
 C       3.053161     0.784491     1.762481      29.78
 C       1.877241     1.178391     2.481970      95.52
 H       2.022834     2.207054     2.966501      23.10
 O       1.440410     0.482481     3.747969     212.50
 H       0.990645    -0.508554     3.667369      22.38
 C       0.601281     1.376331     1.508283      84.73
 H       1.152264     1.656023     0.541034      21.18
 C      -0.552283     2.454644     1.942864     105.06
 O      -0.050321     3.837483     2.284376     309.53
 H       0.637156     3.676422     1.599273      29.71
 H      -0.982734     2.026846     2.769218      26.97
 H      -1.130685     2.450264     1.000593      25.54
 C      -2.015793    -2.302122    -0.702368      54.50
 H      -2.624909    -3.192818    -0.485078      22.50
 C      -1.587535    -0.335376    -2.208982      49.43
 H      -1.752507     0.289400    -2.972218      24.58
 C      -0.755819     0.270265    -1.161737       4.44
 O      -0.100023     1.492616    -1.203438     239.00
 C      -0.373185     2.456092    -2.123880     120.77
 H      -0.065310     3.613160    -1.916665      23.75
 H       0.137646     2.006781    -2.886159      27.00
 H      -1.446023     2.553826    -2.410591      26.83
 C      -0.673039    -0.298889     0.205469     -12.61
 O       0.006374     0.036201     1.422201     137.75
 C      -1.396501    -1.656639     0.391308      10.53
 H      -1.448116    -2.113412     1.548325      22.72
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 C      -2.304421    -1.609315    -1.952119      20.96
 C      -3.126019    -2.103255    -3.199226      73.69
 H      -2.891471    -1.410701    -4.013759      25.71
 O      -3.048565    -3.633346    -3.507927     246.65
 H      -2.284142    -3.995898    -3.674128      31.86
 C      -4.752445    -2.018523    -2.839719      64.59
 H      -4.773662    -2.757099    -2.022073      25.82
 O      -5.072217    -0.618295    -2.306282     164.82
 H      -4.454652    -0.310828    -1.518438      28.64
 C      -5.834961    -2.249358    -4.039288     102.45
 O      -6.211782    -3.577732    -3.790666     317.76
 H      -6.097491    -4.035694    -4.628902      29.41
 H      -5.357434    -2.093481    -4.954337      26.83
 H      -6.700627    -1.587028    -3.753599      24.94
55
name = lig-ACN-frame_663
 C       3.124865     0.530851     0.367154      43.84
 H       2.223977     0.781358    -0.274922      21.19
 C       4.205955     0.242508     2.558050      47.89
 H       4.188138     0.484828     3.550814      21.10
 C       5.325500    -0.271401     1.960355      17.76
 O       6.480505    -0.561335     2.662328     255.50
 C       6.606339     0.134255     3.891149     120.93
 H       7.766947     0.161222     4.163095      24.88
 H       6.089060    -0.320185     4.768878      28.61
 H       6.381505     1.067595     3.849845      34.10
 C       5.403965    -0.532453     0.540993      13.34
 O       6.501377    -1.282060    -0.081097     155.46
 H       7.106477    -1.537425     0.710579      22.21
 C       4.273408    -0.129319    -0.218525      53.47
 H       4.317751    -0.241196    -1.355952      22.45
 C       3.125390     0.577408     1.781800      24.84
 C       1.769067     1.176077     2.552754      91.02
 H       2.135674     2.252967     2.830917      23.15
 O       1.487669     0.488007     3.779958     294.74
 H       1.276217    -0.379949     3.516166      29.05
 C       0.650866     1.535937     1.507237      70.97
 H       0.991402     1.948024     0.468594      17.93
 C      -0.469330     2.451013     1.970611     109.58
 O      -0.121418     3.816525     2.289531     288.54
 H       0.603553     4.501812     1.993083      28.47
 H      -0.847470     2.111990     2.848915      27.04
 H      -1.494420     2.426491     1.395157      24.26
 C      -2.067424    -2.271729    -0.800792      38.22
 H      -2.697043    -3.211299    -0.626108      21.10
 C      -1.534287    -0.301507    -2.176842      45.84
 H      -1.691660     0.033870    -3.099952      24.84
 C      -0.752431     0.294199    -1.107141      -6.02
 O      -0.011854     1.480688    -1.015627     203.18
 C      -0.471410     2.427819    -2.132561     102.72
 H       0.121336     3.458073    -1.667489      21.24
 H      -0.114496     2.362777    -3.113594      27.64
 H      -1.527017     2.411600    -2.173335      27.73
 C      -0.737236    -0.381082     0.242903      17.36
 O      -0.001941     0.057574     1.342283     128.26
 C      -1.457818    -1.477289     0.324844      44.68
 H      -1.584689    -2.024320     1.407216      23.25
 C      -2.192509    -1.590201    -2.026511      19.38
 C      -3.240206    -2.240214    -3.184375      91.43
 H      -3.050444    -1.721586    -4.131242      24.75
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 O      -3.028403    -3.577298    -3.531536     280.38
 H      -2.025461    -3.438029    -3.614744      25.78
 C      -4.667676    -1.925818    -2.836684      86.57
 H      -5.113999    -2.662522    -2.205641      25.73
 O      -5.056495    -0.666542    -2.335148     277.79
 H      -4.308631    -0.249028    -2.258323      36.10
 C      -5.801013    -2.107300    -4.084984      71.52
 O      -6.283353    -3.676711    -3.749243     228.44
 H      -6.461305    -4.071145    -4.577425      30.18
 H      -5.733993    -2.060136    -5.147203      26.21
 H      -6.694245    -1.406866    -3.941732      25.52
55
name = lig-ACN-frame_664
 C       3.195088     0.418236     0.385626      49.02
 H       2.309550     0.385349    -0.193850      22.10
 C       4.154724     0.294316     2.593778      50.43
 H       4.178720     0.265497     3.683919      18.13
 C       5.371533    -0.260382     1.920677       6.02
 O       6.472031    -0.603436     2.638403     253.22
 C       6.669241     0.123955     3.913907     102.74
 H       7.717555    -0.193296     4.266359      24.53
 H       5.876521    -0.240802     4.571940      29.10
 H       6.517641     1.080819     3.772224      33.43
 C       5.408618    -0.548173     0.541492      20.17
 O       6.402728    -1.271352    -0.104467     218.11
 H       7.168291    -1.437615     0.414743      27.18
 C       4.345098    -0.121472    -0.248516      53.32
 H       4.259351    -0.622106    -1.260347      23.31
 C       2.950471     0.485174     1.806306      25.00
 C       1.827140     1.260648     2.522984      92.32
 H       2.194598     2.276789     2.982668      23.06
 O       1.522387     0.547191     3.756780     294.53
 H       1.404779    -0.355511     3.655960      29.67
 C       0.639173     1.507600     1.591444      69.72
 H       1.217962     1.959647     0.694483      20.48
 C      -0.459010     2.454997     2.123919     104.18
 O      -0.188060     3.851020     2.357686     263.76
 H       0.243831     4.017605     1.428717      27.90
 H      -0.675782     2.056175     3.036671      26.41
 H      -1.223984     2.370556     1.145629      21.51
 C      -2.176803    -2.103157    -0.818733      33.71
 H      -2.466129    -3.210487    -0.626318      18.96
 C      -1.468700    -0.297096    -2.132475      59.83
 H      -1.208782     0.349975    -2.912088      19.25
 C      -0.773286     0.246792    -1.000921      16.72
 O      -0.021335     1.462004    -1.067389     240.99
 C      -0.502345     2.443284    -2.075980     108.37
 H      -0.168726     3.605707    -1.655983      22.77
 H      -0.240362     2.216970    -3.079191      26.07
 H      -1.506936     2.515795    -1.928987      29.28
 C      -0.757786    -0.364697     0.182630      10.82
 O      -0.004403     0.166885     1.225587     152.19
 C      -1.600083    -1.605031     0.285358      59.86
 H      -1.534453    -2.056576     1.343104      24.17
 C      -2.127998    -1.581489    -2.134239      43.80
 C      -3.208038    -2.113894    -3.181406      74.19
 H      -2.991353    -1.431062    -4.010590      26.33
 O      -2.988237    -3.552760    -3.481075     209.78
 H      -2.142453    -3.859574    -4.168628      23.82
 C      -4.854219    -1.959024    -2.957313      88.20
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 H      -5.048457    -2.625274    -2.157942      27.57
 O      -4.955695    -0.613193    -2.327543     192.40
 H      -4.263280     0.032853    -2.689307      29.03
 C      -5.793654    -2.263732    -4.007827     101.22
 O      -6.330135    -3.605005    -3.776858     231.70
 H      -6.715236    -3.959921    -4.721955      28.35
 H      -5.176228    -2.123289    -4.914694      27.04
 H      -6.593843    -1.498016    -3.746295      25.25
55
name = lig-ACN-frame_665
 C       3.106150     0.209768     0.392763      60.48
 H       2.466372     0.599837    -0.290672      23.46
 C       4.141909     0.223297     2.525006      51.49
 H       3.988414     0.392907     3.656123      20.76
 C       5.342209    -0.235364     1.945701       5.65
 O       6.543626    -0.640062     2.652130     244.75
 C       6.714027     0.035555     3.926587     135.67
 H       7.669661    -0.311325     4.295674      25.72
 H       5.969697    -0.112327     4.693038      29.31
 H       6.862997     1.062317     3.831230      29.95
 C       5.404107    -0.536230     0.538933      21.93
 O       6.363153    -1.271457    -0.111542     187.09
 H       7.141043    -1.111914     0.477701      25.22
 C       4.298506    -0.188455    -0.228497      51.83
 H       4.336636    -0.249151    -1.340710      23.48
 C       3.035468     0.543083     1.768295      35.86
 C       1.866754     1.193282     2.506846     101.02
 H       2.216722     2.300821     2.566928      24.27
 O       1.536771     0.645368     3.787466     255.28
 H       1.188357    -0.340641     3.503542      24.03
 C       0.641108     1.486052     1.601931      81.14
 H       0.918003     2.022571     0.650642      20.62
 C      -0.547191     2.383839     2.278301      88.56
 O      -0.177679     3.864925     2.346325     264.05
 H      -0.041343     4.290909     1.520628      31.06
 H      -1.034460     2.021466     3.216067      25.31
 H      -1.594636     2.243939     1.574111      22.62
 C      -2.292534    -2.123931    -0.863741       7.79
 H      -3.037852    -3.030129    -0.889193      23.23
 C      -1.373015    -0.281143    -2.216260      44.86
 H      -1.538993     0.118113    -3.265214      22.87
 C      -0.796012     0.289454    -1.112533      10.08
 O      -0.061193     1.425808    -1.208161     252.31
 C      -0.588654     2.481331    -1.962021     121.10
 H       0.191468     3.441913    -1.846987      22.75
 H      -0.259649     2.227871    -2.976303      26.06
 H      -1.585708     2.567459    -2.079581      28.53
 C      -0.809122    -0.352384     0.290213       8.00
 O       0.013528     0.207620     1.244569     171.25
 C      -1.525762    -1.578594     0.414562      41.84
 H      -1.679990    -2.300613     1.178805      23.13
 C      -2.225635    -1.464478    -2.117890      27.40
 C      -3.110095    -1.986873    -3.291046      67.02
 H      -3.056078    -1.513780    -4.273246      26.43
 O      -3.042972    -3.506892    -3.406135     174.21
 H      -2.176971    -3.582527    -4.113069      23.47
 C      -4.698965    -1.965963    -2.755226      62.71
 H      -4.888834    -2.551164    -1.933901      26.83
 O      -4.903806    -0.529986    -2.334044      65.77
 H      -4.324972    -0.000516    -3.185992      27.66
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 C      -5.792519    -2.333876    -4.002321      90.76
 O      -6.403315    -3.583496    -3.850216     239.57
 H      -6.674735    -3.844420    -4.818161      28.90
 H      -5.335615    -2.416137    -5.051005      24.42
 H      -6.578041    -1.559369    -4.306508      24.48
55
name = lig-ACN-frame_666
 C       2.950600     0.185878     0.318929      53.29
 H       2.097448     0.496354    -0.156335      20.51
 C       4.200384     0.165163     2.542628      63.71
 H       4.259970     0.500747     3.665991      21.95
 C       5.418255    -0.326637     1.961286      14.81
 O       6.544797    -0.642658     2.660166     260.81
 C       6.834755    -0.048804     3.965431     120.80
 H       7.649202    -0.540999     4.338347      26.31
 H       5.959155    -0.208057     4.556911      29.88
 H       6.960281     0.994214     3.823962      29.61
 C       5.343125    -0.541035     0.567221      12.14
 O       6.441867    -1.246188    -0.067650     166.42
 H       7.360660    -1.299191     0.419589      23.59
 C       4.181739    -0.278560    -0.236359      58.83
 H       4.423725    -0.161977    -1.277070      23.34
 C       3.099798     0.507315     1.681532      18.61
 C       1.833797     1.253388     2.414784      80.77
 H       2.225335     2.220397     2.861187      23.73
 O       1.555026     0.723584     3.786070     203.38
 H       1.038272    -0.288407     3.862103      22.87
 C       0.472167     1.527361     1.608430      83.01
 H       0.738368     2.078135     0.730962      21.63
 C      -0.602176     2.384591     2.335733      93.06
 O      -0.181768     3.768200     2.388414     229.83
 H      -0.175348     4.228955     1.470074      28.67
 H      -0.446404     2.264793     3.462820      23.08
 H      -1.687673     2.273793     1.706412      21.62
 C      -2.282784    -2.021355    -0.756376      61.86
 H      -3.048601    -2.793648    -0.445912      21.89
 C      -1.455598    -0.352501    -2.350877      33.39
 H      -1.261606     0.305219    -3.352322      20.36
 C      -0.820525     0.225655    -1.108345       6.02
 O      -0.059393     1.401964    -1.234774     203.27
 C      -0.592418     2.554465    -2.087476     104.19
 H      -0.171680     3.438372    -1.445650      23.34
 H      -0.540755     2.647020    -3.198227      25.16
 H      -1.503007     2.675756    -1.644521      27.64
 C      -0.859478    -0.299344     0.175015       2.53
 O       0.007592     0.095748     1.354538     135.10
 C      -1.554168    -1.580776     0.284366      51.82
 H      -1.427073    -1.831983     1.245143      23.87
 C      -2.298508    -1.369369    -2.061524      28.00
 C      -3.203517    -2.047763    -3.204476      91.56
 H      -2.958985    -1.493323    -4.129538      25.49
 O      -3.075304    -3.394175    -3.380965     291.65
 H      -2.138877    -3.666954    -3.438871      28.34
 C      -4.543865    -1.790692    -2.731092      84.40
 H      -4.676613    -2.428338    -1.934203      25.77
 O      -4.877910    -0.492284    -2.377196     191.26
 H      -4.684718     0.121735    -3.188963      28.02
 C      -5.652390    -2.254851    -4.033658      40.01
 O      -6.534143    -3.677755    -3.896025     237.80
 H      -6.492349    -4.066427    -4.715047      32.14
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 H      -4.880383    -2.331364    -4.925279      24.63
 H      -6.296434    -1.367083    -3.880399      24.35
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name = lig-ACN-frame_667
 C       2.977804     0.225918     0.318996      35.76
 H       2.119245     0.103841    -0.341808      22.11
 C       4.221725     0.215322     2.511002      41.09
 H       4.114960     0.453720     3.633174      19.63
 C       5.351993    -0.390738     1.964457       5.34
 O       6.616709    -0.682486     2.642027     240.40
 C       6.884134    -0.145974     3.981326     121.70
 H       7.702973    -0.618931     4.249955      28.25
 H       6.115505    -0.232808     4.704407      31.13
 H       7.198063     0.943027     3.994856      28.38
 C       5.354697    -0.664854     0.520381       5.68
 O       6.490137    -1.179612    -0.040078     165.20
 H       7.053508    -1.165354     0.772821      21.33
 C       4.168814    -0.357385    -0.269812      48.46
 H       4.094678    -0.812361    -1.236117      23.07
 C       2.919242     0.478261     1.768250      24.84
 C       1.824354     1.311773     2.431519      92.50
 H       2.154659     2.386980     2.384179      24.52
 O       1.560846     0.781690     3.772521     238.34
 H       1.338922    -0.187548     3.459020      25.13
 C       0.397700     1.456623     1.595363      83.23
 H       0.572365     1.816585     0.647026      22.62
 C      -0.550885     2.367442     2.455310     101.95
 O      -0.187596     3.738834     2.412441     257.60
 H      -0.076844     3.895195     1.384015      28.21
 H      -0.687483     1.751759     3.455559      23.61
 H      -1.742083     2.135874     2.141531      23.16
 C      -2.377166    -1.950491    -0.731069      21.26
 H      -2.827807    -2.923942    -0.567939      23.03
 C      -1.485682    -0.308106    -2.213859      58.54
 H      -1.272350     0.100368    -3.371596      17.93
 C      -0.791694     0.300651    -1.242074      29.59
 O      -0.020892     1.422970    -1.359210     264.54
 C      -0.645194     2.629473    -2.000735     107.55
 H       0.040334     3.458978    -1.858983      26.24
 H      -0.502838     2.330171    -3.110656      24.34
 H      -1.719968     2.640930    -1.984850      27.80
 C      -0.764549    -0.278747     0.119641      15.00
 O      -0.123974    -0.009864     1.330493     150.27
 C      -1.486138    -1.411010     0.321724      56.92
 H      -1.602356    -1.966193     1.093437      22.11
 C      -2.332421    -1.486532    -2.013758      51.06
 C      -3.146864    -1.937996    -3.067942      92.29
 H      -2.935575    -1.366724    -3.984033      26.56
 O      -3.087875    -3.425033    -3.345380     278.04
 H      -2.214623    -3.600580    -3.379448      32.16
 C      -4.731657    -1.806339    -2.851727      91.13
 H      -5.004066    -2.233283    -1.926528      25.99
 O      -4.885296    -0.372003    -2.399228     222.50
 H      -4.877017     0.164982    -3.057797      33.98
 C      -5.553883    -2.305589    -3.894076     109.46
 O      -6.513155    -3.573920    -3.920433     267.94
 H      -6.158142    -3.983242    -4.777469      29.01
 H      -5.162826    -2.195367    -5.054100      24.29
 H      -6.418597    -1.690298    -4.108513      24.02
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name = lig-ACN-frame_668
 C       3.085805     0.137972     0.415962      52.03
 H       2.177597     0.449531    -0.232481      21.71
 C       4.066378     0.279875     2.474543      58.63
 H       4.179421     0.504918     3.544051      21.82
 C       5.232202    -0.376032     1.895818      -6.25
 O       6.614274    -0.715952     2.597629     183.84
 C       6.954805    -0.246672     3.973637     108.66
 H       7.749778    -0.780397     4.275809      27.59
 H       6.132914    -0.438261     4.616621      30.37
 H       7.121517     0.902213     3.865181      26.79
 C       5.309633    -0.725287     0.549290      18.07
 O       6.535258    -1.132233     0.010802     187.99
 H       7.261839    -1.250758     0.589862      25.13
 C       4.170560    -0.493732    -0.208285      69.46
 H       4.028794    -0.925757    -1.180263      23.47
 C       2.941067     0.479324     1.731044      42.75
 C       1.738562     1.310003     2.367221     102.13
 H       2.059211     2.347594     2.595820      24.36
 O       1.570341     0.835804     3.717716     282.86
 H       1.500572    -0.036286     3.781592      32.62
 C       0.441844     1.296369     1.596164      98.51
 H       0.536303     1.911325     0.763627      24.50
 C      -0.587689     2.139167     2.539522      77.76
 O      -0.184430     3.716501     2.430625     227.28
 H       0.262880     3.961770     1.636341      31.28
 H      -0.383156     2.274795     3.708238      22.03
 H      -1.650503     2.267619     2.011687      22.46
 C      -2.372460    -2.012181    -0.600115      65.07
 H      -2.982728    -2.849381    -0.466431      24.94
 C      -1.538258    -0.310994    -2.162001      48.95
 H      -1.751437     0.117084    -3.285656      20.55
 C      -0.691982     0.379910    -1.130890      28.13
 O       0.053816     1.525981    -1.481407     256.22
 C      -0.641171     2.587085    -2.082276     108.29
 H      -0.202069     3.424238    -1.695508      27.19
 H      -0.555562     2.665000    -3.281517      23.76
 H      -1.661575     2.738131    -1.575453      25.57
 C      -0.701633    -0.279714     0.089145      24.23
 O      -0.185350     0.083970     1.329171     185.77
 C      -1.623743    -1.448406     0.320938      50.15
 H      -1.417554    -1.655426     1.249257      25.63
 C      -2.248206    -1.414204    -1.945828      21.69
 C      -3.271390    -1.996429    -3.117101      71.92
 H      -3.015221    -1.487143    -4.067069      25.41
 O      -3.083188    -3.442107    -3.279283     235.11
 H      -2.273231    -3.571465    -3.964880      25.35
 C      -4.785060    -1.778993    -2.719414      69.37
 H      -5.111988    -2.417475    -1.904125      26.31
 O      -4.965789    -0.285148    -2.433960     146.54
 H      -4.912010     0.091799    -3.430185      28.52
 C      -5.789830    -2.262823    -4.050553      72.99
 O      -6.354208    -3.452017    -3.905022     264.90
 H      -6.172372    -4.188337    -4.651911      27.40
 H      -4.886503    -2.373248    -4.889072      23.95
 H      -6.368147    -1.348736    -4.019138      24.72
55
name = lig-ACN-frame_669
 C       3.011695     0.050882     0.347998      33.35
 H       2.255701     0.463126    -0.497078      19.99
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 C       4.137045     0.238273     2.587887      65.01
 H       4.083992     0.682806     3.531088      23.55
 C       5.300562    -0.339751     2.021283      18.47
 O       6.461544    -0.712601     2.527047     244.93
 C       6.917612    -0.349885     3.869835     111.82
 H       7.851512    -0.832924     4.029211      26.10
 H       6.171532    -0.560449     4.606990      30.08
 H       7.169622     0.819434     4.070846      26.42
 C       5.354991    -0.755029     0.613291      -3.14
 O       6.534189    -1.131617     0.004304     174.58
 H       7.181138    -1.125816     0.799102      19.79
 C       4.160261    -0.662283    -0.168478      49.87
 H       4.352179    -0.519376    -1.244969      23.47
 C       2.991391     0.586332     1.701647      28.57
 C       1.779306     1.179909     2.319011     107.07
 H       1.989314     2.266222     2.308906      25.28
 O       1.583728     0.873928     3.750390     256.24
 H       1.389055    -0.114791     3.712927      27.40
 C       0.387178     1.417711     1.658680      94.50
 H       0.597864     1.869882     0.711410      22.50
 C      -0.536239     2.211581     2.485270     102.56
 O      -0.186943     3.619500     2.473199     267.37
 H       0.431568     3.600780     1.716884      30.49
 H      -0.510682     1.584715     3.582464      23.06
 H      -1.588461     1.727734     2.289102      24.90
 C      -2.374215    -2.106659    -0.630284      29.65
 H      -3.107728    -2.758113    -0.258729      27.42
 C      -1.506966    -0.194985    -2.123064      39.97
 H      -1.556112     0.575047    -2.993083      20.05
 C      -0.682439     0.355380    -1.180360       6.90
 O       0.165022     1.502256    -1.524613     196.65
 C      -0.663565     2.700020    -2.142694      84.76
 H      -0.188837     3.475906    -1.818977      27.85
 H      -0.846969     2.705850    -3.346840      24.04
 H      -1.768213     2.429635    -1.804195      24.32
 C      -0.775806    -0.306714     0.139926      13.34
 O      -0.184216     0.094639     1.348555     174.68
 C      -1.567821    -1.388450     0.456375      36.72
 H      -1.806070    -1.722173     1.406129      23.52
 C      -2.408227    -1.470750    -1.952229       3.25
 C      -3.338971    -2.055230    -3.012695      84.25
 H      -3.227265    -1.501076    -3.958066      24.54
 O      -3.079631    -3.453970    -3.228409     184.34
 H      -2.428647    -3.533107    -4.166190      22.62
 C      -4.830121    -1.708614    -2.711028      73.83
 H      -5.096915    -2.100447    -1.678046      24.65
 O      -5.061369    -0.335528    -2.497896      90.38
 H      -4.931359     0.152715    -3.545168      26.48
 C      -5.777937    -2.003610    -4.126174      71.63
 O      -6.311287    -3.473396    -3.836034     308.52
 H      -6.079474    -3.881705    -4.627683      32.65
 H      -5.083907    -1.858490    -5.183292      24.59
 H      -6.665590    -1.490326    -4.413236      26.08
55
name = lig-ACN-frame_670
 C       3.012704     0.011720     0.318266      53.26
 H       2.032956     0.049669    -0.383239      21.93
 C       4.169426     0.276692     2.600143      64.07
 H       4.148693     0.420810     3.617049      22.02
 C       5.260875    -0.345944     1.997926      19.07
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 O       6.461505    -0.721875     2.575850     223.72
 C       6.871519    -0.431627     3.826055     106.29
 H       7.858097    -0.990714     3.848517      25.02
 H       6.256659    -0.866660     4.615482      28.86
 H       7.016668     0.784314     3.845423      25.55
 C       5.276931    -0.734923     0.656001      15.40
 O       6.497385    -1.150671     0.048598     144.56
 H       7.344306    -1.141807     0.647547      22.18
 C       4.181652    -0.642356    -0.169427      53.46
 H       4.365892    -0.995430    -1.243683      23.18
 C       3.066469     0.442505     1.641490      19.23
 C       1.825535     1.303015     2.377699      87.09
 H       2.294702     2.247632     2.558577      25.61
 O       1.628158     0.842894     3.762339     194.97
 H       1.167138    -0.197919     3.750622      23.32
 C       0.460969     1.432308     1.530372      83.03
 H       0.532186     2.011256     0.574658      22.10
 C      -0.579871     2.181324     2.499012      93.38
 O      -0.200844     3.518722     2.522446     246.36
 H       0.460249     3.892989     1.814046      29.73
 H      -0.420214     1.871201     3.707968      21.81
 H      -1.608789     2.387629     2.011678      22.90
 C      -2.309747    -1.962035    -0.629692      78.22
 H      -2.826259    -2.895117    -0.578915      23.34
 C      -1.662163    -0.266684    -2.151607      44.38
 H      -1.664772    -0.027082    -3.211195      19.65
 C      -0.662724     0.291097    -1.165084       7.93
 O       0.161352     1.431093    -1.553832     199.84
 C      -0.684937     2.673706    -2.133380      73.66
 H      -0.266906     3.509768    -1.875952      29.81
 H      -0.326120     2.405354    -3.214724      22.25
 H      -1.819453     2.805324    -1.786598      25.42
 C      -0.813200    -0.230518     0.257575       3.36
 O      -0.143570     0.085193     1.394082     151.35
 C      -1.651641    -1.458898     0.381367      54.71
 H      -1.725847    -1.749531     1.459582      23.18
 C      -2.434664    -1.380474    -1.861783      34.66
 C      -3.352722    -1.980363    -2.964050      69.68
 H      -2.960087    -1.472763    -3.852370      25.97
 O      -3.130356    -3.481509    -3.184006     248.37
 H      -2.298371    -3.535145    -3.761591      27.40
 C      -4.985055    -1.671676    -2.888408      87.50
 H      -5.648154    -2.356834    -2.195377      23.35
 O      -5.121217    -0.279572    -2.535839     207.81
 H      -4.868262     0.296868    -3.283240      31.15
 C      -5.763685    -2.011537    -3.992897      98.77
 O      -6.214004    -3.391415    -3.858529     288.30
 H      -6.271009    -3.866892    -4.703878      30.84
 H      -5.165467    -1.924349    -5.054183      24.76
 H      -6.561441    -1.317729    -3.782982      25.06
55
name = lig-ACN-frame_671
 C       3.034330    -0.056942     0.383456      38.43
 H       1.996906    -0.076162    -0.104530      22.10
 C       4.130629     0.267263     2.478519      59.73
 H       4.010263     0.533900     3.509302      23.23
 C       5.264317    -0.384235     1.978235      19.95
 O       6.487689    -0.803051     2.527927     226.21
 C       6.909832    -0.470671     3.944917      97.68
 H       8.043548    -0.754075     4.167990      24.28
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 H       6.164420    -0.893106     4.654592      27.95
 H       6.855897     0.697240     4.291261      26.01
 C       5.319652    -0.708742     0.577653      14.38
 O       6.435537    -1.198748     0.070837     176.42
 H       7.106398    -1.187996     0.747295      22.34
 C       4.183580    -0.583049    -0.252190      62.83
 H       3.947625    -1.269649    -1.130936      23.02
 C       2.950686     0.413176     1.762093      41.15
 C       1.934495     1.342143     2.367263      96.91
 H       2.152380     2.367953     2.535692      26.47
 O       1.653515     0.786941     3.730119     205.82
 H       1.178936    -0.196273     3.537890      24.20
 C       0.501471     1.411721     1.609588      91.85
 H       0.703549     1.867499     0.554696      21.93
 C      -0.585690     2.170471     2.370091      90.70
 O      -0.155706     3.642065     2.629536     234.61
 H       0.287821     3.743810     1.789289      31.67
 H      -0.813091     1.636330     3.489919      24.46
 H      -1.576015     1.782164     1.927509      25.28
 C      -2.410642    -1.975831    -0.616447       7.43
 H      -2.826772    -3.000678    -0.456672      22.78
 C      -1.602350    -0.234288    -2.169457      39.83
 H      -1.542918     0.156256    -3.091365      24.43
 C      -0.792130     0.268494    -1.133055      10.60
 O       0.019265     1.342950    -1.513542     228.53
 C      -0.539667     2.510118    -2.130626      96.83
 H      -0.092092     3.259527    -1.597663      27.20
 H      -0.690230     2.715362    -3.275945      24.99
 H      -1.682954     2.333917    -1.870164      24.85
 C      -0.862231    -0.218349     0.175529      19.60
 O      -0.043819     0.099654     1.411729     152.21
 C      -1.584126    -1.352561     0.454634      42.07
 H      -1.329071    -2.081479     1.351964      23.93
 C      -2.552532    -1.358766    -1.874222      20.99
 C      -3.385737    -1.956114    -2.990359     100.14
 H      -3.156259    -1.514915    -3.966661      24.80
 O      -3.196350    -3.415709    -3.112025     292.22
 H      -2.349058    -3.550951    -3.183651      34.60
 C      -4.871093    -1.668628    -2.839816      70.43
 H      -5.074879    -2.103676    -1.745877      23.54
 O      -5.175751    -0.186097    -2.516116     235.45
 H      -4.656324     0.199234    -3.108288      34.76
 C      -5.874691    -2.028911    -4.078427      81.89
 O      -6.149942    -3.393476    -3.907612     230.12
 H      -6.517794    -3.651722    -4.907362      27.06
 H      -5.387473    -1.743871    -5.165435      23.82
 H      -6.811417    -1.451779    -4.141005      24.28
55
name = lig-ACN-frame_672
 C       2.894074    -0.082561     0.459443      60.99
 H       2.118758    -0.009901    -0.259622      25.28
 C       4.170071     0.204448     2.515542      58.76
 H       4.357089     0.702868     3.515965      23.15
 C       5.315516    -0.403011     1.916400      -4.57
 O       6.551487    -0.835008     2.597701     178.02
 C       6.841422    -0.475133     4.040556      83.18
 H       8.019246    -0.861636     4.031759      23.72
 H       6.272614    -1.205685     4.716427      26.70
 H       6.667208     0.687115     4.108113      25.05
 C       5.306954    -0.674249     0.489219       7.05
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 O       6.474521    -1.301570     0.013802     152.71
 H       7.119496    -1.358219     0.736803      20.43
 C       4.077848    -0.570944    -0.197912      48.46
 H       4.171933    -0.707679    -1.334828      21.57
 C       2.957999     0.459937     1.701482      26.79
 C       1.820884     1.255883     2.410617     113.60
 H       2.356538     2.176368     2.429832      26.77
 O       1.659808     0.747906     3.700601     292.54
 H       1.407375    -0.165507     3.588976      30.49
 C       0.592075     1.446872     1.657608      86.60
 H       0.884287     2.011714     0.643459      23.10
 C      -0.545825     2.238620     2.318061     102.76
 O      -0.173887     3.633453     2.666410     242.83
 H       0.067012     4.164766     1.906613      32.45
 H      -0.721171     1.677379     3.390989      24.51
 H      -1.372704     2.472424     1.590371      25.11
 C      -2.469604    -1.927306    -0.545724      44.92
 H      -3.197276    -2.702452    -0.160385      23.17
 C      -1.662841    -0.282524    -2.194253      44.43
 H      -1.613396     0.304223    -2.991491      25.77
 C      -0.923137     0.352744    -1.097172       9.83
 O       0.008414     1.234769    -1.455544     246.65
 C      -0.537686     2.397646    -2.067822     115.29
 H      -0.008464     3.306899    -1.754245      26.80
 H      -0.098087     2.326748    -3.134112      25.37
 H      -1.643423     2.651482    -1.890635      27.08
 C      -0.792724    -0.222888     0.268604      14.81
 O       0.019227     0.056765     1.284112     165.46
 C      -1.585472    -1.409361     0.395104      41.97
 H      -1.347814    -1.905303     1.484642      23.85
 C      -2.553285    -1.350307    -1.890227      15.10
 C      -3.389449    -1.922950    -3.096439      91.69
 H      -2.986962    -1.471299    -4.011956      24.70
 O      -3.294828    -3.338116    -3.015223     226.63
 H      -2.256725    -3.536352    -3.054221      26.56
 C      -4.903290    -1.543284    -2.729763      68.68
 H      -5.299626    -2.236514    -1.792337      22.89
 O      -5.146769    -0.198652    -2.525031     190.22
 H      -4.344383     0.495351    -2.813993      26.94
 C      -5.876201    -1.948226    -4.086980      66.57
 O      -6.148288    -3.522360    -4.028314     244.31
 H      -6.608234    -3.862799    -4.836449      30.29
 H      -5.218581    -1.743679    -5.045373      24.55
 H      -6.907758    -1.452420    -3.992787      24.02
55
name = lig-ACN-frame_673
 C       2.824007    -0.073153     0.365191      39.68
 H       1.953442     0.182580    -0.061309      20.57
 C       4.250841     0.202648     2.490159      60.10
 H       4.224148     0.450909     3.645576      22.32
 C       5.377649    -0.423819     1.924739      24.12
 O       6.516873    -0.813965     2.634640     229.94
 C       6.755059    -0.523048     3.973277     108.50
 H       7.987595    -0.539890     4.276850      23.66
 H       6.091337    -1.089084     4.773939      26.40
 H       6.522196     0.551670     4.366014      25.86
 C       5.345445    -0.763550     0.563862      12.22
 O       6.453216    -1.369945    -0.106147     130.66
 H       7.313012    -1.339548     0.497755      22.13
 C       4.079057    -0.546420    -0.189488      20.59
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 H       4.108939    -0.538922    -1.311741      23.82
 C       3.065566     0.420065     1.759778      13.74
 C       1.894506     1.186049     2.436196      94.66
 H       2.017625     2.195258     2.761018      27.02
 O       1.619069     0.691634     3.799425     262.30
 H       1.412954    -0.196959     3.756895      31.09
 C       0.569479     1.462135     1.495875      76.24
 H       0.953450     2.088181     0.537228      23.06
 C      -0.521048     2.377224     2.246004     109.93
 O      -0.146754     3.625260     2.737687     230.64
 H      -0.166171     4.251487     1.894576      28.92
 H      -1.137584     1.898665     3.149385      26.17
 H      -1.409026     2.287638     1.509047      26.56
 C      -2.537628    -1.832066    -0.559758      20.09
 H      -3.327159    -2.588943    -0.362607      22.97
 C      -1.755787    -0.212477    -2.108054      51.50
 H      -1.778935    -0.119258    -3.136420      22.01
 C      -0.965631     0.294573    -1.010569       9.30
 O       0.073964     1.242539    -1.340680     205.57
 C      -0.436762     2.431849    -2.110821     103.54
 H      -0.001997     3.368217    -1.567539      25.28
 H      -0.260455     2.303891    -3.235955      25.72
 H      -1.517841     2.397149    -2.167624      27.87
 C      -0.834664    -0.314641     0.207722      17.60
 O       0.128372     0.083445     1.208705     148.85
 C      -1.609734    -1.475544     0.414039      51.06
 H      -1.925322    -1.869190     1.487817      23.30
 C      -2.537645    -1.414829    -1.880493      31.43
 C      -3.438755    -1.862134    -2.952982      82.80
 H      -3.190563    -1.495301    -3.959592      26.47
 O      -3.383729    -3.327205    -2.957837     166.50
 H      -2.355383    -3.679013    -3.350419      25.04
 C      -5.002639    -1.582954    -2.905911      85.06
 H      -5.452372    -2.167456    -1.886870      24.18
 O      -5.119430    -0.119095    -2.510190     108.29
 H      -3.996767     0.095740    -2.248583      24.86
 C      -5.816799    -2.092073    -3.972640     100.56
 O      -6.121414    -3.512294    -4.123876     293.29
 H      -6.298425    -3.520738    -5.014804      30.57
 H      -5.364504    -1.664772    -4.954643      25.56
 H      -6.746490    -1.346850    -3.883659      24.43
55
name = lig-ACN-frame_674
 C       3.054389     0.031511     0.457067      60.69
 H       2.279038     0.031170    -0.230315      26.93
 C       4.275569     0.199772     2.475658      66.18
 H       4.159335     0.373728     3.649392      23.30
 C       5.385622    -0.465783     1.958292      17.78
 O       6.528947    -0.813802     2.593199     190.24
 C       6.636907    -0.461931     4.040799      92.17
 H       7.857482    -0.787346     4.192630      23.02
 H       6.034570    -1.348749     4.541342      25.38
 H       6.280703     0.583239     4.144064      24.47
 C       5.299524    -0.866122     0.523093       5.83
 O       6.361876    -1.387346    -0.215691     156.55
 H       7.241702    -1.252984     0.273537      23.29
 C       4.190005    -0.530985    -0.212953      49.52
 H       4.164092    -1.079741    -1.152467      23.74
 C       3.014366     0.384499     1.769680      31.91
 C       1.914012     1.212930     2.486834      83.09
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 H       2.473396     2.139081     2.549721      26.23
 O       1.556459     0.627171     3.891969     223.65
 H       1.077082    -0.278903     3.648686      25.42
 C       0.622313     1.451643     1.497419      76.17
 H       0.961619     1.902429     0.470296      23.27
 C      -0.597807     2.295357     2.111974      90.47
 O      -0.090139     3.684504     2.760888     200.48
 H      -0.068241     4.341907     2.056592      31.62
 H      -0.781368     1.597543     3.003879      25.98
 H      -1.417147     2.606756     1.398162      26.43
 C      -2.648848    -1.927154    -0.529402      35.71
 H      -3.233367    -2.804045    -0.299871      22.98
 C      -1.796899    -0.158090    -2.077405      62.77
 H      -1.526841     0.537410    -2.882833      21.26
 C      -0.816754     0.298371    -1.131139     -18.38
 O       0.059161     1.314289    -1.256770     192.39
 C      -0.355172     2.398340    -2.165887     117.26
 H       0.046454     3.435000    -1.631832      25.15
 H       0.088470     2.487039    -3.160419      27.03
 H      -1.381169     2.458760    -2.037711      28.73
 C      -0.822139    -0.389523     0.263460      -6.61
 O       0.129777     0.086062     1.114362     154.68
 C      -1.748795    -1.460727     0.532174      46.20
 H      -1.656052    -1.965589     1.564965      25.24
 C      -2.588986    -1.302711    -1.822016      27.18
 C      -3.534829    -1.966633    -2.902880     103.17
 H      -3.101882    -1.460823    -3.775655      25.84
 O      -3.442902    -3.385528    -2.936629     254.29
 H      -2.762136    -3.550687    -3.654544      28.32
 C      -4.945415    -1.635016    -2.755108      66.91
 H      -5.396424    -2.211597    -1.718146      23.47
 O      -5.082839    -0.097966    -2.556049     148.25
 H      -4.537292     0.009527    -1.675519      28.81
 C      -5.868153    -2.061216    -4.086138      87.43
 O      -6.078995    -3.460257    -4.191875     291.94
 H      -6.048467    -3.857433    -5.160183      27.52
 H      -5.417867    -1.664140    -5.040697      24.64
 H      -6.966546    -1.698629    -3.841663      22.53
55
name = lig-ACN-frame_675
 C       3.186351     0.108111     0.388953      40.89
 H       2.232164     0.304424    -0.163584      27.03
 C       4.203275     0.141351     2.553737      56.41
 H       4.472221     0.538374     3.600583      23.73
 C       5.320063    -0.524549     1.853218      17.54
 O       6.595206    -0.803915     2.579421     190.70
 C       6.531161    -0.500973     4.004070     106.44
 H       7.694842    -0.467216     4.495541      24.73
 H       5.779925    -1.081127     4.727713      26.11
 H       6.271969     0.515675     4.303656      26.71
 C       5.379294    -0.865455     0.537417      40.62
 O       6.325664    -1.419900    -0.277749     200.63
 H       7.113985    -1.516127     0.225468      26.20
 C       4.233638    -0.614312    -0.204458      51.27
 H       4.071687    -0.814938    -1.247716      24.24
 C       3.053389     0.392581     1.824259       8.44
 C       1.831977     1.177300     2.537854      92.88
 H       2.125647     2.169525     2.946927      25.71
 O       1.509979     0.662246     3.814946     228.82
 H       1.013287    -0.368749     3.704226      23.81
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 C       0.676846     1.462830     1.527557      73.43
 H       1.207297     2.032852     0.719147      26.10
 C      -0.483490     2.289409     2.093527     115.06
 O      -0.075079     3.592088     2.717122     240.51
 H       0.123611     4.171289     1.989353      32.71
 H      -1.075368     1.874627     2.925906      28.67
 H      -1.284522     2.385309     1.349279      29.15
 C      -2.597603    -1.937332    -0.423444      46.27
 H      -3.193819    -2.804507    -0.383183      25.51
 C      -1.742428    -0.124010    -2.065256      46.39
 H      -2.309062     0.212351    -2.977216      21.28
 C      -0.788112     0.173935    -1.067395      22.26
 O       0.058228     1.395225    -1.235725     203.62
 C      -0.299621     2.431593    -2.147852     122.57
 H       0.221347     3.463015    -1.647570      25.10
 H       0.199400     2.154446    -3.026074      28.92
 H      -1.207283     2.582816    -2.552159      30.00
 C      -0.844552    -0.330885     0.186639      16.65
 O       0.131583     0.006729     1.156533     123.76
 C      -1.807068    -1.374300     0.559574      67.64
 H      -1.581187    -1.904047     1.473985      27.30
 C      -2.692575    -1.224502    -1.724476     -15.18
 C      -3.477527    -1.975302    -2.908804      77.85
 H      -3.298243    -1.707986    -3.959188      25.25
 O      -3.447384    -3.490481    -2.938750     229.70
 H      -2.959096    -3.807087    -3.592672      31.69
 C      -5.054785    -1.568727    -2.659432      62.33
 H      -5.623129    -2.219071    -1.749663      23.85
 O      -5.058892    -0.193533    -2.582312     248.16
 H      -5.351479     0.134979    -1.856854      34.68
 C      -5.941944    -1.938093    -4.111644      66.69
 O      -6.013862    -3.494954    -4.224048     252.12
 H      -6.049168    -3.726193    -5.313707      23.39
 H      -5.349982    -1.372486    -4.822700      26.86
 H      -6.945887    -1.289985    -4.008385      24.47
55
name = lig-ACN-frame_676
 C       3.061078     0.167062     0.421575      31.76
 H       2.334978     0.638771    -0.387966      25.93
 C       4.268803     0.010430     2.560907      71.87
 H       4.180655     0.335162     3.602494      25.92
 C       5.413596    -0.556915     1.982286      14.41
 O       6.560114    -0.765409     2.599466     195.18
 C       6.477962    -0.467545     4.003204     103.77
 H       7.564020    -0.834371     4.436548      24.60
 H       5.677561    -1.246249     4.375644      25.27
 H       6.187649     0.546233     4.057051      26.28
 C       5.365969    -0.858279     0.460659      -5.39
 O       6.438023    -1.494737    -0.280941     133.56
 H       7.241679    -1.749428     0.253467      22.13
 C       4.131892    -0.575655    -0.231586      38.43
 H       4.354882    -0.616589    -1.284016      22.98
 C       3.104395     0.485460     1.804428      23.88
 C       1.851038     1.164185     2.505871     106.36
 H       2.143717     2.240224     2.573449      28.23
 O       1.418666     0.659603     3.772002     241.27
 H       1.228231    -0.462415     3.637507      24.36
 C       0.698476     1.361318     1.598124      95.18
 H       0.973989     1.723878     0.659667      28.09
 C      -0.449406     2.261246     2.117441     123.89
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 O      -0.058280     3.496417     2.624441     216.48
 H       0.504134     3.995485     1.890867      30.44
 H      -0.932028     1.700506     2.845223      29.99
 H      -1.005352     2.476335     1.200124      28.91
 C      -2.580899    -1.835351    -0.463945      62.59
 H      -3.092834    -2.672781    -0.093159      26.50
 C      -1.885506    -0.251325    -2.013614      68.99
 H      -1.648783     0.365919    -2.969028      23.74
 C      -0.861086     0.351855    -1.178780     -17.87
 O       0.003594     1.366904    -1.173242     173.35
 C      -0.196772     2.442847    -2.250019     116.79
 H       0.160255     3.552492    -1.687631      25.26
 H       0.273254     2.418191    -3.124673      30.04
 H      -1.195709     2.478661    -2.169881      29.42
 C      -0.813032    -0.294323     0.287472      -9.36
 O       0.143916    -0.015082     1.248603     149.81
 C      -1.682110    -1.296372     0.569796      64.64
 H      -1.860296    -1.574876     1.545882      26.13
 C      -2.672469    -1.361291    -1.718335      50.36
 C      -3.592058    -2.014070    -2.822431      89.64
 H      -3.121992    -1.463895    -3.675820      25.42
 O      -3.439926    -3.517400    -2.862092     185.40
 H      -2.579105    -3.676037    -3.534909      26.08
 C      -5.130940    -1.667196    -2.828326      96.08
 H      -5.556154    -2.083782    -1.759649      25.18
 O      -5.078918    -0.161965    -2.587071     182.50
 H      -6.013508    -0.064700    -2.096966      28.58
 C      -5.885485    -1.923913    -3.975475     117.45
 O      -5.964280    -3.356652    -4.259714     258.90
 H      -6.390034    -3.384531    -5.166657      27.65
 H      -5.407804    -1.628419    -4.843140      25.97
 H      -7.015720    -1.660149    -4.053792      23.99
55
name = lig-ACN-frame_677
 C       3.062002     0.191807     0.388959      43.59
 H       2.102835     0.644078    -0.199340      21.81
 C       4.219861    -0.025408     2.524014      67.84
 H       4.165057    -0.178059     3.537110      27.59
 C       5.369938    -0.573143     1.827215       9.47
 O       6.610438    -0.767096     2.621008     150.42
 C       6.458279    -0.500881     4.032115     112.04
 H       7.489969    -0.785434     4.513426      25.73
 H       5.602495    -1.041812     4.591309      25.20
 H       6.355418     0.502264     4.366174      26.30
 C       5.321255    -0.887745     0.495825      21.36
 O       6.479058    -1.514897    -0.214614     124.51
 H       7.219606    -1.363899     0.524275      18.41
 C       4.170861    -0.426064    -0.198523      42.98
 H       3.929078    -0.679236    -1.229891      28.70
 C       3.120452     0.447206     1.763055      33.58
 C       1.982538     1.211528     2.437838      86.47
 H       2.381271     2.156814     2.897637      27.34
 O       1.388637     0.645441     3.772602     201.12
 H       1.065293    -0.343978     3.577080      27.12
 C       0.665931     1.240263     1.499761     112.17
 H       0.991574     1.706240     0.667202      28.98
 C      -0.503139     2.106064     2.052683     114.65
 O       0.025944     3.517763     2.574685     203.19
 H       0.772254     3.737552     1.981080      32.40
 H      -0.942333     1.728758     2.844370      31.77
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 H      -1.317113     2.192801     1.392381      29.77
 C      -2.561855    -1.840301    -0.320042      59.45
 H      -3.265173    -2.600097    -0.027453      26.05
 C      -1.843047    -0.209945    -2.060121      29.16
 H      -1.894453    -0.010114    -3.170831      20.40
 C      -1.025268     0.319322    -0.936808      17.52
 O       0.003725     1.415387    -1.287648     193.42
 C      -0.226203     2.439751    -2.225876     120.29
 H       0.367667     3.399901    -1.585009      24.22
 H       0.175441     2.196084    -3.108500      29.98
 H      -1.179693     2.724579    -2.589969      28.77
 C      -0.744507    -0.179656     0.251420      28.51
 O       0.138125    -0.024374     1.344106     181.91
 C      -1.663811    -1.276442     0.557142      57.13
 H      -1.622071    -1.554147     1.549663      28.30
 C      -2.658497    -1.440960    -1.772250     -20.99
 C      -3.609988    -2.072467    -2.788598      98.20
 H      -3.380296    -1.792394    -3.883437      24.54
 O      -3.415066    -3.457550    -2.792771     203.87
 H      -2.268762    -3.545805    -2.995923      24.82
 C      -5.028160    -1.633454    -2.715816      77.92
 H      -5.644757    -2.327012    -1.955535      25.50
 O      -5.160128    -0.160904    -2.576147     140.10
 H      -6.300135     0.110954    -2.658680      25.76
 C      -5.909369    -1.924580    -4.100459      87.52
 O      -5.943659    -3.312471    -4.268755     295.71
 H      -6.346303    -3.579846    -5.041038      29.42
 H      -5.586957    -1.245111    -4.757187      29.17
 H      -6.783380    -1.407955    -3.603318      25.91
55
name = lig-ACN-frame_678
 C       3.153413     0.245890     0.377506      48.78
 H       2.233650     0.264635    -0.376661      24.60
 C       4.197077    -0.093575     2.469460      73.44
 H       4.186735     0.128967     3.469928      27.88
 C       5.346700    -0.553378     1.870705      12.81
 O       6.561072    -0.783688     2.591802     153.48
 C       6.513919    -0.533783     4.129954     107.02
 H       7.468506    -0.943514     4.498705      26.75
 H       5.668581    -1.119354     4.558631      25.48
 H       6.357947     0.526992     4.188357      26.03
 C       5.356971    -0.881906     0.429063      18.21
 O       6.413840    -1.451675    -0.065431     142.95
 H       7.302172    -1.348859     0.370873      23.72
 C       4.220163    -0.394283    -0.304205      47.58
 H       4.205211    -0.746548    -1.359978      22.85
 C       3.045671     0.377286     1.794780      28.15
 C       1.895735     1.135587     2.507865     110.09
 H       2.176494     2.252993     2.608800      27.98
 O       1.459745     0.647910     3.718526     305.15
 H       1.003212    -0.103288     3.553051      33.52
 C       0.722507     1.403720     1.462830      85.66
 H       0.884056     1.671510     0.510406      27.82
 C      -0.491034     2.137447     2.118890     134.79
 O       0.061120     3.434432     2.468316     254.29
 H       0.761621     3.563718     1.870381      34.81
 H      -0.688075     1.693608     2.932753      32.78
 H      -1.222421     2.167101     1.405759      30.78
 C      -2.585820    -1.860380    -0.369240      50.84
 H      -3.204580    -2.717223    -0.007731      23.94
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 C      -1.783912    -0.274131    -1.965006      69.18
 H      -1.926784     0.336053    -2.816544      27.85
 C      -1.000195     0.472708    -1.056317       4.72
 O      -0.091552     1.329508    -1.359723     204.30
 C      -0.281791     2.471932    -2.284578     108.33
 H       0.318599     3.511515    -1.792751      24.43
 H       0.289817     2.362712    -3.127282      28.64
 H      -1.363112     2.698828    -2.342075      27.42
 C      -0.845894    -0.302189     0.337783      -0.62
 O       0.128630    -0.077542     1.326576     115.97
 C      -1.685449    -1.320103     0.627212      67.84
 H      -1.493348    -1.914197     1.488168      28.13
 C      -2.585622    -1.328725    -1.623969      40.57
 C      -3.448312    -1.991320    -2.841823      67.53
 H      -3.055065    -1.551881    -3.846852      25.30
 O      -3.392985    -3.487343    -2.689887     195.34
 H      -2.416265    -3.786784    -2.748289      27.98
 C      -5.115759    -1.588868    -2.703197      82.05
 H      -5.510491    -2.039996    -1.702986      25.05
 O      -5.233444    -0.198899    -2.514374     203.26
 H      -5.997865     0.020544    -3.188859      29.22
 C      -5.907992    -1.791363    -4.020641     111.18
 O      -5.930954    -3.354428    -4.272686     274.50
 H      -6.031612    -3.397256    -5.253578      26.88
 H      -5.550602    -1.460383    -4.864900      28.57
 H      -6.974155    -1.610359    -4.101711      27.01
55
name = lig-ACN-frame_679
 C       3.175714     0.192349     0.293671      46.80
 H       2.316166     0.643569    -0.297025      28.92
 C       4.146209    -0.051019     2.568191      56.68
 H       4.228121     0.301934     3.574321      26.07
 C       5.320179    -0.556770     1.940100      26.98
 O       6.498201    -0.823321     2.629858     199.68
 C       6.552462    -0.590106     4.039539     125.61
 H       7.496383    -0.878101     4.338142      29.61
 H       5.768828    -1.139680     4.543329      26.54
 H       6.452850     0.446692     4.424132      26.96
 C       5.348778    -0.713741     0.553004      13.19
 O       6.456730    -1.454692    -0.062980     176.23
 H       7.076180    -1.476610     0.638905      23.05
 C       4.307962    -0.440843    -0.344033      64.92
 H       4.468471    -0.392098    -1.442391      19.61
 C       3.001354     0.313607     1.689892       1.64
 C       1.825357     1.152945     2.372108      91.96
 H       2.434936     2.050330     2.717671      26.34
 O       1.515822     0.625181     3.728089     253.93
 H       1.119205    -0.232276     3.638402      31.08
 C       0.638086     1.309894     1.494303     112.55
 H       1.100461     1.864448     0.732887      30.09
 C      -0.409659     2.165166     2.149795     141.62
 O       0.092473     3.449983     2.388742     225.95
 H       0.587708     3.819868     1.549663      30.79
 H      -0.651958     1.728256     2.972881      33.04
 H      -1.296626     2.208118     1.675758      31.84
 C      -2.595960    -1.932671    -0.334932      47.16
 H      -3.097886    -2.948697    -0.370409      26.60
 C      -1.815400    -0.169441    -1.949972      40.89
 H      -1.794448     0.198357    -2.900692      25.38
 C      -0.929327     0.308524    -0.904881      11.29
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 O      -0.032157     1.384549    -1.420497     186.72
 C      -0.345765     2.516097    -2.335944     102.02
 H       0.082595     3.454940    -1.647982      24.87
 H      -0.108656     2.383527    -3.364700      27.70
 H      -1.510574     2.598068    -2.455170      26.58
 C      -0.904093    -0.261390     0.320993       9.84
 O       0.142802    -0.030225     1.222008     178.58
 C      -1.754442    -1.485148     0.659825      50.63
 H      -1.697260    -1.973043     1.673501      22.63
 C      -2.674887    -1.299825    -1.647721      11.94
 C      -3.417675    -1.929301    -2.725315      82.97
 H      -2.839865    -1.662641    -3.691742      24.99
 O      -3.388021    -3.448459    -2.603122     244.61
 H      -2.602636    -3.621339    -2.955635      33.30
 C      -5.066158    -1.571300    -2.769510      61.76
 H      -5.444177    -2.274433    -1.958100      26.06
 O      -5.297570    -0.124652    -2.442923     250.12
 H      -5.514184     0.305824    -3.148425      35.93
 C      -5.889718    -1.988319    -4.003709     130.34
 O      -5.903393    -3.292353    -4.236676     292.13
 H      -6.088479    -3.551956    -5.285231      24.22
 H      -5.264101    -1.445228    -4.542546      29.56
 H      -6.729748    -1.341948    -3.885367      28.18
55
name = lig-ACN-frame_680
 C       3.121377     0.125840     0.198742      53.90
 H       2.548342     0.669009    -0.496775      23.30
 C       4.052072     0.061249     2.570350      89.49
 H       3.749722     0.083296     3.669233      23.07
 C       5.227859    -0.512655     2.017614      -1.85
 O       6.461578    -0.868968     2.634984     174.25
 C       6.602815    -0.664712     4.031903     125.50
 H       7.531634    -0.938257     4.243845      31.02
 H       5.961135    -1.256701     4.619673      28.39
 H       6.421345     0.435248     4.204784      25.45
 C       5.445436    -0.740792     0.562507      19.27
 O       6.464672    -1.398679    -0.014895      97.81
 H       7.291451    -1.652135     0.488817      22.75
 C       4.353788    -0.344596    -0.241969      16.87
 H       4.561141    -0.432196    -1.334489      26.07
 C       3.054566     0.281631     1.651822      32.36
 C       1.948327     1.052783     2.332581      97.14
 H       2.035576     2.181282     2.393101      27.92
 O       1.560379     0.591700     3.724245     179.65
 H       1.266991    -0.476234     3.594639      26.05
 C       0.606328     1.260964     1.475881      99.90
 H       0.653037     1.647561     0.455508      26.13
 C      -0.482686     2.142721     2.191282     110.74
 O       0.164793     3.604012     2.341073     173.37
 H       0.258831     3.886769     1.377246      31.11
 H      -0.566953     1.996940     3.165457      31.17
 H      -1.279767     2.101148     1.608689      31.48
 C      -2.593875    -1.995085    -0.392696      51.52
 H      -3.181422    -2.926675    -0.130812      24.19
 C      -1.901824    -0.124849    -1.905888      54.29
 H      -1.835213     0.112481    -2.930799      23.36
 C      -0.924249     0.295442    -1.010193     -25.56
 O       0.094905     1.396313    -1.396096     141.45
 C      -0.535639     2.451543    -2.303450      94.15
 H      -0.028188     3.492384    -2.049277      27.21
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 H       0.066218     2.251081    -3.214501      25.91
 H      -1.727409     2.626365    -2.313847      25.47
 C      -0.933192    -0.343881     0.394579       0.47
 O       0.147498    -0.029554     1.142525     171.18
 C      -1.729611    -1.456989     0.611865      52.36
 H      -1.632642    -1.848905     1.708514      24.11
 C      -2.704871    -1.283932    -1.588181      20.09
 C      -3.556802    -1.963669    -2.707011      96.51
 H      -3.285953    -1.672484    -3.798063      26.66
 O      -3.396549    -3.344756    -2.530737     223.44
 H      -2.662188    -3.612951    -3.097549      28.59
 C      -4.940599    -1.562967    -2.686100      88.66
 H      -5.450488    -1.972956    -1.808043      27.78
 O      -5.342352    -0.135591    -2.372428     164.53
 H      -4.873864     0.362321    -3.146018      31.03
 C      -5.717507    -1.867888    -4.041377     110.66
 O      -5.889160    -3.398761    -4.193682     222.13
 H      -6.460314    -3.424700    -5.105923      26.93
 H      -5.540725    -1.512265    -5.000367      27.89
 H      -6.709877    -1.673189    -3.862251      27.57
55
name = lig-ACN-frame_681
 C       3.160528     0.143435     0.248255      64.39
 H       2.353162     0.175287    -0.345704      24.90
 C       4.093808     0.004895     2.485679      65.97
 H       3.914384     0.134635     3.653543      23.29
 C       5.298786    -0.502550     2.004128      30.93
 O       6.417245    -0.954195     2.640691     211.44
 C       6.660778    -0.711826     4.101546     122.39
 H       7.592465    -0.872543     4.259263      30.94
 H       6.012337    -1.305909     4.627117      27.88
 H       6.397995     0.350523     4.390803      26.10
 C       5.371908    -0.750682     0.657884       7.05
 O       6.503980    -1.357967     0.004947     166.36
 H       7.278026    -1.182136     0.702904      17.73
 C       4.435572    -0.281954    -0.251248      51.05
 H       4.558355    -0.582955    -1.298460      26.92
 C       2.963698     0.384389     1.592254      20.06
 C       1.808585     1.075644     2.296813     102.87
 H       2.478615     1.936172     2.605210      26.72
 O       1.634341     0.556788     3.623060     193.53
 H       1.167101    -0.468342     3.548224      26.60
 C       0.596277     1.309949     1.470833      85.19
 H       1.042405     1.948339     0.640155      26.30
 C      -0.426179     2.258498     2.251350     121.94
 O       0.145498     3.644583     2.236743     229.47
 H       0.282802     3.907747     1.360938      33.93
 H      -0.622393     1.841320     3.236063      29.46
 H      -1.333601     2.375157     1.878679      30.25
 C      -2.557859    -1.948275    -0.350255      25.07
 H      -3.192742    -2.829876    -0.140823      22.09
 C      -1.957541    -0.147070    -1.921329      56.56
 H      -2.187340     0.507208    -2.828765      23.91
 C      -0.877284     0.387136    -1.029140      20.88
 O       0.014637     1.313142    -1.327731     216.63
 C      -0.550081     2.331032    -2.267815      89.56
 H      -0.374609     3.322563    -1.803560      26.59
 H      -0.516586     2.235627    -3.436247      25.24
 H      -1.695834     1.968626    -2.168581      24.37
 C      -0.854566    -0.300533     0.158863      21.05
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 O       0.127245    -0.195669     1.202400     108.23
 C      -1.703195    -1.392824     0.577332      50.16
 H      -1.567547    -2.046688     1.549510      26.09
 C      -2.740346    -1.316341    -1.601293      19.16
 C      -3.526047    -1.881054    -2.700901      80.36
 H      -2.967189    -1.490293    -3.624586      26.67
 O      -3.476633    -3.353865    -2.498993     154.95
 H      -2.415278    -3.638003    -2.806965      25.08
 C      -5.128213    -1.515681    -2.644867     100.78
 H      -5.609877    -2.198123    -2.005946      29.97
 O      -5.288022    -0.163585    -2.367509     147.89
 H      -4.319667     0.484645    -2.484628      26.70
 C      -5.733259    -1.884079    -4.005896      98.59
 O      -5.837375    -3.454739    -4.142385     251.44
 H      -6.288996    -3.596111    -4.956840      29.12
 H      -5.114007    -1.388872    -4.782063      28.49
 H      -6.599218    -1.335361    -3.933673      29.26
55
name = lig-ACN-frame_682
 C       3.160355     0.179106     0.221879      51.29
 H       2.381375     0.180324    -0.428510      26.39
 C       4.077317     0.009178     2.452522      51.72
 H       4.149507     0.335127     3.583020      21.70
 C       5.324462    -0.540122     1.964427     -10.34
 O       6.462975    -1.037673     2.767236     156.58
 C       6.654117    -0.758300     4.128579     132.28
 H       7.608325    -0.899939     4.260725      31.41
 H       6.192565    -1.403690     4.760461      28.71
 H       6.421450     0.287443     4.443964      26.18
 C       5.432396    -0.726981     0.537721      16.32
 O       6.524073    -1.284017     0.068761      61.76
 H       7.338848    -1.367796     0.670728      22.23
 C       4.372962    -0.321880    -0.299987      68.75
 H       4.514410    -0.442271    -1.371719      23.69
 C       3.040778     0.387581     1.643974      32.56
 C       1.844065     1.155145     2.345883      99.96
 H       1.909455     2.305999     2.510814      27.53
 O       1.627523     0.465162     3.568697     255.70
 H       1.066237    -0.301720     3.427314      30.78
 C       0.548874     1.303705     1.520842      89.78
 H       0.720332     1.526109     0.385393      22.47
 C      -0.395429     2.342648     2.219200     127.48
 O       0.117621     3.648706     2.173449     235.25
 H       0.554974     3.735955     1.250167      30.28
 H      -0.225014     2.224691     3.328358      27.34
 H      -1.284730     2.162489     1.840614      30.89
 C      -2.604734    -1.889624    -0.333976      83.77
 H      -3.038811    -2.841503    -0.137411      29.17
 C      -1.959042    -0.090123    -1.935959      49.29
 H      -2.312640     0.356893    -3.027429      19.07
 C      -0.997761     0.273397    -1.031371      14.60
 O      -0.026679     1.319148    -1.363277     213.01
 C      -0.678456     2.212891    -2.199630     105.80
 H      -0.315358     3.223506    -1.901768      27.63
 H      -0.006316     2.108478    -3.228628      23.98
 H      -1.800938     2.346831    -2.157866      26.05
 C      -0.715752    -0.389149     0.202440      29.28
 O       0.130677    -0.120124     1.234966     161.57
 C      -1.633695    -1.356342     0.490053      41.98
 H      -1.348114    -1.623056     1.572143      24.81
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 C      -2.702915    -1.258690    -1.585949      28.53
 C      -3.616884    -1.917228    -2.633596      78.06
 H      -3.333338    -1.728648    -3.706074      25.64
 O      -3.546258    -3.370945    -2.536375     171.33
 H      -2.418970    -3.632498    -2.494388      24.35
 C      -5.141403    -1.601899    -2.641480      85.61
 H      -5.526382    -2.054985    -1.809648      28.14
 O      -5.250840    -0.095959    -2.365039     126.04
 H      -4.428467    -0.070429    -1.583719      25.76
 C      -5.788577    -1.984655    -4.026488     115.05
 O      -5.803729    -3.344344    -4.077644     310.79
 H      -5.887422    -3.534652    -4.988993      31.64
 H      -4.984346    -1.722038    -4.741437      27.46
 H      -6.632534    -1.595401    -4.494613      28.48
55
name = lig-ACN-frame_683
 C       3.137486     0.200173     0.216319      53.01
 H       2.499848     0.830143    -0.363626      24.92
 C       4.215473     0.065145     2.522596      59.20
 H       3.904956     0.149060     3.596201      21.91
 C       5.332421    -0.604915     2.000714      18.60
 O       6.408251    -1.090641     2.730034     192.62
 C       6.663314    -0.786837     4.227518     115.86
 H       7.652762    -0.860624     4.366689      29.76
 H       6.084254    -1.414291     4.765958      29.53
 H       6.289867     0.222575     4.361261      26.90
 C       5.468655    -0.656110     0.548696       2.74
 O       6.640098    -1.265655    -0.009298     157.04
 H       7.133620    -1.554055     0.741769      21.55
 C       4.319853    -0.394517    -0.332354      35.07
 H       4.444077    -0.476182    -1.407777      21.52
 C       3.089839     0.484792     1.620829       9.59
 C       1.934646     1.170089     2.311048      86.89
 H       2.402866     2.158352     2.720855      25.27
 O       1.554211     0.403090     3.597872     213.28
 H       1.113176    -0.298412     3.267755      31.18
 C       0.597324     1.296658     1.466817     103.99
 H       0.777386     2.025548     0.597808      24.58
 C      -0.405179     2.237697     2.250168     102.99
 O       0.113873     3.715554     2.025783     179.07
 H       0.852901     3.774746     1.269230      28.42
 H      -0.627266     1.994204     3.367136      26.96
 H      -1.333505     2.304410     1.919893      29.03
 C      -2.584076    -1.845894    -0.357189      45.17
 H      -3.219610    -2.637055    -0.073665      27.34
 C      -2.012540    -0.123363    -1.935155      73.98
 H      -1.774899     0.410075    -3.084961      18.83
 C      -0.890782     0.246029    -1.033829      11.47
 O      -0.134583     1.248024    -1.339787     204.30
 C      -0.658202     2.366575    -2.260038      86.94
 H      -0.262599     3.290930    -1.954328      27.99
 H      -0.573394     1.998997    -3.470971      22.70
 H      -1.745971     2.253986    -2.305243      24.93
 C      -0.712496    -0.406935     0.241598      17.36
 O       0.140476     0.016135     1.302615     182.77
 C      -1.579052    -1.481584     0.610863      48.48
 H      -1.781757    -1.975035     1.557204      21.52
 C      -2.826391    -1.281010    -1.634424      11.37
 C      -3.717691    -2.037043    -2.661498      81.02
 H      -3.286375    -1.557320    -3.568129      25.79
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 O      -3.592043    -3.427044    -2.524643     240.00
 H      -2.579130    -3.600602    -2.811402      26.83
 C      -5.171347    -1.531027    -2.592333     107.19
 H      -5.795013    -2.094009    -2.034990      29.97
 O      -5.201394    -0.120034    -2.341944     236.73
 H      -5.309154     0.041095    -1.431002      31.45
 C      -5.717295    -1.889213    -4.100471      96.35
 O      -5.826489    -3.407582    -4.036199     241.07
 H      -5.755165    -3.791459    -5.047850      27.52
 H      -5.181598    -1.473328    -4.902357      28.70
 H      -6.701581    -1.499488    -3.850296      26.16
55
name = lig-ACN-frame_684
 C       3.237583     0.312444     0.270197      57.78
 H       2.429912     0.638328    -0.481287      27.05
 C       4.206032     0.096825     2.518035      69.24
 H       4.113960     0.001839     3.548808      22.28
 C       5.345478    -0.569075     2.002544      10.56
 O       6.392284    -1.155751     2.722231     166.68
 C       6.565534    -0.785605     4.178415     121.28
 H       7.614885    -0.953254     4.332941      28.42
 H       6.066489    -1.479868     4.779903      29.37
 H       6.304614     0.173918     4.477935      28.22
 C       5.459823    -0.727279     0.529429      12.20
 O       6.639726    -1.217563    -0.096860     120.30
 H       7.391668    -1.395433     0.524817      23.78
 C       4.374458    -0.409467    -0.260994      64.43
 H       4.479776    -0.671402    -1.313656      22.61
 C       3.212339     0.511819     1.632443      46.85
 C       1.972991     1.119192     2.373380      93.86
 H       2.299281     2.086105     2.875377      25.92
 O       1.503009     0.410200     3.557122     209.20
 H       1.099943    -0.574062     3.389156      24.87
 C       0.717688     1.500865     1.523961      73.26
 H       0.942182     1.674663     0.448947      23.57
 C      -0.396384     2.310943     2.184228     124.29
 O       0.056733     3.685936     1.965175     252.05
 H       0.785626     3.528571     1.340785      31.70
 H      -0.294311     1.976243     3.320833      26.09
 H      -1.226385     2.016753     1.661373      29.51
 C      -2.599110    -1.889758    -0.330628      44.66
 H      -3.266290    -2.686356    -0.106206      23.23
 C      -1.928372    -0.290063    -1.893130      45.08
 H      -2.143874     0.242831    -3.059778      21.76
 C      -0.964235     0.121793    -0.999871      10.68
 O      -0.123944     1.378466    -1.385025     184.85
 C      -0.673241     2.392831    -2.310261     103.90
 H      -0.065660     3.235366    -2.091799      28.01
 H      -0.393502     2.264305    -3.540148      23.87
 H      -1.621746     2.541312    -1.981574      28.47
 C      -0.801638    -0.396750     0.334292       2.35
 O       0.120408     0.024245     1.304918     117.95
 C      -1.633895    -1.571680     0.624750      58.35
 H      -1.386402    -2.007363     1.533064      24.44
 C      -2.835552    -1.280777    -1.609402      42.89
 C      -3.692935    -1.977057    -2.636020      83.57
 H      -3.370025    -1.914266    -3.656796      27.53
 O      -3.605846    -3.525339    -2.513397     179.88
 H      -2.881243    -3.753404    -2.944285      32.09
 C      -5.207155    -1.567233    -2.697069     107.26
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 H      -5.715604    -2.070244    -1.996415      30.01
 O      -5.184381    -0.128258    -2.324389     257.82
 H      -5.957246     0.039473    -1.799454      32.34
 C      -5.819270    -1.796278    -3.998710     102.35
 O      -5.844211    -3.414118    -4.046694     213.86
 H      -5.996260    -3.632405    -5.050084      27.53
 H      -5.251169    -1.400972    -4.752991      30.14
 H      -6.867701    -1.361925    -4.286951      27.10
55
name = lig-ACN-frame_685
 C       3.399906     0.366013     0.272787      40.13
 H       2.385864     0.316405    -0.356874      26.56
 C       4.250594     0.034381     2.508298      54.79
 H       4.148606     0.266878     3.483230      24.81
 C       5.433693    -0.553500     1.936056      20.51
 O       6.367523    -1.165665     2.745950     241.36
 C       6.488951    -0.841863     4.086596     124.16
 H       7.579349    -0.969166     4.354085      25.75
 H       5.830173    -1.441199     4.684928      26.25
 H       6.214141     0.143510     4.183735      26.37
 C       5.523385    -0.828551     0.565678      32.24
 O       6.584881    -1.171820    -0.165756     146.16
 H       7.406639    -1.246975     0.492656      21.38
 C       4.438580    -0.361833    -0.232267      31.23
 H       4.402187    -0.625540    -1.297810      23.53
 C       3.183975     0.569851     1.741823      -4.92
 C       1.947363     1.158368     2.448514     105.18
 H       2.219896     2.166962     2.814774      28.44
 O       1.488602     0.400701     3.558843     196.60
 H       1.068432    -0.528166     3.042556      24.71
 C       0.778908     1.398073     1.477503      90.42
 H       1.021633     1.909978     0.577857      26.03
 C      -0.281235     2.319884     2.056644     118.53
 O      -0.022917     3.705212     1.950587     279.80
 H       0.425697     3.986753     1.175125      33.74
 H      -0.577425     2.325333     3.240528      25.76
 H      -1.234153     2.187129     1.744822      29.36
 C      -2.698291    -2.054267    -0.250928      56.54
 H      -3.115270    -3.061890    -0.106776      28.92
 C      -1.842263    -0.379711    -1.938152      47.36
 H      -2.058852     0.341256    -2.970226      20.77
 C      -0.976619     0.254199    -0.968925      -5.96
 O      -0.103386     1.398866    -1.386655     213.81
 C      -0.644705     2.413023    -2.259112     111.31
 H       0.014533     3.225062    -2.263246      27.88
 H      -0.702976     1.788066    -3.388120      22.63
 H      -1.625223     2.769133    -2.236444      28.20
 C      -0.870390    -0.344201     0.365312      22.22
 O       0.093089    -0.003211     1.295868     161.77
 C      -1.626054    -1.508344     0.588445      45.47
 H      -1.480744    -2.103863     1.406953      23.69
 C      -2.771253    -1.430611    -1.499629       2.75
 C      -3.666544    -2.078809    -2.683531      94.94
 H      -3.165536    -1.631031    -3.503523      27.85
 O      -3.648943    -3.519108    -2.469933     244.55
 H      -2.745982    -3.766912    -2.741584      30.53
 C      -5.157977    -1.585594    -2.603928      81.63
 H      -5.614633    -2.181161    -1.914115      28.51
 O      -5.212269    -0.119839    -2.339900     156.34
 H      -6.365200    -0.064495    -2.423976      27.11
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 C      -5.954394    -1.912023    -4.041380      92.22
 O      -5.906541    -3.257020    -4.132446     284.59
 H      -6.312428    -3.428721    -4.924610      32.38
 H      -5.202591    -1.560968    -4.663167      28.04
 H      -7.057697    -1.437089    -4.188426      25.88
55
name = lig-ACN-frame_686
 C       3.329116     0.350515     0.396560      42.25
 H       2.617585     0.919268    -0.408696      22.08
 C       4.321786     0.039173     2.519436      66.99
 H       4.287000    -0.031727     3.599259      20.76
 C       5.404023    -0.598804     1.960349      21.35
 O       6.424183    -1.226106     2.666491     180.01
 C       6.418284    -0.825730     4.105585     120.46
 H       7.468830    -1.143465     4.543404      26.25
 H       5.656379    -1.393581     4.670108      28.18
 H       6.269543     0.175615     4.325858      29.36
 C       5.506959    -0.745309     0.532257      15.06
 O       6.674780    -1.213586    -0.215015      98.55
 H       7.374661    -1.528015     0.432591      25.57
 C       4.468575    -0.300597    -0.246301      53.13
 H       4.611545    -0.436233    -1.335040      24.95
 C       3.236492     0.562189     1.713634      33.36
 C       1.937137     1.205144     2.411114      90.41
 H       2.179228     2.161366     2.847640      27.25
 O       1.500405     0.366822     3.589998     242.18
 H       0.888511    -0.371597     3.288391      26.96
 C       0.712635     1.261062     1.402892     110.95
 H       1.116742     1.417089     0.487229      26.30
 C      -0.343453     2.314268     2.001172      96.25
 O      -0.047659     3.859495     1.928281     224.80
 H      -0.016079     3.875378     0.888927      28.03
 H      -0.306701     1.835647     3.143461      24.40
 H      -1.121953     2.053070     1.407250      28.30
 C      -2.570215    -2.094004    -0.230404      31.18
 H      -3.156832    -3.014141     0.133522      22.73
 C      -1.883304    -0.409476    -1.821522      41.10
 H      -1.866013    -0.175592    -3.052041      21.78
 C      -1.005669     0.374983    -0.971806      31.44
 O      -0.124331     1.344603    -1.274865     223.47
 C      -0.621823     2.365075    -2.329693      93.48
 H       0.174556     3.118415    -2.407216      25.97
 H      -0.780848     1.933595    -3.476857      23.58
 H      -1.504346     2.576586    -1.686277      23.43
 C      -0.897615    -0.242735     0.251357      14.34
 O       0.121662    -0.009090     1.303087     166.55
 C      -1.690099    -1.508010     0.645307      40.68
 H      -1.441452    -1.773047     1.635458      22.81
 C      -2.685004    -1.532896    -1.591597      34.53
 C      -3.609237    -2.071520    -2.602166      93.50
 H      -3.329649    -1.994555    -3.624256      26.50
 O      -3.676650    -3.496279    -2.475969     188.55
 H      -2.588727    -3.828908    -2.424808      24.18
 C      -5.144710    -1.599994    -2.598345      88.09
 H      -5.667774    -2.092113    -1.846743      27.39
 O      -5.298986    -0.193953    -2.354642     163.34
 H      -6.003599     0.377631    -3.058698      27.05
 C      -5.878354    -1.812704    -3.998702      96.29
 O      -6.030072    -3.296589    -4.265038     235.05
 H      -6.377094    -3.538293    -5.206286      27.61
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 H      -5.659145    -1.183231    -4.824213      28.74
 H      -6.843033    -1.393950    -3.511982      26.75
55
name = lig-ACN-frame_687
 C       3.305076     0.371070     0.301625      35.75
 H       2.620082     1.109219    -0.310459      22.36
 C       4.309241     0.043846     2.580941      53.65
 H       4.014447    -0.002981     3.714066      20.49
 C       5.423039    -0.709191     1.893029       6.83
 O       6.495458    -1.234327     2.678170     177.54
 C       6.396698    -0.874023     4.131414      94.96
 H       7.399979    -1.424121     4.548051      25.00
 H       5.434495    -1.311698     4.559844      26.13
 H       6.414901     0.193221     4.207395      26.81
 C       5.604901    -0.667473     0.441280      21.33
 O       6.715332    -1.263267    -0.169018     174.82
 H       7.253670    -1.654852     0.490379      24.69
 C       4.431588    -0.181216    -0.277258      47.03
 H       4.510044    -0.015089    -1.360623      22.34
 C       3.254529     0.532450     1.812908      19.75
 C       1.933587     1.066377     2.370896     106.52
 H       2.062434     2.095256     2.632912      27.97
 O       1.548391     0.397406     3.608428     272.46
 H       1.043933    -0.260289     3.336108      32.92
 C       0.752827     1.336098     1.363345      84.13
 H       0.975903     1.794933     0.456177      24.60
 C      -0.388325     2.343411     1.879171     101.94
 O      -0.088289     3.789716     1.897060     231.83
 H       0.032142     4.178691     0.956086      29.65
 H      -0.742263     2.313564     3.092540      24.76
 H      -1.363225     2.266194     1.563326      27.09
 C      -2.420348    -2.064124    -0.270501      51.72
 H      -3.154361    -2.881836     0.013592      21.83
 C      -1.916447    -0.355361    -1.884273      44.32
 H      -1.870211    -0.014423    -3.022244      21.07
 C      -1.092984     0.259639    -0.945313       7.64
 O      -0.124693     1.350582    -1.305784     217.64
 C      -0.617297     2.278719    -2.262555     113.64
 H       0.288286     3.007596    -2.412403      25.61
 H      -0.923843     1.745853    -3.292299      23.88
 H      -1.512138     3.065219    -2.157136      25.48
 C      -0.893861    -0.334558     0.394240      35.74
 O       0.064785    -0.057714     1.271327     169.98
 C      -1.647912    -1.338702     0.707540      62.04
 H      -1.681415    -1.720405     1.745544      26.41
 C      -2.576523    -1.544466    -1.510692      29.94
 C      -3.609783    -2.082426    -2.631417      88.84
 H      -3.112919    -1.670344    -3.503487      26.57
 O      -3.707962    -3.554022    -2.440344     172.57
 H      -2.618688    -3.906716    -2.589354      23.81
 C      -5.085432    -1.613825    -2.658337     101.22
 H      -5.626155    -2.279372    -1.966644      26.43
 O      -5.335298    -0.195409    -2.357271     234.91
 H      -5.209855     0.129630    -3.254773      31.61
 C      -5.944010    -1.795622    -3.892010      98.97
 O      -6.100322    -3.317744    -4.389292     223.43
 H      -6.161983    -2.920196    -5.391134      25.61
 H      -5.521066    -1.234667    -4.739052      27.47
 H      -7.039646    -1.590516    -3.710732      25.72
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name = lig-ACN-frame_688
 C       3.381697     0.488382     0.359923      59.69
 H       2.482465     0.541483    -0.296356      25.54
 C       4.309752    -0.102070     2.489507      63.53
 H       4.387942     0.035324     3.694803      20.21
 C       5.423292    -0.657786     1.938969      18.68
 O       6.490219    -1.208368     2.683589     206.56
 C       6.422802    -0.976316     4.070408     111.60
 H       7.291321    -1.551332     4.712161      24.80
 H       5.391589    -1.261457     4.570847      24.88
 H       6.560599     0.121029     4.359673      26.95
 C       5.561421    -0.649147     0.463901      10.04
 O       6.694700    -1.289751    -0.107063     102.71
 H       7.314461    -1.472274     0.680269      21.76
 C       4.554924    -0.047600    -0.338007      59.50
 H       4.676331    -0.071708    -1.420813      23.03
 C       3.180246     0.429080     1.670673      26.89
 C       1.930535     1.100594     2.370754      93.87
 H       2.372303     1.992038     2.718344      26.32
 O       1.574345     0.443244     3.599002     252.04
 H       1.231411    -0.525454     3.495648      26.28
 C       0.668146     1.401553     1.426166     101.06
 H       1.199122     1.656432     0.492994      24.26
 C      -0.480936     2.387795     1.857035     114.91
 O      -0.092148     3.715355     1.841734     304.86
 H       0.357373     3.911423     1.039767      32.53
 H      -0.630058     1.992859     3.054267      24.33
 H      -1.151876     2.071389     1.139649      27.53
 C      -2.402195    -2.042982    -0.242040      34.55
 H      -2.825694    -3.035071    -0.007508      19.53
 C      -1.896658    -0.291547    -1.940115      56.55
 H      -2.203536     0.388527    -2.754310      23.65
 C      -0.989145     0.236246    -0.928168      21.95
 O      -0.242014     1.276542    -1.287102     244.03
 C      -0.596382     2.264112    -2.306019      88.22
 H       0.423689     2.818386    -2.602889      24.76
 H      -0.801935     1.739688    -3.303290      24.19
 H      -1.542332     2.862713    -1.774237      23.59
 C      -0.884254    -0.281284     0.350097      11.97
 O       0.148880     0.047989     1.304591     165.68
 C      -1.762033    -1.433026     0.834079      38.52
 H      -1.688659    -1.871710     1.904070      24.86
 C      -2.631624    -1.457647    -1.603092      25.67
 C      -3.532063    -2.150991    -2.626749      95.64
 H      -3.136581    -2.085437    -3.649862      26.87
 O      -3.689504    -3.573678    -2.444222     243.94
 H      -2.946652    -3.988765    -2.904145      29.95
 C      -5.088611    -1.656158    -2.583103      65.06
 H      -5.445373    -2.030455    -1.542574      26.11
 O      -5.298263    -0.194909    -2.395419     258.98
 H      -4.587334     0.277347    -2.571581      35.44
 C      -6.045838    -1.987254    -3.955387     101.81
 O      -6.092109    -3.179194    -4.481484     290.40
 H      -6.251931    -3.474354    -5.445499      26.59
 H      -5.505751    -1.285462    -4.582371      28.29
 H      -6.921675    -1.302595    -3.667926      26.65
55
name = lig-ACN-frame_689
 C       3.450879     0.474454     0.188946      41.51
 H       2.695427     0.795732    -0.494787      21.90
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 C       4.176228    -0.154079     2.439653      52.89
 H       4.030928     0.025390     3.634857      21.52
 C       5.453028    -0.593633     1.890915      25.31
 O       6.464525    -1.185217     2.621748     205.39
 C       6.452793    -1.039904     4.113372      94.47
 H       7.346835    -1.824224     4.297831      23.56
 H       5.409362    -1.484786     4.518976      23.89
 H       6.683762     0.056967     4.471617      24.47
 C       5.577024    -0.665441     0.530882      27.45
 O       6.637666    -1.286379    -0.022285     176.92
 H       7.459752    -1.346839     0.616557      22.52
 C       4.700734     0.040461    -0.296057      56.55
 H       4.839928    -0.108842    -1.360407      25.58
 C       3.151095     0.337538     1.672652      23.92
 C       1.976125     1.178473     2.413521      95.48
 H       2.261241     2.158218     2.717613      27.28
 O       1.574306     0.477554     3.633821     194.29
 H       1.349407    -0.567528     3.225001      23.80
 C       0.732736     1.415732     1.498964      92.84
 H       0.937930     1.965585     0.489523      22.15
 C      -0.486162     2.243030     1.844112     101.59
 O      -0.058382     3.735232     1.784219     220.62
 H       0.710760     3.652944     1.125116      29.60
 H      -1.193786     2.016756     2.867539      24.71
 H      -1.330855     2.233190     1.189603      26.47
 C      -2.532919    -2.053961    -0.330649      39.66
 H      -2.936119    -3.032941    -0.256860      27.01
 C      -1.978152    -0.257168    -1.857879      69.93
 H      -2.114809     0.195203    -2.761403      19.85
 C      -1.014138     0.211261    -0.980722       6.36
 O      -0.197007     1.294295    -1.249321     185.16
 C      -0.590930     2.200030    -2.365123      97.57
 H       0.358332     2.984669    -2.321838      23.97
 H      -1.018799     1.895362    -3.292126      25.59
 H      -1.445531     3.006248    -1.879836      23.87
 C      -0.925603    -0.335472     0.444877      16.89
 O       0.177897     0.108443     1.304943     146.69
 C      -1.696512    -1.379244     0.747222      50.66
 H      -1.545775    -1.832301     1.806530      22.49
 C      -2.638299    -1.467344    -1.581927      32.61
 C      -3.583252    -2.191661    -2.672354      82.74
 H      -3.285119    -1.880598    -3.695800      24.78
 O      -3.647621    -3.631031    -2.424827     260.74
 H      -3.021754    -3.992492    -2.937184      32.23
 C      -5.101993    -1.681084    -2.561373      70.50
 H      -5.698567    -2.328719    -1.690649      25.24
 O      -5.200944    -0.206711    -2.450409     194.43
 H      -4.453062    -0.083449    -1.681858      26.06
 C      -5.943618    -1.806238    -3.920953      98.46
 O      -6.073858    -3.283050    -4.518194     246.52
 H      -6.391874    -2.955447    -5.317961      31.22
 H      -5.641284    -1.186057    -4.725162      27.97
 H      -7.065041    -1.750342    -3.693775      25.08
55
name = lig-ACN-frame_690
 C       3.433116     0.460202     0.140245      63.70
 H       3.066462     1.230382    -0.413187      23.32
 C       4.113195    -0.160554     2.479693      59.15
 H       3.795876    -0.345967     3.588078      22.56
 C       5.329412    -0.570265     1.990970      13.29
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 O       6.451579    -1.138623     2.629000     207.51
 C       6.512346    -1.182030     4.050265     105.81
 H       7.424610    -1.781102     4.432928      25.19
 H       5.492317    -1.561452     4.620322      24.71
 H       6.664483    -0.031306     4.483190      24.34
 C       5.627805    -0.587452     0.560500      10.78
 O       6.700158    -1.326170    -0.008259     161.78
 H       7.318240    -1.496733     0.712074      23.83
 C       4.716047     0.018032    -0.301398      54.09
 H       5.044972     0.254090    -1.315273      24.17
 C       3.120993     0.460366     1.515773      10.75
 C       1.976307     1.176217     2.402728      90.65
 H       2.486520     2.100304     2.702454      26.94
 O       1.594365     0.512938     3.640571     228.72
 H       1.042223    -0.349215     3.372810      25.78
 C       0.709654     1.414648     1.481630      70.67
 H       1.326754     1.775483     0.510601      22.78
 C      -0.486080     2.345327     1.861363     108.26
 O      -0.039538     3.671774     1.755692     257.41
 H       0.804574     3.940569     1.188861      28.31
 H      -0.797216     2.282449     3.047333      24.65
 H      -1.189433     1.976685     1.057689      25.56
 C      -2.569946    -2.036735    -0.271274      75.71
 H      -3.150178    -2.843716     0.075430      27.04
 C      -2.059533    -0.267384    -1.846825      65.94
 H      -1.943777     0.009117    -2.769987      18.60
 C      -1.068473     0.278574    -0.865817      18.23
 O      -0.139017     1.320797    -1.276694     228.99
 C      -0.587449     2.242539    -2.291787      91.46
 H       0.363512     2.851118    -2.717408      24.80
 H      -0.643480     1.635569    -3.085963      27.72
 H      -1.705759     2.868782    -2.107609      24.14
 C      -0.840730    -0.238434     0.352460      29.75
 O       0.136801    -0.029422     1.263119     156.72
 C      -1.684264    -1.472521     0.576047      43.56
 H      -1.693383    -1.988113     1.595082      22.69
 C      -2.753310    -1.533315    -1.622173      14.87
 C      -3.689102    -2.178233    -2.658504      90.11
 H      -3.148206    -1.928253    -3.600028      25.66
 O      -3.607206    -3.659113    -2.421324     201.25
 H      -2.644616    -3.981162    -2.854787      24.54
 C      -5.109096    -1.688583    -2.700476      96.27
 H      -5.729141    -2.329994    -1.837507      24.94
 O      -5.026488    -0.263293    -2.409863     123.67
 H      -5.188708     0.013340    -1.278355      25.08
 C      -5.925220    -1.803587    -3.890153      97.15
 O      -5.985501    -3.269644    -4.468639     252.39
 H      -6.207547    -3.390442    -5.373028      29.08
 H      -5.489128    -1.017248    -4.555836      28.97
 H      -6.896899    -1.287456    -3.545631      26.84
55
name = lig-ACN-frame_691
 C       3.466199     0.630778     0.178719      57.52
 H       2.785350     1.008250    -0.510816      27.83
 C       4.014372    -0.151460     2.440686      60.62
 H       3.756240    -0.241058     3.489320      22.82
 C       5.314913    -0.635953     1.978797      19.87
 O       6.424322    -1.121715     2.661277     196.49
 C       6.554669    -1.247990     4.063725     102.37
 H       7.480525    -1.846618     4.177371      26.88
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 H       5.583268    -1.903564     4.470955      25.64
 H       6.600689    -0.131988     4.646728      24.47
 C       5.617767    -0.554765     0.592322      13.73
 O       6.776215    -1.317853     0.041976     162.67
 H       7.272238    -1.705510     0.758717      20.59
 C       4.689168    -0.005972    -0.335649      48.48
 H       5.035816     0.035250    -1.399209      21.63
 C       3.141187     0.497608     1.582788      31.72
 C       1.906703     1.125203     2.289189     101.70
 H       2.176325     2.174285     2.609741      25.35
 O       1.627158     0.534015     3.620555     279.89
 H       0.959827    -0.014219     3.492017      32.69
 C       0.697065     1.307509     1.443061      87.25
 H       0.827901     1.591819     0.276522      19.38
 C      -0.345681     2.340222     1.853086     113.14
 O      -0.010424     3.761875     1.742699     271.52
 H       0.467637     3.689068     0.904595      31.04
 H      -0.650633     2.035407     2.976917      26.06
 H      -1.435258     2.340962     1.469223      24.98
 C      -2.639271    -2.048201    -0.299811      42.16
 H      -3.149052    -2.897371     0.109441      22.92
 C      -1.998958    -0.335933    -1.839700      67.89
 H      -2.260941     0.136357    -2.670795      28.01
 C      -1.149747     0.420157    -0.988828      11.12
 O      -0.155837     1.337028    -1.260971     219.29
 C      -0.564114     2.182608    -2.358906     110.95
 H       0.177105     3.101215    -2.299397      24.88
 H      -0.789393     1.814148    -3.252160      29.03
 H      -1.666881     2.729903    -1.879801      23.94
 C      -0.890532    -0.393312     0.275204       5.23
 O       0.169286    -0.081049     1.265819     141.06
 C      -1.605754    -1.493820     0.584797      57.31
 H      -1.328856    -1.875910     1.585998      24.63
 C      -2.838335    -1.431217    -1.556722      23.06
 C      -3.594620    -2.262383    -2.679255      89.34
 H      -3.341695    -2.097744    -3.757850      25.08
 O      -3.572317    -3.648569    -2.450243     179.12
 H      -2.419604    -3.856015    -2.542686      23.55
 C      -5.079076    -1.721703    -2.621954      65.87
 H      -5.608316    -2.167636    -1.603742      23.87
 O      -4.919293    -0.281662    -2.335256     184.59
 H      -5.681108    -0.199226    -1.611879      27.18
 C      -5.958292    -1.843862    -4.075293      84.87
 O      -5.889593    -3.150584    -4.320082     236.49
 H      -5.889169    -3.123798    -5.394846      25.76
 H      -5.375017    -1.374432    -4.925192      24.80
 H      -7.068928    -1.517612    -4.034317      24.52
55
name = lig-ACN-frame_692
 C       3.538689     0.715955     0.219889      56.30
 H       2.730746     0.855893    -0.488369      25.05
 C       4.114247    -0.205312     2.472572      65.14
 H       3.924609    -0.128065     3.459064      26.62
 C       5.300587    -0.649378     1.918017      18.00
 O       6.400724    -1.121908     2.661100     194.30
 C       6.543418    -1.332697     4.108154      99.92
 H       7.522569    -1.719723     4.214156      27.46
 H       5.713320    -2.110095     4.550714      24.97
 H       6.504467    -0.260142     4.823713      23.47
 C       5.616726    -0.665363     0.522641      18.13
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 O       6.746768    -1.218766     0.116566     162.26
 H       7.291987    -1.496554     0.970158      18.60
 C       4.651656     0.022317    -0.283030      55.60
 H       4.538774    -0.304786    -1.346853      22.36
 C       3.134755     0.531507     1.597224       3.44
 C       1.894855     1.164557     2.226819      85.35
 H       2.103684     2.289887     2.306095      25.54
 O       1.630083     0.572844     3.554997     241.75
 H       1.106559    -0.287634     3.396322      27.76
 C       0.622400     1.188026     1.248394      91.41
 H       1.212939     1.726381     0.373840      22.90
 C      -0.367948     2.261946     1.979932      75.38
 O       0.093770     3.826630     1.702170     174.07
 H       0.227037     4.148869     0.824627      30.48
 H      -0.297623     2.378701     3.087990      25.49
 H      -1.390316     2.007022     1.368352      23.90
 C      -2.604052    -2.061849    -0.236946      73.84
 H      -3.077387    -3.043743    -0.349363      28.53
 C      -2.028979    -0.243390    -1.955492      49.95
 H      -2.224704     0.273095    -2.880976      22.40
 C      -1.097721     0.228135    -0.948357      16.23
 O      -0.245643     1.324385    -1.313728     213.32
 C      -0.608065     2.271490    -2.359344      96.48
 H       0.212820     3.084240    -2.383551      25.20
 H      -0.517699     1.727179    -3.234617      26.80
 H      -1.838489     2.738241    -2.216011      24.19
 C      -0.851818    -0.386770     0.249419      33.72
 O       0.095306    -0.114979     1.197471     200.46
 C      -1.626871    -1.562349     0.609855      53.08
 H      -1.415914    -2.154431     1.482082      22.81
 C      -2.774617    -1.413116    -1.505525     -10.72
 C      -3.599564    -2.219328    -2.709167      81.31
 H      -2.920274    -1.825624    -3.493916      24.28
 O      -3.502491    -3.671915    -2.448631     231.18
 H      -2.541436    -4.060278    -2.523386      27.03
 C      -5.099398    -1.660963    -2.657230      83.20
 H      -5.762754    -2.457886    -2.025003      24.12
 O      -4.914733    -0.285284    -2.243392     267.50
 H      -5.644043     0.132882    -2.132908      36.01
 C      -5.848810    -1.733722    -4.042436      87.05
 O      -5.812228    -3.260033    -4.294549     221.98
 H      -5.864862    -3.591223    -5.297853      26.37
 H      -5.333361    -0.954347    -4.740202      26.89
 H      -6.901749    -1.317028    -4.032501      26.97
55
name = lig-ACN-frame_693
 C       3.505208     0.626170     0.290143      54.76
 H       3.003871     1.424149    -0.361831      22.76
 C       4.136308    -0.125577     2.497601      74.54
 H       4.103279    -0.270743     3.477377      24.14
 C       5.334958    -0.658895     1.951966      12.19
 O       6.434583    -1.150833     2.681226     169.72
 C       6.497760    -1.381120     4.090391     112.07
 H       7.469313    -1.695609     4.324242      28.98
 H       5.684052    -2.219934     4.380447      26.37
 H       6.109497    -0.291496     4.669624      23.59
 C       5.509449    -0.679051     0.543312      17.52
 O       6.767324    -1.164443     0.114494     104.96
 H       7.333497    -1.254476     0.954986      21.92
 C       4.610982    -0.029795    -0.317755      52.93
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 H       4.833575     0.037612    -1.429765      22.01
 C       3.230056     0.544404     1.634280      37.68
 C       1.910986     1.166735     2.167292      92.43
 H       2.155720     2.240126     2.521273      26.18
 O       1.585169     0.628488     3.450630     182.49
 H       1.561696    -0.497039     3.301569      26.16
 C       0.682161     1.293424     1.294674      87.10
 H       0.713164     1.487562     0.197948      21.36
 C      -0.300125     2.350572     1.902016     111.27
 O       0.132459     3.735181     1.725979     235.42
 H       0.117582     3.665754     0.681242      28.07
 H      -0.247721     2.095447     2.938327      28.00
 H      -1.530758     2.212871     1.894402      25.26
 C      -2.548895    -2.071656    -0.351967      54.58
 H      -2.980145    -3.001955     0.106854      24.63
 C      -2.081892    -0.233668    -1.868246      69.33
 H      -2.084506     0.134858    -2.977117      21.08
 C      -1.030270     0.142437    -1.099415      15.36
 O      -0.340185     1.319007    -1.318049     213.51
 C      -0.650503     2.283542    -2.377710     102.63
 H       0.080296     3.058864    -2.264586      27.72
 H      -0.558976     1.873896    -3.373178      27.23
 H      -1.897331     2.783063    -2.446054      23.92
 C      -0.921536    -0.499817     0.277272       6.04
 O       0.075237    -0.099875     1.133437     152.70
 C      -1.655589    -1.642205     0.637595      55.20
 H      -1.434363    -2.064534     1.614898      24.01
 C      -2.724902    -1.457681    -1.629681      50.39
 C      -3.545540    -2.108315    -2.583898      94.24
 H      -3.348872    -2.092879    -3.692235      25.01
 O      -3.471231    -3.632202    -2.460951     222.41
 H      -2.737123    -3.727246    -2.919618      31.92
 C      -5.024219    -1.659946    -2.735436      94.91
 H      -5.653515    -2.146926    -1.863870      25.24
 O      -4.982636    -0.280279    -2.138401     201.52
 H      -5.572325     0.227300    -2.781608      31.31
 C      -5.714141    -1.730816    -4.027928      99.02
 O      -5.752829    -3.292155    -4.303264     237.43
 H      -6.019124    -3.298674    -5.184399      30.98
 H      -5.078330    -1.312347    -4.943643      25.86
 H      -6.729304    -1.353835    -3.801354      26.52
55
name = lig-ACN-frame_694
 C       3.498163     0.578796     0.226045      31.32
 H       2.920827     1.479274    -0.290706      23.55
 C       4.196267    -0.083771     2.597409      65.08
 H       3.791678     0.025187     3.554581      23.84
 C       5.346966    -0.675158     2.009452      27.50
 O       6.497218    -1.183569     2.642989     212.83
 C       6.353821    -1.376608     4.059969     106.50
 H       7.372682    -1.572194     4.374003      28.79
 H       5.675636    -2.291622     4.315442      26.46
 H       6.004332    -0.371880     4.799668      22.60
 C       5.563304    -0.693390     0.600643      13.46
 O       6.742946    -1.118526     0.058354     175.21
 H       7.384957    -1.342763     0.699111      24.18
 C       4.596364    -0.071679    -0.348240      41.41
 H       5.091089     0.343455    -1.249535      23.57
 C       3.229379     0.542289     1.674556      11.84
 C       1.995474     1.222441     2.179741      85.56
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 H       2.265426     2.363779     2.284871      25.84
 O       1.527207     0.619945     3.399840     205.89
 H       1.504808    -0.416502     3.282090      27.20
 C       0.638788     1.360367     1.208133      72.59
 H       1.087504     1.867460     0.382337      26.87
 C      -0.278968     2.324235     2.004271     117.47
 O       0.143866     3.620784     1.700407     246.96
 H       0.548782     3.930977     0.848676      29.56
 H      -0.230914     2.266374     3.029733      28.60
 H      -1.326417     2.176019     1.338979      24.74
 C      -2.518160    -2.196371    -0.381147      39.42
 H      -3.351671    -2.970672    -0.464792      28.88
 C      -2.067831    -0.351480    -1.927204      59.00
 H      -2.412302     0.354867    -2.893624      22.01
 C      -1.051078     0.154058    -1.042616      19.63
 O      -0.371022     1.351284    -1.307005     201.16
 C      -0.716723     2.236028    -2.389980      98.30
 H      -0.113173     3.046674    -2.213786      28.06
 H      -0.573020     1.749884    -3.488791      24.88
 H      -1.915087     2.531945    -2.003937      23.67
 C      -0.868465    -0.460343     0.196007      19.92
 O       0.122538    -0.050045     1.185459     135.61
 C      -1.644623    -1.588880     0.572966      52.42
 H      -1.673102    -1.977837     1.625193      21.84
 C      -2.667623    -1.520744    -1.611770       9.98
 C      -3.553341    -2.198586    -2.728658     101.50
 H      -2.972256    -1.685162    -3.555403      25.51
 O      -3.451938    -3.529816    -2.478429     239.12
 H      -2.848163    -4.022058    -3.066100      28.84
 C      -4.950053    -1.618897    -2.497879      89.04
 H      -5.568351    -2.423579    -1.963002      27.41
 O      -5.118426    -0.238300    -2.116161     116.62
 H      -5.122129     0.354669    -3.136907      26.54
 C      -5.610581    -1.910148    -4.080866      77.66
 O      -5.741182    -3.198903    -4.346698     256.86
 H      -6.166889    -3.409076    -5.214330      29.34
 H      -5.000374    -1.246583    -4.936713      26.26
 H      -6.587366    -1.404689    -4.254516      26.43
55
name = lig-ACN-frame_695
 C       3.525284     0.570481     0.247069      61.05
 H       2.733187     0.733107    -0.624405      26.03
 C       4.192633    -0.049149     2.576020      63.20
 H       4.267954     0.015631     3.683101      21.38
 C       5.348119    -0.674539     2.021118       3.02
 O       6.498036    -1.186647     2.664567     168.81
 C       6.284831    -1.377979     4.086341     112.87
 H       7.246031    -1.648701     4.633055      27.93
 H       5.484544    -2.161120     4.255680      27.31
 H       5.752640    -0.286971     4.443268      22.27
 C       5.566422    -0.651333     0.582505      12.70
 O       6.726949    -1.103671    -0.035872     129.24
 H       7.302285    -1.538503     0.666211      21.14
 C       4.689910    -0.025568    -0.233629      63.99
 H       4.803095    -0.188413    -1.317613      23.11
 C       3.244065     0.504659     1.586146      26.91
 C       1.958742     1.249025     2.170189      85.52
 H       2.249651     2.294430     2.572439      25.03
 O       1.500451     0.620045     3.426543     244.33
 H       1.086351    -0.101878     3.134468      32.85
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 C       0.778630     1.323023     1.295425     108.97
 H       0.784883     1.601874     0.315213      24.99
 C      -0.323771     2.218872     1.921416     100.44
 O       0.190930     3.712706     1.717736     209.25
 H       0.820527     3.474681     1.094806      33.22
 H      -0.463703     2.088464     2.906034      29.35
 H      -1.492411     1.897680     1.620699      25.67
 C      -2.497613    -2.240856    -0.393729      79.90
 H      -2.812919    -3.195068     0.130219      24.74
 C      -1.922084    -0.364626    -1.949492      59.21
 H      -2.450435     0.253683    -2.912093      23.01
 C      -1.131254     0.261352    -1.014797      15.73
 O      -0.333090     1.345079    -1.277371     221.76
 C      -0.855506     2.190939    -2.309875     109.40
 H      -0.250648     2.998552    -2.491122      28.93
 H      -0.734910     1.496406    -3.327285      24.80
 H      -2.046160     2.599630    -2.476863      25.98
 C      -0.747427    -0.416566     0.225742      16.86
 O       0.144608     0.034269     1.151224     173.16
 C      -1.652016    -1.545939     0.500810      30.32
 H      -1.483160    -1.897698     1.586712      27.83
 C      -2.624596    -1.617864    -1.653280      43.12
 C      -3.408688    -2.072199    -2.720839      64.68
 H      -3.206312    -2.036272    -3.842048      26.24
 O      -3.500769    -3.593858    -2.546472      92.89
 H      -2.611458    -3.954937    -3.219367      23.61
 C      -5.075966    -1.682725    -2.614225      69.58
 H      -5.408109    -2.059921    -1.631899      26.90
 O      -5.250453    -0.248563    -2.159210      95.17
 H      -4.540267     0.347079    -2.804730      28.82
 C      -5.579356    -1.775310    -4.022688      87.16
 O      -5.724964    -3.300631    -4.418226     183.33
 H      -6.135152    -3.394011    -5.464015      24.33
 H      -4.542956    -1.456301    -4.486306      24.80
 H      -6.472718    -1.180989    -4.090517      27.12
55
name = lig-ACN-frame_696
 C       3.471592     0.476480     0.229045      27.36
 H       2.550012     0.628930    -0.458085      23.02
 C       4.230939    -0.027895     2.421137      60.16
 H       3.879418     0.085830     3.539333      22.91
 C       5.431601    -0.635301     1.934948      39.19
 O       6.440751    -1.189589     2.729697     219.17
 C       6.173092    -1.329518     4.120864     108.73
 H       7.247455    -1.678102     4.494828      26.26
 H       5.414300    -2.091032     4.318035      26.89
 H       5.939053    -0.301896     4.796408      23.12
 C       5.673861    -0.590418     0.604132      33.00
 O       6.726142    -1.157416    -0.083160     173.64
 H       7.440356    -1.617769     0.551304      21.56
 C       4.718479    -0.000574    -0.287207      45.56
 H       4.741709    -0.369590    -1.311211      23.70
 C       3.208647     0.530598     1.679655      25.42
 C       1.999863     1.142810     2.245420      97.11
 H       2.315291     2.283537     2.311797      25.76
 O       1.501043     0.615724     3.469058     262.45
 H       0.799577    -0.059167     3.298445      28.35
 C       0.720912     1.361848     1.251895      87.83
 H       1.234602     1.782926     0.488160      27.13
 C      -0.305223     2.299735     1.878714     118.56
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 O       0.152128     3.656795     1.762120     238.78
 H       0.883999     3.917230     1.114679      29.21
 H      -0.402227     2.028755     2.842236      29.88
 H      -1.235774     2.391413     1.102425      24.89
 C      -2.338178    -2.125612    -0.345674      37.99
 H      -2.894497    -3.064774    -0.209029      31.69
 C      -1.888143    -0.404785    -1.890955      70.97
 H      -1.731846    -0.037727    -3.049833      19.41
 C      -1.055247     0.283344    -0.949442      20.37
 O      -0.346799     1.436311    -1.258393     189.42
 C      -0.943032     2.163714    -2.412852      88.82
 H      -0.294850     3.025531    -2.443168      27.67
 H      -0.994023     1.542189    -3.527017      23.28
 H      -1.941391     2.333151    -1.781174      25.62
 C      -0.844144    -0.371477     0.213584      35.54
 O       0.178082    -0.047091     1.160129     145.46
 C      -1.499457    -1.486628     0.567287      64.66
 H      -1.274335    -2.090223     1.506030      24.28
 C      -2.483407    -1.597834    -1.674575      13.54
 C      -3.575809    -2.213884    -2.703910      88.08
 H      -3.080665    -1.699238    -3.635768      25.24
 O      -3.524486    -3.629315    -2.665819     192.08
 H      -2.493539    -3.916500    -3.041292      25.60
 C      -4.988314    -1.660311    -2.629236     113.10
 H      -5.640024    -2.464213    -2.184876      27.19
 O      -5.308975    -0.285809    -2.274587     261.04
 H      -4.515960     0.145190    -2.104753      33.40
 C      -5.591685    -1.816437    -4.046465      87.56
 O      -5.728164    -3.283793    -4.474833     249.67
 H      -5.903703    -3.034826    -5.459952      25.75
 H      -5.113798    -1.240360    -5.002576      24.74
 H      -6.529430    -1.317481    -4.181518      26.41
55
name = lig-ACN-frame_697
 C       3.400597     0.361358     0.203034      65.08
 H       2.766078     0.889666    -0.508175      26.11
 C       4.277025    -0.022408     2.437368      71.57
 H       4.146480    -0.270083     3.586693      22.61
 C       5.460101    -0.523073     1.949045       3.80
 O       6.363656    -1.172170     2.776886     180.39
 C       6.129638    -1.312324     4.226991     107.29
 H       7.105280    -1.881869     4.640664      25.96
 H       5.272479    -1.917053     4.436684      27.74
 H       5.940725    -0.232093     4.694698      23.68
 C       5.754091    -0.500120     0.439193      19.26
 O       6.779414    -1.268911    -0.107992     125.78
 H       7.537096    -1.318772     0.525963      21.89
 C       4.619217    -0.077322    -0.329306      53.62
 H       4.901097     0.198053    -1.344217      23.48
 C       3.241821     0.476942     1.564403      30.17
 C       1.900967     1.152463     2.276824      93.23
 H       2.232122     2.140292     2.657535      27.18
 O       1.525337     0.609648     3.581061     199.53
 H       1.035122    -0.391048     3.311958      24.87
 C       0.792312     1.315533     1.255313     103.15
 H       0.989996     1.586173     0.277371      27.10
 C      -0.289981     2.368338     1.733941     113.61
 O       0.153377     3.721077     1.872306     222.60
 H       0.546929     3.886877     0.893262      27.95
 H      -0.690561     2.256605     2.631574      30.21
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 H      -1.315240     2.106813     1.132988      26.80
 C      -2.281559    -2.097099    -0.356879      61.91
 H      -2.916480    -2.914389    -0.003152      24.16
 C      -1.770389    -0.362160    -1.963948      45.53
 H      -1.700414    -0.071102    -3.077634      21.01
 C      -0.971346     0.280799    -1.011787       3.77
 O      -0.353765     1.500170    -1.319654     217.68
 C      -1.023153     2.205753    -2.385793      98.90
 H      -0.449739     3.203870    -2.602264      26.73
 H      -1.013677     1.603007    -3.509727      23.50
 H      -2.143707     2.555161    -2.361950      26.60
 C      -0.817385    -0.273143     0.382626     -11.50
 O       0.242277    -0.039426     1.148006     158.99
 C      -1.404687    -1.599039     0.668083      43.12
 H      -1.153723    -1.980881     1.676032      24.87
 C      -2.515430    -1.587831    -1.599398      43.06
 C      -3.483827    -2.207757    -2.650281      80.49
 H      -3.150124    -1.886871    -3.756293      24.07
 O      -3.525765    -3.654604    -2.786501     252.41
 H      -2.657848    -3.893978    -2.994611      31.34
 C      -5.031792    -1.744257    -2.738373      78.66
 H      -5.617169    -2.324968    -1.939851      26.67
 O      -5.260398    -0.349847    -2.343707     221.14
 H      -4.857493    -0.221055    -1.554254      34.28
 C      -5.719895    -1.876194    -4.231548      98.50
 O      -5.719826    -3.176113    -4.538976     331.28
 H      -5.948667    -3.554903    -5.308790      32.77
 H      -5.101421    -1.058198    -4.876805      25.75
 H      -6.626105    -1.594468    -3.821014      26.37
55
name = lig-ACN-frame_698
 C       3.390348     0.355514     0.132541      33.57
 H       2.715942     0.801803    -0.522074      23.60
 C       4.232697    -0.013383     2.443443      49.89
 H       4.048330     0.045182     3.583660      21.37
 C       5.507849    -0.468388     1.866358      13.89
 O       6.353276    -1.176428     2.793074     172.79
 C       6.068415    -1.266929     4.255865     102.79
 H       7.007264    -1.878543     4.671207      24.99
 H       5.146599    -1.737246     4.465129      26.64
 H       6.123143    -0.275926     4.787057      24.86
 C       5.696218    -0.563560     0.464568      21.32
 O       6.815241    -1.301882    -0.114524     130.80
 H       7.559788    -1.297186     0.484624      24.28
 C       4.666413    -0.112625    -0.423512      42.74
 H       4.723768    -0.067005    -1.535004      23.53
 C       3.160196     0.406378     1.650856      10.99
 C       2.022225     1.173569     2.289085      88.60
 H       2.283208     2.200386     2.430946      28.01
 O       1.530019     0.553622     3.625011     192.83
 H       1.530743    -0.527017     3.548004      26.63
 C       0.788987     1.345855     1.297495     103.02
 H       1.373628     1.740633     0.444410      26.56
 C      -0.380520     2.298848     1.697772     100.83
 O       0.178285     3.826492     1.885594     190.31
 H       0.460015     4.189301     1.049941      30.81
 H      -0.720663     1.861633     2.578169      28.87
 H      -1.033029     2.486892     0.788618      25.79
 C      -2.325459    -2.176261    -0.212727      29.42
 H      -2.778595    -3.135254     0.071732      25.32
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 C      -1.702730    -0.436957    -1.991944      61.65
 H      -2.070865     0.096757    -2.794744      25.75
 C      -0.942737     0.251826    -1.008845      -5.10
 O      -0.403722     1.533616    -1.376886     167.35
 C      -1.068581     2.311947    -2.468147      81.00
 H      -0.340041     3.305316    -2.450431      24.47
 H      -0.786496     1.616465    -3.483688      23.41
 H      -2.103446     2.353479    -2.120194      27.31
 C      -0.758429    -0.352222     0.334306      21.96
 O       0.320219     0.019123     1.222733     141.93
 C      -1.394337    -1.536435     0.623880      65.83
 H      -1.297757    -2.037240     1.542343      25.86
 C      -2.542772    -1.506717    -1.589228     -22.40
 C      -3.393254    -2.125741    -2.764633      76.81
 H      -2.850926    -1.685245    -3.708575      23.71
 O      -3.473837    -3.661671    -2.820678     227.99
 H      -2.735010    -3.972007    -3.215247      31.93
 C      -5.073760    -1.817069    -2.814417      76.35
 H      -5.526869    -2.593662    -2.123148      26.35
 O      -5.152668    -0.404643    -2.406206     117.43
 H      -5.358783    -0.515220    -1.313950      27.55
 C      -5.856924    -1.778461    -4.141534      96.70
 O      -5.690821    -3.272635    -4.641945     270.49
 H      -6.130103    -3.079482    -5.483391      27.17
 H      -5.256357    -1.152992    -5.007792      24.94
 H      -6.780789    -1.352414    -4.358237      26.87
55
name = lig-ACN-frame_699
 C       3.452165     0.363733     0.197572      62.40
 H       2.652991     0.456127    -0.428490      25.71
 C       4.235042     0.004817     2.387067      70.74
 H       4.210929     0.304916     3.423018      23.25
 C       5.412679    -0.547273     1.947246      15.43
 O       6.384537    -1.153103     2.763693     219.01
 C       6.042393    -1.199026     4.194276     117.01
 H       6.789804    -2.013767     4.543557      25.98
 H       5.060453    -1.578748     4.350756      27.64
 H       6.176663    -0.295705     4.687798      27.92
 C       5.658881    -0.725987     0.477488       5.50
 O       6.760337    -1.242250    -0.086577     154.50
 H       7.459947    -1.644485     0.579634      22.86
 C       4.653527    -0.127586    -0.385363      50.55
 H       4.769535    -0.617536    -1.370875      22.25
 C       3.176040     0.381456     1.533571      37.63
 C       2.029259     1.166006     2.378184      96.43
 H       2.518718     2.013076     2.722084      27.95
 O       1.610164     0.557906     3.581816     291.21
 H       1.587667    -0.315564     3.437225      32.77
 C       0.846596     1.458701     1.347662      75.19
 H       1.221887     1.836403     0.289062      23.78
 C      -0.301005     2.428205     1.671352     123.93
 O       0.124917     3.774619     1.933103     269.67
 H       0.626635     3.920244     1.138392      32.83
 H      -0.972962     2.291422     2.463106      28.64
 H      -1.070530     2.324797     0.864497      27.14
 C      -2.402348    -2.119625    -0.305689      58.95
 H      -2.939584    -3.080398    -0.106652      23.69
 C      -1.808881    -0.480004    -1.857294      56.21
 H      -1.919883    -0.071866    -2.732429      28.59
 C      -0.910940     0.273534    -1.031747      18.48
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 O      -0.426408     1.507591    -1.356682     197.07
 C      -1.028198     2.280656    -2.490209     107.45
 H      -0.651527     3.429068    -2.234842      25.44
 H      -0.998167     2.164904    -3.705258      25.17
 H      -2.076188     2.448326    -2.354576      28.55
 C      -0.551591    -0.361451     0.167380       3.51
 O       0.265312    -0.003780     1.225694     125.19
 C      -1.446221    -1.510082     0.609441      32.50
 H      -1.080534    -1.846924     1.508962      27.10
 C      -2.558553    -1.635002    -1.540882      27.41
 C      -3.492027    -2.194738    -2.899995      82.16
 H      -3.012940    -1.705061    -3.804410      24.16
 O      -3.347870    -3.559777    -2.819158     216.00
 H      -2.525399    -3.866747    -3.483156      23.76
 C      -4.968308    -1.776907    -2.856755      90.32
 H      -5.487102    -2.515514    -2.195316      27.44
 O      -5.095697    -0.450896    -2.377232     135.12
 H      -5.591655    -0.287071    -1.367951      26.98
 C      -5.787467    -1.885232    -4.193827      88.31
 O      -5.736272    -3.220849    -4.719888     272.26
 H      -6.037856    -3.544522    -5.723501      23.67
 H      -5.187546    -1.056523    -4.879255      24.50
 H      -6.730838    -1.606526    -3.807110      25.87
55
name = lig-ACN-frame_700
 C       3.414128     0.308324     0.119233      51.31
 H       2.738761     0.583983    -0.664008      26.32
 C       4.272226     0.045292     2.422335      49.37
 H       4.124213     0.168217     3.419789      22.62
 C       5.378773    -0.745130     1.907082      31.35
 O       6.411595    -1.102893     2.733418     233.73
 C       6.061817    -1.199197     4.113224     131.56
 H       6.625627    -1.979744     4.647408      28.41
 H       4.997448    -1.317337     4.230198      28.90
 H       6.278446    -0.331205     4.525193      30.84
 C       5.563166    -0.755826     0.585358      33.65
 O       6.724656    -1.241486    -0.060112     166.30
 H       7.308473    -1.646523     0.717843      18.49
 C       4.626343    -0.302962    -0.268123      61.16
 H       4.731261    -0.189134    -1.356803      23.79
 C       3.228197     0.479382     1.571446      17.24
 C       2.053059     1.194451     2.297860     108.18
 H       2.375729     2.135991     2.552989      28.05
 O       1.702195     0.528313     3.556895     265.95
 H       1.103739    -0.175241     3.354335      28.83
 C       0.851296     1.458596     1.421764      72.93
 H       1.291063     1.646580     0.300245      23.36
 C      -0.342032     2.471272     1.712110     124.95
 O       0.131828     3.775594     1.936249     255.69
 H       0.934859     4.123040     1.380297      29.13
 H      -0.781598     2.010523     2.569276      28.51
 H      -0.880037     2.468347     0.797891      27.73
 C      -2.420526    -2.120280    -0.278606      14.08
 H      -3.053425    -2.813456     0.362098      26.10
 C      -1.918608    -0.391781    -1.876723      54.46
 H      -1.935440    -0.128017    -2.803460      26.61
 C      -0.930426     0.195035    -1.069670      10.14
 O      -0.410590     1.490044    -1.417216     198.35
 C      -1.062064     2.315210    -2.423243      99.38
 H      -0.455101     3.335820    -2.222308      25.09
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 H      -0.453220     1.750990    -3.240948      24.61
 H      -2.112011     2.192711    -2.422636      28.33
 C      -0.555927    -0.454492     0.161193      30.30
 O       0.250649     0.072311     1.185157     146.40
 C      -1.409080    -1.478670     0.492705      51.78
 H      -1.465475    -1.840340     1.470485      27.01
 C      -2.623109    -1.619072    -1.745765       7.00
 C      -3.426095    -2.143776    -2.834893     110.61
 H      -3.111027    -1.777863    -3.819158      25.34
 O      -3.244117    -3.598903    -2.867479     185.79
 H      -2.177493    -3.721166    -3.394486      22.02
 C      -4.910093    -1.857617    -2.813619      92.50
 H      -5.362203    -2.467764    -2.022228      27.33
 O      -5.060234    -0.398461    -2.359900     211.18
 H      -5.462677    -0.552407    -1.575119      32.75
 C      -5.664134    -1.925115    -4.222878     100.38
 O      -5.735571    -3.221072    -4.714177     259.48
 H      -6.197460    -3.089444    -5.694229      24.29
 H      -5.662437    -1.070895    -5.085190      22.88
 H      -6.684968    -1.660249    -3.962171      24.68
55
name = lig-ACN-frame_701
 C       3.336426     0.269923     0.189376      53.01
 H       2.721924     0.923167    -0.486927      24.23
 C       4.243343     0.012353     2.443608      60.09
 H       4.072370     0.120401     3.453119      23.22
 C       5.314591    -0.758501     1.997603       8.46
 O       6.469255    -1.132373     2.711235     218.90
 C       6.106232    -1.182117     4.140300     132.06
 H       6.621807    -2.048466     4.428875      29.25
 H       5.047384    -1.422464     4.286586      27.98
 H       6.425530    -0.441247     4.679764      31.10
 C       5.567647    -0.848537     0.525834       2.12
 O       6.705035    -1.297561     0.004072     137.19
 H       7.546168    -1.369592     0.476878      21.44
 C       4.487029    -0.383937    -0.357690      46.74
 H       4.960980    -0.284847    -1.324076      24.34
 C       3.285966     0.573647     1.549493      38.12
 C       2.079552     1.264170     2.240574      91.55
 H       2.298190     2.204078     2.514971      28.95
 O       1.771519     0.517693     3.534940     180.22
 H       0.887174    -0.079943     3.209554      24.68
 C       0.781168     1.376766     1.255786      98.10
 H       1.295340     2.054695     0.407279      24.49
 C      -0.298733     2.347564     1.734259     104.87
 O       0.175428     3.888367     2.000446     180.53
 H       0.868518     3.875746     1.227288      29.43
 H      -0.859317     2.161706     2.657478      27.93
 H      -1.067388     2.354558     1.064851      29.09
 C      -2.431968    -2.053271    -0.404895      68.13
 H      -3.151206    -2.871665    -0.093412      24.29
 C      -1.930359    -0.344287    -2.069477      61.56
 H      -2.203724     0.311081    -2.848257      24.10
 C      -0.965822     0.200696    -1.118272      10.12
 O      -0.370727     1.401539    -1.347949     203.65
 C      -0.969968     2.228139    -2.419973     119.01
 H      -0.818899     3.313174    -2.216239      27.60
 H      -0.731342     2.156564    -3.536533      26.69
 H      -2.061039     2.241689    -2.348182      28.14
 C      -0.651633    -0.352059     0.150895      -5.24
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 O       0.237521     0.084234     1.174456     170.00
 C      -1.440808    -1.571804     0.484164      31.64
 H      -1.375694    -1.782978     1.553553      25.28
 C      -2.573040    -1.499643    -1.596201      40.57
 C      -3.313418    -2.183702    -2.858464      76.73
 H      -2.900694    -1.629226    -3.650613      26.88
 O      -3.196900    -3.666580    -2.921958     203.72
 H      -2.129773    -4.004505    -3.195045      23.89
 C      -4.916556    -1.823132    -2.809816      87.92
 H      -5.439489    -2.613538    -2.273776      28.43
 O      -5.045315    -0.419112    -2.373865     189.08
 H      -5.247307    -0.280110    -1.444458      30.13
 C      -5.714191    -1.837318    -4.112021      91.87
 O      -5.674105    -3.293578    -4.696649     248.30
 H      -6.132766    -3.422552    -5.552684      26.85
 H      -4.818904    -1.308250    -4.663101      24.32
 H      -6.700173    -1.366183    -3.996335      26.23
55
name = lig-ACN-frame_702
 C       3.394043     0.314195     0.187106      40.72
 H       2.517801     0.645609    -0.522024      22.17
 C       4.201850    -0.048802     2.466216      75.98
 H       4.143713     0.224684     3.540045      23.90
 C       5.364346    -0.663699     1.910567      14.78
 O       6.422231    -1.153999     2.745816     215.39
 C       6.245631    -1.290686     4.213929     126.86
 H       6.758666    -2.079892     4.553550      28.69
 H       5.160805    -1.383344     4.416094      26.11
 H       6.454715    -0.411319     4.634830      28.76
 C       5.429149    -0.902146     0.522181      15.23
 O       6.702723    -1.379101    -0.022193     213.12
 H       7.241430    -1.256363     0.753914      21.02
 C       4.475509    -0.426460    -0.382011      62.43
 H       4.282570    -0.691986    -1.394407      24.97
 C       3.264654     0.567246     1.581350      23.55
 C       2.027443     1.288679     2.222471     105.30
 H       2.279043     2.209928     2.540077      29.63
 O       1.787055     0.591307     3.432577     216.62
 H       1.259464    -0.380654     3.374362      25.48
 C       0.840896     1.449786     1.222188      75.82
 H       0.884821     1.397645     0.079266      20.28
 C      -0.297021     2.440151     1.828898     113.62
 O       0.200790     3.795093     1.996305     261.38
 H       0.578620     4.178163     1.234313      32.49
 H      -0.460093     2.011578     2.897334      27.14
 H      -1.059034     2.398995     1.201605      30.12
 C      -2.404459    -2.072713    -0.400732     -13.82
 H      -2.718715    -3.145812    -0.435322      26.65
 C      -1.820698    -0.277807    -2.046306      58.68
 H      -2.220154     0.143278    -3.112338      22.76
 C      -1.002249     0.259541    -1.143864      22.79
 O      -0.290647     1.406598    -1.377345     217.32
 C      -0.945383     2.244488    -2.382854     107.43
 H      -0.505946     3.155509    -2.050679      27.61
 H      -0.489305     1.935799    -3.298830      27.54
 H      -2.075372     2.046929    -2.349372      26.56
 C      -0.839792    -0.387867     0.164027      19.80
 O       0.181587     0.018893     1.070100     112.82
 C      -1.454106    -1.523738     0.569558      55.00
 H      -1.084085    -2.180988     1.410228      24.09
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 C      -2.590807    -1.437782    -1.766271     -16.94
 C      -3.361646    -2.242366    -2.852699      96.33
 H      -3.033613    -1.982612    -3.777564      26.27
 O      -3.219008    -3.659797    -2.914738     261.85
 H      -2.332174    -3.781973    -3.397554      27.32
 C      -4.889036    -1.861709    -2.734826      73.24
 H      -5.267190    -2.370010    -1.859133      25.30
 O      -5.074419    -0.458306    -2.394487      27.91
 H      -4.551444    -0.334245    -1.335333      27.20
 C      -5.573101    -1.886230    -4.189032      95.90
 O      -5.626738    -3.262399    -4.565057     296.77
 H      -5.953911    -3.255165    -5.409201      30.64
 H      -5.123640    -1.150631    -5.024968      25.21
 H      -6.577143    -1.354712    -4.126642      25.85
55
name = lig-ACN-frame_703
 C       3.400634     0.365062     0.181632      57.62
 H       2.507698     0.486012    -0.584496      26.72
 C       4.220259    -0.014361     2.429642      61.09
 H       4.132226     0.028818     3.600549      22.30
 C       5.369393    -0.612152     1.919167      13.02
 O       6.358909    -1.189790     2.745732     200.33
 C       6.316477    -1.348252     4.230013     128.14
 H       7.014669    -2.022317     4.379434      30.04
 H       5.361995    -1.721118     4.642808      27.51
 H       6.697107    -0.528286     4.789547      28.16
 C       5.504027    -0.912085     0.473414      13.22
 O       6.581157    -1.449009    -0.018971     121.98
 H       7.374999    -1.833234     0.518329      22.61
 C       4.395714    -0.491132    -0.348268      48.20
 H       4.420501    -0.949483    -1.322172      22.66
 C       3.228521     0.502049     1.566195      41.49
 C       2.040952     1.255070     2.110279      98.38
 H       2.286588     2.228582     2.271807      29.28
 O       1.700200     0.661401     3.404731     255.32
 H       1.841627    -0.212848     3.179513      32.54
 C       0.747838     1.449578     1.204859      72.67
 H       1.353833     2.151511     0.520256      25.21
 C      -0.229262     2.413010     1.854681     120.90
 O       0.233761     3.745083     2.019809     244.11
 H       0.375797     4.000689     1.072644      31.39
 H      -0.361804     2.075706     3.005059      26.81
 H      -1.167811     2.391053     1.572750      30.56
 C      -2.315178    -2.134019    -0.523935      50.84
 H      -2.595339    -3.134581    -0.220943      24.29
 C      -1.905852    -0.341696    -2.084112      40.13
 H      -1.419132     0.086563    -3.173368      19.82
 C      -1.002489     0.289366    -1.030472      -7.91
 O      -0.205928     1.427516    -1.403739     223.91
 C      -0.830101     2.325889    -2.353650     117.69
 H      -0.536634     3.262609    -2.406583      30.76
 H      -0.611356     1.951583    -3.338267      27.94
 H      -2.018572     2.438155    -2.311226      27.82
 C      -0.851289    -0.290809     0.235343       9.31
 O       0.147917    -0.026465     1.051261     114.07
 C      -1.604158    -1.569844     0.474788      42.17
 H      -1.192659    -2.169674     1.372710      27.48
 C      -2.522448    -1.574869    -1.791415      36.98
 C      -3.412282    -2.182590    -2.891076      97.38
 H      -3.196330    -1.644858    -3.722823      29.92
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 O      -3.255566    -3.669977    -2.838706     256.08
 H      -2.643247    -3.907947    -3.388859      33.48
 C      -4.891318    -1.838913    -2.762935     118.64
 H      -5.475245    -2.662847    -2.390628      31.53
 O      -5.065274    -0.464752    -2.355586     129.05
 H      -3.995153    -0.149824    -1.908659      24.31
 C      -5.492492    -1.921222    -4.149132      92.29
 O      -5.594209    -3.277527    -4.488327     236.45
 H      -5.940416    -3.479048    -5.455124      25.46
 H      -4.816552    -1.339582    -4.916613      25.89
 H      -6.553473    -1.534224    -4.016773      25.37
55
name = lig-ACN-frame_704
 C       3.331006     0.251175     0.114056      45.33
 H       2.577257     0.879075    -0.491956      25.48
 C       4.235183     0.049464     2.395916      69.77
 H       3.990249     0.125806     3.553374      22.58
 C       5.359646    -0.653404     1.977769      31.24
 O       6.331158    -1.236668     2.732284     218.20
 C       6.408722    -1.419102     4.180893     129.15
 H       7.160668    -2.046527     4.240052      30.50
 H       5.517348    -1.922947     4.531244      29.12
 H       6.443955    -0.431232     4.713418      26.84
 C       5.509057    -0.807701     0.589285      18.34
 O       6.533948    -1.604819    -0.127919     172.60
 H       7.125363    -1.874139     0.669318      21.41
 C       4.437243    -0.566743    -0.297910      46.23
 H       4.644681    -0.587373    -1.384426      22.99
 C       3.207127     0.483719     1.489911      31.37
 C       1.999284     1.241828     2.097409     110.95
 H       2.367507     2.184006     2.297334      29.33
 O       1.610747     0.742432     3.393037     247.89
 H       1.684743    -0.171292     3.576056      31.24
 C       0.762224     1.389997     1.226685      97.71
 H       0.697975     1.553105     0.098328      21.76
 C      -0.290205     2.258073     2.010832      95.03
 O       0.278179     3.763017     2.015709     165.32
 H       0.648999     4.070843     1.055492      27.72
 H      -0.352371     1.954041     3.213721      25.46
 H      -1.099874     2.162100     1.456826      29.98
 C      -2.305598    -2.314238    -0.620896      50.25
 H      -3.015046    -3.092268    -0.525228      30.05
 C      -1.779699    -0.379339    -1.984233      62.09
 H      -1.950976    -0.108368    -3.228814      25.29
 C      -1.090047     0.336653    -1.098083      13.71
 O      -0.195533     1.412188    -1.387244     169.12
 C      -0.725996     2.422348    -2.446315     114.22
 H      -0.131235     3.105524    -2.133234      30.85
 H      -0.695638     2.157677    -3.431652      29.76
 H      -1.812154     2.523217    -1.949977      27.32
 C      -0.907971    -0.289628     0.212717       6.33
 O       0.223345     0.088140     1.121616      83.33
 C      -1.566343    -1.485260     0.404932      32.76
 H      -1.733165    -1.842628     1.476052      25.73
 C      -2.429962    -1.635181    -1.842727       5.76
 C      -3.344313    -2.205195    -2.881223      99.30
 H      -2.954906    -2.042210    -3.816806      30.08
 O      -3.326116    -3.633704    -2.782919     204.51
 H      -2.519148    -3.929353    -3.353271      26.61
 C      -4.912030    -1.818529    -2.811478      99.76
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 H      -5.326372    -2.272485    -1.930060      28.03
 O      -5.036474    -0.481445    -2.243000     159.84
 H      -4.295604     0.154765    -2.636978      31.60
 C      -5.544915    -1.882343    -4.189511      95.35
 O      -5.557895    -3.426268    -4.484361     195.27
 H      -6.061703    -3.459794    -5.461588      23.50
 H      -4.781069    -1.327935    -4.875723      26.33
 H      -6.414764    -1.161070    -4.323292      26.39
55
name = lig-ACN-frame_705
 C       3.288621     0.130609     0.087462      45.84
 H       2.759500     0.426446    -0.832648      22.71
 C       4.172853     0.078996     2.411567      61.14
 H       4.078491     0.447612     3.484273      23.34
 C       5.337861    -0.685595     1.984761       1.43
 O       6.396284    -1.311648     2.704720     189.65
 C       6.424001    -1.491500     4.110718     133.16
 H       7.333034    -1.814797     4.438152      29.77
 H       5.612957    -2.097877     4.439182      28.46
 H       6.384282    -0.470383     4.677426      25.62
 C       5.506088    -0.915295     0.516767      18.14
 O       6.451907    -1.696831    -0.089636     121.22
 H       7.330115    -1.724199     0.282544      24.57
 C       4.513023    -0.430252    -0.321988      41.53
 H       4.719194    -0.657901    -1.424769      25.67
 C       3.174669     0.469273     1.484150      39.79
 C       2.038546     1.248288     2.102816     101.14
 H       2.270850     2.254741     2.292877      29.84
 O       1.545554     0.829713     3.458535     170.26
 H       1.180101    -0.196754     3.194575      26.98
 C       0.692027     1.382590     1.282132      82.59
 H       1.048334     2.054967     0.408272      26.74
 C      -0.241422     2.326391     2.028259     116.21
 O       0.230370     3.664912     2.038352     241.66
 H       0.880171     3.618435     1.278936      31.13
 H      -0.407965     1.894818     3.220064      25.92
 H      -1.213750     2.323865     1.755758      29.58
 C      -2.263848    -2.254683    -0.541785      79.76
 H      -2.658660    -3.178778    -0.215614      27.64
 C      -1.758975    -0.421329    -2.127043      46.91
 H      -2.116097     0.421735    -2.942890      25.28
 C      -0.995054     0.337070    -1.073539      17.46
 O      -0.259047     1.399343    -1.488561     244.33
 C      -0.607413     2.478852    -2.358632     135.58
 H       0.045735     3.196006    -2.446054      31.07
 H      -0.608814     2.071549    -3.299956      29.44
 H      -1.619630     3.128809    -2.266673      27.72
 C      -0.808535    -0.260775     0.156586      13.23
 O       0.106346    -0.000822     1.158446     147.21
 C      -1.628881    -1.566616     0.414636      31.81
 H      -1.579814    -1.822116     1.494172      28.56
 C      -2.363540    -1.652002    -1.863402      18.01
 C      -3.304940    -2.278275    -2.920873     102.64
 H      -3.071332    -1.888268    -3.922222      27.98
 O      -3.387641    -3.688241    -2.742192     162.95
 H      -2.374269    -4.166418    -3.060189      23.92
 C      -4.786672    -1.737438    -2.708156      70.48
 H      -5.308935    -2.638655    -2.275150      29.70
 O      -5.009284    -0.411794    -2.194027     241.34
 H      -4.927941     0.104140    -2.878427      35.44
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 C      -5.537314    -1.975212    -4.307543      80.02
 O      -5.599318    -3.411885    -4.519748     257.02
 H      -6.024565    -3.579531    -5.370503      28.62
 H      -4.922196    -1.583764    -5.155282      25.69
 H      -6.651330    -1.779992    -4.363147      24.82
55
name = lig-ACN-frame_706
 C       3.307015     0.111301     0.105553      46.89
 H       2.349403     0.132796    -0.318345      25.11
 C       4.239547     0.026257     2.378081      62.36
 H       4.163483     0.266639     3.413016      24.46
 C       5.332810    -0.743883     1.905778      17.46
 O       6.445120    -1.356412     2.611162     190.62
 C       6.391099    -1.495875     4.123771     116.38
 H       7.392899    -1.832670     4.219380      27.51
 H       5.791762    -2.311827     4.399604      28.76
 H       5.999346    -0.504632     4.667044      23.76
 C       5.446832    -1.003820     0.546417      11.75
 O       6.437762    -1.797506    -0.033952     189.19
 H       7.275845    -1.517072     0.381579      24.23
 C       4.580536    -0.352525    -0.410390      45.25
 H       4.618388    -0.660507    -1.531130      25.12
 C       3.141012     0.411446     1.486050       7.88
 C       1.912437     1.283899     2.174774      95.55
 H       2.445746     2.210931     2.245610      28.52
 O       1.571339     0.830432     3.498133     185.94
 H       0.813345     0.020992     3.401117      25.96
 C       0.683902     1.414917     1.327989      81.65
 H       0.883686     1.628202     0.225669      24.83
 C      -0.341113     2.323491     2.059556     113.45
 O       0.239424     3.633628     2.069125     265.18
 H       0.840199     3.910971     1.437983      33.18
 H      -0.216962     2.002067     3.288852      24.49
 H      -1.279504     2.210883     1.602598      29.29
 C      -2.242292    -2.150242    -0.548209       2.19
 H      -2.568942    -3.178297    -0.415298      27.34
 C      -1.785570    -0.356337    -2.130749      60.51
 H      -1.921593     0.019337    -3.221952      24.20
 C      -0.967148     0.214304    -1.221461      15.95
 O      -0.220343     1.467710    -1.485644     170.92
 C      -0.522129     2.522382    -2.443388     119.29
 H       0.295381     3.014582    -2.195871      29.80
 H      -0.725226     2.307890    -3.452982      28.89
 H      -1.487770     3.052626    -1.944672      27.20
 C      -0.805526    -0.424348     0.136109      15.09
 O       0.012642    -0.013230     1.187309     109.99
 C      -1.507392    -1.463374     0.532081      75.33
 H      -1.239857    -2.085142     1.339740      28.57
 C      -2.334117    -1.658789    -1.873396      39.41
 C      -3.289459    -2.244323    -2.883760      81.86
 H      -2.857446    -2.122151    -3.945168      27.67
 O      -3.417909    -3.783412    -2.726800     169.52
 H      -2.440401    -4.113993    -2.930523      28.14
 C      -4.803890    -1.795480    -2.891661      82.63
 H      -5.368417    -2.287998    -1.995942      25.84
 O      -4.956439    -0.405626    -2.200492     146.63
 H      -5.534133     0.224206    -2.774998      29.58
 C      -5.511044    -2.047962    -4.274704     114.67
 O      -5.634942    -3.450776    -4.557424     284.05
 H      -5.926915    -3.540426    -5.433014      28.89
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 H      -5.078192    -1.405184    -5.027298      27.01
 H      -6.379009    -1.402139    -3.947969      25.80
55
name = lig-ACN-frame_707
 C       3.281303     0.146787     0.176877      47.51
 H       2.645000     0.337368    -0.610182      28.17
 C       4.288285    -0.052804     2.369000      71.09
 H       4.182566     0.029478     3.373613      25.72
 C       5.359731    -0.824968     1.861569      13.05
 O       6.394531    -1.339672     2.582991     177.78
 C       6.368165    -1.531600     4.016003     127.19
 H       7.381157    -1.495396     4.529408      27.98
 H       5.760548    -2.354933     4.240231      30.14
 H       5.926293    -0.560012     4.569762      24.09
 C       5.422262    -0.993784     0.402053      13.73
 O       6.465037    -1.867625     0.020812      68.99
 H       7.188285    -2.010576     0.775612      19.64
 C       4.458917    -0.423330    -0.410819      67.40
 H       4.724947    -0.438999    -1.542101      20.98
 C       3.167025     0.338657     1.588550      22.09
 C       1.964755     1.157137     2.178616      89.44
 H       2.159074     2.234108     2.408598      27.74
 O       1.620643     0.821142     3.559947     252.83
 H       1.139151     0.035287     3.561474      32.63
 C       0.579450     1.341732     1.293644      97.20
 H       0.720127     1.889160     0.344369      27.56
 C      -0.371201     2.265863     2.035814      97.09
 O       0.241494     3.743705     2.137915     180.93
 H       0.329578     3.754122     1.123989      30.60
 H      -0.791732     1.920267     3.149191      27.04
 H      -1.333191     2.317301     1.518765      29.16
 C      -2.219820    -2.154376    -0.525705      65.02
 H      -2.891275    -3.042510    -0.373765      26.44
 C      -1.794077    -0.389823    -2.211521      56.59
 H      -1.720502    -0.072997    -3.226426      24.67
 C      -0.863531     0.238829    -1.249766      16.08
 O      -0.162313     1.378277    -1.406431     158.17
 C      -0.474716     2.568807    -2.482704      99.33
 H       0.308259     3.282413    -2.518271      29.03
 H      -0.621269     2.303387    -3.503204      28.14
 H      -1.402749     3.129863    -1.980433      27.03
 C      -0.736059    -0.316188     0.082968     -18.26
 O       0.029710     0.076847     1.252732     149.65
 C      -1.463603    -1.616782     0.443602      55.09
 H      -1.294138    -1.865032     1.434907      27.97
 C      -2.418470    -1.572706    -1.828540      22.26
 C      -3.301632    -2.362795    -2.866781     112.45
 H      -2.760876    -2.138666    -3.889269      27.50
 O      -3.392320    -3.762541    -2.707266     259.80
 H      -2.670896    -4.089115    -3.017573      34.69
 C      -4.758889    -1.843627    -2.893285      98.67
 H      -5.284551    -2.725328    -2.230142      27.34
 O      -4.887460    -0.452438    -2.321245     112.29
 H      -5.908912    -0.090454    -2.755499      26.45
 C      -5.551025    -1.931810    -4.177238     106.05
 O      -5.681781    -3.481593    -4.590208     192.38
 H      -6.011569    -3.333081    -5.597840      24.36
 H      -4.958106    -1.599515    -4.937638      27.20
 H      -6.609045    -1.680768    -4.331214      25.39
55
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name = lig-ACN-frame_708
 C       3.281301     0.194079     0.173841      57.72
 H       2.671669     0.913461    -0.244294      24.71
 C       4.236450    -0.174721     2.443276      77.60
 H       4.303116     0.042028     3.444155      26.21
 C       5.298919    -0.815190     1.783289      15.01
 O       6.413987    -1.346793     2.541217     214.94
 C       6.273980    -1.498633     3.956829     120.88
 H       7.434450    -1.606785     4.184715      26.05
 H       5.898762    -2.466783     4.238153      29.23
 H       5.625059    -0.650751     4.445045      23.37
 C       5.502941    -1.061391     0.416130      28.02
 O       6.477045    -1.890216     0.000265     143.39
 H       6.922492    -2.158990     0.874361      18.97
 C       4.376084    -0.542742    -0.383175      25.22
 H       4.320903    -0.464041    -1.508426      23.44
 C       3.166957     0.317608     1.594478       6.74
 C       1.984117     1.125857     2.205971      85.04
 H       2.535259     2.141350     2.100753      26.50
 O       1.676615     0.757004     3.624577     246.42
 H       1.751791    -0.148117     3.646981      33.27
 C       0.666324     1.383594     1.401227      86.77
 H       1.093475     1.719534     0.474234      28.53
 C      -0.389477     2.393952     2.026232     107.26
 O       0.148385     3.686338     2.162279     214.06
 H       0.222415     4.318899     1.302354      27.75
 H      -0.542511     2.012502     3.142706      26.74
 H      -1.383603     2.298399     1.380747      26.96
 C      -2.325837    -2.226992    -0.562276       1.21
 H      -2.875608    -3.098256    -0.037341      24.71
 C      -1.640040    -0.409304    -2.195063      56.81
 H      -1.905580     0.093177    -3.005583      27.97
 C      -0.870678     0.238703    -1.193794      -0.65
 O      -0.041385     1.439014    -1.477376     185.01
 C      -0.449152     2.490835    -2.415197     113.12
 H       0.470154     3.123870    -2.397347      27.21
 H      -0.626184     1.845053    -3.287524      26.54
 H      -1.446875     3.038260    -2.204940      27.93
 C      -0.739234    -0.368794     0.122960      30.18
 O      -0.031638     0.071516     1.163448     159.92
 C      -1.311449    -1.563878     0.305167      61.37
 H      -1.447760    -1.910490     1.270764      28.65
 C      -2.516597    -1.579415    -1.819555      11.42
 C      -3.294754    -2.319014    -2.898542      99.22
 H      -3.021554    -2.064060    -3.999621      26.05
 O      -3.338821    -3.776262    -2.650421     177.71
 H      -2.639706    -4.227746    -3.288211      26.74
 C      -4.797496    -1.922287    -2.757089      59.24
 H      -5.432553    -2.599665    -1.943255      26.03
 O      -4.839968    -0.553781    -2.488835     192.27
 H      -5.866894    -0.344223    -2.532757      29.98
 C      -5.558072    -2.024027    -4.307933      84.76
 O      -5.732377    -3.369757    -4.597945     229.82
 H      -6.131767    -3.640104    -5.582934      23.10
 H      -5.074762    -1.370726    -4.911193      27.88
 H      -6.459938    -1.378887    -4.003405      26.46
55
name = lig-ACN-frame_709
 C       3.353364     0.252017     0.242867      55.69
 H       2.686792     0.548747    -0.560103      30.54
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 C       4.136868    -0.275710     2.421672      68.05
 H       4.039564    -0.049113     3.495223      25.56
 C       5.313277    -0.835249     1.848670      21.87
 O       6.396887    -1.338283     2.455899     173.08
 C       6.251961    -1.525394     3.931254     109.35
 H       7.331714    -1.377254     4.517718      24.97
 H       5.698527    -2.470321     4.088946      26.22
 H       5.747487    -0.675949     4.494449      23.24
 C       5.318479    -1.089542     0.424556       2.68
 O       6.474201    -1.900014    -0.070537      93.31
 H       7.180443    -1.947224     0.554296      23.22
 C       4.349638    -0.604066    -0.404606      63.76
 H       4.451139    -0.965548    -1.418383      22.85
 C       3.130963     0.285868     1.616436      10.68
 C       2.028525     1.152674     2.328527      95.84
 H       2.351056     2.230276     2.664314      26.76
 O       1.773987     0.706065     3.634850     196.16
 H       1.948721    -0.375951     3.709452      26.16
 C       0.785324     1.431082     1.411423      79.32
 H       0.955602     1.824231     0.432237      26.90
 C      -0.315589     2.377639     2.004609     108.82
 O       0.066693     3.738125     2.221757     251.69
 H       0.277705     4.131940     1.382987      32.08
 H      -0.626973     2.071863     3.069920      27.38
 H      -1.363651     2.208122     1.421032      26.83
 C      -2.296373    -2.139817    -0.578668      48.98
 H      -2.823147    -3.171848    -0.498446      25.13
 C      -1.657317    -0.464431    -2.087699      66.99
 H      -1.780907    -0.064296    -2.951691      30.36
 C      -0.819679     0.306093    -1.196387      28.30
 O       0.025237     1.407904    -1.442465     229.18
 C      -0.447222     2.284342    -2.434652     127.92
 H       0.271455     3.276545    -2.404835      26.58
 H      -0.427698     2.187704    -3.479309      28.60
 H      -1.382982     2.783971    -2.009519      28.18
 C      -0.694862    -0.341946     0.010373     -13.26
 O      -0.026160     0.077505     1.184645      89.70
 C      -1.413491    -1.669005     0.290971      46.02
 H      -0.933365    -2.131264     1.125558      28.71
 C      -2.402888    -1.606668    -1.892859      36.80
 C      -3.398976    -2.277740    -2.862845      95.03
 H      -2.935896    -2.051385    -3.865143      27.14
 O      -3.247894    -3.802460    -2.625263     108.93
 H      -2.482979    -4.094584    -3.455373      24.33
 C      -4.891709    -2.024533    -2.902150     105.66
 H      -5.345709    -2.535870    -1.919258      25.85
 O      -4.838703    -0.558972    -2.592735     260.82
 H      -5.592232    -0.232195    -2.396273      36.58
 C      -5.540953    -2.023772    -4.200441     113.96
 O      -5.813207    -3.355670    -4.645879     267.30
 H      -6.139514    -3.270585    -5.565405      28.36
 H      -4.956539    -1.605487    -4.896631      27.66
 H      -6.607068    -1.553229    -4.190527      25.24
55
name = lig-ACN-frame_710
 C       3.321614     0.194135     0.130366      64.57
 H       2.420409     0.569239    -0.459229      25.00
 C       4.099979    -0.323082     2.435519      64.57
 H       3.986411    -0.405015     3.597753      24.46
 C       5.237689    -0.906687     1.842611      13.54
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 O       6.421525    -1.333406     2.532539     212.29
 C       6.257085    -1.507995     3.911443     116.67
 H       7.416606    -1.766954     4.338092      24.12
 H       5.703850    -2.491892     4.188388      27.00
 H       5.685628    -0.675216     4.276427      24.32
 C       5.354351    -1.215339     0.461027      29.17
 O       6.352006    -1.826543    -0.140431     174.10
 H       7.196817    -1.557485     0.301167      24.41
 C       4.332001    -0.623020    -0.366661      44.80
 H       4.230574    -0.728407    -1.408152      25.19
 C       3.144802     0.355089     1.606480      -9.66
 C       2.085589     1.191716     2.363414      75.66
 H       2.523838     2.302597     2.395193      26.65
 O       1.853130     0.617692     3.708460     195.86
 H       1.218417    -0.332758     3.441175      23.94
 C       0.751464     1.407756     1.367327      88.07
 H       1.342323     1.865062     0.608643      27.88
 C      -0.289412     2.251444     2.072708     100.09
 O       0.027030     3.841033     2.246013     192.30
 H       0.471695     4.045734     1.397143      31.14
 H      -0.554272     1.780576     2.982990      28.72
 H      -1.171944     2.383966     1.242666      25.63
 C      -2.262361    -2.204478    -0.632225      31.66
 H      -2.694796    -3.239857    -0.408860      27.67
 C      -1.678694    -0.322811    -2.227803      60.98
 H      -1.590178    -0.063208    -3.165117      21.35
 C      -0.793082     0.193513    -1.200658      -5.59
 O       0.066171     1.269709    -1.435666     180.42
 C      -0.471598     2.309118    -2.481005      87.58
 H       0.181712     3.319161    -2.225425      24.81
 H      -0.393634     1.649943    -3.336517      25.90
 H      -1.582736     2.340367    -2.368437      28.25
 C      -0.666703    -0.411088     0.140309      22.47
 O       0.064498     0.111826     1.236367     164.93
 C      -1.326398    -1.581709     0.365007      41.52
 H      -1.135408    -2.289232     1.214637      25.63
 C      -2.396701    -1.596498    -1.870606       1.05
 C      -3.316097    -2.405263    -2.890205      96.50
 H      -3.091990    -2.133956    -3.939983      27.68
 O      -3.158396    -3.769135    -2.673362     235.08
 H      -2.355238    -4.042143    -3.238460      27.70
 C      -4.881202    -1.926466    -2.833801      78.33
 H      -5.546501    -2.740773    -2.325854      25.26
 O      -4.837221    -0.496257    -2.645832     216.54
 H      -5.826376    -0.202976    -2.372625      29.25
 C      -5.625450    -2.036471    -4.247832      90.21
 O      -5.911577    -3.436632    -4.715429     283.15
 H      -6.093339    -3.423528    -5.622462      28.66
 H      -4.944316    -1.550634    -4.803897      28.74
 H      -6.482808    -1.241999    -4.197321      26.22
55
name = lig-ACN-frame_711
 C       3.178123     0.126917     0.215980      23.72
 H       2.605834     0.756623    -0.594316      22.90
 C       4.117432    -0.333229     2.387059      51.68
 H       3.914950    -0.199765     3.577323      23.45
 C       5.241047    -1.052425     1.860065      20.58
 O       6.393656    -1.323920     2.547806     178.50
 C       6.273951    -1.527286     3.997186     108.20
 H       7.475670    -1.718438     4.333417      24.91
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 H       5.529352    -2.426217     4.175158      25.05
 H       6.092872    -0.717175     4.626985      26.35
 C       5.231273    -1.147039     0.464706      12.30
 O       6.365518    -1.779704    -0.235048     102.21
 H       7.204263    -1.836289     0.414035      21.28
 C       4.266115    -0.616098    -0.368220      58.51
 H       4.593580    -0.709400    -1.363234      26.39
 C       3.226757     0.364408     1.556682      35.14
 C       2.070215     1.145501     2.291940      85.06
 H       2.511705     2.225105     2.676340      25.80
 O       1.872695     0.615571     3.692460     208.84
 H       1.148587    -0.147099     3.636586      26.45
 C       0.850878     1.394343     1.474284      96.89
 H       0.803827     1.703010     0.444557      24.07
 C      -0.298357     2.381308     2.063385     104.22
 O      -0.001123     3.751020     2.250680     231.49
 H       0.717332     4.161344     1.574878      27.83
 H      -0.548927     2.091792     3.025603      28.66
 H      -1.402182     2.069633     1.532764      25.64
 C      -2.069863    -2.172720    -0.605923      28.46
 H      -2.602203    -3.087622    -0.314373      22.69
 C      -1.669011    -0.367344    -2.229878      51.73
 H      -1.768376     0.203231    -3.106638      24.38
 C      -0.779066     0.074625    -1.201756       3.49
 O       0.048687     1.218878    -1.476387     205.67
 C      -0.492322     2.129104    -2.472045     119.41
 H       0.079637     3.279195    -2.337021      24.66
 H       0.068566     2.156350    -3.442185      25.95
 H      -1.524881     2.399633    -2.530152      28.57
 C      -0.642462    -0.387545     0.209721      -6.88
 O       0.196460     0.097513     1.242878     138.79
 C      -1.330077    -1.649067     0.411491      50.42
 H      -1.467868    -1.839534     1.538241      25.06
 C      -2.440478    -1.536282    -1.911162      16.30
 C      -3.258174    -2.329629    -2.954385      93.43
 H      -2.876221    -2.104808    -3.925892      26.72
 O      -3.095418    -3.822042    -2.739918     242.01
 H      -2.286969    -3.960285    -2.985791      34.05
 C      -4.846895    -1.931736    -2.846645      72.67
 H      -5.170206    -2.063319    -1.798674      22.99
 O      -4.862199    -0.445728    -2.614963     114.49
 H      -5.977801    -0.150620    -2.498893      26.49
 C      -5.619250    -2.087901    -4.411690      84.45
 O      -6.000716    -3.421931    -4.684497     264.20
 H      -6.091773    -3.565922    -5.704356      26.76
 H      -5.168986    -1.621182    -5.204711      26.25
 H      -6.643320    -1.647222    -4.210831      24.81
55
name = lig-ACN-frame_712
 C       3.165931     0.114364     0.163855      50.40
 H       2.337828     0.665092    -0.460676      23.75
 C       4.173328    -0.286643     2.390258      58.21
 H       4.268301     0.036900     3.552019      22.07
 C       5.202728    -1.049349     1.862729      -0.18
 O       6.364292    -1.353703     2.587827     163.32
 C       6.354588    -1.541098     4.094228     107.96
 H       7.377216    -2.163799     4.363209      25.77
 H       5.457860    -2.301663     4.426103      26.97
 H       6.113031    -0.620028     4.482877      26.95
 C       5.281907    -1.161987     0.394866       7.48
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 O       6.375713    -1.689983    -0.251372     116.03
 H       6.891647    -2.144799     0.445681      21.89
 C       4.210788    -0.604040    -0.394043      62.72
 H       4.214794    -0.565819    -1.478310      23.56
 C       3.141033     0.286704     1.609926      23.25
 C       2.132795     1.134996     2.326786      77.49
 H       2.542734     2.321011     2.400784      24.68
 O       1.831702     0.695636     3.619621     261.80
 H       1.750604    -0.219605     3.519755      31.10
 C       0.738717     1.462054     1.453126      72.49
 H       1.372494     1.999070     0.733887      26.35
 C      -0.310689     2.337140     2.170230     108.44
 O       0.031349     3.741943     2.221102     257.57
 H       0.542191     3.951060     1.383232      30.35
 H      -0.513251     1.947817     3.075334      28.93
 H      -1.280154     2.328039     1.339012      24.05
 C      -2.071898    -2.180744    -0.633231      36.81
 H      -2.609896    -3.082339    -0.514356      27.18
 C      -1.628174    -0.439373    -2.068703      59.36
 H      -1.968671     0.151832    -2.985845      23.81
 C      -0.704979     0.118386    -1.162437      31.62
 O      -0.005102     1.172814    -1.521711     239.33
 C      -0.391405     2.109734    -2.516044     103.89
 H      -0.216097     3.024288    -1.776475      23.67
 H      -0.100898     1.786027    -3.620302      24.57
 H      -1.462744     1.938449    -2.565934      27.84
 C      -0.593491    -0.385151     0.148409      10.19
 O       0.256272    -0.028145     1.244964     123.56
 C      -1.319938    -1.531804     0.490090      42.49
 H      -1.371445    -2.144792     1.497831      23.88
 C      -2.338828    -1.632108    -1.858981      28.54
 C      -3.265609    -2.233087    -2.957150      99.04
 H      -2.898952    -1.921393    -3.888819      27.73
 O      -3.090001    -3.795291    -2.815528     192.05
 H      -2.061793    -3.875402    -3.026192      27.06
 C      -4.747409    -1.856479    -3.019519      84.31
 H      -5.270982    -2.761175    -2.552895      25.84
 O      -4.869550    -0.405955    -2.621904     231.01
 H      -5.814122    -0.228328    -2.788880      31.33
 C      -5.665024    -2.105482    -4.319240      96.53
 O      -6.048848    -3.492096    -4.626491     216.08
 H      -6.212652    -3.511843    -5.740923      24.02
 H      -4.983704    -1.775536    -5.041891      27.20
 H      -6.488199    -1.352235    -4.250625      27.72
55
name = lig-ACN-frame_713
 C       3.166723     0.113897     0.230112      56.29
 H       2.275861     0.279567    -0.407743      26.00
 C       4.182096    -0.192345     2.420109      48.94
 H       4.314196     0.079792     3.544700      21.11
 C       5.241472    -0.964752     1.800014       1.31
 O       6.361831    -1.461702     2.630481     164.90
 C       6.338021    -1.534788     4.060987     112.01
 H       7.388865    -2.037373     4.287337      26.04
 H       5.364786    -2.133476     4.518618      26.22
 H       6.533053    -0.666776     4.617163      27.40
 C       5.256975    -1.140445     0.385649      18.00
 O       6.417168    -1.626602    -0.241297     154.19
 H       7.031394    -2.015969     0.365137      25.72
 C       4.220184    -0.595666    -0.426799      49.32
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 H       4.247773    -0.858851    -1.517283      22.76
 C       3.055167     0.218368     1.611055       3.66
 C       2.030587     1.264485     2.289527      88.63
 H       2.782319     2.234013     2.402619      23.04
 O       1.792921     0.731178     3.623406     247.01
 H       1.964476    -0.193280     3.654936      29.28
 C       0.801645     1.400692     1.478270      96.23
 H       0.698700     1.778931     0.411218      21.08
 C      -0.348919     2.194936     2.175428      88.13
 O       0.126749     3.772202     2.201326     223.54
 H       0.220717     3.951305     1.306971      31.75
 H      -0.584316     1.868977     3.108606      27.70
 H      -1.486334     2.157197     1.585827      23.51
 C      -2.169244    -2.308814    -0.449380      64.31
 H      -2.423455    -3.247543    -0.085128      27.13
 C      -1.639313    -0.451279    -2.022427      43.93
 H      -1.620511     0.053998    -3.141741      19.86
 C      -0.718760     0.118151    -1.104531       5.58
 O       0.138756     1.190883    -1.513572     207.07
 C      -0.458271     2.116272    -2.530343     108.50
 H      -0.127688     3.254781    -2.658615      24.94
 H       0.414120     1.966581    -3.383534      23.63
 H      -1.491615     2.146055    -2.821716      27.06
 C      -0.543938    -0.446488     0.211201      22.93
 O       0.316425     0.011537     1.179215     155.75
 C      -1.392735    -1.546747     0.377413      49.85
 H      -0.949931    -2.028127     1.343512      25.38
 C      -2.270427    -1.685452    -1.818665      15.82
 C      -3.163446    -2.251184    -2.990073      91.79
 H      -2.695424    -1.922823    -3.878776      26.89
 O      -3.132686    -3.634833    -2.924087     190.78
 H      -2.098722    -3.920407    -3.407815      23.23
 C      -4.783873    -1.888189    -3.062738      90.69
 H      -5.247964    -2.375044    -2.099428      25.00
 O      -4.887476    -0.498646    -2.647952     267.40
 H      -5.594836    -0.099001    -2.962231      35.33
 C      -5.541448    -2.039781    -4.350306     107.37
 O      -6.079186    -3.512572    -4.505940     210.22
 H      -6.219676    -3.569679    -5.575485      26.74
 H      -5.172470    -1.750364    -5.333606      26.29
 H      -6.468587    -1.485801    -4.216456      27.47
55
name = lig-ACN-frame_714
 C       3.114088    -0.009038     0.217647      40.62
 H       2.408359     0.429477    -0.418823      24.70
 C       4.175174    -0.155011     2.397092      71.66
 H       4.104379     0.068986     3.463224      24.77
 C       5.298690    -0.848507     1.889941       8.81
 O       6.294903    -1.539564     2.528419     189.49
 C       6.362584    -1.508039     4.032424     108.51
 H       7.082628    -2.316859     4.273113      25.18
 H       5.277609    -1.928199     4.461508      24.95
 H       6.427020    -0.470093     4.356807      25.21
 C       5.313332    -1.054904     0.442825      -1.61
 O       6.464433    -1.600630    -0.240378      89.56
 H       7.209331    -1.523528     0.476935      19.68
 C       4.253027    -0.624326    -0.352878      48.16
 H       4.336923    -0.739659    -1.491536      24.11
 C       3.106880     0.319568     1.633355      29.67
 C       2.075856     1.192973     2.233400      78.16
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 H       2.213173     2.406182     2.433889      24.65
 O       1.748864     0.818308     3.672499     176.28
 H       1.401027    -0.246798     3.520965      25.40
 C       0.666380     1.369860     1.382473      83.26
 H       1.110184     2.018955     0.491808      24.23
 C      -0.318379     2.247100     2.181327     101.98
 O       0.140615     3.612016     2.203062     232.42
 H       0.228840     4.090974     1.284898      28.74
 H      -0.299917     2.085049     3.214802      27.11
 H      -1.446256     2.010573     1.605436      24.05
 C      -2.211233    -2.318322    -0.435626      36.64
 H      -2.721819    -3.249039    -0.292327      26.42
 C      -1.596020    -0.517886    -1.998954      31.67
 H      -1.594804    -0.193743    -3.240388      21.61
 C      -0.701535     0.203038    -1.125037       2.62
 O       0.192036     1.288846    -1.482003     171.90
 C      -0.338694     2.156663    -2.663759      82.62
 H      -0.206527     3.069352    -1.977966      22.89
 H      -0.060917     1.742367    -3.823281      22.47
 H      -1.393168     1.805216    -2.627708      26.24
 C      -0.573813    -0.391163     0.176552      -8.88
 O       0.355444    -0.028991     1.173926     143.27
 C      -1.284698    -1.692650     0.518932      26.69
 H      -1.317950    -2.069073     1.598482      21.36
 C      -2.379813    -1.707842    -1.742193      25.90
 C      -3.139788    -2.171928    -2.984421      87.35
 H      -2.797309    -1.663070    -3.888348      26.38
 O      -3.167290    -3.634763    -3.073354     198.57
 H      -2.274043    -3.957176    -3.606740      26.59
 C      -4.693048    -1.876356    -2.937525      67.75
 H      -5.213222    -2.669392    -2.197592      26.48
 O      -4.856988    -0.508809    -2.660840     163.03
 H      -5.681555    -0.152048    -3.329545      26.19
 C      -5.553146    -2.149750    -4.433860      76.16
 O      -6.047724    -3.437299    -4.394248     279.30
 H      -6.174942    -3.757504    -5.248108      31.56
 H      -4.835682    -1.774777    -5.204824      26.68
 H      -6.372790    -1.446903    -4.292845      28.84
55
name = lig-ACN-frame_715
 C       3.100277    -0.047970     0.223479      52.18
 H       2.408227     0.310204    -0.428712      25.00
 C       4.200597    -0.112775     2.483339      66.60
 H       4.116358     0.030227     3.526336      23.00
 C       5.284705    -0.806157     1.842082       8.62
 O       6.270607    -1.615034     2.508426     209.11
 C       6.300460    -1.487216     3.915292     119.42
 H       7.070774    -2.064839     4.321630      28.26
 H       5.208388    -1.666369     4.430379      25.64
 H       6.719506    -0.473835     4.229853      26.47
 C       5.442638    -0.943173     0.473964      29.09
 O       6.482380    -1.533933    -0.146750     143.33
 H       7.399195    -1.562267     0.337837      23.86
 C       4.276719    -0.651338    -0.276296      31.27
 H       4.390685    -0.633255    -1.415330      21.66
 C       3.187500     0.420018     1.538627       1.42
 C       1.951817     1.204349     2.296501      85.16
 H       2.626048     2.245181     2.288535      23.32
 O       1.706974     0.851180     3.642041     211.65
 H       0.931885     0.030260     3.617323      24.43
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 C       0.739935     1.335112     1.387235      86.33
 H       1.009123     1.755507     0.319527      21.84
 C      -0.298935     2.213403     2.164008     106.92
 O       0.148473     3.539348     2.204803     255.81
 H       0.395266     3.843017     1.224339      27.66
 H      -0.283045     1.736555     3.083959      26.73
 H      -1.559374     2.306737     1.919537      23.04
 C      -2.173560    -2.229197    -0.436894      39.03
 H      -2.835685    -3.056374    -0.122027      23.81
 C      -1.495624    -0.535302    -2.008559      38.64
 H      -1.677970    -0.095044    -3.217132      21.08
 C      -0.680119     0.192511    -1.178460      -3.87
 O       0.141460     1.288098    -1.511396     207.65
 C      -0.313856     2.098586    -2.611266     107.21
 H      -0.032239     3.235058    -2.673194      24.65
 H       0.318988     1.999162    -3.715885      23.02
 H      -1.465591     2.206387    -2.696818      25.61
 C      -0.640199    -0.515399     0.247555      -5.51
 O       0.295026    -0.063805     1.133099     153.03
 C      -1.261838    -1.723630     0.528480      69.51
 H      -1.176886    -2.052533     1.579759      24.35
 C      -2.374223    -1.600359    -1.677263      34.49
 C      -3.247482    -2.164553    -2.904748      76.57
 H      -2.688687    -1.640568    -3.744415      25.13
 O      -3.163319    -3.682937    -3.262552     200.64
 H      -2.270875    -3.720302    -3.433164      31.45
 C      -4.692315    -1.884448    -2.991474      92.28
 H      -5.221396    -2.626025    -2.200116      25.57
 O      -4.842161    -0.437740    -2.640590     117.86
 H      -5.747289    -0.163680    -3.306628      25.58
 C      -5.410660    -2.131081    -4.285555      99.05
 O      -6.036535    -3.477364    -4.315561     241.15
 H      -6.056879    -3.711908    -5.279971      29.59
 H      -4.753379    -2.273149    -5.188768      25.48
 H      -6.125221    -1.371674    -4.569266      28.20
55
name = lig-ACN-frame_716
 C       3.204210     0.015465     0.251281      48.43
 H       2.341452    -0.071839    -0.325418      24.67
 C       4.229883    -0.043334     2.426813      57.88
 H       4.171324     0.066036     3.496658      21.79
 C       5.295744    -0.848794     1.898934      13.68
 O       6.223855    -1.651698     2.494860     217.85
 C       6.309019    -1.419833     3.908146     116.34
 H       6.858881    -2.189871     4.209880      28.53
 H       5.246476    -1.585439     4.448306      27.34
 H       6.608732    -0.313398     4.165528      26.78
 C       5.425279    -0.833672     0.463788       7.19
 O       6.569614    -1.476562    -0.100512     144.69
 H       7.089491    -1.730418     0.668138      22.57
 C       4.333483    -0.610694    -0.358211      44.46
 H       4.386004    -1.055862    -1.382003      20.97
 C       3.130132     0.382146     1.672023      33.46
 C       2.051828     1.233565     2.227967      88.70
 H       2.191072     2.445705     2.534602      22.10
 O       1.646415     0.837383     3.610286     252.47
 H       1.189953     0.010204     3.602559      30.05
 C       0.729890     1.292430     1.370287      87.93
 H       0.890257     1.845629     0.379095      21.47
 C      -0.342465     2.064214     2.133579      83.37
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 O       0.197866     3.570743     2.231801     214.75
 H       0.641059     3.765246     1.417218      30.56
 H      -0.567714     1.943220     3.210366      24.95
 H      -1.336939     1.852517     1.376222      23.11
 C      -2.212122    -2.182295    -0.393607      42.47
 H      -2.747409    -3.157016    -0.122479      22.03
 C      -1.498492    -0.486801    -2.112089      41.89
 H      -1.508227     0.088011    -3.265344      19.76
 C      -0.680059     0.023067    -1.080845      23.32
 O       0.052199     1.236105    -1.477359     205.35
 C      -0.286227     2.143245    -2.653273      82.22
 H       0.286996     3.024818    -2.225997      23.13
 H       0.052809     1.322468    -3.470282      21.80
 H      -1.442952     2.179540    -2.955543      24.19
 C      -0.540385    -0.441283     0.155354      25.07
 O       0.243911    -0.091417     1.201953     181.77
 C      -1.313422    -1.671217     0.482155      50.62
 H      -0.941514    -2.257248     1.293383      26.24
 C      -2.342737    -1.586851    -1.723308      19.62
 C      -3.208136    -2.249893    -2.879865      58.70
 H      -2.903771    -1.628944    -3.830661      25.47
 O      -3.099069    -3.606620    -3.369028     257.04
 H      -2.237803    -3.824748    -3.464568      30.97
 C      -4.795321    -1.794567    -2.876784      81.73
 H      -5.451074    -2.216217    -2.029983      25.03
 O      -4.844968    -0.383178    -2.637471     252.18
 H      -5.670481     0.043549    -2.791593      31.26
 C      -5.257068    -2.211411    -4.338076      72.02
 O      -6.049042    -3.526279    -4.223435     196.11
 H      -6.120243    -3.729537    -5.338224      26.06
 H      -4.254227    -2.078443    -4.925225      25.67
 H      -5.983834    -1.437718    -4.535935      27.15
55
name = lig-ACN-frame_717
 C       3.233735     0.050995     0.263645      72.02
 H       2.278637     0.271573    -0.259586      22.87
 C       4.282636    -0.045715     2.478005      62.72
 H       4.293758     0.256504     3.572505      20.73
 C       5.247949    -0.797064     1.809227      15.09
 O       6.180582    -1.647065     2.529583     199.59
 C       6.319611    -1.413476     3.998274     109.53
 H       7.019330    -1.993874     4.413435      29.46
 H       5.273245    -1.484952     4.445848      27.45
 H       6.785624    -0.318877     4.164577      26.40
 C       5.476273    -0.890120     0.434274      28.69
 O       6.594855    -1.403223    -0.051373     159.41
 H       7.235370    -1.781175     0.547527      25.42
 C       4.340251    -0.498544    -0.374587      47.70
 H       4.177048    -0.754389    -1.416850      22.68
 C       3.175604     0.332167     1.625607      12.02
 C       2.012934     1.226407     2.235762      82.71
 H       2.531077     2.368714     2.138122      23.70
 O       1.624217     0.767899     3.577419     263.67
 H       1.710126    -0.121179     3.436376      32.12
 C       0.736483     1.261083     1.420061     104.17
 H       0.967437     1.669224     0.427037      24.63
 C      -0.329487     2.162619     2.049220      99.56
 O       0.154581     3.475127     2.249101     277.46
 H       0.622523     3.835047     1.478463      30.48
 H      -0.715457     1.601019     2.993431      25.45
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 H      -1.400572     2.257403     1.372822      24.10
 C      -2.274258    -2.149747    -0.529947      24.33
 H      -2.746091    -3.192157    -0.349669      25.32
 C      -1.597576    -0.564622    -2.079337      53.77
 H      -1.624554    -0.122716    -3.254352      21.48
 C      -0.678571     0.088794    -1.246235       6.94
 O      -0.031563     1.211617    -1.359222     167.30
 C      -0.230675     1.985831    -2.680002     109.91
 H       0.359512     2.891297    -2.549886      27.03
 H       0.112896     1.974603    -3.771609      24.35
 H      -1.298972     2.494982    -2.427599      25.13
 C      -0.521916    -0.543181     0.191519       4.43
 O       0.270367    -0.079219     1.312916     163.29
 C      -1.266161    -1.599411     0.453705      50.55
 H      -1.175633    -2.053709     1.420553      22.78
 C      -2.326384    -1.718575    -1.832455      40.18
 C      -3.242913    -2.124667    -2.913486      72.75
 H      -2.953434    -1.358267    -3.763853      22.88
 O      -3.070344    -3.542560    -3.353549     173.33
 H      -2.027415    -3.467422    -3.609809      25.07
 C      -4.779238    -1.800642    -2.743136      74.93
 H      -5.445878    -2.454036    -2.160179      26.46
 O      -4.805519    -0.292660    -2.632899     274.19
 H      -5.685657    -0.225166    -2.505292      31.90
 C      -5.285856    -2.280744    -4.302873      82.24
 O      -5.971169    -3.492786    -4.215724     246.82
 H      -6.344838    -3.984875    -5.039155      29.28
 H      -4.429646    -2.635903    -5.089203      23.41
 H      -5.818550    -1.511267    -4.889337      26.12
55
name = lig-ACN-frame_718
 C       3.179716     0.101861     0.251844      40.82
 H       2.568396     0.631545    -0.576811      22.57
 C       4.244286    -0.056540     2.456622      55.98
 H       4.337433     0.179117     3.604686      20.59
 C       5.309395    -0.823142     1.870144       9.64
 O       6.174689    -1.615280     2.624227     198.88
 C       6.332180    -1.364953     4.024761     125.54
 H       7.028776    -2.112704     4.226499      26.37
 H       5.476564    -1.533214     4.705903      27.88
 H       6.677219    -0.245773     4.255364      26.30
 C       5.382983    -0.929186     0.418943       4.84
 O       6.649799    -1.385921    -0.132650     100.49
 H       7.285248    -1.415983     0.688043      21.07
 C       4.368075    -0.415621    -0.389474      49.78
 H       4.640764    -0.239422    -1.386854      22.73
 C       3.194031     0.391561     1.645654      28.40
 C       2.048350     1.137940     2.260115      92.14
 H       2.480926     2.257238     2.632644      22.68
 O       1.671830     0.687149     3.537621     215.17
 H       1.821833    -0.380024     3.717208      25.71
 C       0.763445     1.300228     1.361378      90.54
 H       1.052189     1.604793     0.394153      24.99
 C      -0.388268     2.202688     1.927178      93.67
 O       0.130196     3.472752     2.329725     245.46
 H       0.448101     3.905538     1.397899      27.44
 H      -0.738829     1.783055     3.000336      24.02
 H      -1.307174     2.221666     1.128534      24.13
 C      -2.190753    -2.270061    -0.536579      68.16
 H      -2.940436    -3.019998    -0.101313      22.65
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 C      -1.571206    -0.556857    -2.131563      51.36
 H      -1.807761    -0.001351    -3.149548      20.92
 C      -0.722339    -0.017114    -1.112799      12.86
 O       0.000111     1.305765    -1.431065     195.17
 C      -0.183163     2.016791    -2.587559     102.20
 H       0.549742     2.774966    -2.532858      25.70
 H      -0.173635     1.075229    -3.233523      23.53
 H      -1.386131     2.361342    -2.877091      23.78
 C      -0.514726    -0.504807     0.134958      -1.43
 O       0.245037    -0.134436     1.307860     126.26
 C      -1.414852    -1.722663     0.392740      27.25
 H      -1.601174    -1.902173     1.439063      26.10
 C      -2.317755    -1.716997    -1.859937      30.09
 C      -3.285721    -2.053206    -2.984674      76.36
 H      -2.998932    -1.434660    -3.954651      25.07
 O      -3.047273    -3.426597    -3.300281     127.60
 H      -1.901184    -3.596634    -3.526417      21.37
 C      -4.739892    -1.831011    -2.925166     105.15
 H      -4.975324    -2.150731    -1.953085      26.15
 O      -4.820550    -0.343132    -2.612380     165.36
 H      -5.833309    -0.003079    -2.264486      26.59
 C      -5.276146    -2.269211    -4.277690      80.01
 O      -6.009471    -3.547512    -4.139759     287.65
 H      -6.062632    -3.622302    -5.023191      33.30
 H      -4.194027    -2.354757    -4.824990      23.61
 H      -5.936268    -1.442272    -4.646091      26.14
55
name = lig-ACN-frame_719
 C       3.270394     0.238039     0.177870      55.53
 H       2.339141     0.704482    -0.352013      20.94
 C       4.231134    -0.115215     2.392086      40.74
 H       4.047804    -0.002987     3.541308      18.72
 C       5.258911    -0.880535     1.899695      24.74
 O       6.200180    -1.565917     2.675873     236.21
 C       6.377801    -1.340692     4.094197     118.83
 H       7.229139    -1.946717     4.469979      27.10
 H       5.470090    -1.579250     4.531874      31.03
 H       6.708374    -0.237398     4.345824      27.58
 C       5.447176    -0.964256     0.485669      20.17
 O       6.583845    -1.341508    -0.198011     130.86
 H       7.436772    -1.475116     0.425908      21.82
 C       4.422089    -0.346779    -0.343617      52.92
 H       4.509519    -0.243084    -1.410574      24.63
 C       3.178110     0.411876     1.582668      16.63
 C       2.036109     1.150704     2.323912      83.29
 H       2.174554     2.351010     2.409941      23.04
 O       1.718772     0.551449     3.629847     195.33
 H       1.490135    -0.519881     3.264141      22.29
 C       0.761631     1.276326     1.310182      82.10
 H       1.036785     1.758551     0.419488      22.98
 C      -0.375450     2.120990     1.878618      79.45
 O       0.117047     3.556751     2.352117     211.01
 H       0.424392     4.242299     1.644436      27.59
 H      -1.029464     1.661143     2.811046      24.14
 H      -1.266447     2.140901     1.079363      24.22
 C      -2.236061    -2.407211    -0.634279      38.19
 H      -3.016863    -3.190702    -0.425309      20.44
 C      -1.470709    -0.484186    -2.079917      56.31
 H      -1.675067     0.135683    -2.939146      23.07
 C      -0.658662     0.126052    -1.125559       6.67
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 O       0.000472     1.275692    -1.297208     175.66
 C      -0.199565     1.923193    -2.686508      97.96
 H       0.582439     2.575575    -2.896569      27.02
 H       0.051425     1.351544    -3.654151      24.74
 H      -1.235407     2.651161    -2.803821      23.65
 C      -0.622846    -0.631378     0.206764      24.38
 O       0.174337    -0.153133     1.178090     165.38
 C      -1.435324    -1.676568     0.458572      53.34
 H      -1.393227    -2.161050     1.452240      24.02
 C      -2.333342    -1.607427    -1.845139       7.96
 C      -3.105119    -2.030388    -3.057730      76.13
 H      -2.709985    -1.329929    -3.916218      24.39
 O      -3.035952    -3.423772    -3.285309     168.32
 H      -1.901174    -3.645273    -3.269640      22.97
 C      -4.715648    -1.756012    -2.880982      91.28
 H      -5.296455    -2.523602    -2.429244      25.94
 O      -4.846879    -0.406605    -2.639048     217.07
 H      -5.927586    -0.354473    -2.281992      25.10
 C      -5.339553    -2.221124    -4.213370      89.02
 O      -6.044435    -3.524527    -4.157225     261.07
 H      -6.115019    -4.028605    -4.999030      30.62
 H      -4.749197    -2.272515    -5.293777      24.51
 H      -6.144948    -1.496241    -4.516157      26.68
55
name = lig-ACN-frame_720
 C       3.371200     0.405707     0.184559      57.40
 H       2.677223     0.534035    -0.709659      23.21
 C       4.117972    -0.189555     2.409496      50.89
 H       4.003202    -0.129658     3.522511      19.62
 C       5.258242    -0.949740     1.892305      11.80
 O       6.303425    -1.552738     2.690945     212.28
 C       6.372474    -1.275883     4.161977     105.05
 H       7.339574    -1.906282     4.435487      25.98
 H       5.617620    -1.590986     4.761319      31.08
 H       6.457167    -0.182742     4.331113      28.52
 C       5.455503    -0.869254     0.482030      25.71
 O       6.545383    -1.332283    -0.243802     165.51
 H       7.138853    -1.861077     0.319714      24.76
 C       4.474076    -0.313383    -0.313062      53.22
 H       4.591924    -0.730231    -1.338465      21.77
 C       3.180818     0.444289     1.576237      21.23
 C       1.918197     1.145313     2.299411      87.72
 H       2.388184     2.108426     2.691524      23.13
 O       1.749391     0.404572     3.625395     241.63
 H       1.134857    -0.372946     3.465916      25.52
 C       0.724303     1.207296     1.403168      95.49
 H       1.182786     1.493637     0.455681      22.87
 C      -0.342796     2.218107     1.884681     100.80
 O       0.038540     3.505596     2.352632     295.47
 H       0.305302     3.769757     1.507784      32.07
 H      -0.821115     1.580465     2.878905      23.29
 H      -1.010431     2.380782     1.103240      26.54
 C      -2.253538    -2.278297    -0.649722      44.56
 H      -2.521118    -3.314168    -0.742447      21.56
 C      -1.504969    -0.409295    -2.049941      61.63
 H      -1.462077    -0.077951    -2.976427      23.82
 C      -0.660281     0.107355    -1.029898      17.33
 O       0.027255     1.308310    -1.282181     165.05
 C      -0.118284     1.887585    -2.785758      86.41
 H       0.612243     2.617220    -2.549843      25.04
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 H      -0.259488     1.156562    -3.553640      25.15
 H      -1.251610     2.283779    -2.531415      23.61
 C      -0.720925    -0.555150     0.139716       1.39
 O       0.205760    -0.117394     1.152387     166.89
 C      -1.527183    -1.834312     0.415446      53.13
 H      -1.151343    -2.349479     1.328049      25.70
 C      -2.235696    -1.536931    -1.826225      40.93
 C      -3.090928    -2.007126    -3.012920      80.23
 H      -2.749970    -1.490987    -3.979529      24.24
 O      -2.986388    -3.500188    -3.301824     211.54
 H      -2.002794    -3.721765    -3.393519      26.64
 C      -4.577503    -1.878825    -2.949443      77.62
 H      -4.718815    -2.299024    -1.968381      24.32
 O      -4.940018    -0.418257    -2.621052     254.90
 H      -5.831044    -0.411322    -2.441163      31.21
 C      -5.544666    -2.171429    -4.363222      59.29
 O      -6.067081    -3.494208    -4.128618     252.08
 H      -5.839555    -3.790504    -5.194723      24.37
 H      -4.730760    -2.097318    -5.286149      23.62
 H      -6.302554    -1.378615    -4.242557      25.55
55
name = lig-ACN-frame_721
 C       3.429848     0.480178     0.160153      45.93
 H       2.708145     1.072756    -0.397009      23.22
 C       4.083962    -0.317575     2.441660      45.27
 H       3.911119    -0.307998     3.482822      21.92
 C       5.304124    -0.912007     1.949237      11.87
 O       6.324775    -1.520033     2.690272     245.78
 C       6.364534    -1.206279     4.142567     108.92
 H       7.448814    -1.626191     4.514850      25.58
 H       5.586294    -1.659080     4.548634      31.58
 H       6.387690    -0.167954     4.359545      29.41
 C       5.499396    -0.808658     0.519754      18.71
 O       6.550194    -1.404966    -0.237892     183.91
 H       7.098104    -1.925361     0.377340      24.11
 C       4.491416    -0.316382    -0.352401      49.58
 H       4.570971    -0.312364    -1.498629      20.49
 C       3.169705     0.472437     1.611451      17.85
 C       1.976301     0.966539     2.386701     107.89
 H       1.982023     2.060357     2.629691      24.09
 O       1.716519     0.329177     3.568203     318.75
 H       1.344470    -0.447414     3.356815      30.80
 C       0.730340     1.238842     1.417215      76.24
 H       1.069472     1.802228     0.471383      22.29
 C      -0.415579     2.146555     1.938225      97.84
 O       0.011788     3.479540     2.304209     272.73
 H       0.613741     4.047187     1.759383      29.32
 H      -1.071939     1.841065     3.006300      23.48
 H      -1.202112     2.069777     1.294275      27.65
 C      -2.259680    -2.251272    -0.684143      40.47
 H      -2.653029    -3.237026    -0.585468      25.39
 C      -1.530244    -0.306325    -2.116136      52.59
 H      -1.553722     0.045424    -3.082898      22.18
 C      -0.776181     0.158695    -1.073754      -4.48
 O       0.083576     1.300341    -1.370778     211.68
 C      -0.105919     1.879531    -2.610918     130.10
 H       0.600282     2.573883    -3.066740      26.16
 H       0.338666     1.126385    -3.322322      26.62
 H      -1.032327     2.338461    -3.142264      25.67
 C      -0.729655    -0.484983     0.317704      11.73
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 O       0.204085    -0.181710     1.236566     152.17
 C      -1.341352    -1.749724     0.396065      37.08
 H      -1.363936    -2.487705     1.239598      21.09
 C      -2.312177    -1.598861    -1.943749      16.00
 C      -3.050171    -2.105193    -3.130918      86.55
 H      -2.631332    -1.503488    -3.979899      24.74
 O      -2.911199    -3.534809    -3.297719     266.03
 H      -2.098122    -3.603066    -3.554377      33.57
 C      -4.642604    -1.825124    -2.995215      84.38
 H      -5.104206    -2.654776    -2.378568      25.00
 O      -4.962121    -0.465367    -2.617617     278.24
 H      -5.848671    -0.560850    -2.406201      30.40
 C      -5.514584    -2.159706    -4.172151      91.79
 O      -6.083980    -3.484926    -4.212071     261.60
 H      -6.199529    -4.052876    -5.055732      27.77
 H      -5.034048    -1.862155    -5.271562      24.71
 H      -6.399621    -1.497914    -4.172077      27.26
55
name = lig-ACN-frame_722
 C       3.425486     0.526234     0.284174      66.27
 H       2.942231     1.190612    -0.328057      24.44
 C       4.110323    -0.398038     2.449622      61.69
 H       3.830742    -0.552945     3.418256      22.71
 C       5.337971    -0.811182     1.904043       1.99
 O       6.320147    -1.454355     2.679183     241.17
 C       6.345473    -1.157313     4.072848     125.56
 H       7.395467    -1.571811     4.566651      24.37
 H       5.668671    -1.661002     4.620235      31.12
 H       6.187970    -0.172908     4.226523      30.58
 C       5.505051    -0.850880     0.462933       8.61
 O       6.559544    -1.514047    -0.135768     128.01
 H       7.452121    -1.573209     0.440536      24.82
 C       4.495771    -0.186646    -0.332346      46.77
 H       4.821290    -0.048625    -1.415272      19.78
 C       3.282634     0.337424     1.631564      31.34
 C       1.973010     1.056792     2.348639      89.37
 H       2.463965     1.910549     2.755686      24.92
 O       1.627017     0.213052     3.569118     246.90
 H       1.699610    -0.782738     3.374873      25.94
 C       0.704050     1.187711     1.519440      87.07
 H       0.986039     1.523558     0.422271      20.51
 C      -0.493984     2.041317     2.022114      91.65
 O      -0.007894     3.507960     2.293592     227.05
 H       0.460104     3.465713     1.329619      26.47
 H      -0.781140     1.488127     3.156910      22.43
 H      -1.169097     1.995785     1.294835      27.09
 C      -2.158116    -2.222711    -0.721536      38.84
 H      -2.891362    -2.915567    -0.402747      21.91
 C      -1.640649    -0.384720    -2.146845      54.47
 H      -1.760913     0.325605    -3.013634      22.11
 C      -0.844072     0.256934    -1.055781      -0.95
 O       0.071377     1.283182    -1.320281     177.83
 C       0.049305     1.863404    -2.713876     104.27
 H       0.456437     2.761869    -2.241298      24.10
 H       0.286005     1.158348    -3.532962      25.99
 H      -1.065361     2.019524    -2.768192      25.65
 C      -0.675843    -0.418505     0.219594      -1.60
 O       0.218483    -0.166558     1.346790     132.67
 C      -1.308543    -1.678952     0.320740      41.96
 H      -1.097444    -2.038981     1.357645      22.64
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 C      -2.345495    -1.561847    -1.992311      23.14
 C      -3.146010    -2.156239    -3.225472      82.26
 H      -2.860810    -1.645559    -4.137214      25.45
 O      -2.841890    -3.567342    -3.329802     239.47
 H      -1.893700    -3.747937    -3.366637      27.89
 C      -4.699799    -1.901224    -2.979388      85.98
 H      -4.980584    -2.474056    -2.011740      22.13
 O      -4.925638    -0.522963    -2.593342     184.79
 H      -5.909699    -0.476624    -2.046904      23.69
 C      -5.553357    -2.148166    -4.196816      79.97
 O      -6.085690    -3.541158    -4.218595     296.04
 H      -6.076815    -3.510365    -5.139516      29.32
 H      -5.025388    -1.843570    -5.247195      24.01
 H      -6.375183    -1.506707    -3.876752      26.13
55
name = lig-ACN-frame_723
 C       3.505934     0.533523     0.329730      51.84
 H       2.819208     1.049152    -0.217651      22.40
 C       4.168118    -0.425655     2.461486      47.86
 H       4.096508    -0.619120     3.497183      20.20
 C       5.359789    -0.846063     1.843955       7.89
 O       6.347015    -1.407288     2.600309     218.66
 C       6.309953    -1.115753     4.067331     117.85
 H       7.457682    -1.393365     4.248756      24.35
 H       5.592911    -1.672800     4.560272      31.16
 H       6.218508    -0.098432     4.269607      31.13
 C       5.467724    -0.875039     0.451913      23.21
 O       6.597294    -1.596441    -0.048981     183.09
 H       7.248177    -1.447201     0.737853      21.88
 C       4.651821    -0.055100    -0.295282      66.93
 H       4.659242    -0.010277    -1.397229      22.48
 C       3.124936     0.308710     1.723571      22.10
 C       2.061567     0.988057     2.435312     103.77
 H       2.208036     1.946035     2.779092      25.22
 O       1.555636     0.178985     3.544150     229.57
 H       1.551199    -0.920112     3.207368      19.77
 C       0.697093     1.164514     1.561536      78.82
 H       1.042109     1.738938     0.545112      19.68
 C      -0.403840     2.035585     2.170018     102.07
 O      -0.077083     3.374805     2.223365     289.10
 H       0.281552     3.899830     1.437615      27.64
 H      -0.897531     1.629839     3.347371      22.40
 H      -1.307191     1.915413     1.698989      25.74
 C      -2.142533    -2.205685    -0.723924      33.96
 H      -2.517753    -3.233857    -0.523673      21.84
 C      -1.667701    -0.266300    -2.083496      59.36
 H      -1.868368     0.211461    -3.190715      18.70
 C      -0.832205     0.225257    -1.083913      26.08
 O       0.061209     1.262865    -1.302788     210.00
 C       0.085359     1.928358    -2.667323     116.24
 H       0.629643     2.904290    -2.809604      25.33
 H       0.679367     1.496561    -3.493887      26.73
 H      -0.896345     2.188634    -3.047177      25.32
 C      -0.571885    -0.430798     0.099426      18.41
 O       0.139059    -0.168530     1.311545     161.82
 C      -1.343879    -1.577679     0.276843      54.84
 H      -1.292835    -2.249611     1.147361      23.62
 C      -2.344241    -1.579145    -2.004233      20.97
 C      -3.204774    -2.150474    -3.139932      76.94
 H      -3.031966    -1.551816    -4.022117      24.57
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 O      -2.839129    -3.615597    -3.384923     173.02
 H      -1.721052    -3.496773    -3.228695      22.73
 C      -4.684549    -2.029211    -2.874656      72.55
 H      -4.909649    -2.794544    -2.005336      23.17
 O      -4.826341    -0.529282    -2.549936     170.62
 H      -5.806045    -0.674562    -1.892499      22.06
 C      -5.702721    -2.197059    -4.168446      90.09
 O      -6.043490    -3.556191    -4.224419     331.51
 H      -6.119792    -3.904484    -5.013133      33.48
 H      -4.972050    -1.881427    -5.055648      25.35
 H      -6.511080    -1.519645    -4.289668      28.11
55
name = lig-ACN-frame_724
 C       3.495410     0.539597     0.400187      60.69
 H       2.825072     1.026741    -0.265923      22.82
 C       4.138801    -0.372529     2.482426      52.40
 H       4.020096    -0.291421     3.599982      18.77
 C       5.257318    -0.938796     1.861075       7.83
 O       6.412586    -1.381263     2.563278     239.51
 C       6.390629    -1.130581     3.986624     109.46
 H       7.285110    -1.497348     4.574674      25.70
 H       5.582388    -1.683513     4.426258      30.90
 H       6.193199     0.009007     4.190811      27.61
 C       5.575891    -0.890147     0.456152       5.03
 O       6.614318    -1.614773     0.017292     165.01
 H       7.213804    -2.056271     0.589866      23.99
 C       4.694214    -0.000873    -0.293399      55.22
 H       4.845943     0.124933    -1.345912      22.27
 C       3.225792     0.280074     1.724595      30.36
 C       1.870099     0.872033     2.478311     103.83
 H       2.231970     1.736002     2.863480      25.99
 O       1.524228     0.147931     3.598585     269.37
 H       1.057173    -0.801048     3.248256      22.49
 C       0.755852     1.185098     1.562433      75.10
 H       0.938592     1.784817     0.522080      19.93
 C      -0.386326     1.949708     2.272970      91.25
 O      -0.134351     3.400738     2.230806     258.36
 H       0.177343     3.473913     1.376679      32.50
 H      -0.138300     1.837591     3.544135      21.55
 H      -1.273306     1.589939     1.760553      25.40
 C      -2.155181    -2.248469    -0.765751      65.55
 H      -2.296009    -3.394894    -0.753860      21.83
 C      -1.743558    -0.233870    -2.107151      49.30
 H      -1.707051     0.469547    -3.152856      18.54
 C      -0.702785     0.217248    -1.207378      -4.30
 O       0.087344     1.400497    -1.393801     192.97
 C       0.121846     2.026966    -2.650171     123.56
 H       0.630935     2.940215    -2.225142      24.41
 H       0.562857     1.224816    -3.162063      28.04
 H      -0.786279     2.166783    -3.153122      27.02
 C      -0.593005    -0.533528     0.138260       8.95
 O       0.104322    -0.136722     1.199118     151.14
 C      -1.423728    -1.680922     0.282336      59.46
 H      -1.267608    -2.075543     1.300011      23.77
 C      -2.339008    -1.529796    -1.958235      24.35
 C      -3.145840    -2.198816    -3.085192      75.40
 H      -2.943506    -1.584659    -3.947372      24.97
 O      -2.860690    -3.551889    -3.411732     185.15
 H      -1.726181    -3.819781    -3.583889      22.86
 C      -4.784333    -2.001726    -2.840496      79.10
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 H      -5.376268    -2.633279    -2.066999      24.09
 O      -4.747584    -0.647771    -2.450245     244.46
 H      -5.707527    -0.344845    -2.119070      26.03
 C      -5.609764    -2.257250    -4.069794      96.05
 O      -6.043856    -3.670451    -4.149057     309.93
 H      -5.978972    -3.718417    -4.982009      34.11
 H      -5.091193    -1.978577    -5.061780      25.46
 H      -6.495681    -1.688226    -3.815138      27.71
55
name = lig-ACN-frame_725
 C       3.540262     0.498346     0.306355      51.67
 H       2.891930     1.203693    -0.303068      22.45
 C       4.161023    -0.355449     2.572088      49.29
 H       3.998425    -0.391489     3.738963      17.60
 C       5.307262    -0.997298     1.949171      18.42
 O       6.477865    -1.399456     2.560604     223.93
 C       6.433250    -1.191382     3.954872     108.85
 H       7.401759    -1.568353     4.224522      27.02
 H       5.541379    -1.635218     4.490403      29.83
 H       6.427923    -0.006315     4.159841      27.92
 C       5.538292    -0.828407     0.542534      10.00
 O       6.649055    -1.627516    -0.048457     143.41
 H       6.940517    -1.931658     0.832969      20.05
 C       4.706265    -0.062799    -0.225807      67.58
 H       5.015107     0.275769    -1.167396      22.89
 C       3.158882     0.328282     1.713483      27.53
 C       1.943423     0.830601     2.391225      78.01
 H       2.114220     1.723997     2.806058      25.91
 O       1.445766     0.043413     3.711489     232.84
 H       1.059263    -0.776824     3.522530      27.09
 C       0.641606     1.172546     1.482828      85.87
 H       1.234806     1.717946     0.616339      21.38
 C      -0.323297     1.916068     2.403586      90.96
 O      -0.202762     3.441544     2.211584     221.51
 H       0.251929     3.673153     1.331111      27.32
 H      -0.246597     1.283679     3.542024      21.22
 H      -1.437147     1.711108     2.274319      23.83
 C      -2.107964    -2.342982    -0.792937      26.62
 H      -2.891610    -3.238791    -0.721745      20.76
 C      -1.661931    -0.252714    -2.137138      46.44
 H      -2.183866     0.339275    -3.103996      19.70
 C      -0.644144     0.172625    -1.216804      21.25
 O       0.009353     1.431668    -1.311073     203.91
 C       0.192001     2.100190    -2.706674     122.16
 H       0.690145     3.079978    -2.642032      27.03
 H       0.708321     1.886763    -3.538603      29.08
 H      -0.781419     2.413096    -2.903475      26.98
 C      -0.713414    -0.466408    -0.028519      -2.96
 O       0.171746    -0.128365     1.159028     125.14
 C      -1.406591    -1.785509     0.342845      30.94
 H      -1.365363    -2.293300     1.316870      22.13
 C      -2.321987    -1.496850    -1.961553      16.50
 C      -3.171201    -2.155343    -3.088150      87.75
 H      -3.068814    -1.571298    -3.984489      26.79
 O      -2.875781    -3.549804    -3.417312     212.50
 H      -1.874708    -3.548903    -3.689549      26.97
 C      -4.648504    -2.031280    -2.793059      92.97
 H      -4.742132    -2.764890    -1.900289      25.65
 O      -4.715211    -0.655251    -2.346797     303.53
 H      -5.556730    -0.494994    -2.278890      33.65
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 C      -5.614598    -2.317633    -3.992103     102.18
 O      -6.016350    -3.770039    -4.083792     297.04
 H      -6.184812    -4.093435    -4.920731      31.11
 H      -5.193433    -1.876699    -4.922613      27.93
 H      -6.531813    -1.699305    -3.964659      28.74
55
name = lig-ACN-frame_726
 C       3.503356     0.484363     0.355364      53.01
 H       2.905118     1.142134    -0.427316      20.49
 C       4.184189    -0.369747     2.518674      53.40
 H       3.935981    -0.508667     3.650643      19.96
 C       5.343931    -0.876002     1.971047      12.63
 O       6.465311    -1.476462     2.580024     245.37
 C       6.582649    -1.246476     4.033147     122.90
 H       7.386329    -1.737468     4.437809      26.21
 H       5.659350    -1.755634     4.540491      28.40
 H       6.604365    -0.080240     4.346228      27.47
 C       5.555460    -0.930447     0.578931      14.97
 O       6.572459    -1.540429    -0.023647     183.09
 H       7.488873    -1.809834     0.384786      23.70
 C       4.711836    -0.072006    -0.233182      54.44
 H       4.988879    -0.033426    -1.275723      22.77
 C       3.234584     0.238750     1.711474      36.25
 C       1.890708     0.828159     2.461170      84.56
 H       2.181517     1.706404     2.832682      25.53
 O       1.447404     0.021270     3.666487     284.25
 H       1.522958    -0.831411     3.420912      29.44
 C       0.667785     1.100671     1.509643      71.75
 H       0.566813     1.792537     0.613115      19.65
 C      -0.325363     1.994667     2.413895      80.43
 O      -0.276516     3.403935     2.256077     199.00
 H       0.469218     3.622075     1.500939      26.77
 H       0.146873     2.164880     3.545792      20.74
 H      -1.475659     1.607343     2.145733      21.97
 C      -2.128843    -2.306676    -0.785447      65.92
 H      -2.744771    -3.271835    -0.473279      21.97
 C      -1.590056    -0.354889    -2.212028      48.48
 H      -1.819939     0.404357    -3.107447      20.44
 C      -0.763651     0.221809    -1.265115     -10.83
 O       0.002598     1.423683    -1.331615     149.53
 C       0.140606     2.254661    -2.686450     109.60
 H       0.723574     2.984084    -2.195898      26.13
 H       0.436681     1.429484    -3.168857      28.39
 H      -0.735351     2.498740    -3.133874      28.40
 C      -0.687924    -0.539149     0.145031      12.64
 O       0.166071    -0.207528     1.023439     161.49
 C      -1.331517    -1.722813     0.187846      68.34
 H      -1.177164    -2.200168     1.154533      22.92
 C      -2.236029    -1.621194    -1.994574      29.91
 C      -3.099475    -2.062308    -3.194538      89.19
 H      -2.925075    -1.408791    -4.052400      25.60
 O      -2.845211    -3.526637    -3.413513     246.17
 H      -1.996512    -3.620645    -3.505485      33.03
 C      -4.548828    -2.095858    -2.671673      66.99
 H      -4.800918    -2.917986    -1.909430      24.62
 O      -4.733221    -0.630120    -2.278592     278.89
 H      -5.585039    -0.681345    -1.903115      28.86
 C      -5.679053    -2.422265    -3.958588      86.34
 O      -5.971762    -3.793104    -3.976120     244.36
 H      -5.997662    -3.811630    -5.084711      23.94
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 H      -5.064238    -2.247950    -4.815037      25.04
 H      -6.578966    -1.786198    -3.842153      26.91
55
name = lig-ACN-frame_727
 C       3.537779     0.436260     0.364622      48.10
 H       2.589890     0.907644    -0.179784      21.09
 C       4.193879    -0.417378     2.525798      73.38
 H       4.078576    -0.433720     3.648219      23.75
 C       5.480809    -0.840348     1.979996      11.54
 O       6.444723    -1.543120     2.703977     239.03
 C       6.691258    -1.348017     4.126718     118.75
 H       7.576739    -1.830884     4.272362      24.80
 H       5.748635    -1.709867     4.814223      26.01
 H       6.748922    -0.198422     4.338562      26.57
 C       5.517830    -0.861058     0.558955      26.92
 O       6.594499    -1.511894    -0.092991     185.34
 H       7.285600    -1.365920     0.620549      24.90
 C       4.649041    -0.145956    -0.209976      66.87
 H       4.732235    -0.138446    -1.310421      22.75
 C       3.166743     0.232470     1.740563      22.49
 C       1.919103     0.793308     2.445295     100.78
 H       2.169895     1.687341     2.849044      26.03
 O       1.509557     0.042144     3.516413     279.15
 H       1.562962    -1.032255     3.425906      22.85
 C       0.642250     1.132926     1.593888      93.68
 H       1.222455     1.598848     0.790641      23.41
 C      -0.320201     1.978211     2.480014      96.88
 O      -0.318452     3.450950     2.193181     223.92
 H       0.373928     3.644180     1.516451      28.91
 H      -0.239793     1.470221     3.595420      23.00
 H      -1.493223     1.501124     2.330886      22.53
 C      -2.165085    -2.261148    -0.826291      21.46
 H      -2.403609    -3.396388    -0.770378      21.33
 C      -1.504334    -0.424247    -2.266407      59.40
 H      -1.446320    -0.128126    -3.344569      19.76
 C      -0.852480     0.267126    -1.139215      27.31
 O      -0.084286     1.410177    -1.368010     242.89
 C       0.054153     2.195745    -2.542987     138.95
 H       0.780000     2.915065    -2.410318      28.62
 H       0.630426     1.808089    -3.327022      28.93
 H      -0.703070     2.743663    -2.931325      29.30
 C      -0.662808    -0.421886    -0.067980      12.16
 O       0.295338    -0.253232     1.117814     103.51
 C      -1.280464    -1.736968     0.180862      33.90
 H      -1.065338    -2.314480     1.085964      20.41
 C      -2.142345    -1.634312    -2.130079      30.40
 C      -3.006679    -2.168128    -3.175756      82.94
 H      -2.971999    -1.553401    -4.092095      26.27
 O      -2.796814    -3.493310    -3.474379     242.76
 H      -1.834870    -3.760390    -3.308849      27.39
 C      -4.656751    -1.993802    -2.744893      79.74
 H      -4.609950    -2.622425    -1.818177      24.77
 O      -4.775472    -0.716549    -2.213379     253.01
 H      -5.680288    -0.554863    -1.656857      26.26
 C      -5.528280    -2.404820    -3.811305     107.29
 O      -5.981004    -3.823708    -3.925253     227.16
 H      -5.927467    -4.385116    -4.966660      24.55
 H      -5.254326    -1.999643    -4.732738      27.92
 H      -6.445939    -1.786662    -3.658443      28.08
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name = lig-ACN-frame_728
 C       3.378939     0.371517     0.401126      51.05
 H       2.785426     0.889895    -0.454094      21.32
 C       4.247246    -0.406337     2.582722      36.33
 H       4.102955    -0.485177     3.629489      22.67
 C       5.417808    -0.867017     2.044141       9.31
 O       6.434524    -1.603710     2.774472     229.59
 C       6.752273    -1.396184     4.188750     117.42
 H       7.646549    -1.959409     4.354530      26.73
 H       5.951234    -1.906318     4.968465      27.01
 H       6.992940    -0.343544     4.493924      27.78
 C       5.625288    -0.787140     0.544934       3.84
 O       6.665036    -1.456000    -0.113810     186.34
 H       7.357817    -1.837946     0.416851      24.93
 C       4.518755    -0.217488    -0.241125      53.17
 H       4.726893    -0.125933    -1.353823      22.22
 C       3.239674     0.215947     1.773847      42.19
 C       2.000393     0.825351     2.407454     105.99
 H       2.300325     1.702264     2.812437      26.43
 O       1.571339    -0.032441     3.544723     206.05
 H       1.265911    -1.003281     2.999882      21.68
 C       0.789343     1.140453     1.592103      83.52
 H       0.781783     1.847677     0.791336      23.29
 C      -0.373981     1.861206     2.440022      79.80
 O      -0.344436     3.422052     2.162667     209.89
 H       0.169555     3.516063     1.404216      32.73
 H      -0.063817     2.011360     3.542156      23.53
 H      -1.545938     1.728841     1.978336      20.99
 C      -2.024675    -2.270718    -0.892320      68.53
 H      -2.657734    -3.185920    -0.785608      22.28
 C      -1.373073    -0.390496    -2.353414      76.74
 H      -1.250426     0.073699    -3.266561      25.49
 C      -0.878773     0.323439    -1.324484      -8.78
 O      -0.150350     1.422127    -1.311143     206.59
 C       0.027163     2.215433    -2.518083     131.90
 H       0.567582     2.906569    -2.045529      27.64
 H       0.138341     1.661604    -3.423140      27.81
 H      -0.884292     2.536075    -2.653026      30.52
 C      -0.588198    -0.522392     0.116285     -13.98
 O       0.318946    -0.198110     1.139308     140.50
 C      -1.278210    -1.700432     0.144266      71.87
 H      -1.041677    -2.283173     1.047156      24.48
 C      -2.107128    -1.623838    -2.097814      29.51
 C      -3.088400    -2.158138    -3.211625      89.30
 H      -2.878741    -1.555190    -4.115302      25.60
 O      -2.748931    -3.627115    -3.569092     115.54
 H      -1.597987    -3.564526    -3.335377      23.06
 C      -4.443210    -2.080766    -2.668865      80.52
 H      -4.768531    -2.925496    -2.048872      25.04
 O      -4.782131    -0.685796    -2.194813     160.36
 H      -5.917733    -0.908610    -2.152767      22.51
 C      -5.592253    -2.357690    -3.851650      79.95
 O      -5.980803    -3.809110    -3.854662     258.63
 H      -5.634551    -3.967324    -4.872196      25.34
 H      -5.221907    -2.042076    -4.742111      27.95
 H      -6.547558    -1.907830    -3.498091      27.71
55
name = lig-ACN-frame_729
 C       3.369327     0.233760     0.331969      50.93
 H       2.494337     0.798642     0.010876      21.68
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 C       4.246749    -0.346012     2.640571      34.48
 H       4.008646    -0.477400     3.622434      18.97
 C       5.454242    -0.961697     2.005584      20.31
 O       6.401323    -1.631650     2.763229     248.47
 C       6.810700    -1.442305     4.221281      82.74
 H       7.683822    -2.139989     4.376555      26.38
 H       5.762171    -1.681685     4.804934      27.24
 H       6.955264    -0.398301     4.422703      29.50
 C       5.638969    -0.806496     0.626415      23.85
 O       6.722346    -1.347738    -0.116327     204.76
 H       7.117322    -2.037311     0.515487      23.35
 C       4.567874    -0.292229    -0.198363      55.03
 H       4.692096    -0.294798    -1.325225      21.58
 C       3.286361     0.237959     1.775213      21.42
 C       2.096017     0.859417     2.534824      80.91
 H       2.324962     1.718906     3.093912      25.46
 O       1.634118    -0.094992     3.571460     258.89
 H       1.039801    -0.806356     3.201355      24.78
 C       0.738164     1.187668     1.529300      87.89
 H       1.070128     1.639251     0.644312      23.54
 C      -0.357872     1.941994     2.325099     100.05
 O      -0.345203     3.315960     2.128295     239.91
 H      -0.017145     3.590032     1.178407      27.21
 H      -0.427941     1.711581     3.418506      24.93
 H      -1.236853     1.062450     2.116239      22.53
 C      -1.917618    -2.277218    -0.933245      39.71
 H      -2.589197    -3.013302    -0.581258      23.07
 C      -1.348610    -0.385070    -2.455843      53.35
 H      -1.599726     0.099808    -3.258817      21.84
 C      -0.687464     0.122585    -1.150818      -8.53
 O      -0.130495     1.493672    -1.217554     185.79
 C      -0.139996     2.315919    -2.501304     124.22
 H       0.628514     2.953737    -2.614420      28.72
 H       0.415786     1.605633    -3.101532      26.20
 H      -0.874764     2.796124    -2.857796      29.99
 C      -0.601808    -0.453078     0.072659      27.40
 O       0.287077    -0.157985     1.101633     154.03
 C      -1.223591    -1.746432     0.235023      30.23
 H      -1.280594    -2.339389     1.169387      22.16
 C      -2.077297    -1.592644    -2.217789      24.73
 C      -2.966484    -2.176216    -3.232637      73.71
 H      -3.104715    -1.509508    -4.128855      24.99
 O      -2.700831    -3.670965    -3.626487     118.87
 H      -1.573758    -3.882495    -3.727104      23.28
 C      -4.525082    -2.175687    -2.718732      78.78
 H      -4.403744    -2.744673    -1.806832      24.73
 O      -4.733203    -0.749460    -2.238412     175.17
 H      -5.817926    -0.484396    -2.104347      25.40
 C      -5.631721    -2.364400    -3.812831     108.49
 O      -5.945567    -3.709277    -3.869332     345.67
 H      -5.825238    -4.105294    -4.606432      35.47
 H      -5.404118    -2.036321    -4.729914      29.09
 H      -6.448789    -1.611140    -3.633843      28.42
55
name = lig-ACN-frame_730
 C       3.433435     0.126945     0.413527      55.59
 H       2.838978     0.239911    -0.431603      22.22
 C       4.331834    -0.361341     2.579420      64.96
 H       4.273406    -0.274666     3.606756      25.31
 C       5.423775    -0.947318     2.104296      14.19
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 O       6.449075    -1.706316     2.730634     242.29
 C       6.704166    -1.422955     4.118087     128.74
 H       7.613792    -2.182712     4.317470      25.11
 H       5.927877    -1.696269     4.997595      26.84
 H       7.153034    -0.502289     4.248182      28.04
 C       5.580509    -0.887118     0.613072      17.39
 O       6.743784    -1.257933    -0.046021     159.55
 H       7.452526    -1.712017     0.590598      24.53
 C       4.622966    -0.345969    -0.172896      60.07
 H       4.817552    -0.493718    -1.255740      22.70
 C       3.281258     0.282215     1.821725      42.49
 C       2.003410     0.787958     2.571904      97.75
 H       2.259060     1.753646     3.010523      25.51
 O       1.681329    -0.095431     3.623207     308.73
 H       1.290225    -0.757278     3.211575      31.49
 C       0.843020     1.195117     1.550087      83.92
 H       1.261429     1.864259     0.881148      24.90
 C      -0.363522     1.824356     2.220220     106.14
 O      -0.377719     3.298603     2.079749     200.05
 H      -0.155904     3.393892     1.057605      27.40
 H      -0.127902     1.662667     3.243169      26.40
 H      -1.460885     1.834102     1.795626      21.00
 C      -1.895482    -2.257219    -0.913483      50.87
 H      -2.192993    -3.226875    -1.043212      23.51
 C      -1.342362    -0.366582    -2.256357      69.67
 H      -1.429729     0.261732    -3.011651      22.95
 C      -0.522340     0.183126    -1.322338      -3.97
 O      -0.133297     1.601334    -1.158136     216.71
 C      -0.154094     2.264846    -2.500038     125.55
 H       0.291236     3.091919    -2.109218      26.53
 H      -0.089777     1.711492    -3.459503      26.55
 H      -1.084847     2.456976    -2.586296      30.87
 C      -0.567117    -0.525840     0.073458      -9.70
 O       0.274467    -0.125088     1.122833     127.90
 C      -1.224313    -1.762340     0.176679      70.01
 H      -1.228568    -2.166383     1.202807      22.26
 C      -1.935121    -1.666987    -2.204454      22.23
 C      -2.963346    -2.289304    -3.329492      65.39
 H      -2.726055    -1.686665    -4.270338      23.48
 O      -2.672824    -3.607369    -3.656907     274.38
 H      -1.724684    -3.629770    -3.802578      29.53
 C      -4.563249    -2.097229    -2.740256      83.02
 H      -4.925076    -2.908430    -2.082185      25.39
 O      -4.622846    -0.805941    -2.323147     301.59
 H      -5.471737    -0.780907    -1.928410      30.83
 C      -5.575183    -2.310434    -3.813906     105.85
 O      -6.002795    -3.750289    -3.872410     284.30
 H      -6.066852    -3.798198    -4.859257      29.18
 H      -5.139196    -1.904810    -4.603690      29.28
 H      -6.523025    -1.906950    -3.430772      27.30
55
name = lig-ACN-frame_731
 C       3.427988     0.080174     0.407844      48.88
 H       2.558634     0.374860    -0.031229      24.36
 C       4.311605    -0.276761     2.675222      79.91
 H       4.288665    -0.170858     3.768159      19.60
 C       5.497562    -0.991298     2.006753      31.66
 O       6.437279    -1.753755     2.685730     269.30
 C       6.715150    -1.418901     4.044633     110.15
 H       7.478236    -2.269557     4.527762      24.66
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 H       5.667855    -1.395643     4.539564      27.06
 H       7.000825    -0.423963     4.152185      29.99
 C       5.679335    -0.975790     0.682995      23.87
 O       6.819171    -1.245432     0.049058     213.10
 H       7.594922    -1.242251     0.617806      24.79
 C       4.623961    -0.432577    -0.156570      62.14
 H       4.692559    -0.347840    -1.228860      22.88
 C       3.289413     0.219055     1.821709      26.79
 C       2.006970     0.768136     2.505186      88.73
 H       2.227359     1.736370     3.035948      23.85
 O       1.661850    -0.088300     3.688992     206.20
 H       1.600597    -1.121832     3.485373      24.26
 C       0.858874     1.092593     1.565678      95.47
 H       1.234318     1.517463     0.663304      23.16
 C      -0.423245     1.844712     2.192964      87.01
 O      -0.360591     3.348348     2.029438     244.97
 H      -0.124453     3.611027     1.180727      31.94
 H      -0.683607     1.731935     3.160284      26.68
 H      -1.126837     1.014201     1.683919      22.88
 C      -1.876564    -2.433197    -0.962896      32.00
 H      -2.214051    -3.363065    -0.697359      21.85
 C      -1.325208    -0.300380    -2.227270      51.15
 H      -1.561371     0.074032    -3.204222      20.64
 C      -0.485020     0.260429    -1.147164      20.24
 O      -0.088610     1.539011    -1.234054     243.93
 C      -0.297728     2.318669    -2.398468     118.73
 H       0.153992     3.277543    -2.559698      26.38
 H       0.347100     1.810819    -3.210118      25.98
 H      -1.204484     2.430486    -2.621782      30.97
 C      -0.368483    -0.489718    -0.019291      26.20
 O       0.289552    -0.171363     1.135664     159.35
 C      -1.201949    -1.683383     0.145072      28.33
 H      -1.067959    -2.323590     1.028610      23.64
 C      -1.911462    -1.701979    -2.185120      22.65
 C      -2.961759    -2.221189    -3.265484      87.59
 H      -3.047535    -1.448512    -4.111790      24.66
 O      -2.635665    -3.621834    -3.680007     259.23
 H      -1.771527    -3.693482    -3.692144      32.27
 C      -4.379605    -2.196960    -2.832207      86.75
 H      -4.400987    -2.811082    -1.920213      25.93
 O      -4.539049    -0.736740    -2.319165     271.22
 H      -5.281613    -0.634407    -1.812955      31.88
 C      -5.621903    -2.309185    -3.881513      94.98
 O      -6.029891    -3.766544    -3.961774     185.38
 H      -6.441853    -4.060857    -5.017099      25.33
 H      -5.518081    -2.080224    -4.848772      27.63
 H      -6.348477    -1.536375    -3.614084      27.25
55
name = lig-ACN-frame_732
 C       3.391049     0.040576     0.456657      56.26
 H       2.817676     0.501154    -0.298698      23.24
 C       4.432590    -0.301135     2.676956      63.15
 H       4.175288    -0.233430     3.801996      17.85
 C       5.415983    -0.978806     2.123539      14.06
 O       6.462155    -1.788610     2.636216     239.34
 C       6.650317    -1.359776     4.030499     106.27
 H       7.511692    -2.189907     4.482939      26.04
 H       5.757091    -1.474971     4.690852      28.91
 H       7.176283    -0.443015     4.077598      29.36
 C       5.637737    -0.899764     0.589521      -8.30
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 O       6.976547    -1.290109     0.077966     163.48
 H       7.502102    -1.478169     0.876318      22.56
 C       4.581125    -0.501658    -0.165841      62.84
 H       4.822695    -0.472080    -1.197339      23.28
 C       3.314998     0.102723     1.856003      35.90
 C       2.091182     0.707233     2.547110      81.66
 H       2.384073     1.758196     2.965243      23.68
 O       1.612800    -0.044562     3.727079     170.62
 H       1.800383    -1.140258     3.443383      23.01
 C       0.763749     1.017963     1.585941      81.33
 H       1.091385     1.733511     0.800222      23.32
 C      -0.436538     1.906847     2.111481     109.09
 O      -0.370997     3.321364     1.994938     261.41
 H       0.159219     3.437843     1.176693      29.77
 H      -0.532358     1.637100     3.089408      27.22
 H      -1.478439     1.913833     1.495353      21.51
 C      -1.731661    -2.420435    -0.893240      64.37
 H      -2.445012    -3.153054    -0.700548      23.19
 C      -1.338860    -0.451539    -2.256802      56.22
 H      -1.458351     0.399515    -3.058109      20.09
 C      -0.677756     0.250878    -1.203619      -4.58
 O       0.028809     1.555604    -1.221416     190.07
 C      -0.382630     2.382359    -2.473053     100.87
 H      -0.112891     3.308673    -1.901043      23.85
 H       0.175590     1.906090    -3.354706      25.43
 H      -1.269657     2.312397    -2.798399      30.18
 C      -0.312396    -0.574350     0.005265       8.82
 O       0.367089    -0.336231     1.194058     148.29
 C      -1.070318    -1.758006     0.054852      50.59
 H      -0.969650    -2.089723     1.090739      22.28
 C      -1.976290    -1.625778    -2.145778      34.27
 C      -2.810464    -2.108613    -3.288463      81.60
 H      -2.561576    -1.541442    -4.246833      24.93
 O      -2.606251    -3.593686    -3.703038     188.85
 H      -1.590020    -3.804950    -3.474870      25.92
 C      -4.370082    -2.148864    -2.840586      61.34
 H      -4.559126    -2.920668    -2.075821      25.24
 O      -4.442163    -0.702773    -2.328300     196.77
 H      -5.468382    -0.744014    -1.868738      25.64
 C      -5.581960    -2.438748    -3.976208      95.65
 O      -6.088105    -3.728777    -4.012327     212.13
 H      -6.334323    -3.880445    -5.169600      24.45
 H      -5.130017    -2.001244    -4.776513      27.70
 H      -6.401843    -1.927486    -3.499601      26.38
55
name = lig-ACN-frame_733
 C       3.452697    -0.019622     0.428078      43.46
 H       2.519601     0.329824    -0.071218      22.61
 C       4.364287    -0.383103     2.685557      63.13
 H       4.467005    -0.377406     3.861641      16.57
 C       5.528874    -1.032504     1.951011      25.93
 O       6.443976    -1.740144     2.698588     269.39
 C       6.703485    -1.371543     4.052883      94.26
 H       7.615218    -2.183627     4.422277      24.74
 H       5.847025    -1.395165     4.672920      29.02
 H       6.947760    -0.288292     4.092369      28.71
 C       5.729681    -0.918361     0.643550      26.15
 O       6.914637    -1.291161     0.140568     215.60
 H       7.488137    -1.961144     0.680676      21.48
 C       4.583312    -0.508628    -0.222456      60.81
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 H       4.509274    -0.505839    -1.284322      22.74
 C       3.278041     0.067311     1.879379      20.50
 C       1.988066     0.734247     2.596318      86.89
 H       2.459212     1.741987     3.027002      22.76
 O       1.613428    -0.002730     3.743527     265.89
 H       1.424567    -0.960370     3.480087      26.41
 C       0.799655     1.002267     1.593946      84.54
 H       1.269075     1.265673     0.599548      20.87
 C      -0.523163     1.848367     2.078256      90.37
 O      -0.271285     3.356610     1.961733     203.47
 H       0.453723     3.625802     1.209660      25.81
 H      -0.604741     1.789908     3.113928      25.66
 H      -1.475780     1.243528     1.632449      23.29
 C      -1.766758    -2.335563    -0.943026      39.32
 H      -2.155136    -3.366911    -0.796910      22.15
 C      -1.308486    -0.338187    -2.245358      44.10
 H      -1.575934    -0.019254    -3.407344      16.70
 C      -0.607503     0.227441    -1.162591      18.95
 O      -0.012490     1.470321    -1.301605     231.09
 C      -0.383666     2.396193    -2.459915     104.59
 H      -0.394340     3.511506    -2.225111      24.74
 H       0.173980     2.583479    -3.429008      24.48
 H      -1.278973     2.173976    -2.505504      30.63
 C      -0.400474    -0.585352    -0.007679       6.98
 O       0.438283    -0.418381     1.198292     108.48
 C      -0.847542    -1.937404     0.163252      39.34
 H      -0.951090    -2.492868     1.088627      20.33
 C      -1.982042    -1.677064    -2.116262      15.78
 C      -2.775481    -2.219999    -3.350058      73.76
 H      -2.561102    -1.408408    -4.126411      23.89
 O      -2.546756    -3.502622    -3.688068     204.12
 H      -1.396349    -3.759872    -3.503978      21.38
 C      -4.350962    -2.033262    -2.904047      86.15
 H      -4.427968    -2.735135    -2.043390      24.60
 O      -4.458683    -0.769589    -2.347263     183.09
 H      -5.526991    -0.448784    -2.099557      25.42
 C      -5.423235    -2.348107    -3.922321      98.99
 O      -6.123793    -3.776487    -4.112791     241.58
 H      -6.038428    -3.987720    -5.150051      26.97
 H      -5.259784    -2.185661    -4.965378      25.21
 H      -6.193530    -1.606833    -3.802221      28.04
55
name = lig-ACN-frame_734
 C       3.421556    -0.054772     0.496713      41.95
 H       2.595169    -0.021804    -0.321353      21.64
 C       4.322137    -0.553174     2.569648      67.96
 H       4.204130    -0.438151     3.704686      24.13
 C       5.460195    -0.979055     2.064384      18.38
 O       6.473304    -1.725128     2.740930     248.81
 C       6.755659    -1.344367     4.111407     121.36
 H       7.764427    -1.992856     4.494252      23.81
 H       5.991950    -1.672499     4.711780      28.98
 H       7.061937    -0.236839     4.284931      25.20
 C       5.653691    -0.938663     0.579925       5.65
 O       6.908444    -1.334526     0.034688     155.96
 H       7.373709    -1.813205     0.797084      23.10
 C       4.653632    -0.493660    -0.187548      61.10
 H       4.816039    -0.634637    -1.256664      22.25
 C       3.256519     0.072697     1.871334      39.39
 C       1.978832     0.756352     2.563399      85.06
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 H       2.052850     1.903637     2.981278      23.74
 O       1.586118     0.007482     3.799326     278.65
 H       1.044505    -0.607716     3.519113      32.19
 C       0.831362     0.945203     1.569431      86.41
 H       1.145776     1.778129     0.819279      22.78
 C      -0.394618     1.770648     2.086815      96.73
 O      -0.192605     3.315011     1.916445     179.39
 H       0.365926     3.330521     1.066413      28.39
 H      -0.807305     1.592136     3.147806      25.33
 H      -1.217046     1.649336     1.336178      24.55
 C      -1.751892    -2.470957    -0.847877      41.49
 H      -2.040007    -3.576835    -0.971158      21.40
 C      -1.368490    -0.362229    -2.230136      51.95
 H      -1.135868     0.386714    -3.181452      18.78
 C      -0.499441     0.144387    -1.187867      -3.11
 O       0.013314     1.440774    -1.393980     203.76
 C      -0.483148     2.384033    -2.378649     105.12
 H      -0.244014     3.265107    -1.714242      24.09
 H       0.264658     1.993617    -3.078908      24.52
 H      -1.274152     2.363440    -2.917151      28.86
 C      -0.374081    -0.653218     0.135133      10.57
 O       0.456525    -0.365803     1.154921     152.54
 C      -0.884639    -2.030629     0.075185      49.00
 H      -0.314043    -2.658046     0.751534      22.37
 C      -1.888197    -1.591307    -2.181817      26.64
 C      -2.837560    -2.102787    -3.271830      91.38
 H      -2.785042    -1.570883    -4.256399      24.78
 O      -2.457336    -3.544271    -3.696923     138.84
 H      -1.282675    -3.519640    -3.740154      22.19
 C      -4.263109    -2.146537    -2.903298      77.51
 H      -4.456515    -2.945261    -2.130015      24.92
 O      -4.516310    -0.712904    -2.362144     236.95
 H      -5.445813    -0.635246    -2.454903      31.53
 C      -5.415348    -2.288878    -4.080993      79.34
 O      -6.064017    -3.727345    -4.120951     291.10
 H      -6.021301    -3.899183    -4.970896      33.68
 H      -4.743266    -2.091728    -4.974568      25.60
 H      -6.193422    -1.615478    -3.844814      27.94
55
name = lig-ACN-frame_735
 C       3.376630    -0.082209     0.364703      51.52
 H       2.540036     0.427729    -0.274192      19.43
 C       4.175513    -0.569132     2.675805      24.48
 H       3.999158    -0.815939     3.727418      20.87
 C       5.505246    -1.043525     2.058115      10.72
 O       6.524205    -1.674888     2.760496     222.33
 C       6.808092    -1.349723     4.200236     103.58
 H       7.878647    -1.891291     4.275728      24.11
 H       6.114222    -1.651027     4.885780      29.28
 H       6.803658    -0.160618     4.308108      25.47
 C       5.704009    -0.988156     0.687953      20.29
 O       6.863698    -1.400127    -0.058632     217.11
 H       7.645819    -1.364958     0.478992      27.37
 C       4.579219    -0.463672    -0.125966      50.94
 H       4.686781    -0.402157    -1.238794      24.31
 C       3.213183     0.069021     1.819060      16.60
 C       2.013473     0.703425     2.561164      80.98
 H       2.603261     1.747392     2.891936      22.20
 O       1.553908     0.059004     3.804509     246.15
 H       0.886487    -0.721078     3.510537      24.66
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 C       0.849643     1.009609     1.561572      95.00
 H       1.392686     1.321526     0.587501      20.32
 C      -0.326444     1.824184     2.027842     114.98
 O      -0.091280     3.169487     1.914769     297.59
 H       0.161468     3.392448     1.071207      32.04
 H      -0.549257     1.449758     3.123453      24.45
 H      -1.205351     1.453867     1.403570      25.35
 C      -1.701607    -2.519684    -1.090852      32.41
 H      -2.183232    -3.588626    -0.986985      18.33
 C      -1.257399    -0.381059    -2.159449      55.70
 H      -1.661192     0.238571    -3.071891      16.66
 C      -0.512397     0.060506    -1.134890      26.27
 O       0.037802     1.319552    -1.283962     221.91
 C      -0.432923     2.352500    -2.379416     103.55
 H      -0.343209     3.370073    -1.978242      26.08
 H       0.156723     2.611995    -3.239786      25.27
 H      -1.408980     2.249364    -2.471551      28.27
 C      -0.355606    -0.685225     0.001106      20.18
 O       0.476591    -0.337561     1.129292     160.64
 C      -0.841211    -1.998070     0.046709      45.46
 H      -0.495359    -2.719946     0.797671      21.54
 C      -1.954996    -1.708781    -2.077124      45.12
 C      -2.775341    -2.114892    -3.296565      68.21
 H      -2.629931    -1.310940    -4.028387      27.91
 O      -2.396107    -3.532967    -3.694957     199.20
 H      -1.344437    -3.588599    -3.671245      26.66
 C      -4.392731    -2.157693    -2.862783      72.37
 H      -4.684329    -2.952915    -2.103123      25.98
 O      -4.581896    -0.743797    -2.391223     264.04
 H      -5.481123    -0.596355    -2.400326      32.23
 C      -5.320986    -2.370581    -4.168121     101.72
 O      -5.925541    -3.571330    -4.116438     314.18
 H      -6.292329    -3.867096    -4.883913      34.18
 H      -4.932352    -2.042466    -5.234849      26.72
 H      -6.097894    -1.617191    -4.145359      27.80
55
name = lig-ACN-frame_736
 C       3.332555     0.018588     0.409627      38.39
 H       2.727154     0.578008    -0.362486      22.51
 C       4.228278    -0.630315     2.648512      38.15
 H       3.967648    -0.652420     3.654795      18.88
 C       5.420535    -1.102019     2.146656      13.54
 O       6.572295    -1.624516     2.830347     247.34
 C       6.826930    -1.326440     4.190979     112.80
 H       7.856719    -1.690380     4.538310      26.38
 H       6.102618    -1.834469     4.743771      30.68
 H       6.825682    -0.138274     4.427995      26.95
 C       5.680316    -0.967814     0.661491      14.05
 O       6.754601    -1.439413    -0.092558     168.37
 H       7.658032    -1.298808     0.328779      23.13
 C       4.615722    -0.503809    -0.125059      40.12
 H       4.876550    -0.374573    -1.221953      21.46
 C       3.181730    -0.114614     1.812215      30.06
 C       2.049990     0.674626     2.527917      81.67
 H       2.425074     1.764636     3.032401      22.24
 O       1.524020     0.120570     3.751535     197.80
 H       1.205355    -0.960373     3.476551      22.85
 C       0.981053     0.997081     1.466264      71.95
 H       1.337747     1.744747     0.682796      22.37
 C      -0.322198     1.717210     1.972326      98.45
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 O      -0.003780     3.177641     1.955328     211.70
 H       0.254747     3.424163     0.997686      28.05
 H      -0.475327     1.687924     3.149510      23.46
 H      -1.249932     1.425488     1.470179      25.21
 C      -1.541622    -2.578209    -1.044016      51.01
 H      -2.100180    -3.583165    -0.913963      21.17
 C      -1.354897    -0.528014    -2.202967      51.36
 H      -1.633194     0.136775    -3.015664      21.02
 C      -0.547683     0.111630    -1.171189       7.12
 O       0.143478     1.344399    -1.184527     221.73
 C      -0.406676     2.335484    -2.275476     109.35
 H      -0.273994     3.188806    -1.708043      26.39
 H      -0.005043     2.036285    -3.199376      26.58
 H      -1.370949     2.023444    -2.503572      28.24
 C      -0.245105    -0.740407    -0.012025       7.08
 O       0.442606    -0.413354     1.109604     112.09
 C      -0.859517    -2.070388    -0.023629      60.28
 H      -1.021940    -2.447381     0.983389      23.62
 C      -1.999994    -1.727526    -2.148860      49.23
 C      -2.831160    -2.234964    -3.230968     105.82
 H      -2.737633    -1.616725    -4.136451      28.08
 O      -2.402713    -3.455038    -3.718676     283.09
 H      -1.552205    -3.596554    -3.414348      31.10
 C      -4.412088    -2.053396    -2.997463      86.97
 H      -4.619389    -2.846454    -2.206693      25.23
 O      -4.648027    -0.819284    -2.406483     187.80
 H      -5.729391    -0.607705    -2.158835      25.56
 C      -5.229900    -2.221367    -4.225785      83.24
 O      -5.847786    -3.617904    -4.089566     209.73
 H      -6.303555    -3.588343    -5.125330      27.46
 H      -4.407775    -2.409899    -5.039145      25.06
 H      -5.877432    -1.381999    -4.258576      27.56
55
name = lig-ACN-frame_737
 C       3.505867     0.035183     0.463334      64.83
 H       2.700081     0.403873    -0.100575      26.57
 C       4.235664    -0.713717     2.649337      64.36
 H       4.325176    -0.502418     3.655154      20.48
 C       5.520702    -1.156296     2.082617      17.51
 O       6.600321    -1.571410     2.804513     235.42
 C       6.775067    -1.281641     4.257071     122.07
 H       7.758302    -1.675876     4.364756      25.39
 H       6.092348    -1.799124     4.961218      27.66
 H       6.637920    -0.130823     4.506391      26.35
 C       5.562211    -1.008463     0.704255      16.43
 O       6.677351    -1.459949    -0.075410     141.05
 H       7.376089    -1.697548     0.664320      22.33
 C       4.581880    -0.449408    -0.133510      69.83
 H       4.826524    -0.459523    -1.225154      21.47
 C       3.169755    -0.191603     1.837151      28.50
 C       2.049080     0.665766     2.459867      80.49
 H       2.523057     1.826599     2.625084      22.31
 O       1.494574     0.105634     3.684275     244.45
 H       1.490961    -0.905908     3.580753      25.79
 C       0.896258     0.903214     1.435492      95.75
 H       1.341706     1.293308     0.527229      23.73
 C      -0.237560     1.713629     2.022696     109.47
 O       0.035187     3.219558     1.974924     209.80
 H       0.527118     3.418014     1.033977      26.36
 H      -0.405474     1.090059     3.007795      24.00
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 H      -1.117577     1.637939     1.413575      26.36
 C      -1.603760    -2.662563    -1.022635      41.53
 H      -1.919069    -3.711899    -0.889004      21.04
 C      -1.391760    -0.366311    -2.234837      92.54
 H      -1.395464     0.052623    -3.130166      22.24
 C      -0.509417     0.033645    -1.196460      -6.73
 O       0.163498     1.370519    -1.172092     215.14
 C      -0.387251     2.206154    -2.130352     137.88
 H      -0.048308     3.173743    -2.116013      28.51
 H       0.182846     2.068870    -2.989543      27.55
 H      -1.361258     2.349382    -2.216623      30.75
 C      -0.231350    -0.803462    -0.062350      19.91
 O       0.479761    -0.445017     1.095610     154.09
 C      -0.815462    -2.028669     0.084241      54.28
 H      -0.620947    -2.636210     0.994603      22.01
 C      -1.925720    -1.846518    -2.122027      30.50
 C      -2.916949    -2.133641    -3.308974      81.46
 H      -2.680571    -1.308866    -3.973841      27.29
 O      -2.485268    -3.544641    -3.749697     232.68
 H      -1.612047    -3.585202    -3.598134      29.51
 C      -4.375249    -2.102881    -2.981954      83.05
 H      -4.793514    -2.993178    -2.454535      24.58
 O      -4.699829    -0.747504    -2.351692     201.69
 H      -5.708234    -1.165818    -2.024564      24.93
 C      -5.117770    -2.254193    -4.347072      85.15
 O      -5.831569    -3.575509    -4.112221     195.20
 H      -6.045251    -4.138007    -5.155248      25.73
 H      -4.433285    -2.136454    -5.329272      26.74
 H      -5.891286    -1.620962    -4.696159      27.10
55
name = lig-ACN-frame_738
 C       3.419739     0.025060     0.513912      47.11
 H       2.804265     0.500050    -0.133313      20.76
 C       4.301320    -0.757271     2.711643      51.89
 H       4.058302    -0.842008     3.760305      21.12
 C       5.438872    -1.119291     2.063977       2.48
 O       6.645470    -1.537842     2.775762     208.76
 C       6.711967    -1.247674     4.263001     117.93
 H       7.641604    -1.499072     4.593760      25.43
 H       5.838135    -1.831394     4.780093      27.09
 H       6.629543    -0.127341     4.409251      27.68
 C       5.590979    -1.140411     0.623286      22.15
 O       6.705401    -1.510222     0.015828     222.92
 H       7.264880    -2.145883     0.428225      28.16
 C       4.646047    -0.437410    -0.149551      48.16
 H       4.635639    -0.339792    -1.242872      23.25
 C       3.287500    -0.127309     1.898799      29.34
 C       2.028205     0.594195     2.374589      87.35
 H       2.483964     1.680532     2.822915      21.77
 O       1.510087     0.091696     3.638991     286.91
 H       1.465442    -0.768543     3.535694      32.03
 C       0.912455     0.822824     1.392474      95.34
 H       1.193725     1.427051     0.580081      23.15
 C      -0.226087     1.789840     1.976996     103.25
 O       0.086660     3.169131     2.056226     257.23
 H       0.671972     3.338669     1.298810      30.95
 H      -0.529498     1.800538     3.152966      22.82
 H      -1.096920     1.539414     1.420764      26.19
 C      -1.643348    -2.607639    -0.930715      56.98
 H      -1.984118    -3.585788    -1.026114      24.98
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 C      -1.359607    -0.459043    -2.169489      71.58
 H      -1.609234     0.117199    -2.893960      25.38
 C      -0.420176     0.031466    -1.199298      25.00
 O       0.078507     1.231729    -1.130067     229.54
 C      -0.266452     2.273811    -2.190046     116.39
 H       0.171989     3.021345    -1.701122      27.22
 H      -0.338724     1.899500    -3.140813      27.51
 H      -1.271895     2.218520    -2.018138      29.69
 C      -0.291043    -0.777218    -0.027518       0.76
 O       0.503743    -0.515910     1.071999     158.81
 C      -0.826552    -2.163397     0.075919      43.83
 H      -0.276797    -2.763461     0.824378      21.83
 C      -1.870962    -1.688608    -2.124623      34.00
 C      -2.740992    -2.126785    -3.278218      88.51
 H      -2.659942    -1.537187    -4.185181      24.48
 O      -2.644411    -3.569686    -3.796189     183.62
 H      -1.606308    -3.699667    -3.997694      25.49
 C      -4.406175    -2.064866    -3.024232      53.67
 H      -4.495820    -2.796926    -2.198830      23.96
 O      -4.779296    -0.796667    -2.299425     281.85
 H      -5.581618    -0.698592    -1.778500      28.72
 C      -5.135382    -2.384996    -4.467639      80.79
 O      -5.802231    -3.531242    -4.201518     271.37
 H      -5.793825    -4.106138    -5.115482      27.65
 H      -4.353528    -2.634316    -5.351373      23.49
 H      -5.673694    -1.454056    -4.448268      24.93
55
name = lig-ACN-frame_739
 C       3.481199    -0.009561     0.468021      70.99
 H       2.755062     0.551998    -0.003825      20.84
 C       4.235699    -0.713505     2.744170      37.56
 H       4.075150    -1.013280     3.835995      17.52
 C       5.507243    -1.164210     2.103707      -5.05
 O       6.658610    -1.511389     2.759682     224.72
 C       6.619451    -1.211234     4.158969     131.80
 H       7.435928    -1.615588     4.557960      26.89
 H       5.718946    -1.794176     4.735413      27.43
 H       6.407069    -0.184983     4.348364      30.13
 C       5.576436    -1.152784     0.650796      -1.57
 O       6.871787    -1.635480    -0.003119     166.98
 H       7.284789    -2.071858     0.775941      25.18
 C       4.600795    -0.478837    -0.126126      59.66
 H       4.952953    -0.354943    -1.126333      23.00
 C       3.317404    -0.037813     1.896115      28.66
 C       2.077733     0.601012     2.486562      90.67
 H       2.250143     1.814159     2.689268      21.85
 O       1.536241     0.027188     3.648004     258.73
 H       1.005718    -0.860261     3.420361      23.74
 C       0.933086     0.876210     1.427322      70.51
 H       1.362639     1.319369     0.577401      22.97
 C      -0.316084     1.757399     1.996903      97.67
 O       0.208632     3.170974     2.088066     239.48
 H       0.531588     3.499841     1.260975      30.20
 H      -0.476257     1.199605     3.084902      23.09
 H      -1.199149     1.807355     1.389338      25.34
 C      -1.684685    -2.537947    -1.006098      60.74
 H      -2.148703    -3.453285    -0.981885      24.88
 C      -1.263559    -0.454230    -2.159257      59.37
 H      -1.639953     0.240153    -2.786387      22.14
 C      -0.495413    -0.082161    -1.128808       2.87
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 O       0.113380     1.231948    -1.173977     219.25
 C      -0.273981     2.258268    -2.154541     139.29
 H       0.390998     3.074530    -2.194872      27.49
 H       0.106780     2.026132    -3.077567      28.24
 H      -1.154573     2.786720    -2.265753      29.40
 C      -0.337288    -0.926403     0.092414      14.50
 O       0.510281    -0.556738     1.059501     147.53
 C      -0.773316    -2.179203     0.002576      73.81
 H      -0.766713    -2.871756     0.860437      23.65
 C      -1.926353    -1.761450    -2.083932      28.70
 C      -2.769630    -2.164976    -3.297803      95.55
 H      -2.253664    -1.480048    -3.994962      24.09
 O      -2.769034    -3.528505    -3.785543     140.61
 H      -1.630411    -3.831215    -3.949194      24.27
 C      -4.302646    -2.014040    -3.030361      86.18
 H      -4.619260    -2.992639    -2.603645      24.57
 O      -4.789958    -0.836049    -2.327151     310.26
 H      -5.559326    -1.167063    -2.128310      33.19
 C      -5.046407    -2.306696    -4.343800      86.55
 O      -5.880208    -3.636864    -4.269142     236.15
 H      -6.199381    -3.769380    -5.202119      30.51
 H      -4.138753    -2.460049    -5.126520      24.58
 H      -5.690569    -1.701424    -4.970103      25.43
55
name = lig-ACN-frame_740
 C       3.533980     0.052627     0.485998      37.69
 H       2.902591     0.438089    -0.350563      25.15
 C       4.293917    -0.706910     2.647033      51.20
 H       4.139177    -0.462338     3.788297      17.46
 C       5.462172    -1.174825     2.051873      20.70
 O       6.644814    -1.517864     2.744366     242.45
 C       6.541798    -1.229940     4.153227     128.78
 H       7.463795    -1.470497     4.548639      26.15
 H       5.600457    -1.841881     4.620823      26.34
 H       6.531826    -0.240158     4.321152      30.44
 C       5.767815    -1.176729     0.674133      12.23
 O       6.846899    -1.707762     0.091969     160.19
 H       7.775341    -1.612131     0.602032      21.26
 C       4.717824    -0.620697    -0.142684      41.42
 H       4.734527    -0.478904    -1.198131      22.39
 C       3.277525    -0.026082     1.872438      22.58
 C       2.022122     0.732164     2.543747      77.29
 H       2.515587     1.630103     3.120698      22.60
 O       1.544531    -0.083577     3.735805     191.39
 H       0.907496    -0.842174     3.135899      21.39
 C       0.877091     0.863324     1.469346      95.46
 H       1.234864     1.365413     0.549677      23.16
 C      -0.234269     1.717934     1.975192      96.87
 O       0.291497     3.128113     2.158859     209.86
 H       0.279624     3.298979     1.103005      26.75
 H      -0.693346     1.423353     3.114565      23.45
 H      -1.083645     1.596069     1.263331      25.34
 C      -1.733291    -2.663334    -1.073783      55.63
 H      -2.266320    -3.585665    -0.913497      20.03
 C      -1.343637    -0.517771    -2.204649      48.18
 H      -1.221742     0.002814    -3.142631      19.91
 C      -0.542779    -0.003918    -1.049206      -1.74
 O       0.123931     1.262200    -1.164972     202.18
 C      -0.131694     2.236225    -2.247630     103.05
 H       0.474127     2.939114    -1.737794      25.03
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 H      -0.117095     1.740096    -3.139422      26.95
 H      -1.194746     2.464776    -2.152367      27.51
 C      -0.249784    -0.896055     0.058562      -6.97
 O       0.571854    -0.530831     1.188794     148.45
 C      -0.863404    -2.283640     0.051333      38.65
 H      -0.755679    -2.894207     0.979403      23.10
 C      -1.965720    -1.767638    -2.171053      36.63
 C      -2.838617    -2.094873    -3.317907     101.14
 H      -2.828601    -1.463962    -4.259797      26.19
 O      -2.777746    -3.525232    -3.742134     146.48
 H      -1.743388    -3.845501    -3.525984      26.54
 C      -4.306806    -2.055263    -3.059527      94.62
 H      -4.400944    -2.811660    -2.271462      24.91
 O      -4.770686    -0.901760    -2.371760     218.11
 H      -5.818562    -0.895814    -2.125771      26.01
 C      -5.004184    -2.305918    -4.404353      69.17
 O      -5.913417    -3.649338    -4.273453     269.41
 H      -6.392710    -3.554083    -4.975406      36.20
 H      -4.273970    -2.633862    -5.272651      26.39
 H      -5.667411    -1.369799    -4.462254      26.04
55
name = lig-ACN-frame_741
 C       3.661564    -0.000839     0.418925      63.91
 H       2.893436     0.526821    -0.267583      25.32
 C       4.304165    -0.589924     2.559481      44.19
 H       4.404178    -0.544655     3.719394      15.63
 C       5.520557    -1.157905     2.022800      12.63
 O       6.595071    -1.550070     2.775692     236.86
 C       6.562766    -1.258923     4.209605     129.74
 H       7.410042    -1.756987     4.682632      25.30
 H       5.648013    -1.804811     4.747709      27.49
 H       6.314690    -0.300693     4.361644      32.65
 C       5.758188    -1.137843     0.635306      12.02
 O       6.896212    -1.807220     0.163878     194.02
 H       7.714131    -1.333364     0.460940      24.60
 C       4.742410    -0.654192    -0.130883      71.64
 H       4.898173    -0.909432    -1.160072      20.10
 C       3.260472    -0.001474     1.796591      29.94
 C       2.065086     0.642725     2.602090      95.69
 H       2.133771     1.740749     2.927544      22.85
 O       1.543029    -0.140801     3.735498     232.40
 H       1.208964    -1.153601     3.473453      22.87
 C       0.967272     0.857597     1.586678      78.67
 H       1.395306     1.391136     0.656555      23.32
 C      -0.235575     1.747976     2.022103      97.83
 O       0.307506     3.019275     2.156286     244.40
 H       0.523473     3.754629     1.482003      27.53
 H      -0.708128     1.489240     3.194469      22.85
 H      -1.059965     1.792281     1.238035      24.66
 C      -1.728112    -2.702299    -1.059515      42.01
 H      -2.185395    -3.733922    -1.223769      19.51
 C      -1.307123    -0.506465    -2.141276      47.31
 H      -1.292505    -0.057090    -3.202857      21.31
 C      -0.565743     0.027449    -1.118276      12.18
 O       0.117318     1.190795    -1.098090     213.76
 C      -0.052643     2.147115    -2.283759     113.16
 H       0.479250     3.113726    -2.388086      26.15
 H       0.260785     1.917605    -3.249844      27.60
 H      -1.134710     2.478540    -2.282796      26.69
 C      -0.254723    -0.917120     0.005273     -19.11
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 O       0.552688    -0.551414     1.267681      86.37
 C      -0.943731    -2.173555     0.035271      55.73
 H      -0.556885    -2.905950     0.778251      24.27
 C      -1.936649    -1.787084    -2.180981      14.13
 C      -2.900416    -2.091614    -3.402477      85.34
 H      -2.472523    -1.432456    -4.249355      25.60
 O      -2.674576    -3.537769    -3.693401     240.02
 H      -1.873485    -3.710676    -3.393351      33.58
 C      -4.435682    -2.199758    -2.982969      66.08
 H      -4.681626    -3.145935    -2.457205      25.73
 O      -4.745214    -0.858973    -2.424013     163.95
 H      -5.832080    -0.887566    -1.934129      23.39
 C      -5.144634    -2.456512    -4.417028      85.57
 O      -5.909914    -3.496782    -4.218411     267.41
 H      -6.178996    -3.977665    -5.087462      28.36
 H      -4.512391    -2.419839    -5.400657      25.67
 H      -5.713610    -1.461926    -4.652311      26.23
55
name = lig-ACN-frame_742
 C       3.551840    -0.009708     0.323192      30.78
 H       2.826348     0.451050    -0.477494      21.23
 C       4.415221    -0.521050     2.606221      24.98
 H       3.979009    -0.671948     3.629755      16.15
 C       5.571589    -1.034737     2.086296       7.00
 O       6.574402    -1.608595     2.871422     224.93
 C       6.529833    -1.336078     4.284771     133.14
 H       7.599487    -1.625263     4.564992      24.16
 H       5.688287    -1.930260     4.755596      28.00
 H       6.621183    -0.329516     4.559375      30.47
 C       5.781212    -1.209213     0.676717      16.80
 O       6.925975    -1.877374     0.159081     119.52
 H       7.712511    -1.738122     0.689531      25.14
 C       4.754191    -0.662153    -0.244509      26.97
 H       4.821961    -0.614644    -1.348395      22.91
 C       3.411613     0.019779     1.771627      24.97
 C       2.073237     0.486701     2.574632      94.30
 H       2.530797     1.377658     3.029836      24.54
 O       1.613500    -0.169455     3.736938     298.68
 H       1.435717    -1.024078     3.463722      30.49
 C       0.926462     0.763983     1.598802      75.41
 H       1.521258     1.221923     0.685981      23.13
 C      -0.223672     1.736807     2.033945      95.72
 O       0.356767     3.089182     2.254692     259.71
 H       0.440429     3.106046     1.342252      31.77
 H      -0.628529     1.206630     3.118037      23.61
 H      -1.103994     1.589272     1.233601      24.11
 C      -1.672885    -2.572656    -1.103005      57.82
 H      -1.927931    -3.685785    -0.895519      20.63
 C      -1.312902    -0.521670    -2.221973      70.58
 H      -1.717173     0.437057    -2.813060      16.49
 C      -0.463202    -0.075656    -1.080001      -4.47
 O       0.156953     1.248324    -1.128301     184.58
 C      -0.012115     2.055973    -2.332118      95.67
 H       0.595549     2.802794    -1.782682      23.96
 H       0.319712     1.332288    -2.964686      28.32
 H      -1.065962     2.350010    -2.779818      24.70
 C      -0.321420    -0.834953     0.090490      24.71
 O       0.418046    -0.612452     1.156428     162.50
 C      -0.901868    -2.111611    -0.018547      48.62
 H      -0.784398    -2.771934     0.872154      24.02
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 C      -1.966314    -1.784898    -2.146008      49.63
 C      -2.870652    -2.261079    -3.247871      94.60
 H      -2.925826    -1.462661    -4.092441      27.77
 O      -2.530144    -3.574563    -3.698328     251.63
 H      -1.609243    -3.679392    -3.632781      30.38
 C      -4.453759    -2.144643    -3.103206      92.45
 H      -4.730710    -2.860452    -2.317659      25.13
 O      -4.734782    -0.868843    -2.470148     230.75
 H      -5.626610    -1.011937    -1.825746      24.80
 C      -5.205671    -2.305043    -4.385999      96.90
 O      -6.103431    -3.574943    -4.175045     205.27
 H      -5.745269    -4.187176    -5.101374      27.49
 H      -4.370349    -2.672956    -5.011167      27.19
 H      -5.926752    -1.540246    -4.827890      25.85
55
name = lig-ACN-frame_743
 C       3.575472    -0.095907     0.302563      65.59
 H       2.705788     0.216429    -0.361463      20.87
 C       4.437019    -0.473882     2.658437      38.02
 H       4.376990    -0.476347     3.729398      16.81
 C       5.673764    -1.006840     2.117760      -5.66
 O       6.579870    -1.657719     2.938346     230.81
 C       6.591722    -1.412001     4.386488     113.00
 H       7.492379    -2.019095     4.884253      23.31
 H       5.788090    -1.887894     4.896653      29.47
 H       6.327693    -0.362680     4.527554      29.21
 C       5.761342    -1.221491     0.622271       5.49
 O       6.874119    -1.881571     0.144545     138.31
 H       7.395129    -2.318420     0.917720      27.07
 C       4.782225    -0.644047    -0.209566      65.47
 H       5.100639    -0.618409    -1.290292      21.72
 C       3.411632    -0.023402     1.700803      29.62
 C       2.152085     0.460641     2.453405      88.58
 H       2.254353     1.474366     2.791506      24.08
 O       1.741445    -0.262816     3.753442     256.71
 H       1.175846    -0.911521     3.548132      29.19
 C       0.894196     0.674710     1.497555      91.66
 H       1.081532     1.275715     0.496133      19.40
 C      -0.145326     1.603426     2.130520      79.78
 O       0.347268     3.086773     2.267690     211.30
 H       0.858784     3.577074     1.605311      29.30
 H      -0.695378     1.454224     3.260176      22.90
 H      -1.007733     1.909001     1.358731      22.43
 C      -1.564087    -2.565873    -1.029643      39.52
 H      -2.184680    -3.532500    -1.099818      19.93
 C      -1.342694    -0.450097    -2.165674      49.34
 H      -1.846324     0.260164    -3.063537      18.63
 C      -0.408956    -0.015491    -1.211789      18.46
 O       0.083680     1.208102    -1.105462     245.89
 C       0.140111     1.919570    -2.390409     112.33
 H       0.582447     2.946092    -2.540678      25.31
 H       0.625230     1.655438    -3.266906      27.51
 H      -1.010792     2.203452    -2.499438      23.63
 C      -0.413201    -0.803335     0.055550      -0.88
 O       0.359407    -0.583633     1.192571     156.49
 C      -0.842426    -2.142850     0.045714      59.45
 H      -0.837866    -2.709685     0.988980      21.84
 C      -1.971394    -1.684372    -2.166023      22.92
 C      -2.909775    -2.280595    -3.246849      89.45
 H      -2.440212    -1.719021    -4.114795      24.49
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 O      -2.402988    -3.674091    -3.719920     117.42
 H      -1.290431    -3.486666    -3.771301      24.23
 C      -4.452569    -2.104224    -3.026125      93.53
 H      -4.881846    -2.972402    -2.507159      25.38
 O      -4.697525    -0.810893    -2.496762     270.55
 H      -5.483513    -0.823341    -1.978780      28.09
 C      -5.265596    -2.364207    -4.402703      67.10
 O      -6.263775    -3.647045    -4.157402     207.10
 H      -6.009303    -4.202076    -4.991055      28.39
 H      -4.794041    -2.545840    -5.336550      27.15
 H      -5.688406    -1.272484    -4.496622      26.48
55
name = lig-ACN-frame_744
 C       3.639890    -0.212518     0.371953      46.34
 H       2.886476     0.074779    -0.351459      22.52
 C       4.516317    -0.423321     2.558372      36.11
 H       4.368016    -0.117181     3.514987      16.92
 C       5.626194    -1.070790     2.113442      20.55
 O       6.649701    -1.712185     2.953358     226.52
 C       6.552911    -1.495490     4.459937     109.56
 H       7.648832    -1.851900     4.821827      24.65
 H       5.732424    -1.981697     4.751991      29.58
 H       6.722252    -0.398985     4.828532      26.99
 C       5.793969    -1.160521     0.756515      21.82
 O       6.781491    -1.893947     0.113480     150.63
 H       7.327710    -2.346536     0.893811      21.70
 C       4.862133    -0.644819    -0.162711      50.72
 H       4.951502    -0.868949    -1.267490      22.73
 C       3.390906    -0.129952     1.784856      36.00
 C       2.124446     0.521217     2.335932      95.72
 H       2.404302     1.465666     2.695002      26.03
 O       1.908438    -0.267599     3.670227     199.51
 H       1.319103    -1.087698     3.398218      24.81
 C       0.929964     0.712536     1.506589      85.67
 H       1.452611     1.151580     0.540724      22.84
 C      -0.101699     1.725628     2.162188      99.70
 O       0.331665     3.032778     2.344582     196.93
 H       1.001099     3.068477     1.476959      26.34
 H      -0.170409     1.212394     3.284611      24.44
 H      -1.165856     1.384249     1.589693      24.10
 C      -1.629883    -2.631721    -1.064494      55.64
 H      -1.934549    -3.680749    -1.080118      20.03
 C      -1.456419    -0.370453    -2.212056      66.18
 H      -1.249459     0.208769    -3.324168      18.43
 C      -0.531373    -0.020366    -1.186261      -2.19
 O       0.137497     1.273102    -1.172304     182.80
 C       0.215264     1.934059    -2.515535      84.00
 H       0.713078     2.810796    -2.032166      24.56
 H       0.609325     1.083270    -2.995680      28.00
 H      -0.872026     2.070915    -3.125474      22.61
 C      -0.342437    -0.866848    -0.017412       1.49
 O       0.284192    -0.561046     1.243131     146.50
 C      -0.880042    -2.152949     0.091270      52.48
 H      -0.468248    -2.766531     0.893523      23.81
 C      -1.894877    -1.752694    -2.053063      20.03
 C      -2.788951    -2.246956    -3.391072      59.07
 H      -2.897136    -1.468399    -4.211861      24.97
 O      -2.382064    -3.696490    -3.684538     103.42
 H      -1.196706    -3.769530    -3.393035      21.52
 C      -4.423778    -2.281272    -3.070015      65.35
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 H      -4.626322    -2.842797    -2.171015      25.67
 O      -4.627127    -0.728334    -2.531166     233.32
 H      -5.381429    -0.697666    -2.105808      31.23
 C      -5.403198    -2.501576    -4.345686     102.46
 O      -6.318989    -3.561966    -4.162352     333.43
 H      -6.523492    -3.939571    -4.898640      37.80
 H      -4.829607    -2.556264    -5.189721      28.74
 H      -6.304476    -1.766791    -4.442041      23.78
55
name = lig-ACN-frame_745
 C       3.614809    -0.283465     0.360463      82.01
 H       2.881740    -0.043106    -0.320342      25.47
 C       4.510231    -0.372879     2.654171      47.77
 H       4.430404    -0.337157     3.709520      17.05
 C       5.682304    -1.164048     2.215281       5.45
 O       6.675491    -1.685394     2.964797     219.31
 C       6.572684    -1.566122     4.409320     114.11
 H       7.383399    -2.336374     4.825761      24.84
 H       5.738108    -1.951767     4.839015      31.16
 H       6.463654    -0.406411     4.675807      26.90
 C       5.885866    -1.175511     0.746927      20.08
 O       6.770891    -1.970187     0.126474     182.52
 H       7.695881    -1.891345     0.413522      23.13
 C       4.866431    -0.685849    -0.084694      58.68
 H       5.023255    -0.847606    -1.181323      22.05
 C       3.406511    -0.153611     1.700826      27.79
 C       2.252719     0.501109     2.450725     105.12
 H       2.569707     1.425244     2.732736      26.60
 O       2.012021    -0.179957     3.553636     201.02
 H       1.608929    -1.232222     3.338206      22.32
 C       0.954626     0.818947     1.476411      78.84
 H       1.189600     1.292058     0.462785      22.61
 C      -0.084358     1.598883     2.240427      97.50
 O       0.371737     3.022086     2.357787     192.83
 H       0.737489     3.423336     1.476402      28.42
 H      -0.139834     1.168127     3.385795      24.77
 H      -1.229220     1.842337     1.839310      22.78
 C      -1.660865    -2.708227    -1.013321      46.69
 H      -1.871831    -3.720735    -1.057332      23.35
 C      -1.402860    -0.496962    -2.170938      39.60
 H      -1.688560     0.148491    -3.242315      18.84
 C      -0.640945     0.090345    -1.056534      13.34
 O       0.106172     1.263003    -1.240399     218.61
 C       0.315183     1.870641    -2.580391     102.48
 H       0.969614     2.783599    -2.592594      26.08
 H       1.028401     1.462939    -3.320061      25.87
 H      -0.617522     2.428136    -3.199496      22.49
 C      -0.270377    -0.861651     0.008896      -0.71
 O       0.222869    -0.515487     1.221375     136.28
 C      -0.890480    -2.199144    -0.015529      62.18
 H      -0.624035    -2.881443     0.792070      24.31
 C      -1.990679    -1.762440    -2.284144      16.53
 C      -2.758243    -2.311795    -3.367910      98.12
 H      -2.357431    -1.790484    -4.280034      26.30
 O      -2.410153    -3.614948    -3.661817     187.76
 H      -1.420685    -3.933100    -3.235930      24.54
 C      -4.358368    -2.235970    -3.094973      85.79
 H      -4.538851    -3.014236    -2.344817      26.94
 O      -4.514331    -0.808099    -2.665115     210.97
 H      -5.313490    -0.828578    -2.055014      26.72
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 C      -5.473744    -2.470957    -4.226117      92.88
 O      -6.405849    -3.640730    -4.121012     234.52
 H      -6.774743    -3.561713    -5.102539      29.66
 H      -4.950858    -2.725941    -5.088953      28.13
 H      -5.673274    -1.370727    -4.335042      27.49
55
name = lig-ACN-frame_746
 C       3.573510    -0.300511     0.297820      47.94
 H       2.790224    -0.107389    -0.343177      20.46
 C       4.544854    -0.525113     2.689936      49.49
 H       4.257327    -0.290468     3.747551      19.53
 C       5.688579    -1.077235     2.192418      13.93
 O       6.710664    -1.676400     2.971436     226.94
 C       6.535150    -1.647553     4.375803     119.53
 H       7.412207    -2.194203     4.881744      23.61
 H       5.557041    -1.966621     4.547651      29.59
 H       6.831251    -0.551347     4.854570      25.30
 C       5.850844    -1.248613     0.816734      24.68
 O       6.927559    -2.065915     0.111848     166.76
 H       7.764660    -1.579496     0.226406      24.13
 C       4.877451    -0.782770    -0.103143      29.68
 H       5.231352    -0.787537    -1.140463      22.60
 C       3.563616    -0.091531     1.776095      19.38
 C       2.333019     0.609983     2.308775      85.71
 H       2.542763     1.536609     2.630332      28.94
 O       1.998022    -0.157110     3.647790     136.83
 H       1.450774    -1.084265     3.266847      23.65
 C       0.938298     0.790301     1.497669      86.99
 H       1.124587     1.405715     0.610142      24.36
 C      -0.076257     1.629364     2.336701      89.91
 O       0.452833     3.040118     2.399221     225.94
 H       0.155089     3.382918     1.601158      31.37
 H      -0.211513     1.319168     3.457656      25.60
 H      -1.093727     1.304330     1.672368      24.35
 C      -1.693085    -2.655241    -1.187656      60.26
 H      -2.218658    -3.507318    -1.078315      23.19
 C      -1.354055    -0.558904    -2.128882      50.81
 H      -1.765690     0.368497    -2.819249      19.25
 C      -0.661742     0.014533    -1.128552       8.72
 O       0.046236     1.272477    -1.309449     202.40
 C       0.477326     1.881908    -2.684411      65.10
 H       0.955199     2.706743    -2.166909      25.21
 H       0.698787     0.987593    -3.340773      25.58
 H      -0.708716     2.040031    -2.953227      21.18
 C      -0.402754    -0.810439     0.007545      -7.40
 O       0.277068    -0.444579     1.230802     149.24
 C      -0.807119    -2.172947    -0.095973      54.84
 H      -0.711793    -2.752186     0.828085      22.99
 C      -1.964803    -1.862977    -2.140310      33.49
 C      -2.818262    -2.303775    -3.461327      81.34
 H      -2.742664    -1.546042    -4.273745      27.03
 O      -2.450399    -3.724839    -3.670978     232.12
 H      -1.558380    -3.736604    -3.417943      31.24
 C      -4.285957    -2.216883    -3.123573     108.92
 H      -4.501294    -2.867359    -2.263828      26.18
 O      -4.427361    -0.907997    -2.746143     213.40
 H      -5.286518    -0.711490    -2.005537      23.77
 C      -5.297768    -2.396957    -4.232280      90.02
 O      -6.505821    -3.666494    -4.048947      82.18
 H      -6.997329    -3.658337    -5.108258      28.13
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 H      -4.895196    -2.597486    -5.185869      28.37
 H      -6.192078    -1.762692    -4.295694      25.52
55
name = lig-ACN-frame_747
 C       3.745463    -0.314204     0.402750      71.59
 H       2.995257     0.085824    -0.250478      23.88
 C       4.520726    -0.588197     2.653770      56.94
 H       4.471239    -0.376946     3.803629      20.41
 C       5.806683    -1.111790     2.165114      -0.10
 O       6.773319    -1.653170     2.920315     202.64
 C       6.522596    -1.683995     4.421876      96.43
 H       7.115892    -2.551511     4.682052      24.91
 H       5.513299    -2.021538     4.777577      26.29
 H       6.619706    -0.572938     4.916685      23.88
 C       5.904320    -1.392494     0.678602       5.82
 O       6.991187    -2.029656     0.192814     162.74
 H       7.971228    -1.914676     0.593917      22.77
 C       4.875146    -0.906274    -0.175467      69.27
 H       4.928147    -1.080716    -1.236953      23.64
 C       3.555713    -0.029892     1.703079      36.14
 C       2.264758     0.638866     2.330157      92.03
 H       2.530421     1.611951     2.529037      27.46
 O       1.950658    -0.066935     3.687350     202.46
 H       1.322776    -0.807805     3.506624      27.72
 C       0.984776     0.814807     1.562145      90.90
 H       1.213696     1.299934     0.654134      26.11
 C       0.021872     1.685823     2.395027     106.24
 O       0.430521     3.025623     2.433699     190.21
 H      -0.013682     3.585697     1.679721      26.97
 H      -0.039748     1.233325     3.433339      26.80
 H      -1.140738     1.876459     1.976439      24.05
 C      -1.611593    -2.724185    -1.064898      43.93
 H      -1.948434    -3.730772    -0.977680      23.29
 C      -1.477991    -0.488229    -2.262194      42.31
 H      -1.538054     0.010398    -3.313138      22.20
 C      -0.474592    -0.025545    -1.219080       1.19
 O      -0.007081     1.237752    -1.293448     209.06
 C       0.373137     1.770134    -2.646690     118.22
 H       1.256633     2.412407    -2.592137      27.53
 H       1.126169     1.045203    -3.145914      26.55
 H      -0.117128     2.456350    -3.416501      25.19
 C      -0.441829    -0.749710     0.045545      15.92
 O       0.319303    -0.492442     1.184320     137.64
 C      -0.836762    -2.147567    -0.085502      44.23
 H      -0.464968    -2.792782     0.745867      22.80
 C      -1.978713    -1.757040    -2.300838      16.43
 C      -2.789947    -2.336157    -3.437011      87.22
 H      -2.568013    -1.828028    -4.367548      26.93
 O      -2.495051    -3.807041    -3.730672     223.29
 H      -1.651164    -3.948849    -3.833867      34.21
 C      -4.337257    -2.350519    -3.124267      77.22
 H      -4.596343    -3.056834    -2.299167      26.82
 O      -4.378385    -0.790421    -2.717462      94.83
 H      -5.375120    -0.818785    -2.120500      23.19
 C      -5.360657    -2.538066    -4.364724      81.95
 O      -6.467250    -3.614287    -3.976259     237.95
 H      -6.756724    -3.894149    -4.933547      29.53
 H      -4.814843    -2.402515    -5.272448      28.42
 H      -5.819523    -1.506792    -4.241544      28.14
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name = lig-ACN-frame_748
 C       3.840985    -0.242613     0.347045      32.77
 H       3.152565     0.110612    -0.485259      26.19
 C       4.614200    -0.536607     2.544963      45.51
 H       4.479831    -0.537763     3.693551      18.31
 C       5.706313    -1.185112     2.009860      14.26
 O       6.835706    -1.627986     2.967233     218.65
 C       6.525667    -1.762554     4.387771     106.13
 H       7.177244    -2.402346     4.875118      26.30
 H       5.354987    -1.921644     4.396355      26.40
 H       6.878885    -0.740439     4.908155      26.67
 C       5.950010    -1.407481     0.675012      15.41
 O       7.107467    -2.043916     0.229833     170.99
 H       7.564156    -2.161887     1.155461      17.36
 C       4.919622    -1.085444    -0.201204      47.44
 H       4.847455    -1.384565    -1.226409      21.21
 C       3.520055    -0.089948     1.827847      21.74
 C       2.270588     0.570156     2.471131     103.23
 H       2.533904     1.557804     2.745003      26.63
 O       1.904271     0.074354     3.678045     297.47
 H       1.508519    -0.689585     3.536112      33.37
 C       0.969987     0.832891     1.478543      77.74
 H       1.220857     1.373222     0.642291      27.27
 C       0.007718     1.694968     2.424413      91.59
 O       0.444883     3.118863     2.505669     165.45
 H       0.226948     3.664381     1.615754      27.20
 H       0.135315     1.415432     3.446870      27.21
 H      -1.175258     1.351390     2.028701      25.01
 C      -1.579586    -2.598464    -1.135040      52.70
 H      -1.507658    -3.698059    -1.312919      23.16
 C      -1.417677    -0.474500    -2.393241      54.18
 H      -1.446124     0.196158    -3.230971      19.86
 C      -0.543598    -0.069089    -1.312295      -4.37
 O      -0.018063     1.297910    -1.312595     246.26
 C       0.476274     1.654517    -2.580154     102.53
 H       1.112541     2.457427    -2.274458      26.26
 H       0.507152     0.736909    -3.311229      25.94
 H      -0.564547     1.979101    -2.899045      23.58
 C      -0.356989    -0.758326    -0.068952     -13.55
 O       0.381053    -0.528161     1.167880     112.31
 C      -0.878883    -2.109343     0.028457      41.16
 H      -0.424690    -2.801939     0.794283      22.92
 C      -1.918771    -1.898332    -2.249682      23.32
 C      -2.782067    -2.528798    -3.429356      90.55
 H      -2.648301    -1.854172    -4.248177      27.24
 O      -2.559753    -3.854141    -3.782888     209.39
 H      -1.470876    -3.882576    -3.832411      25.92
 C      -4.359105    -2.298103    -3.174539      72.26
 H      -4.652094    -2.968666    -2.322151      27.01
 O      -4.421407    -0.832047    -2.691523     219.99
 H      -5.226268    -0.632446    -2.056206      25.67
 C      -5.416512    -2.583176    -4.345595     110.29
 O      -6.323160    -3.512733    -3.982298     306.49
 H      -6.451985    -4.091724    -4.586897      36.76
 H      -5.123367    -3.196733    -5.157536      25.97
 H      -5.946183    -1.611874    -4.667201      27.69
55
name = lig-ACN-frame_749
 C       3.804826    -0.261334     0.312667      68.76
 H       2.935714     0.094757    -0.392915      25.90
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 C       4.648977    -0.528064     2.580972      48.12
 H       4.596484    -0.298650     3.669129      19.10
 C       5.792142    -1.261280     2.118463       7.83
 O       6.829646    -1.602738     2.896263     225.09
 C       6.544988    -1.752565     4.316220     116.80
 H       7.050110    -2.588382     4.562271      27.28
 H       5.437645    -2.141103     4.664281      25.58
 H       6.640161    -0.768711     4.919482      25.97
 C       5.998511    -1.488724     0.681163       0.19
 O       7.163068    -2.080005     0.280854     208.55
 H       7.814024    -2.396170     0.870217      22.13
 C       4.853539    -1.097761    -0.162239      56.45
 H       5.102033    -1.264654    -1.201778      22.59
 C       3.573491    -0.163539     1.651985      26.34
 C       2.314268     0.645662     2.356743      73.61
 H       2.733653     1.647793     2.549226      25.25
 O       1.828593     0.097650     3.776539     167.47
 H       1.710308    -0.916998     3.633700      26.79
 C       1.017485     0.830587     1.516165      89.85
 H       1.242608     1.348514     0.644407      27.27
 C       0.014786     1.690135     2.402464      96.06
 O       0.415217     3.172333     2.529184     212.96
 H       0.603515     3.363320     1.639106      32.01
 H       0.097788     1.308639     3.342701      28.61
 H      -1.244514     1.668367     2.087310      24.51
 C      -1.476715    -2.629064    -1.151706      44.67
 H      -1.987731    -3.688445    -0.965248      21.80
 C      -1.297278    -0.646135    -2.385735      63.83
 H      -1.813718    -0.074341    -3.018544      24.63
 C      -0.669435     0.024230    -1.252986       0.69
 O      -0.011098     1.190306    -1.231924     204.39
 C       0.399885     1.668805    -2.619988      94.24
 H       1.301571     2.259587    -2.680105      27.68
 H       1.001977     0.782343    -3.113789      26.29
 H      -0.257711     2.245066    -3.299003      25.36
 C      -0.262924    -0.831809    -0.116406       1.00
 O       0.446766    -0.441157     1.081095     125.27
 C      -0.893944    -2.078349    -0.020161      56.43
 H      -0.843842    -2.650507     0.951399      24.30
 C      -1.856549    -1.888443    -2.327357      24.40
 C      -2.860981    -2.474059    -3.434409      80.01
 H      -2.567063    -1.945427    -4.324680      27.08
 O      -2.575059    -3.951982    -3.816728     117.91
 H      -1.431378    -4.238971    -3.579948      23.60
 C      -4.379494    -2.192900    -3.157625      93.38
 H      -4.778935    -2.922339    -2.400194      25.76
 O      -4.461977    -0.932630    -2.712993     302.49
 H      -5.135053    -0.969819    -2.141012      31.12
 C      -5.232597    -2.547240    -4.456811      82.90
 O      -6.363739    -3.539343    -3.832622     187.16
 H      -6.255834    -4.369054    -4.542059      27.38
 H      -4.380405    -2.716344    -5.070239      28.19
 H      -5.800972    -1.778890    -5.024286      28.06
55
name = lig-ACN-frame_750
 C       3.723215    -0.446014     0.249803      21.87
 H       2.955854    -0.065432    -0.587179      20.98
 C       4.614985    -0.561562     2.577270      65.21
 H       4.559963    -0.103627     3.517382      22.60
 C       5.775009    -1.190824     2.115356      12.60
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 O       6.872138    -1.618355     2.902740     231.24
 C       6.583218    -1.777071     4.302698     103.04
 H       7.258477    -2.427156     4.717650      26.25
 H       5.376049    -1.993567     4.290484      23.91
 H       6.874924    -0.850984     4.826739      26.19
 C       5.926781    -1.555214     0.787311      17.74
 O       7.090787    -2.133355     0.212826     192.87
 H       7.826190    -1.778912     0.779952      21.95
 C       4.982255    -1.050032    -0.151265      31.90
 H       5.059348    -1.066877    -1.240922      22.25
 C       3.591443    -0.128071     1.705908      25.45
 C       2.373285     0.599743     2.264053      76.95
 H       2.631384     1.657067     2.651392      25.99
 O       1.874789     0.125193     3.757188      71.50
 H       1.575859    -0.981490     3.512878      24.28
 C       1.058954     0.929573     1.484610      70.40
 H       1.323002     1.592690     0.679411      26.63
 C       0.034749     1.737896     2.390492     110.15
 O       0.370122     3.117516     2.490374     224.40
 H       1.032250     3.436744     1.841482      30.29
 H      -0.143685     1.332033     3.312101      28.67
 H      -0.979789     1.736790     1.629571      24.67
 C      -1.563628    -2.805603    -1.146322      35.93
 H      -2.375521    -3.638667    -0.762691      18.48
 C      -1.310957    -0.604272    -2.339889      41.53
 H      -1.340627    -0.010966    -3.180994      22.36
 C      -0.628408    -0.077038    -1.169931       8.95
 O       0.006836     1.236663    -1.292659     197.20
 C       0.445933     1.663470    -2.646142      95.24
 H       1.026727     2.477721    -2.211491      25.42
 H       0.703151     0.688375    -3.251672      25.46
 H      -0.405718     2.010348    -3.161486      26.42
 C      -0.245621    -0.759936    -0.063731      18.40
 O       0.500230    -0.395886     1.002015     143.52
 C      -0.840531    -2.140090    -0.084598      26.92
 H      -0.905259    -2.598986     0.935731      24.17
 C      -1.815642    -2.037614    -2.358284      22.15
 C      -2.750618    -2.437832    -3.468439      88.88
 H      -2.579190    -1.884703    -4.389525      27.17
 O      -2.615762    -3.970557    -3.788816     119.80
 H      -1.655235    -4.140287    -3.251111      26.32
 C      -4.348119    -2.325143    -3.192499      76.67
 H      -4.616633    -3.075566    -2.412247      25.40
 O      -4.509075    -0.865455    -2.683586     244.46
 H      -5.164985    -0.664049    -2.141560      30.01
 C      -5.068065    -2.594325    -4.462522      92.83
 O      -6.282877    -3.539755    -3.824108      92.62
 H      -6.426674    -4.548316    -4.350438      26.83
 H      -4.864687    -3.360674    -5.213028      25.75
 H      -5.526005    -1.655539    -4.727651      28.79
55
name = lig-ACN-frame_751
 C       3.746625    -0.599050     0.343510      64.45
 H       2.967595    -0.340364    -0.489814      22.91
 C       4.586252    -0.495634     2.590181      47.52
 H       4.510516    -0.368883     3.601451      21.80
 C       5.775312    -1.183375     2.113230      -6.92
 O       6.909539    -1.629383     2.904174     214.23
 C       6.647975    -1.731141     4.348124     116.44
 H       7.165273    -2.583295     4.710616      26.56
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 H       5.531033    -2.067401     4.651615      25.54
 H       6.725919    -0.796710     4.826590      27.08
 C       5.895585    -1.518260     0.710023      10.59
 O       6.977561    -2.160704     0.202860     191.61
 H       7.909345    -1.702435     0.282642      24.17
 C       4.967035    -0.991947    -0.185817      46.36
 H       5.354374    -1.300822    -1.167516      20.97
 C       3.516657    -0.175139     1.638825      22.59
 C       2.332287     0.608719     2.376428      96.38
 H       2.938295     1.616132     2.552460      24.22
 O       2.006441     0.106054     3.581713     226.89
 H       1.286165    -0.726262     3.539181      24.28
 C       1.120281     0.980589     1.419166      75.51
 H       1.318652     1.543517     0.484269      25.15
 C      -0.004449     1.725487     2.196407     103.18
 O       0.379269     3.118900     2.492085     181.08
 H       1.142875     3.299517     1.744296      27.40
 H      -0.157613     1.368994     3.155314      28.27
 H      -1.047590     1.486365     1.561395      25.42
 C      -1.687273    -2.737188    -1.098033      47.52
 H      -1.971322    -3.965641    -1.135123      22.39
 C      -1.315832    -0.684893    -2.263588      58.69
 H      -1.289196    -0.208762    -3.258613      23.50
 C      -0.491561    -0.053016    -1.314728      -6.78
 O      -0.015522     1.228517    -1.345595     234.19
 C       0.403389     1.689690    -2.608295     126.37
 H       1.109947     2.503293    -2.736830      27.34
 H       1.055327     1.018395    -3.268040      27.42
 H      -0.451161     2.034129    -3.141321      27.48
 C      -0.368588    -0.865325    -0.025000     -11.12
 O       0.583946    -0.370547     1.014321     100.42
 C      -0.797306    -2.213824    -0.053528      48.78
 H      -0.397551    -2.876862     0.742430      23.35
 C      -1.775600    -2.042721    -2.265471      27.50
 C      -2.671634    -2.532759    -3.496834     103.15
 H      -2.397254    -1.894299    -4.364861      27.29
 O      -2.619824    -3.891974    -3.718316     267.87
 H      -1.883888    -4.251106    -3.411043      34.64
 C      -4.109722    -2.331640    -3.144412      66.99
 H      -4.392016    -2.953220    -2.270991      27.60
 O      -4.492321    -0.876810    -2.747545     230.43
 H      -5.183799    -1.146459    -2.163884      28.39
 C      -5.164498    -2.836073    -4.365792      95.26
 O      -6.199120    -3.482347    -3.854242     319.66
 H      -6.308839    -4.121831    -4.511959      31.95
 H      -4.447142    -3.243279    -5.232975      25.68
 H      -5.492690    -1.928768    -4.920580      28.05
55
name = lig-ACN-frame_752
 C       3.649727    -0.567613     0.289830      39.19
 H       2.705554    -0.526207    -0.300383      25.58
 C       4.640447    -0.508504     2.565626      60.10
 H       4.412391    -0.297360     3.566882      21.94
 C       5.793178    -1.207187     2.145716      16.39
 O       6.828484    -1.614450     2.901419     203.96
 C       6.659553    -1.663678     4.406402     114.72
 H       7.423523    -2.428281     4.720219      26.00
 H       5.574946    -1.911526     4.558076      27.41
 H       6.994021    -0.817953     4.861269      29.09
 C       5.981846    -1.345876     0.717203      25.33
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 O       6.938767    -2.229556     0.155580     206.80
 H       7.842545    -1.969325     0.495132      21.74
 C       4.917431    -1.084019    -0.204814      44.36
 H       4.795557    -1.138196    -1.288619      23.28
 C       3.527835    -0.288173     1.716637      11.47
 C       2.394090     0.690177     2.217690      78.57
 H       2.790394     1.791545     2.575324      23.98
 O       2.049814     0.031310     3.535799     241.21
 H       1.526521    -0.661659     3.241050      30.77
 C       1.106117     0.923182     1.344603      81.09
 H       1.652310     1.442556     0.493257      25.26
 C      -0.030963     1.698678     2.039309     106.10
 O       0.410708     3.100555     2.436630     211.46
 H       0.729876     3.610576     1.641113      29.12
 H      -0.278347     1.063820     2.895492      27.71
 H      -0.961879     2.012123     1.445594      25.32
 C      -1.598039    -2.713147    -0.972134      43.87
 H      -1.680354    -3.989640    -1.070848      21.26
 C      -1.206265    -0.723660    -2.371259      51.36
 H      -1.702623    -0.084535    -3.223090      21.60
 C      -0.481274    -0.162971    -1.263798      13.63
 O      -0.000725     1.188503    -1.333848     170.50
 C       0.375314     1.776198    -2.748574     105.05
 H       0.809578     2.648147    -2.224135      26.02
 H       0.932322     0.907881    -3.061238      27.80
 H      -0.352657     1.932130    -3.431945      28.24
 C      -0.309405    -0.783912    -0.065236     -11.46
 O       0.595635    -0.463067     1.003930     123.27
 C      -0.811570    -2.277054     0.038361      33.61
 H      -0.275499    -2.957717     0.698434      24.11
 C      -1.852677    -1.953544    -2.216824      29.05
 C      -2.551197    -2.454606    -3.398552      89.14
 H      -2.192132    -1.999845    -4.348978      27.41
 O      -2.562892    -3.962232    -3.680626     204.91
 H      -1.650630    -4.144775    -3.699643      31.45
 C      -4.116600    -2.258460    -3.145720     105.00
 H      -4.152395    -2.935303    -2.281250      26.92
 O      -4.412913    -1.008276    -2.846447     229.91
 H      -5.269815    -0.783476    -2.128376      23.70
 C      -4.946628    -2.787696    -4.318082      78.39
 O      -6.257669    -3.579678    -3.844778     270.66
 H      -6.757179    -3.954553    -4.514276      34.90
 H      -4.381347    -3.755703    -4.781452      23.68
 H      -5.294418    -1.924837    -4.927630      27.20
55
name = lig-ACN-frame_753
 C       3.604510    -0.553012     0.315091      81.27
 H       2.872339    -0.362164    -0.404751      26.76
 C       4.618086    -0.555376     2.580315      59.67
 H       4.734486    -0.126446     3.596807      21.49
 C       5.796354    -1.142128     2.050744       5.80
 O       6.788388    -1.623238     2.974107     210.87
 C       6.689939    -1.577863     4.379466     124.61
 H       7.278652    -2.503626     4.785683      25.75
 H       5.720876    -1.760387     4.829437      28.13
 H       6.950210    -0.659753     4.690831      29.01
 C       5.964314    -1.325857     0.625140      10.32
 O       6.972422    -2.232496     0.142808     172.16
 H       7.628090    -2.369078     0.801450      20.13
 C       4.763717    -1.117819    -0.153631      40.03
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 H       5.116183    -1.510293    -1.099384      20.78
 C       3.552597    -0.213312     1.648800      37.02
 C       2.428674     0.593324     2.154541      83.73
 H       2.807343     1.765764     2.336526      24.73
 O       2.009897     0.003241     3.508277     201.53
 H       1.872926    -0.876677     3.388658      31.55
 C       1.153919     0.814140     1.219427      83.45
 H       1.151960     1.298803     0.180917      23.00
 C       0.010578     1.764051     1.901559     104.19
 O       0.437778     3.034616     2.376547     275.07
 H       0.373269     3.587337     1.642460      32.17
 H      -0.490978     1.426748     2.820234      27.10
 H      -0.734091     1.678264     1.014317      26.36
 C      -1.462422    -2.747861    -1.006406      44.85
 H      -2.153457    -3.822000    -0.803659      20.56
 C      -1.161954    -0.681838    -2.355010      52.81
 H      -1.258189     0.126212    -3.267225      20.54
 C      -0.515161    -0.122666    -1.284112       6.07
 O      -0.013108     1.162804    -1.396865     221.04
 C       0.351009     1.738626    -2.696256     130.61
 H       0.714363     2.770237    -2.607765      27.75
 H       1.161237     1.466563    -3.308738      28.89
 H      -0.518687     1.855339    -3.200861      28.00
 C      -0.183051    -0.921340    -0.016927      28.23
 O       0.591871    -0.519428     0.991301     167.51
 C      -0.738160    -2.110589     0.107648      64.75
 H      -0.629036    -2.574698     1.083115      25.49
 C      -1.785618    -1.972778    -2.103389      24.58
 C      -2.613483    -2.502489    -3.360685      85.09
 H      -2.365106    -1.764494    -4.194185      26.06
 O      -2.400226    -3.987710    -3.612290     104.36
 H      -1.316677    -4.253814    -3.867066      24.48
 C      -4.123573    -2.425752    -3.113010      88.31
 H      -4.538605    -3.035965    -2.314979      26.81
 O      -4.365793    -0.905269    -2.879622     161.18
 H      -5.259292    -0.849331    -2.142117      23.45
 C      -4.848047    -2.889962    -4.341660      73.93
 O      -6.277321    -3.630338    -3.795128     172.22
 H      -6.633985    -3.422064    -4.834497      27.56
 H      -4.323669    -3.780478    -4.985307      24.59
 H      -4.955679    -2.086639    -5.133407      27.13
55
name = lig-ACN-frame_754
 C       3.641732    -0.547860     0.277340      43.37
 H       2.895484    -0.216044    -0.336748      24.35
 C       4.618094    -0.511396     2.487963      68.57
 H       4.418094    -0.246935     3.606290      20.83
 C       5.807234    -1.102571     2.065668      22.20
 O       6.772288    -1.660228     2.883388     228.49
 C       6.648958    -1.450228     4.410094     112.97
 H       7.356579    -2.346669     4.807866      24.29
 H       5.691378    -1.538797     4.677501      29.06
 H       7.109514    -0.605796     4.745540      27.11
 C       5.892749    -1.528648     0.671936      18.34
 O       6.965101    -2.144921     0.152349     192.98
 H       7.559685    -2.348978     0.960529      24.02
 C       4.852995    -1.221618    -0.213572      60.71
 H       4.600238    -1.605632    -1.168728      23.57
 C       3.596140    -0.110779     1.631765      28.21
 C       2.303938     0.525051     2.198042      96.00
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 H       2.729150     1.642490     2.570423      23.25
 O       1.966125     0.065997     3.439918     232.86
 H       1.736518    -1.005576     3.384714      25.50
 C       1.174029     0.758548     1.206739      93.85
 H       1.792053     1.155612     0.308890      25.42
 C       0.036761     1.698619     1.742514     101.74
 O       0.469454     3.000186     2.281085     224.36
 H       0.646460     3.759570     1.545549      26.21
 H      -0.448359     0.953816     2.501141      25.89
 H      -0.705519     2.022748     1.015787      25.74
 C      -1.434177    -2.694567    -0.928805      38.38
 H      -2.184089    -3.694987    -0.686619      20.76
 C      -1.214825    -0.743043    -2.232990      59.12
 H      -1.264109    -0.507597    -3.417129      19.68
 C      -0.391605    -0.081873    -1.242750      35.30
 O       0.073944     1.196020    -1.419352     240.72
 C       0.243710     1.777200    -2.679048     129.88
 H       0.352345     2.821934    -2.349815      26.69
 H       1.022060     1.145947    -3.062936      28.60
 H      -0.467604     1.695744    -3.375707      28.97
 C      -0.109429    -0.834237    -0.147320       2.34
 O       0.629970    -0.542328     1.061958     139.05
 C      -0.773098    -2.174115     0.106048      44.85
 H      -0.797578    -2.522457     1.140883      23.66
 C      -1.656460    -2.013415    -2.217662      31.79
 C      -2.615001    -2.649391    -3.210747      99.28
 H      -2.496361    -2.114787    -4.229765      25.79
 O      -2.209469    -3.946664    -3.569082     113.41
 H      -1.011629    -3.894655    -3.381084      22.09
 C      -4.153639    -2.469072    -3.050291      69.07
 H      -4.457976    -2.908237    -2.102058      27.07
 O      -4.349432    -0.907606    -2.883005     214.93
 H      -5.091411    -0.937210    -2.253026      27.24
 C      -4.951326    -3.128367    -4.371008      86.36
 O      -6.149948    -3.547033    -3.899951     189.81
 H      -7.089549    -3.495738    -4.555462      27.06
 H      -4.156751    -3.897090    -4.785301      24.74
 H      -5.234382    -2.227045    -4.984630      25.80
55
name = lig-ACN-frame_755
 C       3.773238    -0.502806     0.208353      68.76
 H       3.005055    -0.491295    -0.506931      26.80
 C       4.627324    -0.400116     2.480192      46.89
 H       4.395133    -0.342229     3.637181      18.45
 C       5.730140    -1.202021     2.051617      14.43
 O       6.787649    -1.664442     2.871568     216.08
 C       6.634824    -1.360935     4.317824     114.56
 H       7.128882    -2.288180     4.896301      24.95
 H       5.706760    -1.364729     4.641387      30.85
 H       7.021638    -0.381394     4.477173      27.33
 C       5.786570    -1.653159     0.715184       5.33
 O       7.025272    -2.115627     0.189037     136.29
 H       7.865055    -2.112487     0.775383      24.79
 C       4.781454    -1.312821    -0.251273      52.21
 H       5.072698    -1.605040    -1.230443      21.71
 C       3.558093    -0.101489     1.560224       6.29
 C       2.341151     0.674613     2.251717      90.10
 H       2.504958     1.885146     2.451023      22.70
 O       1.870827     0.037831     3.510656     185.97
 H       1.157709    -0.848888     3.185392      21.65
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 C       1.246084     0.786269     1.219445      81.74
 H       1.690386     1.138031     0.214827      24.84
 C       0.055680     1.685085     1.560157     102.59
 O       0.508437     2.935685     2.223977     225.12
 H       1.137812     3.304675     1.413035      26.15
 H      -0.379373     1.279282     2.587149      24.83
 H      -0.667611     1.673449     0.776078      26.86
 C      -1.578470    -2.730427    -0.904120      48.06
 H      -1.896502    -3.900202    -0.776974      20.51
 C      -1.150584    -0.738140    -2.295173      39.17
 H      -1.524964     0.088477    -3.032602      20.59
 C      -0.316292    -0.149961    -1.308395      -7.61
 O       0.120185     1.244413    -1.308599     166.27
 C       0.181652     1.814225    -2.766944     121.27
 H       0.420417     2.867434    -2.672576      27.67
 H       1.100308     1.589961    -3.234979      28.58
 H      -0.660358     1.645965    -3.293843      27.61
 C      -0.086402    -0.882297    -0.030075      20.20
 O       0.630160    -0.567772     1.019461     163.76
 C      -0.741796    -2.076307     0.066491      57.04
 H      -0.383065    -2.709702     0.920937      23.78
 C      -1.648762    -2.152475    -2.108787      27.28
 C      -2.541410    -2.618796    -3.245742      74.23
 H      -2.353037    -1.860701    -4.083361      25.49
 O      -2.018824    -4.002784    -3.513511     171.87
 H      -1.029516    -4.205460    -3.050618      24.27
 C      -4.190733    -2.467320    -3.006192      81.79
 H      -4.613385    -3.009932    -2.150196      26.95
 O      -4.356139    -1.083409    -2.899326     305.31
 H      -4.977775    -0.791362    -2.323397      31.57
 C      -4.856870    -3.113812    -4.306491      94.21
 O      -6.218462    -3.568538    -3.903448     290.02
 H      -6.705698    -3.631329    -4.719908      32.33
 H      -4.456640    -4.113872    -4.741097      25.44
 H      -4.654629    -2.473190    -5.214208      27.15
55
name = lig-ACN-frame_756
 C       3.697061    -0.481161     0.136077      29.51
 H       2.935521    -0.079714    -0.581122      22.43
 C       4.603375    -0.420531     2.468105      51.64
 H       4.653000     0.182095     3.469430      18.60
 C       5.633437    -1.320884     2.090042       8.50
 O       6.750509    -1.655539     2.878787     242.92
 C       6.614498    -1.270063     4.214175     122.99
 H       7.290897    -1.961058     4.879480      25.62
 H       5.670637    -1.326377     4.560213      31.03
 H       7.056499    -0.282307     4.425487      27.84
 C       5.878798    -1.682620     0.690057       9.14
 O       7.063288    -2.136425     0.218546     188.23
 H       7.634715    -1.723319     0.840939      25.36
 C       4.843776    -1.397948    -0.202181      48.85
 H       5.051684    -1.464951    -1.253044      23.10
 C       3.588381    -0.058684     1.571722       7.87
 C       2.394544     0.715438     2.228002      73.15
 H       2.966803     1.647191     2.750644      21.71
 O       1.792295     0.065334     3.535680     160.15
 H       1.182494    -0.742763     3.099075      22.47
 C       1.220567     0.811447     1.152985      91.30
 H       1.584929     1.191429     0.167968      23.71
 C       0.077736     1.679354     1.595681     105.35
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 O       0.546881     2.891993     2.074979     316.13
 H       1.224282     3.452529     1.722189      29.66
 H      -0.782479     1.069492     2.276288      24.47
 H      -0.454746     1.966986     0.759261      26.56
 C      -1.558744    -2.776353    -0.833252      37.36
 H      -1.950570    -3.813374    -0.654317      22.23
 C      -1.082907    -0.783524    -2.278924      58.62
 H      -1.684082    -0.269701    -3.028576      22.70
 C      -0.267099    -0.176690    -1.266511       3.29
 O       0.145067     1.246641    -1.375993     179.01
 C       0.179331     1.884907    -2.746749     124.65
 H       0.022364     2.925065    -2.562942      27.43
 H       0.851319     1.446441    -3.406591      28.26
 H      -0.728861     1.624474    -3.191941      27.74
 C      -0.158174    -0.886875    -0.095084       7.80
 O       0.741685    -0.536538     1.040644     117.42
 C      -0.727843    -2.198901     0.102554      46.84
 H      -0.343744    -2.759357     1.026418      22.56
 C      -1.768304    -1.951043    -2.104877      14.45
 C      -2.449614    -2.635349    -3.252998      89.51
 H      -2.277549    -2.122508    -4.251170      26.23
 O      -2.004482    -4.048100    -3.515746     183.85
 H      -1.031176    -4.188301    -3.313949      25.73
 C      -4.066254    -2.628258    -3.060928      95.88
 H      -4.348042    -3.214799    -2.153186      26.33
 O      -4.381440    -1.178689    -2.922880     197.82
 H      -5.190135    -1.257452    -2.180151      24.69
 C      -4.681957    -3.135893    -4.218538      78.22
 O      -6.347761    -3.561461    -3.934603     197.67
 H      -6.517353    -3.874290    -4.774012      31.14
 H      -4.010748    -4.024669    -4.281735      25.44
 H      -4.812990    -2.407444    -5.045916      25.83
55
name = lig-ACN-frame_757
 C       3.703915    -0.561001     0.256487      60.29
 H       3.123321    -0.163535    -0.666680      23.46
 C       4.622914    -0.486282     2.422065      62.95
 H       4.719099     0.078046     3.376065      19.86
 C       5.654759    -1.360997     2.056504      17.70
 O       6.691915    -1.666779     2.847297     204.94
 C       6.644803    -1.156475     4.282833     105.45
 H       7.384621    -1.846430     4.762080      26.09
 H       5.694630    -1.339244     4.658636      29.68
 H       6.814407    -0.023852     4.290588      27.12
 C       5.827720    -1.643790     0.706686      12.06
 O       7.121833    -2.164696     0.286531     165.85
 H       7.974584    -2.007287     0.747636      20.85
 C       4.788425    -1.261414    -0.224233      52.88
 H       4.839620    -1.631497    -1.251447      20.82
 C       3.596373    -0.089076     1.522968      33.59
 C       2.387670     0.623451     2.199913      99.07
 H       2.576817     1.782049     2.459852      24.15
 O       1.786190     0.153925     3.417875     267.81
 H       1.658437    -0.773232     3.398735      30.16
 C       1.266011     0.843711     1.179589      80.67
 H       1.780830     1.264632     0.308110      27.39
 C       0.027551     1.737025     1.501331      97.83
 O       0.558126     2.961295     2.115100     296.28
 H       0.890271     3.248511     1.274173      30.59
 H      -0.523147     1.179346     2.538167      23.47
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 H      -0.572712     1.836219     0.673591      27.27
 C      -1.527781    -2.705510    -0.885044      60.66
 H      -2.126656    -3.535167    -0.772885      25.73
 C      -1.096240    -0.712251    -2.281056      41.42
 H      -0.829632    -0.388617    -3.232592      23.72
 C      -0.312655    -0.093051    -1.278627      -0.65
 O       0.196145     1.168078    -1.492068     212.39
 C       0.034084     1.872657    -2.690708     138.62
 H       0.370276     2.867490    -2.428937      27.16
 H       0.939111     1.666692    -3.224210      28.12
 H      -0.792570     1.782218    -3.301170      27.60
 C      -0.061216    -0.898397     0.006223      -9.78
 O       0.788239    -0.571115     0.953107     123.16
 C      -0.659146    -2.252763     0.161534      53.57
 H      -0.635790    -2.770516     1.191073      22.56
 C      -1.821445    -2.020176    -2.007062      24.75
 C      -2.422314    -2.696658    -3.288325     103.01
 H      -2.169787    -2.009474    -4.142700      25.84
 O      -2.070531    -4.048318    -3.515001     242.73
 H      -1.248417    -4.093423    -3.677367      33.17
 C      -3.857938    -2.657146    -2.999294      81.97
 H      -3.948807    -3.214972    -2.030506      25.74
 O      -4.434042    -1.299397    -2.863725     176.07
 H      -5.328868    -1.174190    -2.164572      23.85
 C      -4.785908    -3.380472    -4.230447      85.94
 O      -6.251449    -3.504632    -4.014227     227.67
 H      -6.668621    -4.213001    -4.758236      27.90
 H      -4.558535    -4.198127    -4.869044      25.70
 H      -4.683868    -2.513322    -4.962005      26.27
55
name = lig-ACN-frame_758
 C       3.669460    -0.589426     0.228352      33.15
 H       2.631850    -0.591083    -0.342364      21.93
 C       4.611660    -0.505544     2.469303      45.67
 H       4.430771    -0.466659     3.498694      18.39
 C       5.701754    -1.249326     2.008502      11.74
 O       6.708963    -1.684868     2.962495     232.87
 C       6.652542    -1.120351     4.275391     123.70
 H       7.493927    -1.377464     4.828830      27.71
 H       5.828470    -1.474886     4.952822      29.09
 H       6.699838     0.072783     4.297495      28.05
 C       5.915877    -1.629153     0.623848      11.74
 O       7.073876    -2.216248     0.282511     131.74
 H       7.549581    -1.994853     1.200974      20.69
 C       4.881757    -1.233229    -0.243841      57.00
 H       4.956406    -1.507446    -1.332699      21.14
 C       3.540047    -0.155521     1.641095       8.35
 C       2.333578     0.688790     2.116711     102.62
 H       2.819741     1.748080     2.316606      24.46
 O       1.845877     0.196061     3.364828     288.74
 H       1.914042    -0.715553     3.343972      31.27
 C       1.256114     0.799681     1.090509     100.89
 H       1.627686     1.193742     0.185206      25.43
 C       0.052405     1.746740     1.573788      81.80
 O       0.527041     3.034813     2.091017     291.83
 H       0.789213     3.929968     1.721549      27.58
 H      -0.629176     1.193177     2.548720      22.81
 H      -0.671040     1.864145     0.769629      25.49
 C      -1.547646    -2.695539    -0.779268      46.91
 H      -1.881000    -3.583786    -0.622086      25.24
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 C      -1.114393    -0.763110    -2.304004      60.58
 H      -0.912305    -0.437388    -3.231087      22.63
 C      -0.404750    -0.193196    -1.190606       4.03
 O       0.257646     1.055400    -1.475497     165.87
 C       0.044782     1.932712    -2.722539     112.18
 H      -0.022474     2.929564    -2.350066      26.82
 H       0.657198     1.666431    -3.600270      26.24
 H      -1.004431     1.803176    -2.983369      26.18
 C      -0.067540    -0.932551    -0.081158      38.07
 O       0.891300    -0.546513     0.913233     167.47
 C      -0.663390    -2.105594     0.124676      53.15
 H      -0.380499    -2.673039     1.066021      22.16
 C      -1.629413    -1.984780    -2.159610      16.76
 C      -2.400181    -2.605006    -3.272205      84.47
 H      -2.280468    -1.978346    -4.190509      26.79
 O      -2.128262    -4.063751    -3.542186     174.93
 H      -1.134245    -4.281691    -3.480086      27.68
 C      -4.012849    -2.781940    -2.944469      59.33
 H      -4.170368    -3.356432    -1.980170      26.15
 O      -4.442582    -1.444377    -2.804260     269.15
 H      -5.137209    -1.585333    -2.186445      29.47
 C      -4.831679    -3.499338    -4.376560      83.92
 O      -6.178069    -3.456231    -4.011939     213.76
 H      -6.659449    -4.174375    -4.784181      25.51
 H      -4.411311    -4.426282    -4.533292      27.25
 H      -4.540287    -2.737210    -5.148183      26.81
55
name = lig-ACN-frame_759
 C       3.683629    -0.630465     0.270316      49.51
 H       2.840421    -0.643260    -0.536704      24.29
 C       4.548667    -0.571182     2.566365      44.19
 H       4.396340    -0.414155     3.562687      18.43
 C       5.789276    -1.135701     2.091751       8.07
 O       6.709261    -1.695538     2.996539     202.67
 C       6.662290    -1.078466     4.343217     126.88
 H       7.614010    -1.233684     4.696797      25.05
 H       5.834938    -1.674852     4.856844      27.18
 H       6.213658     0.026695     4.290441      26.55
 C       5.918260    -1.477796     0.662381      13.29
 O       7.073991    -2.287697     0.295769     135.03
 H       7.818115    -2.478975     0.931618      22.77
 C       4.891862    -1.225316    -0.277133      57.89
 H       5.079055    -1.373504    -1.379926      22.14
 C       3.509749    -0.245835     1.574962      35.70
 C       2.447903     0.753542     2.063677      85.08
 H       2.832190     1.780168     2.333914      25.26
 O       1.915159     0.240334     3.399002     183.03
 H       1.482593    -0.773736     3.162176      23.29
 C       1.201985     0.913735     1.012000      85.26
 H       1.550432     1.326060     0.111439      25.11
 C       0.113381     1.797100     1.612560      94.06
 O       0.447936     3.062012     2.177713     271.44
 H       0.808646     3.265430     1.195086      25.81
 H      -0.452072     1.148246     2.601117      22.67
 H      -0.642685     2.003661     0.841461      25.18
 C      -1.534728    -2.687176    -0.860845      52.28
 H      -1.885496    -3.574095    -0.693029      25.28
 C      -1.053749    -0.756710    -2.347149      51.44
 H      -1.612766    -0.192972    -3.016117      24.12
 C      -0.371632    -0.107711    -1.334804      11.77
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 O       0.360635     1.020388    -1.485935     198.78
 C      -0.058532     1.891425    -2.640572     117.05
 H       0.320676     2.907844    -2.449829      26.63
 H       0.443860     1.618966    -3.562201      27.14
 H      -1.137613     1.727580    -2.869749      26.36
 C      -0.033295    -0.823160    -0.090689      -7.67
 O       0.890386    -0.566797     0.829699     133.38
 C      -0.737914    -2.110296     0.164494      41.40
 H      -0.337250    -2.666857     1.022626      23.14
 C      -1.590570    -2.189594    -2.159587       9.72
 C      -2.560654    -2.727872    -3.255819      93.55
 H      -2.513339    -2.109708    -4.161457      26.23
 O      -2.113956    -4.063311    -3.587171     142.54
 H      -1.076932    -4.211106    -3.066598      23.81
 C      -4.090496    -2.894567    -3.101582      98.15
 H      -4.364690    -3.703885    -2.362326      26.58
 O      -4.516479    -1.562328    -2.705681     285.67
 H      -5.269925    -1.371755    -2.251859      31.09
 C      -4.619805    -3.437160    -4.326226     100.23
 O      -6.222640    -3.467476    -4.004802     257.04
 H      -6.781773    -3.619145    -4.784135      30.61
 H      -4.274517    -4.435276    -4.361060      27.66
 H      -4.548658    -3.185830    -5.376619      25.97
55
name = lig-ACN-frame_760
 C       3.731565    -0.679764     0.176685      38.60
 H       3.128114    -0.107368    -0.545317      22.39
 C       4.507341    -0.608863     2.531495      51.22
 H       4.354770    -0.182527     3.475381      17.99
 C       5.745604    -1.139244     2.147046      20.33
 O       6.719822    -1.630457     2.985910     239.17
 C       6.607972    -1.125267     4.379314     124.97
 H       7.572598    -0.969239     4.844622      25.83
 H       6.040649    -1.821110     5.190416      26.22
 H       6.239505    -0.047214     4.393152      27.14
 C       6.012689    -1.412096     0.800969      15.72
 O       7.021949    -2.318979     0.280015     203.75
 H       7.760600    -2.060017     0.815690      26.71
 C       4.971523    -1.201534    -0.171939      42.19
 H       5.105947    -1.563774    -1.218185      21.76
 C       3.585989    -0.260757     1.577204      15.99
 C       2.441512     0.694842     2.071101     104.19
 H       2.949950     1.654784     2.221356      26.24
 O       1.978121     0.305834     3.369625     216.99
 H       1.163856    -0.471364     3.147619      23.39
 C       1.366323     1.004857     1.118814      76.22
 H       1.712591     1.454160     0.190977      24.21
 C       0.017898     1.737945     1.671155      77.64
 O       0.433410     3.078644     2.184182     271.66
 H       1.071694     3.722925     1.830096      28.76
 H      -0.349558     1.023585     2.658891      23.26
 H      -0.837703     1.700261     0.874059      24.80
 C      -1.455332    -2.804911    -0.883355      39.96
 H      -2.082534    -3.600118    -0.681020      23.27
 C      -1.161234    -0.842164    -2.389611      47.55
 H      -1.562104    -0.280853    -3.286407      22.92
 C      -0.227532    -0.184862    -1.422945      -8.73
 O       0.419206     1.107505    -1.565921     197.09
 C      -0.074821     1.833072    -2.598617     121.47
 H       0.212339     2.895455    -2.407988      25.85
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 H       0.299361     1.419631    -3.516331      26.73
 H      -1.245608     1.985877    -2.771657      25.72
 C      -0.154539    -0.884839    -0.140729      12.09
 O       0.860162    -0.436806     0.768195     107.97
 C      -0.750907    -2.067964     0.126217      65.19
 H      -0.771505    -2.488966     1.090611      24.78
 C      -1.737315    -2.137673    -2.179332       1.73
 C      -2.588713    -2.861881    -3.266145      99.26
 H      -2.396071    -2.153121    -4.062449      27.28
 O      -2.055641    -4.138810    -3.649337     143.05
 H      -0.991921    -4.248695    -3.133138      22.16
 C      -4.107898    -2.865835    -3.065639      91.16
 H      -4.348052    -3.539372    -2.168407      26.35
 O      -4.577905    -1.595513    -2.633009     199.74
 H      -5.573217    -2.035078    -2.369758      23.82
 C      -4.765089    -3.475879    -4.356952     100.15
 O      -6.156541    -3.473684    -4.047235     342.72
 H      -6.410653    -3.305952    -4.870229      32.14
 H      -4.325030    -4.502283    -4.551409      25.32
 H      -4.420680    -2.695610    -5.037323      27.30
55
name = lig-ACN-frame_761
 C       3.809847    -0.540423     0.175716      63.64
 H       3.095217    -0.466638    -0.595167      26.05
 C       4.540168    -0.567961     2.512509      52.77
 H       4.263172    -0.428735     3.591261      19.30
 C       5.733906    -1.248218     2.181530      14.60
 O       6.757326    -1.533442     3.084264     232.22
 C       6.602498    -1.146974     4.429289     131.01
 H       7.688201    -1.061188     4.774231      26.46
 H       5.922508    -2.067694     4.959444      27.58
 H       6.000550    -0.285966     4.544140      31.42
 C       5.993826    -1.521407     0.786575      41.07
 O       7.021824    -2.254893     0.346313     166.85
 H       8.004311    -2.034202     0.491876      13.09
 C       5.073590    -1.204190    -0.108975      57.64
 H       5.386795    -1.559458    -1.090907      22.18
 C       3.539660    -0.236648     1.497589      23.15
 C       2.522644     0.670127     2.104080     102.09
 H       3.037405     1.588453     2.308895      25.09
 O       1.989793     0.357369     3.375540     281.20
 H       1.444824    -0.445186     3.327223      28.41
 C       1.277587     0.988782     1.129838      89.74
 H       1.740802     1.677559     0.385407      24.91
 C       0.163413     1.746040     1.726415      95.57
 O       0.350262     3.072385     2.238349     297.41
 H       0.960473     3.274587     1.580985      32.12
 H      -0.398614     1.282064     2.745233      23.50
 H      -0.650673     1.800219     0.881157      25.45
 C      -1.495363    -2.830279    -0.919687      49.67
 H      -1.896880    -3.829477    -0.561369      22.60
 C      -1.213274    -0.853398    -2.414098      54.39
 H      -0.981321    -0.568122    -3.535727      22.60
 C      -0.223423    -0.333701    -1.526663       4.44
 O       0.389670     0.984045    -1.552500     125.56
 C      -0.060795     1.918328    -2.785773      94.74
 H       0.320842     3.003746    -2.663943      25.39
 H       0.128795     1.620916    -3.777031      27.35
 H      -1.180186     1.611541    -2.549866      25.01
 C      -0.065442    -0.782102    -0.215215      -8.79
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 O       0.801754    -0.312664     0.743329     157.27
 C      -0.820841    -2.109862     0.090950      31.01
 H      -0.737260    -2.343629     1.106804      25.07
 C      -1.821627    -2.104099    -2.123521      31.75
 C      -2.470727    -2.788149    -3.311852      82.47
 H      -2.493738    -2.321788    -4.264311      27.17
 O      -2.007380    -4.257292    -3.677026     127.77
 H      -0.971695    -4.370454    -3.519702      25.71
 C      -4.038448    -3.000350    -2.913503      74.56
 H      -4.134778    -3.708552    -2.039419      25.90
 O      -4.665800    -1.637264    -2.613762     149.14
 H      -5.776776    -1.604046    -2.418297      23.65
 C      -4.783679    -3.364422    -4.313285      89.10
 O      -6.193548    -3.487497    -4.141286     271.14
 H      -6.898269    -3.492349    -4.968810      26.91
 H      -4.399771    -4.241837    -4.979652      23.39
 H      -4.665561    -2.569402    -5.050124      25.26
55
name = lig-ACN-frame_762
 C       3.884574    -0.469243     0.143532      50.84
 H       3.134014    -0.458564    -0.569415      25.28
 C       4.555685    -0.596130     2.483906      44.46
 H       4.292280    -0.404432     3.607563      17.57
 C       5.751774    -1.300540     2.233591      19.71
 O       6.805503    -1.455361     3.095413     239.16
 C       6.553625    -1.187874     4.535853     136.74
 H       7.586700    -1.125380     5.144302      26.14
 H       5.977594    -2.168504     5.088003      26.66
 H       6.088529    -0.308016     4.749543      31.43
 C       5.983008    -1.619448     0.886929      16.35
 O       7.169226    -2.278652     0.385729     161.43
 H       8.028132    -1.807698     0.838760      21.03
 C       5.034029    -1.173924    -0.222467      46.66
 H       5.192232    -1.295704    -1.277145      22.26
 C       3.623809    -0.218717     1.565911      30.16
 C       2.447500     0.775129     2.056862      96.05
 H       2.852320     1.724544     2.171697      25.83
 O       1.998710     0.337455     3.467550     273.88
 H       1.914456    -0.525889     3.407554      31.49
 C       1.311684     1.017566     1.114398      82.81
 H       1.515814     1.393242     0.084794      22.35
 C       0.096143     1.761762     1.840210      93.77
 O       0.363148     3.100685     2.248462     266.25
 H       0.661998     3.858065     1.613972      27.35
 H      -0.227208     0.929479     2.609641      23.65
 H      -0.722704     1.764219     0.982838      24.78
 C      -1.596404    -2.698136    -0.897147      33.90
 H      -1.835201    -3.909893    -0.988782      21.49
 C      -1.110739    -0.907407    -2.465409      53.35
 H      -1.414396    -0.456909    -3.579089      22.71
 C      -0.273517    -0.225849    -1.543991      10.67
 O       0.381158     0.890165    -1.740719     173.98
 C      -0.074103     1.839675    -2.902156      88.80
 H       0.309236     2.803483    -2.349981      24.28
 H       0.529091     1.511135    -3.593933      27.85
 H      -1.254105     2.001844    -3.315892      23.63
 C      -0.078585    -0.904672    -0.221375      23.96
 O       0.728640    -0.301052     0.738859     162.88
 C      -0.733131    -1.993684     0.091746      66.58
 H      -0.511014    -2.624688     0.905167      23.82
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 C      -1.745991    -2.182240    -2.184884      24.82
 C      -2.516396    -2.866026    -3.323605      83.81
 H      -2.316979    -2.115677    -4.069447      27.40
 O      -1.990179    -4.265372    -3.638073     221.29
 H      -1.128995    -4.244569    -3.595983      32.63
 C      -4.072096    -3.033029    -3.011183      90.38
 H      -4.167230    -3.814074    -2.250187      26.85
 O      -4.627598    -1.715172    -2.588246     230.42
 H      -5.499245    -1.879852    -2.408599      29.81
 C      -4.729406    -3.232028    -4.314844      86.05
 O      -6.358821    -3.518607    -4.125561     211.68
 H      -6.185249    -3.836488    -5.197316      22.29
 H      -4.255595    -4.203134    -4.729877      23.21
 H      -4.486430    -2.284146    -4.754006      25.87
55
name = lig-ACN-frame_763
 C       3.854872    -0.467611     0.204217      50.97
 H       3.333709     0.170663    -0.440100      22.86
 C       4.561482    -0.654830     2.594821      60.45
 H       4.477709    -0.071898     3.608175      19.13
 C       5.763473    -1.285771     2.185093     -18.09
 O       6.862820    -1.403237     3.165378     186.24
 C       6.534218    -1.232739     4.623870      94.63
 H       7.628436    -1.223026     5.123703      25.21
 H       5.759887    -2.068267     4.975130      26.65
 H       6.027100    -0.297878     4.771369      28.06
 C       6.023299    -1.684779     0.719610       3.78
 O       7.252319    -2.257935     0.476921     197.27
 H       7.942383    -2.026555     1.169655      23.92
 C       5.111508    -1.202806    -0.169158      61.83
 H       5.405913    -1.450131    -1.168951      20.98
 C       3.642814    -0.097943     1.539215       4.63
 C       2.454979     0.796548     2.097221      90.61
 H       2.788481     1.724426     2.298145      26.34
 O       2.036873     0.346751     3.444018     213.35
 H       2.047269    -0.720081     3.438060      24.45
 C       1.205931     1.007871     1.038197      74.71
 H       1.730639     1.708327     0.300948      23.13
 C       0.028806     1.765825     1.757818      97.17
 O       0.400143     3.148740     2.335240     227.40
 H       0.324514     3.687529     1.434122      27.11
 H      -0.161227     1.451754     2.832462      23.34
 H      -1.048911     1.678705     1.311357      24.93
 C      -1.570565    -2.614541    -0.889867      47.49
 H      -2.133887    -3.641474    -0.375531      22.48
 C      -1.070717    -0.980532    -2.548140      63.87
 H      -1.480542    -0.174945    -3.326797      20.98
 C      -0.404482    -0.268952    -1.509908      17.49
 O       0.349378     0.922028    -1.986471     239.91
 C       0.058930     1.766346    -2.974219     119.76
 H       0.071354     2.914550    -2.686111      25.18
 H       0.690499     1.806668    -3.737207      28.01
 H      -1.074187     1.508455    -3.488471      22.72
 C      -0.071301    -0.761672    -0.266272       0.48
 O       0.697107    -0.408008     0.813208     131.17
 C      -0.739602    -2.159823     0.049604      29.93
 H      -0.413809    -2.483755     1.042957      21.75
 C      -1.659673    -2.178823    -2.266678      44.01
 C      -2.537814    -2.935073    -3.276211     108.64
 H      -2.535995    -2.506059    -4.265708      27.05
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 O      -2.027408    -4.198543    -3.584271     245.92
 H      -1.113987    -4.249301    -3.389745      30.43
 C      -4.043840    -2.953625    -3.066396     101.73
 H      -4.354616    -3.782769    -2.414759      27.11
 O      -4.512784    -1.797344    -2.501984     273.03
 H      -5.381777    -1.946764    -2.112094      28.85
 C      -4.874543    -3.242048    -4.380037      95.02
 O      -6.266232    -3.524156    -4.135442     269.39
 H      -6.963032    -3.860109    -4.915081      26.59
 H      -4.410660    -4.042218    -5.050902      24.26
 H      -4.930607    -2.422802    -5.071986      26.05
55
name = lig-ACN-frame_764
 C       3.974429    -0.457438     0.270953      57.21
 H       3.352863    -0.292236    -0.648358      22.85
 C       4.588381    -0.592543     2.540045      42.66
 H       4.528517    -0.420128     3.658117      17.22
 C       5.798327    -1.240626     2.205924      20.40
 O       6.849378    -1.393527     3.166660     259.22
 C       6.509181    -1.230669     4.559360     123.06
 H       7.477780    -1.545868     5.266243      25.09
 H       5.766370    -1.932167     4.815993      29.03
 H       6.212777    -0.177833     4.923545      27.34
 C       6.088909    -1.615639     0.923463      19.41
 O       7.209869    -2.276515     0.490800     181.08
 H       7.988096    -2.065861     1.016108      25.61
 C       5.078378    -1.215451    -0.149341      60.99
 H       5.209025    -1.301866    -1.227038      22.63
 C       3.661335    -0.088688     1.633399      32.10
 C       2.466911     0.798839     2.111699     105.00
 H       2.798116     1.729130     2.228101      27.04
 O       2.077030     0.342357     3.376498     215.70
 H       1.749384    -0.770819     3.285354      21.77
 C       1.124237     0.976532     1.132672      83.78
 H       1.266562     1.226091     0.017956      22.61
 C       0.023063     1.813984     1.885595     103.03
 O       0.392033     3.140956     2.276025     293.85
 H       0.528594     3.758767     1.613853      31.96
 H      -0.146592     1.039640     2.651890      25.21
 H      -0.914585     1.968511     1.141200      25.05
 C      -1.558432    -2.737407    -0.961228      39.49
 H      -2.608508    -3.402201    -0.678210      22.28
 C      -1.112603    -0.947058    -2.572066      49.79
 H      -1.019446    -0.809384    -3.715033      24.45
 C      -0.360844    -0.156306    -1.639140      -8.20
 O       0.405145     0.858210    -1.983761     153.59
 C       0.073042     1.826602    -3.248876      84.38
 H      -0.223192     2.792408    -2.717303      25.36
 H       0.871834     1.747260    -3.839068      27.57
 H      -0.918643     1.343978    -3.778055      22.84
 C      -0.162097    -0.839958    -0.194313       1.48
 O       0.720439    -0.395512     0.844791     134.03
 C      -0.627002    -2.023501     0.003174      62.32
 H      -0.779051    -2.506190     0.976725      23.08
 C      -1.723299    -2.211799    -2.226778      14.41
 C      -2.519937    -2.834774    -3.377151      80.84
 H      -2.306675    -2.117667    -4.154798      27.35
 O      -2.057625    -4.282429    -3.521902      89.95
 H      -1.000179    -4.335781    -3.090110      24.11
 C      -4.106342    -3.061000    -3.063310      52.99
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 H      -4.192986    -3.962553    -2.468688      26.37
 O      -4.413446    -1.740669    -2.353688     136.41
 H      -5.390025    -1.653555    -1.739512      23.55
 C      -4.985213    -3.264029    -4.658717      83.29
 O      -6.234553    -3.557038    -4.006392     321.48
 H      -6.706715    -3.457152    -4.811347      29.06
 H      -4.538136    -4.173485    -5.117359      23.67
 H      -4.863459    -2.314494    -5.141090      26.27
55
name = lig-ACN-frame_765
 C       3.998560    -0.449145     0.271914      62.82
 H       3.037767    -0.364789    -0.353568      24.99
 C       4.638961    -0.484061     2.613943      37.91
 H       4.179087    -0.410309     3.569423      16.84
 C       5.842961    -1.143682     2.315894      15.22
 O       6.838773    -1.405952     3.147975     220.87
 C       6.492189    -1.258889     4.531596     116.77
 H       7.356423    -1.871383     5.024429      26.21
 H       5.567560    -1.596971     4.739477      34.19
 H       6.531341    -0.054641     4.769747      28.70
 C       6.065093    -1.508276     0.908633      29.86
 O       7.106258    -2.332476     0.466856     191.42
 H       8.026673    -1.919281     0.572403      18.92
 C       5.151074    -1.215168     0.026054      66.97
 H       5.397356    -1.615970    -0.981016      22.93
 C       3.675321    -0.137013     1.574242      20.51
 C       2.459869     0.812880     1.995825      99.40
 H       2.810550     1.739004     2.164687      26.25
 O       2.055495     0.301931     3.380952     221.63
 H       1.484174    -0.545952     3.153212      24.39
 C       1.187497     0.940539     1.171970      72.27
 H       1.477728     1.745152     0.351175      22.46
 C       0.018486     1.781174     1.923308      93.50
 O       0.401704     3.132047     2.276185     248.47
 H       0.954710     3.360259     1.478869      29.02
 H      -0.574749     1.636886     2.805900      24.70
 H      -0.789632     1.723260     1.007291      24.53
 C      -1.547726    -2.759760    -0.969414      56.05
 H      -1.876973    -3.865870    -0.614367      22.37
 C      -1.091517    -0.974309    -2.557571      57.47
 H      -0.881293    -0.701638    -3.551647      25.33
 C      -0.277935    -0.256942    -1.604234      13.39
 O       0.518973     0.946308    -2.023779     129.87
 C       0.043753     1.748822    -3.370842     102.15
 H      -0.119143     2.772762    -3.010312      26.83
 H       1.033746     1.950997    -3.749349      27.25
 H      -0.670488     1.479255    -4.227751      24.75
 C      -0.157355    -0.679824    -0.314066     -16.67
 O       0.676410    -0.405045     0.862415     127.06
 C      -0.850660    -2.132286    -0.043493      23.54
 H      -0.458835    -2.425926     0.940769      22.98
 C      -1.799942    -2.130776    -2.259781      32.49
 C      -2.537615    -2.885615    -3.365412      91.91
 H      -2.389056    -2.527341    -4.384165      27.67
 O      -2.098047    -4.320830    -3.501231      85.14
 H      -0.947643    -4.360631    -3.106536      22.21
 C      -4.076081    -2.982506    -3.243113      93.11
 H      -4.373476    -3.766843    -2.575191      27.90
 O      -4.332149    -1.748787    -2.276274     137.37
 H      -5.303383    -2.016963    -1.868518      25.89
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 C      -4.856836    -3.253320    -4.489939      98.46
 O      -6.312087    -3.569798    -3.978598     305.49
 H      -7.006599    -3.577895    -4.522406      32.12
 H      -4.579782    -4.013382    -5.212919      25.63
 H      -4.962990    -2.397978    -5.168959      26.81
55
name = lig-ACN-frame_766
 C       3.873840    -0.507873     0.228527      50.29
 H       3.357401    -0.155774    -0.766018      20.97
 C       4.585711    -0.384002     2.685652      58.44
 H       4.518115    -0.009237     3.620877      22.38
 C       5.843507    -1.008265     2.279946       5.47
 O       6.876684    -1.478222     3.177945     228.69
 C       6.514220    -1.259793     4.561706     128.56
 H       7.031556    -2.002128     5.277255      26.46
 H       5.556587    -1.384074     4.750265      33.13
 H       6.878459    -0.155533     4.962058      26.81
 C       6.142845    -1.437898     0.986157      18.34
 O       7.040169    -2.382725     0.469786     183.56
 H       8.026241    -2.018706     0.619917      21.21
 C       5.088260    -1.174314    -0.060853      31.98
 H       5.248001    -1.749970    -1.017508      21.29
 C       3.692639    -0.072205     1.594045      30.20
 C       2.492451     0.678147     2.075932     116.18
 H       2.844151     1.638974     2.215132      26.45
 O       2.011634     0.292471     3.352517     304.84
 H       1.608354    -0.470741     3.298711      32.62
 C       1.196037     0.978033     1.239231      68.90
 H       1.466107     1.453619     0.191440      22.84
 C      -0.018192     1.750353     1.892037      94.01
 O       0.463011     3.129907     2.214083     233.67
 H       1.294937     3.503213     1.644938      26.60
 H      -0.233302     1.103875     2.670882      26.75
 H      -0.998432     1.861122     1.132089      24.39
 C      -1.593160    -2.765263    -1.038107      29.99
 H      -1.484964    -3.890579    -1.136126      22.39
 C      -1.018308    -0.938088    -2.542334      54.45
 H      -1.474291    -0.358910    -3.224385      25.64
 C      -0.155754    -0.210255    -1.659312     -13.08
 O       0.500338     0.987555    -2.148951     196.58
 C       0.197637     1.705079    -3.321722     118.18
 H      -0.485175     2.509417    -3.132824      27.38
 H       1.104211     1.905450    -4.046349      25.45
 H      -0.361728     0.960369    -3.803657      25.25
 C      -0.196325    -0.812988    -0.231766      20.61
 O       0.589477    -0.378189     0.756860     152.35
 C      -0.858160    -1.939840    -0.009730      55.98
 H      -0.568702    -2.628333     0.766671      23.79
 C      -1.808328    -2.150670    -2.306134      -8.45
 C      -2.502854    -3.020753    -3.452137      96.24
 H      -2.179610    -2.435846    -4.332700      26.90
 O      -2.130077    -4.358052    -3.448917     161.34
 H      -0.987781    -4.393808    -3.543707      23.31
 C      -4.013434    -2.871819    -3.143349     100.32
 H      -4.089538    -3.830877    -2.621360      28.57
 O      -4.331966    -1.833473    -2.346060     284.09
 H      -5.125362    -1.939821    -2.046784      35.33
 C      -4.972238    -3.160972    -4.334012     106.91
 O      -6.299946    -3.571979    -3.931363     259.94
 H      -6.476738    -3.658468    -4.999826      22.59
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 H      -4.369246    -3.996381    -4.600985      26.10
 H      -5.027328    -2.318790    -5.081715      26.23
55
name = lig-ACN-frame_767
 C       3.862845    -0.540187     0.259247      51.89
 H       3.032843    -0.223302    -0.493358      23.46
 C       4.705243    -0.328007     2.546879      53.35
 H       4.376811    -0.050978     3.545152      23.49
 C       5.917764    -0.983297     2.286587       8.64
 O       6.835131    -1.502366     3.219127     216.69
 C       6.564972    -1.271226     4.661826     113.38
 H       6.981448    -2.157169     5.072929      25.62
 H       5.551610    -1.177270     4.736397      30.21
 H       7.061042    -0.202127     5.059386      26.00
 C       6.010592    -1.413969     0.854040      41.89
 O       7.036826    -2.365671     0.535325      90.13
 H       7.853345    -2.280236     1.106947      22.38
 C       5.051347    -1.174995    -0.104675      62.57
 H       5.224462    -1.335960    -1.195667      23.98
 C       3.642481    -0.070873     1.595721      23.91
 C       2.387865     0.726071     2.153049      94.83
 H       2.725003     1.681933     2.388347      26.95
 O       1.954035     0.237331     3.439900     277.33
 H       1.937900    -0.713919     3.357437      29.64
 C       1.125797     0.944991     1.027864      88.65
 H       1.559188     1.497532     0.102593      24.77
 C       0.135176     1.764886     1.831267     105.44
 O       0.486516     3.090074     2.196368     288.78
 H       1.188461     3.307453     1.580334      31.59
 H      -0.115871     1.328430     2.754242      27.00
 H      -0.979106     1.826884     1.253020      25.50
 C      -1.492339    -2.699892    -1.064417      61.14
 H      -1.996851    -3.586529    -0.761635      26.69
 C      -1.140817    -0.844316    -2.590346      68.90
 H      -1.385788    -0.417353    -3.481123      26.80
 C      -0.205430    -0.211825    -1.727255      16.10
 O       0.554619     0.943942    -2.038848     197.32
 C       0.207062     1.552933    -3.374297     114.36
 H      -0.435628     2.358547    -3.220673      28.61
 H       1.282496     2.181903    -3.563389      25.12
 H      -0.118858     1.015189    -4.147345      28.79
 C      -0.137906    -0.720171    -0.354555     -21.39
 O       0.604411    -0.340764     0.807413     138.31
 C      -0.911620    -2.039701    -0.059739      41.15
 H      -0.899260    -2.252732     0.983511      25.14
 C      -1.621421    -2.166072    -2.384891      40.26
 C      -2.403090    -2.856282    -3.471232      69.96
 H      -2.239203    -2.567475    -4.542811      28.88
 O      -2.120196    -4.456782    -3.431950     110.22
 H      -1.184773    -4.532254    -3.554991      30.02
 C      -4.026122    -3.052592    -3.021297      78.95
 H      -4.084021    -3.816037    -2.255881      26.82
 O      -4.359402    -1.730200    -2.358868     191.75
 H      -5.327504    -1.764579    -2.007377      27.84
 C      -4.928173    -3.139885    -4.234953      96.90
 O      -6.288758    -3.554323    -3.945926     228.18
 H      -7.029204    -3.999967    -4.688325      23.28
 H      -4.629587    -3.872662    -4.952647      25.34
 H      -4.863934    -2.219085    -4.905984      25.09
55
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name = lig-ACN-frame_768
 C       3.762458    -0.505539     0.301761      47.90
 H       2.897289    -0.620271    -0.370009      24.15
 C       4.756380    -0.271193     2.482932      36.42
 H       4.600517    -0.145979     3.625737      19.23
 C       5.875870    -1.053192     2.167155      19.47
 O       6.779632    -1.481260     3.209793     228.92
 C       6.602120    -1.293241     4.660082     127.22
 H       6.954348    -2.109727     5.159138      29.32
 H       5.571570    -1.147891     5.097102      29.02
 H       7.291664    -0.365920     4.979906      26.35
 C       6.011080    -1.519925     0.859556      17.09
 O       7.033081    -2.291657     0.582975     153.71
 H       7.626696    -2.122693     1.289817      27.22
 C       5.014227    -1.137754    -0.136515      53.85
 H       5.360042    -1.390769    -1.157548      21.52
 C       3.607694    -0.058973     1.638806      24.81
 C       2.335385     0.782285     2.062564      87.06
 H       2.556994     1.804326     2.353428      25.99
 O       1.896969     0.164393     3.524978     138.88
 H       1.763313    -0.954040     3.390465      22.23
 C       1.234712     0.948511     1.030571      86.80
 H       1.541122     1.482766     0.082089      24.31
 C       0.124654     1.758499     1.802115      96.88
 O       0.573903     3.115489     2.153165     275.17
 H       0.918995     3.664607     1.476764      31.34
 H      -0.035019     1.182096     2.627279      27.17
 H      -0.896630     1.706005     1.070335      25.56
 C      -1.472478    -2.739198    -1.055830      24.38
 H      -2.264870    -3.271768    -0.829253      26.15
 C      -1.189999    -0.767402    -2.719143      60.73
 H      -1.024104    -0.419746    -3.730636      24.47
 C      -0.308349    -0.188244    -1.682979       7.73
 O       0.553976     0.839017    -1.973594     152.91
 C       0.276206     1.541670    -3.349760      94.36
 H      -0.616453     2.052357    -3.263107      28.11
 H       1.340792     2.231567    -3.502905      24.03
 H       0.226690     0.906914    -4.145020      28.04
 C      -0.143383    -0.794461    -0.397494      31.08
 O       0.593554    -0.372011     0.759218     137.60
 C      -0.799456    -1.896055    -0.082428      47.38
 H      -1.077326    -2.101839     0.914187      25.52
 C      -1.487215    -2.138786    -2.498243       4.53
 C      -2.473804    -2.987324    -3.350571      87.78
 H      -2.516077    -2.473792    -4.377413      29.88
 O      -2.092138    -4.423969    -3.466663     182.29
 H      -1.279532    -4.461012    -3.157147      34.27
 C      -3.973676    -3.038216    -2.952205      56.28
 H      -4.206286    -3.810283    -2.199768      27.25
 O      -4.376403    -1.621040    -2.356907      80.30
 H      -5.451906    -1.768929    -1.945904      24.74
 C      -4.864128    -3.259712    -4.314536      97.03
 O      -6.321445    -3.510577    -3.868726     258.46
 H      -6.666459    -3.841176    -4.721219      27.49
 H      -4.383031    -3.766540    -5.067684      25.21
 H      -4.936380    -2.162215    -4.346091      24.37
55
name = lig-ACN-frame_769
 C       3.757504    -0.558435     0.277096      51.75
 H       3.064693    -0.319505    -0.475033      23.65
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 C       4.662515    -0.233707     2.569914      50.14
 H       4.792007     0.426240     3.539226      21.04
 C       5.712967    -1.081261     2.234783       9.26
 O       6.733410    -1.486704     3.112568     198.64
 C       6.669612    -1.291194     4.590496     118.00
 H       7.032380    -2.161163     4.928915      28.04
 H       5.501742    -1.037842     4.799110      25.29
 H       7.313299    -0.372023     4.917162      26.75
 C       5.931007    -1.520779     0.880983      15.85
 O       7.121609    -2.286018     0.552201     163.66
 H       7.987014    -2.059568     1.056821      24.28
 C       4.960516    -1.132999    -0.077060      58.42
 H       4.895106    -1.560409    -1.061460      20.92
 C       3.613551     0.010973     1.640094      22.77
 C       2.413623     0.657677     2.160867      99.94
 H       2.747007     1.711844     2.407849      24.32
 O       1.866277     0.188586     3.447657     197.75
 H       1.382364    -0.857082     3.240188      22.40
 C       1.246896     0.968507     1.123304      76.44
 H       1.714238     1.330648     0.228071      25.43
 C       0.116729     1.780782     1.712672     101.37
 O       0.654420     3.137045     2.119942     241.68
 H       0.375003     3.579300     1.210523      26.40
 H      -0.251879     1.365554     2.569347      27.34
 H      -0.857943     2.063269     0.967223      24.42
 C      -1.479577    -2.578015    -1.169138      65.81
 H      -1.768083    -3.474703    -0.925291      26.74
 C      -1.021767    -0.870256    -2.747754      48.89
 H      -1.346992    -0.313627    -3.726462      23.42
 C      -0.382568    -0.181101    -1.723038      10.59
 O       0.544921     0.842133    -2.033923     213.74
 C       0.387076     1.534160    -3.181083     117.28
 H      -0.578065     1.890288    -3.399567      27.54
 H       1.096492     2.594130    -3.343443      23.36
 H       0.650738     0.801043    -3.970849      27.01
 C      -0.125489    -0.752601    -0.379234      -9.50
 O       0.637156    -0.387677     0.669257     135.15
 C      -0.888660    -1.968674    -0.074283      49.75
 H      -0.695197    -2.414326     0.906950      25.57
 C      -1.623950    -2.204130    -2.417361      43.17
 C      -2.545120    -3.057787    -3.313869     107.50
 H      -2.417265    -2.575738    -4.346005      29.66
 O      -2.059551    -4.367874    -3.489257     202.76
 H      -1.112078    -4.405701    -3.109568      27.34
 C      -4.032477    -2.907136    -2.885941     103.78
 H      -4.226559    -3.657869    -2.066346      27.95
 O      -4.363964    -1.645109    -2.408301     249.34
 H      -5.256444    -1.756677    -1.953833      29.20
 C      -4.863486    -3.168677    -4.166011     102.30
 O      -6.232490    -3.526222    -3.873771     325.37
 H      -6.777111    -3.494116    -4.571228      32.47
 H      -4.573087    -4.060225    -4.655696      26.49
 H      -4.774606    -2.502480    -5.066854      27.05
55
name = lig-ACN-frame_770
 C       3.762297    -0.500576     0.316791      58.40
 H       3.086547    -0.161325    -0.369980      24.72
 C       4.589522    -0.226010     2.613999      60.36
 H       4.313107     0.302862     3.607886      20.07
 C       5.659827    -1.107705     2.305711       7.08
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 O       6.732398    -1.494927     3.031996     224.34
 C       6.691063    -1.276900     4.414454     140.13
 H       6.981306    -2.130537     4.896044      29.43
 H       5.583811    -1.149809     4.940495      27.16
 H       7.323796    -0.406061     4.708073      27.78
 C       5.935066    -1.522097     0.905496      13.58
 O       7.092710    -2.246944     0.492444     159.40
 H       7.908048    -1.678986     0.812119      22.77
 C       4.947678    -1.298896    -0.048231      51.02
 H       5.266996    -1.534729    -1.056694      22.70
 C       3.634457    -0.042620     1.642761      22.13
 C       2.366530     0.719950     2.213204      90.22
 H       2.769843     1.761828     2.560022      23.86
 O       1.821036     0.220961     3.378672     235.15
 H       1.580274    -0.895311     3.292489      22.44
 C       1.246664     0.916008     1.113330      85.46
 H       1.658277     1.607518     0.445717      26.84
 C       0.108026     1.887957     1.685632      98.13
 O       0.683051     3.130480     2.033939     272.78
 H       0.598078     3.943678     1.447756      28.75
 H      -0.504021     1.494432     2.467995      26.91
 H      -0.628649     1.897837     0.678038      25.42
 C      -1.562643    -2.702583    -1.036608      30.44
 H      -1.622063    -3.691651    -1.019979      25.47
 C      -0.978631    -1.047565    -2.738831      62.30
 H      -1.164703    -0.473768    -3.808168      23.69
 C      -0.256081    -0.245680    -1.722226      -3.07
 O       0.553516     0.872915    -1.911754     167.93
 C       0.441527     1.591190    -3.245516      97.49
 H      -0.604263     1.792570    -3.448614      26.37
 H       1.011903     2.553220    -2.759737      23.85
 H       1.020903     1.302981    -4.206894      25.62
 C      -0.269761    -0.721045    -0.399531      -1.79
 O       0.769280    -0.353241     0.668196     106.71
 C      -0.853978    -1.950117    -0.081767      48.89
 H      -0.464723    -2.643163     0.731070      23.55
 C      -1.791366    -2.079466    -2.447103      19.20
 C      -2.532911    -2.870556    -3.411749      69.06
 H      -2.577753    -2.498854    -4.486648      30.47
 O      -2.050293    -4.406122    -3.461745      31.39
 H      -0.880235    -4.330437    -3.555599      22.30
 C      -4.118602    -2.892395    -2.920264      89.05
 H      -4.354188    -3.704578    -2.162809      27.79
 O      -4.347564    -1.549303    -2.402424     252.80
 H      -5.054465    -1.514770    -1.902758      33.83
 C      -4.836674    -3.298960    -4.121582     107.13
 O      -6.220941    -3.523542    -3.852557     246.40
 H      -6.821742    -2.916991    -4.554135      24.24
 H      -4.265106    -4.149659    -4.191917      26.44
 H      -4.556333    -2.579419    -4.922921      26.71
55
name = lig-ACN-frame_771
 C       3.832190    -0.515358     0.278353      44.40
 H       3.076712    -0.487952    -0.457654      26.08
 C       4.601332    -0.365183     2.680701      40.85
 H       4.503776    -0.395476     3.751403      20.68
 C       5.718621    -1.100589     2.197738      24.21
 O       6.770728    -1.531697     3.001429     243.11
 C       6.726134    -1.265169     4.405993     125.79
 H       7.287095    -2.051756     4.893786      27.35
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 H       5.594226    -1.083054     4.723662      26.23
 H       7.261423    -0.356637     4.611711      28.29
 C       5.879461    -1.546120     0.934549      29.59
 O       7.006854    -2.148554     0.467526     204.33
 H       7.846208    -1.865322     0.855876      25.39
 C       4.891862    -1.342664    -0.045053      51.19
 H       5.130148    -1.547416    -1.095288      23.15
 C       3.508367    -0.025488     1.695487       1.73
 C       2.344178     0.828539     2.063267      85.62
 H       2.571623     1.997388     2.288196      23.43
 O       1.749928     0.197964     3.450593     154.56
 H       1.792279    -0.804362     3.284384      25.97
 C       1.218739     1.039849     1.091299      87.30
 H       1.617418     1.331973     0.214623      27.37
 C       0.078007     1.913504     1.548096     101.77
 O       0.711890     3.185589     2.013651     262.19
 H       0.882937     3.616550     1.194415      31.22
 H      -0.407513     1.481897     2.441480      26.59
 H      -0.694428     2.207289     0.647515      25.73
 C      -1.651890    -2.758802    -1.065399      68.55
 H      -2.191689    -3.647945    -0.756378      26.88
 C      -0.939883    -0.914601    -2.701779      52.66
 H      -0.584873    -0.847644    -3.860283      24.22
 C      -0.140544    -0.339506    -1.724603     -23.35
 O       0.553249     0.865721    -1.880408     124.22
 C       0.481856     1.753905    -3.195547      89.65
 H      -0.568745     1.662401    -3.666175      25.75
 H       0.694806     2.871767    -3.070463      25.87
 H       1.192243     1.150478    -3.952463      25.91
 C      -0.231859    -0.684935    -0.262937     -17.83
 O       0.807865    -0.376617     0.594667     111.89
 C      -0.782229    -2.038772    -0.124718      19.98
 H      -0.523978    -2.274170     0.994973      22.81
 C      -1.779949    -2.136871    -2.246152       7.13
 C      -2.613421    -2.878308    -3.431128      87.81
 H      -2.392474    -2.304429    -4.389519      28.45
 O      -2.101764    -4.306414    -3.463236      10.17
 H      -0.886437    -4.087882    -3.508778      22.31
 C      -4.013962    -2.866624    -2.918392      82.68
 H      -3.977997    -3.441356    -1.942670      26.36
 O      -4.342217    -1.407411    -2.409886     121.14
 H      -5.162120    -1.524492    -1.704592      25.36
 C      -4.808739    -3.509293    -4.168358      89.02
 O      -6.290973    -3.505612    -3.861260     256.77
 H      -6.599947    -2.718556    -4.546449      23.45
 H      -4.603435    -4.334448    -4.711205      26.43
 H      -4.825069    -2.731377    -4.945263      25.94
55
name = lig-ACN-frame_772
 C       3.699745    -0.519208     0.382515      54.71
 H       2.979858    -0.115178    -0.386354      24.59
 C       4.521983    -0.550656     2.638447      72.97
 H       4.353798    -0.143015     3.560255      24.25
 C       5.751337    -1.092507     2.227410       5.02
 O       6.834630    -1.580372     2.996101     209.19
 C       6.797294    -1.208290     4.458424     119.02
 H       7.355470    -2.077149     4.930438      26.12
 H       5.797051    -1.427486     4.945881      26.83
 H       7.120285    -0.219888     4.654683      27.44
 C       5.848841    -1.552564     0.793686      10.36
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 O       7.028238    -2.115635     0.410301     192.23
 H       7.514667    -2.169070     1.238105      23.74
 C       4.839960    -1.271872    -0.069857      73.82
 H       4.780524    -1.838296    -1.019125      23.13
 C       3.577174    -0.074818     1.640210      23.01
 C       2.259305     0.795190     2.135652      71.04
 H       2.807757     1.822148     2.557631      23.77
 O       1.743680     0.298886     3.403380     270.61
 H       1.534921    -0.556352     3.311398      32.40
 C       1.184620     1.031331     0.850692      78.68
 H       1.632795     1.620864     0.168023      28.08
 C       0.060277     1.994761     1.464022      93.73
 O       0.706464     3.228805     1.954323     219.96
 H       1.436036     3.644622     1.290793      27.48
 H      -0.517024     1.497430     2.381749      26.11
 H      -0.802064     2.213317     0.670712      26.83
 C      -1.603375    -2.633412    -0.948746      19.63
 H      -2.442778    -3.348126    -0.579625      23.58
 C      -0.944217    -1.003896    -2.556323      68.73
 H      -0.894206    -0.654624    -3.708988      24.75
 C      -0.146925    -0.231149    -1.633378       9.05
 O       0.604956     0.959562    -1.944822     194.24
 C       0.429857     1.718686    -3.083309     109.92
 H      -0.639583     1.603524    -3.634936      24.27
 H       0.577726     2.689368    -2.702373      27.36
 H       1.399811     1.580425    -3.952480      25.19
 C      -0.087575    -0.858740    -0.370217      -5.77
 O       0.792364    -0.376053     0.605600     132.54
 C      -0.773679    -2.056414    -0.002291      62.29
 H      -0.903205    -2.679412     0.987459      23.34
 C      -1.637512    -2.124556    -2.352451      42.09
 C      -2.446483    -2.811250    -3.252476     106.12
 H      -2.475322    -2.317204    -4.301358      27.83
 O      -2.169384    -4.136651    -3.527670     112.73
 H      -1.163747    -4.428846    -3.005273      23.40
 C      -3.980998    -2.851851    -2.931405      71.93
 H      -4.181554    -3.553354    -2.051423      27.50
 O      -4.355459    -1.421150    -2.530102     172.03
 H      -5.218919    -1.643499    -1.799440      25.01
 C      -4.962074    -3.480003    -4.176294     100.39
 O      -6.330006    -3.496840    -3.901319     328.13
 H      -6.842967    -3.000013    -4.387567      32.06
 H      -4.605468    -4.447029    -4.127535      26.15
 H      -4.528681    -2.969564    -5.034144      25.47
55
name = lig-ACN-frame_773
 C       3.591928    -0.510141     0.314420      41.18
 H       2.830627    -0.084170    -0.473156      23.26
 C       4.484202    -0.585246     2.635594      56.23
 H       4.456407    -0.291786     3.606424      23.39
 C       5.722824    -1.207854     2.174413      11.42
 O       6.844672    -1.571410     3.051499     222.12
 C       6.844006    -1.240584     4.464575     122.71
 H       7.819055    -1.676209     4.992308      25.28
 H       5.893211    -1.466949     4.872617      29.20
 H       7.031573    -0.230730     4.560620      29.29
 C       5.884941    -1.466699     0.821855      11.79
 O       7.071920    -2.141225     0.354815     152.39
 H       7.676139    -2.445567     1.148847      19.02
 C       4.718567    -1.227346    -0.120338      39.74
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 H       4.949698    -1.481123    -1.198811      21.85
 C       3.487781    -0.114928     1.719671      32.80
 C       2.342563     0.716147     2.114191      94.84
 H       2.620802     1.937182     2.192380      24.02
 O       1.694582     0.409228     3.329938     272.53
 H       1.354482    -0.493283     3.252023      29.45
 C       1.215439     1.019469     0.892717      84.51
 H       1.623769     1.244784    -0.018553      26.19
 C       0.104873     2.051209     1.371564      98.72
 O       0.659561     3.256189     1.867892     239.21
 H       1.540523     3.574898     1.314595      26.84
 H      -0.397947     1.547676     2.365428      24.80
 H      -0.684432     2.322914     0.555875      25.97
 C      -1.623942    -2.508123    -0.902439      58.86
 H      -2.249492    -3.563443    -0.755768      25.39
 C      -0.838031    -0.891834    -2.595846      54.78
 H      -1.354185    -0.316058    -3.416442      25.04
 C      -0.194952    -0.184440    -1.603649      -0.48
 O       0.634708     0.886980    -1.872937     179.96
 C       0.349125     1.772772    -3.049364     100.92
 H      -0.742529     1.549351    -3.576471      23.59
 H       0.229028     2.739323    -2.724903      28.10
 H       1.275496     1.756725    -3.958439      24.26
 C       0.140777    -0.926947    -0.369564      -2.20
 O       0.771522    -0.332526     0.666873     137.98
 C      -0.773033    -2.011723     0.112964      27.79
 H      -0.498277    -2.208198     1.255487      23.62
 C      -1.487204    -2.125749    -2.184679      30.38
 C      -2.495157    -2.715137    -3.329102      65.95
 H      -2.265650    -1.978978    -4.195646      27.08
 O      -2.159794    -4.159602    -3.593533     177.13
 H      -1.453948    -4.380019    -3.021097      31.86
 C      -4.124542    -2.774008    -2.949955     102.00
 H      -4.322673    -3.465575    -2.068802      27.79
 O      -4.401571    -1.525139    -2.645904     275.02
 H      -5.168445    -1.354233    -2.100870      30.64
 C      -4.885389    -3.399357    -4.086619      98.71
 O      -6.405739    -3.486276    -3.910026     282.71
 H      -6.710174    -3.057245    -4.782720      25.93
 H      -4.643527    -4.444176    -4.022203      27.55
 H      -4.856915    -3.280725    -5.140433      26.33
55
name = lig-ACN-frame_774
 C       3.643820    -0.506243     0.315227      45.92
 H       2.819567    -0.405526    -0.500435      25.60
 C       4.546924    -0.568897     2.658291      62.28
 H       4.331515    -0.574420     3.688715      22.55
 C       5.669595    -1.286171     2.240197       4.25
 O       6.791791    -1.574246     3.014691     210.65
 C       6.824014    -1.180611     4.439412     115.01
 H       7.802749    -1.783005     4.841967      24.96
 H       6.140084    -1.663455     5.001553      30.42
 H       6.701088    -0.146249     4.599149      29.22
 C       5.882524    -1.496140     0.753037      18.19
 O       7.003697    -2.133511     0.292503     175.34
 H       7.774965    -2.012318     0.949855      22.02
 C       4.832637    -1.173817    -0.089743      65.00
 H       4.993331    -1.108616    -1.182065      24.00
 C       3.410491    -0.256484     1.655850      12.55
 C       2.326281     0.866509     1.996183      79.19
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 H       3.042444     1.839650     2.325158      23.89
 O       1.609136     0.479912     3.313490     168.86
 H       1.491553    -0.640707     3.189448      24.70
 C       1.329689     0.999860     0.994986     100.81
 H       1.849938     1.510562     0.197037      27.36
 C       0.191489     2.002605     1.296502      96.03
 O       0.652905     3.318229     1.801989     267.43
 H       1.088708     3.744589     1.033496      30.42
 H      -0.659329     1.559575     2.119093      25.73
 H      -0.402138     2.087747     0.341280      28.16
 C      -1.562919    -2.577087    -0.765280     -10.66
 H      -2.234942    -3.602775    -0.452684      23.09
 C      -0.921508    -0.824833    -2.606216      66.83
 H      -0.975332    -0.426414    -3.598991      26.40
 C      -0.030906    -0.279763    -1.583034       7.15
 O       0.663659     0.895912    -1.830003     179.72
 C       0.209589     1.846905    -2.978279      93.25
 H      -0.706755     1.312434    -3.531411      24.60
 H       0.136197     2.803012    -2.657935      28.46
 H       1.242736     1.641070    -3.741156      24.66
 C       0.087573    -0.790617    -0.287386      35.49
 O       0.767529    -0.330308     0.824100     142.19
 C      -0.665834    -1.875996     0.117763      46.69
 H      -0.689075    -2.218367     1.227570      22.60
 C      -1.614963    -2.026538    -2.268666     -22.05
 C      -2.564449    -2.745555    -3.310577      89.71
 H      -2.516892    -2.277612    -4.366778      27.54
 O      -2.150236    -4.149338    -3.664648     178.52
 H      -1.305973    -4.175553    -3.453277      35.13
 C      -4.060695    -2.806294    -2.979401      90.71
 H      -4.060046    -3.374620    -2.025912      26.31
 O      -4.519822    -1.345802    -2.701850     233.96
 H      -5.290984    -1.502422    -2.292414      31.84
 C      -4.925446    -3.521270    -4.115977      97.46
 O      -6.412473    -3.414247    -3.922403     200.98
 H      -6.871201    -3.359088    -4.984635      20.75
 H      -4.499217    -4.564453    -4.316619      23.86
 H      -4.515655    -2.786518    -4.803741      24.62
55
name = lig-ACN-frame_775
 C       3.743022    -0.598319     0.343706      53.31
 H       3.050454    -0.154434    -0.403468      24.36
 C       4.424848    -0.600304     2.599170      58.87
 H       4.266251    -0.202068     3.637993      22.48
 C       5.655481    -1.269674     2.187046      20.75
 O       6.730271    -1.595835     2.980538     220.02
 C       6.737467    -1.188190     4.399984     117.55
 H       7.869509    -1.300704     4.743061      25.33
 H       6.065813    -1.700055     4.891214      30.18
 H       6.646710    -0.097422     4.491205      27.17
 C       5.840614    -1.573696     0.856081      16.55
 O       6.980356    -2.104090     0.235730     214.26
 H       7.751762    -1.678396     0.576614      27.75
 C       4.962967    -1.059692    -0.154269      36.34
 H       5.231521    -1.423620    -1.144112      21.44
 C       3.493489    -0.263052     1.708487      27.34
 C       2.411014     0.802685     2.198092      91.21
 H       2.941175     1.944654     2.332060      24.85
 O       1.589267     0.535621     3.272506     228.82
 H       1.522455    -0.593412     3.332900      24.09
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 C       1.392785     1.108878     0.979965      83.89
 H       1.812968     1.214150    -0.055674      25.00
 C       0.206901     2.018558     1.225302      99.46
 O       0.656504     3.325977     1.700994     272.95
 H       0.567462     3.984251     1.001768      30.63
 H      -0.618438     1.538664     2.072461      24.57
 H      -0.255376     2.127727     0.259261      27.60
 C      -1.455447    -2.520628    -0.972766      51.14
 H      -2.099639    -3.420412    -0.386863      22.87
 C      -0.979688    -0.926560    -2.495170       9.16
 H      -0.771550    -0.732818    -3.464792      25.69
 C       0.045637    -0.258733    -1.619021     -31.88
 O       0.680835     1.003842    -1.851970     182.92
 C       0.179491     1.777754    -2.867511     115.42
 H      -0.869956     1.626638    -3.292815      26.95
 H       0.003494     2.690971    -2.357607      28.07
 H       0.928722     2.128642    -3.866042      24.94
 C      -0.038748    -0.626899    -0.162527     -32.96
 O       0.801417    -0.276117     0.934572      80.76
 C      -0.721067    -1.895625     0.084593      36.31
 H      -0.621024    -2.340502     1.118343      24.29
 C      -1.844362    -2.035847    -2.166252      41.23
 C      -2.562280    -2.772931    -3.353758     103.63
 H      -2.511876    -1.981484    -4.182096      27.77
 O      -2.119822    -4.107879    -3.677250     147.26
 H      -1.117757    -4.060663    -3.953921      26.98
 C      -4.056621    -2.823252    -2.867492      68.72
 H      -4.306875    -3.265791    -1.908713      26.87
 O      -4.601967    -1.298451    -2.781809     123.29
 H      -5.598071    -1.423276    -2.283179      25.40
 C      -4.949434    -3.454663    -4.186789      80.75
 O      -6.315493    -3.351148    -3.960846     261.62
 H      -6.852505    -3.645876    -4.790367      26.33
 H      -4.685407    -4.576731    -4.523552      24.41
 H      -4.814425    -2.920641    -5.147364      24.31
55
name = lig-ACN-frame_776
 C       3.740517    -0.515239     0.289127      49.31
 H       3.114788    -0.156838    -0.471996      23.00
 C       4.466166    -0.671446     2.683572      51.29
 H       4.607102    -0.170493     3.743798      17.37
 C       5.630047    -1.238948     2.211806      10.71
 O       6.709541    -1.625850     3.000605     232.09
 C       6.643871    -1.149947     4.326069     121.44
 H       7.652140    -1.330016     4.819272      25.20
 H       6.015753    -1.671544     4.886533      32.21
 H       6.179695    -0.126649     4.362251      28.07
 C       5.876197    -1.557657     0.769909       9.56
 O       7.028343    -2.101530     0.235318     206.40
 H       7.929779    -1.850201     0.635624      27.03
 C       4.974065    -1.106238    -0.114834      57.30
 H       5.136769    -1.131445    -1.178594      20.93
 C       3.515532    -0.151653     1.673476      11.94
 C       2.447525     0.792615     2.138524      81.73
 H       3.132776     1.759746     2.576249      23.08
 O       1.603517     0.502906     3.360768     247.68
 H       1.311213    -0.402311     3.337378      29.37
 C       1.444143     1.078823     0.981706      81.20
 H       2.103543     1.429280     0.055112      23.12
 C       0.249367     2.105216     1.140339      97.46
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 O       0.608308     3.352218     1.650760     247.20
 H       0.598396     4.007742     0.776978      26.22
 H      -0.384866     1.517797     2.078049      23.77
 H      -0.441759     2.158086     0.359193      26.89
 C      -1.558140    -2.605617    -0.920548      21.04
 H      -1.884825    -3.787985    -0.956382      20.54
 C      -0.860590    -0.921115    -2.441074      73.65
 H      -1.070226    -0.504940    -3.324660      27.48
 C      -0.143057    -0.189874    -1.478461      -8.55
 O       0.715108     0.923799    -1.881375     178.61
 C       0.049406     1.952873    -2.818834      89.75
 H      -0.812742     1.405433    -3.091897      26.35
 H      -0.036474     3.013370    -2.446098      25.05
 H       0.789711     1.877481    -3.843646      23.31
 C      -0.049348    -0.606512    -0.105334      21.34
 O       0.744783    -0.216729     0.896902     141.99
 C      -0.731699    -1.870296     0.022766      46.83
 H      -0.512112    -2.422770     0.937289      25.43
 C      -1.774105    -1.977090    -2.185396       1.22
 C      -2.628074    -2.663217    -3.241044      78.52
 H      -2.500039    -2.110524    -4.228842      29.14
 O      -2.106690    -4.036416    -3.689406      36.56
 H      -0.902639    -3.880850    -3.726830      22.23
 C      -4.259791    -2.734917    -3.044027     107.40
 H      -4.391905    -3.393232    -2.195226      28.16
 O      -4.603783    -1.432794    -2.864638     210.95
 H      -5.539106    -1.293030    -2.236175      25.29
 C      -4.850942    -3.340446    -4.233085     100.76
 O      -6.311047    -3.293117    -3.941223     289.85
 H      -6.710716    -3.515318    -4.673489      32.62
 H      -4.470384    -4.468531    -4.096618      24.43
 H      -4.424352    -2.831823    -5.101031      25.72
55
name = lig-ACN-frame_777
 C       3.740954    -0.355499     0.313143      60.20
 H       3.012104    -0.209073    -0.370329      25.36
 C       4.523253    -0.598284     2.622688      51.31
 H       4.035243    -0.611980     3.749062      18.84
 C       5.712594    -1.332011     2.144236       9.21
 O       6.708283    -1.657908     2.995816     221.41
 C       6.534457    -1.128190     4.383026     105.60
 H       7.518454    -1.128833     4.774430      26.77
 H       5.877333    -1.736944     4.873058      29.47
 H       6.378780     0.035149     4.403230      26.54
 C       5.970804    -1.460353     0.748938      11.86
 O       7.130129    -2.130999     0.273084     183.24
 H       7.700894    -2.122427     1.153636      20.13
 C       4.835398    -1.144270    -0.143916      45.56
 H       5.107259    -1.181030    -1.200691      24.19
 C       3.575870    -0.164028     1.685196      28.42
 C       2.357892     0.837548     2.110674      75.67
 H       2.876883     1.981687     2.264135      24.07
 O       1.687581     0.424678     3.432367     260.23
 H       1.337153    -0.357804     3.173682      31.68
 C       1.428603     1.114237     0.954418      80.13
 H       2.019744     1.355131    -0.077025      22.74
 C       0.294649     2.062412     1.192347     102.65
 O       0.531302     3.487409     1.596154     233.05
 H       1.385698     3.859012     1.031805      27.00
 H      -0.477269     1.689108     2.099859      24.38
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 H      -0.146012     2.026957     0.269862      27.62
 C      -1.603494    -2.617405    -0.853532      46.55
 H      -1.839744    -3.663589    -0.539464      26.73
 C      -0.909231    -0.773751    -2.473348      37.41
 H      -0.841314    -0.262790    -3.373640      26.90
 C      -0.239468    -0.014581    -1.408473     -12.10
 O       0.680928     0.853985    -1.911443     177.73
 C      -0.048648     1.985328    -2.794649      85.49
 H      -1.031890     1.968246    -3.058056      27.84
 H       0.060006     2.998985    -2.171829      24.63
 H       0.644254     2.077455    -3.807062      24.15
 C      -0.094733    -0.704896    -0.209068       5.93
 O       0.700921    -0.185388     0.837513     114.04
 C      -0.767700    -2.026838     0.091882      40.48
 H      -0.464545    -2.492423     1.027458      24.92
 C      -1.634763    -1.993951    -2.191739       4.13
 C      -2.656493    -2.571026    -3.264962     104.20
 H      -2.595465    -1.805032    -4.112516      28.06
 O      -2.115451    -3.903589    -3.650629      72.60
 H      -1.066870    -4.042453    -3.090243      24.28
 C      -4.148413    -2.746982    -3.077981     101.69
 H      -4.579477    -3.285430    -2.249414      27.61
 O      -4.659995    -1.376449    -2.898836     261.83
 H      -5.243051    -1.469501    -2.209416      32.32
 C      -4.842077    -3.349889    -4.311449      90.80
 O      -6.276434    -3.239000    -3.974394     245.47
 H      -6.825861    -3.131611    -4.866254      24.85
 H      -4.398091    -4.463811    -4.569096      24.38
 H      -4.722807    -2.800478    -5.248971      25.34
55
name = lig-ACN-frame_778
 C       3.789661    -0.339654     0.312032      46.72
 H       3.078443     0.006272    -0.376318      24.55
 C       4.547494    -0.617572     2.501366      50.23
 H       4.359849    -0.826773     3.682511      18.11
 C       5.692653    -1.262289     2.102016       9.68
 O       6.737544    -1.687068     3.055862     210.49
 C       6.544635    -1.131567     4.420239     103.02
 H       7.368886    -1.339893     4.965968      27.41
 H       5.654159    -1.566451     4.934548      29.64
 H       6.106649    -0.054304     4.282838      27.73
 C       5.934538    -1.453156     0.704350      16.01
 O       7.174025    -2.097605     0.367993     176.06
 H       7.733717    -2.430850     1.068750      19.37
 C       4.887529    -1.111376    -0.182634      63.40
 H       4.761380    -1.609523    -1.164502      23.15
 C       3.525784    -0.025928     1.698262      33.47
 C       2.382546     0.808738     2.176191      95.04
 H       2.709541     1.954569     2.447914      23.99
 O       1.823414     0.377118     3.363929     267.05
 H       1.417332    -0.626092     3.300176      24.46
 C       1.322076     1.060551     0.977311      78.38
 H       1.876217     1.411324    -0.048560      23.40
 C       0.212726     2.176109     1.230244     107.93
 O       0.531781     3.551452     1.553008     287.62
 H       1.373134     3.742120     1.125104      31.16
 H      -0.489517     1.662259     2.092691      25.32
 H      -0.424451     2.227935     0.422659      28.31
 C      -1.531783    -2.556498    -0.915038      58.30
 H      -2.372079    -3.162038    -0.799175      26.38
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 C      -1.119296    -0.712180    -2.432379      46.48
 H      -1.103374    -0.574234    -3.499177      25.93
 C      -0.296779    -0.124858    -1.543237      -6.60
 O       0.563996     0.970467    -1.985479     195.97
 C      -0.006960     2.037371    -2.695226     103.55
 H      -0.986201     1.801007    -2.761348      28.81
 H       0.299492     3.017074    -1.974056      23.26
 H       0.456364     2.157105    -3.753694      25.13
 C      -0.130333    -0.768136    -0.166029       5.90
 O       0.656514    -0.252051     0.782101     156.11
 C      -0.698029    -2.007141     0.178299      52.92
 H      -0.616018    -2.490330     1.190247      22.04
 C      -1.679173    -1.970133    -2.148021      31.12
 C      -2.484997    -2.503550    -3.302804      87.81
 H      -2.393252    -1.834543    -4.226166      25.41
 O      -2.132464    -3.806961    -3.626323     188.05
 H      -1.298746    -4.013267    -3.096865      28.15
 C      -4.035649    -2.708750    -3.020927      54.54
 H      -4.028487    -3.335636    -2.135948      25.82
 O      -4.718594    -1.263047    -2.906283     231.27
 H      -5.233440    -1.173117    -2.129549      29.70
 C      -4.910566    -3.340820    -4.469580      65.71
 O      -6.240373    -3.241033    -4.039795     242.22
 H      -6.783647    -2.800613    -4.956291      22.39
 H      -4.779460    -4.509168    -4.770359      22.81
 H      -4.612361    -2.651154    -5.286306      23.72
55
name = lig-ACN-frame_779
 C       3.815573    -0.332457     0.253139      53.43
 H       3.216537     0.000845    -0.614323      22.12
 C       4.472803    -0.632193     2.569546      63.75
 H       4.386485    -0.179679     3.640511      18.40
 C       5.767721    -1.169257     2.118614      11.00
 O       6.680688    -1.675497     3.060219     229.89
 C       6.510734    -1.165479     4.406930     122.26
 H       7.362155    -1.368824     4.905537      26.08
 H       5.641931    -1.770197     4.898831      26.22
 H       6.587293    -0.002610     4.494515      26.10
 C       5.969900    -1.533750     0.739498      11.93
 O       7.132789    -2.061831     0.374463     212.46
 H       7.586897    -2.003902     1.224047      25.95
 C       4.974114    -1.106781    -0.161175      46.40
 H       5.051003    -1.382805    -1.267626      20.83
 C       3.642726     0.006711     1.569500      16.69
 C       2.360038     0.831707     2.087119      80.13
 H       2.938879     1.849507     2.321301      23.67
 O       1.893137     0.296989     3.375478     185.47
 H       1.815095    -0.843768     3.138672      21.24
 C       1.197487     1.057046     1.024708      82.43
 H       1.859005     1.370974     0.074064      22.92
 C       0.032132     2.217330     1.261051      96.34
 O       0.591755     3.542092     1.578259     249.15
 H       0.884638     3.949081     0.697677      28.08
 H      -0.479190     2.037239     2.340885      23.47
 H      -0.657314     2.171354     0.480665      26.50
 C      -1.544324    -2.560236    -0.862712      65.75
 H      -1.887873    -3.474776    -0.613200      27.73
 C      -1.230264    -0.696447    -2.495404      39.47
 H      -1.495487     0.048198    -3.345332      22.79
 C      -0.218709    -0.196198    -1.562954      12.23
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 O       0.500173     0.938140    -1.927659     233.63
 C      -0.032627     2.157134    -2.601543     110.88
 H      -1.067445     2.257900    -2.785695      28.28
 H       0.167317     3.293003    -2.153632      23.98
 H       0.383144     2.161476    -3.665016      25.24
 C      -0.109072    -0.679719    -0.271145      -0.62
 O       0.693474    -0.277505     0.846519     135.38
 C      -0.746305    -1.953428     0.040168      39.50
 H      -0.624691    -2.299458     1.134607      19.81
 C      -1.827503    -1.863129    -2.155392      35.25
 C      -2.504189    -2.453285    -3.336937      86.57
 H      -2.166169    -1.797410    -4.206756      25.94
 O      -2.090789    -3.874199    -3.643709     210.85
 H      -1.241043    -3.971898    -3.607268      33.06
 C      -4.054376    -2.512015    -3.158136      92.61
 H      -4.323563    -3.157400    -2.321099      26.33
 O      -4.670424    -1.279359    -2.920900     236.79
 H      -5.255507    -1.320293    -1.954587      23.89
 C      -4.829061    -3.242723    -4.383826      85.77
 O      -6.284261    -3.221124    -4.116444     282.24
 H      -6.867407    -2.890189    -4.888830      26.08
 H      -4.321479    -4.315672    -4.547073      24.49
 H      -4.520108    -2.603794    -5.255854      25.44
55
name = lig-ACN-frame_780
 C       3.921364    -0.356231     0.104320      51.41
 H       3.129602     0.041210    -0.637327      21.92
 C       4.502419    -0.447974     2.548202      50.72
 H       4.214500    -0.165636     3.559089      18.20
 C       5.656236    -1.145460     2.208777      16.93
 O       6.639549    -1.622412     3.026261     241.50
 C       6.581792    -1.235607     4.429597     117.60
 H       7.362860    -1.772459     4.847541      25.38
 H       5.491022    -1.516180     4.936726      26.59
 H       6.461364    -0.116889     4.501175      28.19
 C       5.901506    -1.471382     0.869176      27.35
 O       7.157852    -2.094235     0.389611     194.10
 H       8.090628    -1.761171     0.698066      20.81
 C       5.038501    -1.110456    -0.187943      58.42
 H       5.563050    -1.094738    -1.148746      26.04
 C       3.621903    -0.054939     1.512200      15.41
 C       2.390027     0.874132     2.021521      79.74
 H       2.516700     1.973244     2.352771      22.97
 O       1.963551     0.233764     3.351659     172.10
 H       1.725718    -0.850997     3.220312      21.16
 C       1.150982     1.128806     1.063640      82.73
 H       1.423481     1.548066     0.017005      21.74
 C      -0.003409     2.153189     1.436645     102.65
 O       0.614317     3.510058     1.545865     203.84
 H       0.688595     3.891473     0.538766      25.77
 H      -0.720318     1.857264     2.306980      24.82
 H      -0.649835     2.233126     0.575793      25.49
 C      -1.651080    -2.580011    -0.960803      55.72
 H      -1.643089    -3.546559    -0.970805      27.18
 C      -1.187555    -0.575210    -2.399944      47.65
 H      -1.652470     0.065453    -3.336255      21.93
 C      -0.226853    -0.069481    -1.602272      26.65
 O       0.517880     1.004449    -1.832767     204.52
 C      -0.088600     2.258722    -2.610997      86.98
 H      -1.201791     2.301472    -2.691315      26.91
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 H       0.561232     2.825202    -1.782775      21.75
 H       0.417812     2.233730    -3.510509      26.71
 C      -0.030101    -0.672814    -0.271399      12.23
 O       0.683506    -0.279346     0.854965     145.32
 C      -0.773919    -1.821776    -0.048221      43.51
 H      -0.398329    -2.383494     0.917690      22.04
 C      -1.935538    -1.896425    -2.154103      -3.59
 C      -2.632392    -2.547361    -3.427200      81.46
 H      -2.458731    -1.888465    -4.354312      26.57
 O      -2.067716    -3.921114    -3.655478     184.90
 H      -1.184229    -3.715480    -3.946905      28.69
 C      -4.143546    -2.501990    -3.246253     109.57
 H      -4.263333    -3.206909    -2.410545      27.36
 O      -4.602896    -1.173909    -2.930689     220.49
 H      -5.248713    -1.374122    -2.019814      24.48
 C      -4.765152    -3.078991    -4.350263     100.36
 O      -6.264314    -3.219254    -4.142553     298.67
 H      -6.483509    -3.248263    -4.983841      31.78
 H      -4.354894    -4.166397    -4.316572      25.41
 H      -4.700603    -2.713123    -5.390835      25.90
55
name = lig-ACN-frame_781
 C       3.889462    -0.322485     0.121477      48.22
 H       3.341044    -0.030984    -0.872203      22.18
 C       4.502148    -0.239493     2.488944      55.02
 H       4.237366    -0.210894     3.468741      21.00
 C       5.586869    -1.189632     2.238721       2.39
 O       6.636069    -1.575028     3.066750     220.56
 C       6.599992    -1.291974     4.447030     118.87
 H       7.417876    -1.827206     5.002656      25.92
 H       5.533781    -1.740320     4.910959      26.79
 H       6.926022    -0.273538     4.694094      28.82
 C       6.013732    -1.436364     0.832269      17.39
 O       7.119905    -2.124477     0.434163     211.98
 H       7.814666    -1.427372     0.668513      23.00
 C       5.165694    -1.067136    -0.180401      28.60
 H       5.241385    -1.501704    -1.187308      22.24
 C       3.503663     0.023942     1.407049      15.31
 C       2.361492     0.839988     2.050426      98.86
 H       3.024807     1.694982     2.301937      22.35
 O       2.008791     0.249311     3.266040     289.37
 H       1.528462    -0.533369     3.016380      27.34
 C       1.151721     1.102245     1.076782      90.92
 H       1.664717     1.557787     0.205533      23.35
 C       0.040240     2.083937     1.536740     107.88
 O       0.568569     3.427309     1.567713     268.55
 H       0.950968     3.764922     0.702936      28.25
 H      -0.401888     1.876880     2.586946      24.70
 H      -0.798391     1.927512     0.807296      25.39
 C      -1.588766    -2.510041    -1.078399      50.39
 H      -2.147283    -3.334208    -0.891746      22.45
 C      -1.324419    -0.633651    -2.374895      43.15
 H      -1.216189    -0.158933    -3.511167      22.55
 C      -0.277698     0.012102    -1.458951      -5.37
 O       0.558518     1.207809    -1.830619     216.89
 C       0.052396     2.279477    -2.525074     120.68
 H      -1.128144     2.181934    -2.440522      25.70
 H       0.090467     3.419757    -2.177451      24.44
 H       0.208542     2.382362    -3.507212      28.11
 C      -0.075399    -0.671451    -0.287745      19.73
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 O       0.659420    -0.229100     0.811930     181.22
 C      -0.801059    -1.942199    -0.091971      45.89
 H      -0.583382    -2.550574     0.902010      23.34
 C      -1.898164    -1.797695    -2.320811      40.59
 C      -2.612896    -2.539196    -3.432567      87.54
 H      -2.436413    -2.012333    -4.423839      26.66
 O      -2.122940    -3.890135    -3.678810     131.74
 H      -0.949148    -3.909480    -3.642380      23.03
 C      -4.151160    -2.546376    -3.113696      67.16
 H      -4.496989    -3.110613    -2.225667      25.75
 O      -4.529127    -1.028879    -2.920410     236.60
 H      -5.216337    -0.887027    -2.286536      28.73
 C      -4.902676    -3.151094    -4.533741      90.03
 O      -6.210652    -3.213848    -4.166983     298.46
 H      -6.896232    -3.405123    -4.810545      30.40
 H      -4.440839    -4.175312    -4.797839      24.78
 H      -4.505997    -2.382677    -5.182939      26.19
55
name = lig-ACN-frame_782
 C       3.894044    -0.323516     0.079851      62.98
 H       3.120513    -0.172799    -0.753126      23.22
 C       4.510104    -0.280080     2.392064      52.52
 H       4.367465     0.205233     3.244615      21.46
 C       5.679541    -1.075910     2.126370      32.08
 O       6.622608    -1.546295     3.087659     214.00
 C       6.629762    -1.345140     4.555204     103.04
 H       7.388422    -2.195602     4.775036      25.06
 H       5.535831    -1.514666     5.115536      25.28
 H       6.789347    -0.322573     4.795414      26.90
 C       5.982464    -1.396904     0.816442      46.83
 O       7.155570    -2.151245     0.516782     195.57
 H       8.014561    -1.896584     0.829092      18.59
 C       5.045399    -0.979824    -0.169784      61.44
 H       5.256891    -1.376494    -1.140944      21.17
 C       3.605031     0.081558     1.415906      32.33
 C       2.378658     0.851785     1.980242     102.36
 H       2.543767     1.954814     2.232060      24.66
 O       1.957554     0.276418     3.255468     282.94
 H       1.640727    -0.534263     3.145513      30.75
 C       1.243001     1.097126     1.062082      87.18
 H       1.585281     1.477656     0.134959      23.80
 C       0.112996     1.988348     1.625403     112.52
 O       0.517207     3.379420     1.606720     275.78
 H       1.071900     3.486741     0.855243      31.06
 H       0.067440     1.700114     2.687123      25.51
 H      -0.959976     1.829059     1.259402      25.47
 C      -1.604896    -2.493949    -1.144507      52.94
 H      -2.196381    -3.316289    -0.784730      23.97
 C      -1.120010    -0.420313    -2.534109      36.29
 H      -1.207470     0.152962    -3.566233      21.18
 C      -0.413531     0.101384    -1.487747     -10.96
 O       0.603796     1.232708    -1.729399     169.74
 C      -0.007643     2.383505    -2.548972      95.05
 H      -1.235665     2.398080    -2.606010      24.80
 H       0.579184     3.234594    -2.007634      23.41
 H       0.349635     2.223582    -3.440820      27.42
 C      -0.197213    -0.681664    -0.215998       0.94
 O       0.626105    -0.251624     0.786852     141.65
 C      -0.724024    -2.002397    -0.127204      53.06
 H      -0.804282    -2.487065     0.915198      21.72
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 C      -1.770291    -1.826930    -2.336495      15.04
 C      -2.615727    -2.479687    -3.427599      89.39
 H      -2.609632    -1.778039    -4.317133      26.18
 O      -2.187070    -3.864058    -3.691618      94.38
 H      -1.178061    -4.079808    -3.068963      22.55
 C      -4.200167    -2.528219    -3.173490      78.33
 H      -4.519106    -3.007572    -2.214834      25.57
 O      -4.416735    -1.024509    -2.971425     248.60
 H      -5.101066    -1.035728    -2.415685      30.51
 C      -4.843007    -3.102054    -4.514493      88.74
 O      -6.308636    -3.225633    -4.120403     216.85
 H      -6.743605    -3.083788    -5.196496      23.81
 H      -4.456188    -3.973360    -5.096199      24.67
 H      -4.945324    -2.341069    -5.271123      24.56
55
name = lig-ACN-frame_783
 C       3.770726    -0.276132     0.082147      42.73
 H       2.965689    -0.111304    -0.653982      20.28
 C       4.628463    -0.306737     2.434989      71.30
 H       4.571235    -0.015736     3.430885      23.16
 C       5.815062    -0.922778     2.167749      22.06
 O       6.605432    -1.514287     3.079631     241.61
 C       6.594269    -1.369946     4.574261     104.44
 H       7.420144    -2.137600     5.090411      24.38
 H       5.516860    -1.691789     4.953567      25.36
 H       7.045413    -0.493359     4.910198      26.31
 C       6.030783    -1.374724     0.776469      14.09
 O       7.138962    -2.186152     0.539574     164.62
 H       7.684977    -1.941433     1.321178      26.72
 C       5.052940    -1.044857    -0.266706      51.46
 H       5.362839    -1.007407    -1.273757      25.78
 C       3.667645     0.164651     1.412401      27.44
 C       2.423241     0.897143     1.944131      83.09
 H       2.772443     1.899644     2.284909      24.37
 O       1.889562     0.320868     3.277069     214.69
 H       1.871964    -0.667710     3.111726      25.20
 C       1.173206     1.026091     0.903707      96.42
 H       1.429558     1.500578     0.064126      23.56
 C       0.217284     1.871420     1.815631      99.31
 O       0.462157     3.361438     1.634960     239.21
 H       1.187208     3.637722     0.931704      27.66
 H       0.158701     1.544473     2.820230      24.22
 H      -0.746473     1.801873     1.184688      23.29
 C      -1.575669    -2.458872    -1.101837      49.82
 H      -1.946212    -3.492588    -1.381800      21.82
 C      -0.988473    -0.474414    -2.638765      47.84
 H      -1.118868     0.114382    -3.477320      23.13
 C      -0.322701     0.147998    -1.493104      16.96
 O       0.448008     1.189707    -1.608219     192.08
 C       0.072990     2.393855    -2.569429     101.31
 H      -1.090109     2.726055    -2.427346      24.99
 H       0.498572     3.280859    -2.047347      24.75
 H       0.279835     2.360418    -3.520176      27.44
 C      -0.261113    -0.603967    -0.276104      17.47
 O       0.611274    -0.320492     0.804707     166.79
 C      -0.740746    -1.930441    -0.120089      40.96
 H      -0.359570    -2.474354     0.772656      20.43
 C      -1.629976    -1.664498    -2.407013      13.68
 C      -2.624179    -2.435004    -3.456696      89.27
 H      -2.309610    -2.016017    -4.457536      26.43
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 O      -2.258641    -3.826270    -3.701470     196.98
 H      -1.451361    -3.996974    -3.051694      26.82
 C      -4.096789    -2.406719    -3.305984     105.05
 H      -4.346463    -3.196111    -2.537362      26.23
 O      -4.368572    -1.102998    -3.046591     238.42
 H      -5.226916    -0.898334    -2.396877      24.16
 C      -4.940078    -2.912161    -4.401712     101.24
 O      -6.365070    -3.268336    -4.126408     229.65
 H      -6.941268    -2.819792    -5.033277      24.52
 H      -4.404997    -3.857164    -4.471491      27.01
 H      -4.695252    -2.268346    -5.264749      27.11
55
name = lig-ACN-frame_784
 C       3.902972    -0.324274     0.143263      58.13
 H       3.274301    -0.005246    -0.637915      24.01
 C       4.680540    -0.134093     2.520114      47.09
 H       4.187366    -0.212059     3.487651      20.54
 C       5.833407    -0.903218     2.102629      -5.26
 O       6.735240    -1.531790     3.119826     213.44
 C       6.553150    -1.376352     4.516026      98.73
 H       7.278676    -2.368202     4.815805      23.61
 H       5.499402    -1.528489     4.913140      27.92
 H       6.736743    -0.394026     4.846920      27.99
 C       6.011671    -1.324078     0.704150       8.28
 O       7.076794    -2.181535     0.536967     156.56
 H       7.731872    -2.218439     1.335126      26.73
 C       5.044223    -1.001999    -0.257032      57.99
 H       5.177663    -1.453982    -1.236937      23.20
 C       3.677700     0.128403     1.483200      28.51
 C       2.433088     0.871517     1.955178     103.07
 H       2.711546     1.925393     2.108234      25.13
 O       1.913498     0.387032     3.214873     217.84
 H       1.605234    -0.717880     3.111399      21.51
 C       1.213373     0.985148     1.061876     100.47
 H       1.372449     1.366034     0.143010      24.19
 C       0.193608     1.884357     1.772009     111.17
 O       0.418872     3.335934     1.724342     263.37
 H       1.110750     3.373004     0.951918      28.16
 H       0.365840     1.724979     2.753480      25.46
 H      -0.924414     1.510218     1.752559      24.91
 C      -1.472412    -2.352344    -1.266685      53.77
 H      -1.714596    -3.453502    -0.855655      20.31
 C      -0.924566    -0.543047    -2.626964      53.08
 H      -0.744295    -0.185612    -3.523847      25.03
 C      -0.265009     0.034223    -1.566002      11.91
 O       0.329626     1.356762    -1.602627     222.74
 C       0.156008     2.359110    -2.482749     111.82
 H      -1.039737     2.483998    -2.553367      24.63
 H       0.765958     3.173653    -2.178700      26.44
 H       0.463388     2.048735    -3.389113      27.74
 C      -0.208882    -0.593473    -0.257114      10.71
 O       0.613774    -0.322943     0.781983     170.04
 C      -0.806633    -1.850623    -0.136815      52.71
 H      -0.389360    -2.496404     0.587444      23.38
 C      -1.741693    -1.746449    -2.454472      43.61
 C      -2.389745    -2.361503    -3.646360      80.11
 H      -2.293611    -1.720355    -4.587926      26.47
 O      -2.294156    -3.834841    -3.668765     231.54
 H      -1.478404    -4.065042    -3.586150      33.47
 C      -4.065137    -2.349649    -3.233232      62.11
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 H      -4.105439    -2.790185    -2.208155      25.03
 O      -4.410638    -0.933546    -3.036089     182.25
 H      -5.326718    -1.090069    -2.330544      22.92
 C      -4.991840    -2.940783    -4.439910      98.09
 O      -6.369013    -3.233038    -4.131513     312.22
 H      -7.005873    -2.772040    -4.627924      31.56
 H      -4.629191    -3.871326    -4.810433      26.69
 H      -5.023616    -2.320811    -5.408752      25.77
55
name = lig-ACN-frame_785
 C       3.996737    -0.263718     0.203319      52.99
 H       3.196545    -0.106785    -0.448935      24.07
 C       4.704288    -0.107419     2.501161      63.10
 H       4.632821     0.224399     3.620563      22.02
 C       5.779386    -0.905391     2.175724      23.32
 O       6.822715    -1.505820     2.974066     211.60
 C       6.475263    -1.381320     4.451293     111.70
 H       7.245236    -2.052921     5.237797      24.67
 H       5.470836    -1.682705     4.587280      28.67
 H       6.777349    -0.415447     4.857364      27.41
 C       6.043299    -1.299338     0.846385      27.08
 O       7.014573    -2.199662     0.453429     192.07
 H       7.754246    -2.041193     1.070132      23.95
 C       5.124467    -1.029230    -0.191365      50.72
 H       5.019368    -1.581486    -1.153119      22.65
 C       3.723459     0.070345     1.535710      33.76
 C       2.434041     0.839189     1.984746     101.04
 H       2.689599     1.880504     2.190364      25.10
 O       2.002577     0.383813     3.242665     235.04
 H       1.365814    -0.537578     3.009511      22.02
 C       1.204923     1.035814     1.073128      89.80
 H       1.675552     1.551609     0.285400      23.61
 C       0.101099     1.901848     1.897337      98.73
 O       0.404397     3.303142     1.746830     287.32
 H       0.603279     3.679626     0.923539      30.61
 H       0.149649     1.677717     2.891784      25.18
 H      -0.980908     1.761374     1.369973      23.07
 C      -1.467750    -2.470113    -1.267563      40.33
 H      -2.212608    -3.460875    -1.284099      18.56
 C      -0.919869    -0.580517    -2.702259      53.01
 H      -0.901693    -0.140696    -3.623051      25.21
 C      -0.211419     0.083290    -1.562637       4.78
 O       0.305390     1.357696    -1.449107     189.80
 C       0.158997     2.348249    -2.621819     120.86
 H      -0.809579     2.833714    -2.880359      26.73
 H       0.709021     3.111337    -2.187006      27.33
 H       0.568261     1.995212    -3.445884      29.33
 C      -0.112409    -0.599881    -0.288203      17.91
 O       0.679956    -0.293230     0.849453     186.90
 C      -0.811214    -1.803771    -0.211187      57.23
 H      -0.997878    -2.270069     0.703977      24.71
 C      -1.642330    -1.770750    -2.570052      22.69
 C      -2.488753    -2.381407    -3.686704      81.01
 H      -2.208826    -1.994530    -4.732812      25.83
 O      -2.252054    -3.835151    -3.704417     198.28
 H      -1.389156    -3.991471    -4.097921      28.90
 C      -4.007933    -2.208798    -3.300618      65.48
 H      -4.115374    -2.908139    -2.439746      24.40
 O      -4.482620    -0.763973    -3.010646     237.07
 H      -5.239089    -0.698799    -2.281152      24.19
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 C      -4.958354    -3.029226    -4.511856      83.15
 O      -6.395078    -3.198681    -4.046266     308.64
 H      -6.727255    -2.472674    -4.496845      31.12
 H      -4.453466    -3.834922    -4.905998      27.53
 H      -4.939324    -2.040647    -5.107530      25.14
55
name = lig-ACN-frame_786
 C       3.938835    -0.233666     0.211930      63.58
 H       3.196596    -0.235214    -0.573951      22.69
 C       4.764150    -0.161954     2.589504      53.81
 H       4.767443     0.654764     3.481039      21.62
 C       5.885537    -0.969669     2.183651      12.04
 O       6.859020    -1.434031     2.994833     224.77
 C       6.462418    -1.373483     4.350868      99.01
 H       7.292992    -2.197611     4.844986      24.08
 H       5.500201    -1.717618     4.485133      29.63
 H       6.333685    -0.316360     4.694534      25.55
 C       6.033042    -1.377812     0.847139      27.57
 O       7.038951    -2.225006     0.410654     195.95
 H       7.923348    -1.961570     0.657293      20.62
 C       5.097832    -1.013821    -0.081756      59.44
 H       5.582842    -1.233382    -1.089028      26.39
 C       3.704666     0.152289     1.538945       9.38
 C       2.485427     0.905452     2.056592      95.00
 H       2.922303     1.858129     2.277010      25.47
 O       2.067258     0.307051     3.384544     209.32
 H       1.640967    -0.601153     3.193038      25.19
 C       1.201301     1.127841     1.138057      80.80
 H       1.197696     1.607781     0.142363      19.20
 C       0.075345     1.919056     1.846811      99.97
 O       0.390314     3.357195     1.821374     274.78
 H       0.131474     3.439052     0.861058      27.36
 H      -0.306056     1.635887     2.811900      25.09
 H      -0.913785     1.656637     1.221444      23.19
 C      -1.550879    -2.477121    -1.358789      42.34
 H      -2.182087    -3.495051    -1.057028      19.42
 C      -0.843458    -0.459174    -2.703928      62.54
 H      -1.234819     0.249355    -3.450553      21.59
 C      -0.226526     0.095888    -1.571711      -0.62
 O       0.249882     1.399083    -1.451129     210.83
 C       0.233897     2.332301    -2.717810     107.06
 H      -0.783544     2.305466    -2.845178      27.31
 H       0.670692     3.237755    -2.458370      27.48
 H       0.718580     1.916292    -3.533670      29.04
 C      -0.049309    -0.695319    -0.359852     -10.48
 O       0.714444    -0.264866     0.841887     130.27
 C      -0.882688    -1.913137    -0.227973      41.12
 H      -0.947637    -2.081518     0.818531      21.28
 C      -1.420544    -1.812559    -2.597543      18.75
 C      -2.562147    -2.401819    -3.652193      77.22
 H      -2.405974    -1.833340    -4.660570      25.73
 O      -2.250289    -3.838303    -3.779970      94.08
 H      -1.114903    -3.812545    -4.116385      23.73
 C      -4.113857    -2.176623    -3.399761      89.45
 H      -4.353253    -2.615948    -2.409218      25.18
 O      -4.459398    -0.751562    -3.079271     314.29
 H      -4.961506    -0.897108    -2.388533      30.97
 C      -4.923029    -2.818249    -4.431941     106.41
 O      -6.291549    -3.162891    -4.002592     207.58
 H      -7.098414    -2.385224    -4.212241      26.84
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 H      -4.606999    -3.792998    -4.542746      28.67
 H      -4.972401    -2.547342    -5.596739      25.03
55
name = lig-ACN-frame_787
 C       3.861589    -0.305425     0.238568      42.69
 H       3.210586     0.197591    -0.544815      20.85
 C       4.782232    -0.155067     2.462500      61.44
 H       4.667998     0.017596     3.681022      20.64
 C       5.888345    -0.960485     2.150149       9.79
 O       6.935240    -1.359863     3.042030     231.49
 C       6.432531    -1.415769     4.378899     117.38
 H       7.343758    -1.890875     5.139303      25.40
 H       5.616487    -2.000162     4.461681      29.22
 H       6.409358    -0.425076     4.968033      25.34
 C       6.022350    -1.476466     0.810630       8.62
 O       7.125230    -2.267466     0.370425     187.99
 H       7.967532    -1.779451     0.708953      26.95
 C       5.060869    -0.930278    -0.118259      39.23
 H       5.139897    -0.958019    -1.254644      18.76
 C       3.784095     0.193922     1.611782      27.56
 C       2.489452     0.988569     2.192213      89.27
 H       2.540368     1.943788     2.543739      26.88
 O       2.130762     0.261049     3.475676     247.36
 H       2.025853    -0.573254     3.274211      31.61
 C       1.220730     1.132755     1.241681      52.87
 H       1.812082     1.709773     0.394674      20.93
 C      -0.009203     1.926357     1.785462      97.71
 O       0.330420     3.369624     1.864014     233.46
 H       0.244477     4.095582     1.113030      26.44
 H      -0.008129     1.578246     2.841381      23.85
 H      -0.912160     1.773848     1.082459      23.09
 C      -1.501465    -2.380211    -1.346709      36.81
 H      -2.133651    -3.392889    -1.380012      19.94
 C      -0.875367    -0.458779    -2.648977      42.67
 H      -1.061868     0.260360    -3.625013      19.53
 C      -0.166610     0.093937    -1.570416       1.23
 O       0.233757     1.501008    -1.564969     219.90
 C       0.230068     2.207983    -2.747992     128.99
 H      -0.603662     2.363387    -3.274669      28.90
 H       0.547717     3.185690    -2.448263      26.28
 H       0.892914     1.684564    -3.411725      28.17
 C      -0.033602    -0.767008    -0.303566      13.92
 O       0.661169    -0.317348     0.731487     140.41
 C      -0.834946    -1.897685    -0.184895      65.71
 H      -0.820904    -2.738295     0.519708      22.86
 C      -1.480190    -1.800643    -2.640497      32.24
 C      -2.432003    -2.315113    -3.650878      73.48
 H      -2.317687    -1.771244    -4.665847      25.49
 O      -2.279479    -3.792312    -3.893873     114.71
 H      -1.145564    -4.055800    -3.564343      22.93
 C      -4.138129    -2.124295    -3.300537      67.13
 H      -4.443939    -2.837657    -2.499421      25.67
 O      -4.375652    -0.774906    -3.208057     306.30
 H      -5.002257    -0.483575    -2.577494      28.71
 C      -4.985654    -2.790912    -4.452136     100.65
 O      -6.233252    -3.107758    -3.950822     237.47
 H      -6.866889    -2.194460    -4.043324      26.95
 H      -4.410735    -3.638247    -4.402573      28.80
 H      -4.821764    -2.317036    -5.554335      25.99
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name = lig-ACN-frame_788
 C       3.862784    -0.216722     0.349744      44.91
 H       3.075847     0.071337    -0.487216      21.72
 C       4.829220    -0.195990     2.474996      43.05
 H       4.498398    -0.167554     3.637714      22.41
 C       5.943536    -1.021814     2.058315       5.41
 O       6.939596    -1.266984     3.034611     167.18
 C       6.471338    -1.470081     4.570859      92.79
 H       7.440240    -1.969488     5.102663      24.86
 H       5.671931    -2.128130     4.577892      28.26
 H       5.984183    -0.466367     4.827008      23.42
 C       6.030264    -1.458710     0.691395      11.48
 O       7.151295    -2.235935     0.343958     171.77
 H       7.962231    -2.050274     0.966409      24.82
 C       5.036234    -0.947449    -0.214285      47.91
 H       5.125396    -1.384233    -1.237987      20.61
 C       3.695925     0.263595     1.622217      16.93
 C       2.418302     0.893431     2.346364     106.53
 H       2.782740     1.792526     2.498425      27.66
 O       2.196262     0.258428     3.548608     273.92
 H       1.825396    -0.629801     3.300260      27.51
 C       1.266798     1.068468     1.198470      72.38
 H       1.694208     1.603946     0.197723      20.50
 C       0.029248     1.982242     1.717926     101.25
 O       0.266467     3.383203     1.969684     294.14
 H       0.436043     3.559318     1.042781      29.65
 H      -0.480204     1.627007     2.730241      23.60
 H      -0.912640     1.780631     1.161645      24.44
 C      -1.454428    -2.365060    -1.349218      76.15
 H      -1.977492    -3.354916    -1.173458      23.21
 C      -0.908480    -0.485086    -2.645113      47.64
 H      -0.721538    -0.002615    -3.774558      20.24
 C      -0.166643     0.057181    -1.557645      20.87
 O       0.193673     1.426636    -1.537475     223.73
 C       0.279184     2.152554    -2.899356     112.58
 H      -0.666925     2.230316    -3.238734      27.57
 H       0.678648     3.151118    -2.656772      26.38
 H       0.996443     1.747749    -3.602819      27.84
 C      -0.070289    -0.580680    -0.344228       5.06
 O       0.740711    -0.311830     0.803401     146.07
 C      -0.737547    -1.959055    -0.248331      42.63
 H      -0.429015    -2.474491     0.735372      18.78
 C      -1.618386    -1.634780    -2.545002      37.68
 C      -2.457832    -2.287692    -3.699185      74.68
 H      -2.172350    -1.734815    -4.665030      25.60
 O      -2.268391    -3.694725    -3.991409     223.44
 H      -1.665962    -4.156954    -3.324050      27.83
 C      -3.964196    -2.172252    -3.310359      75.18
 H      -4.054591    -2.432446    -2.235137      24.49
 O      -4.291266    -0.655317    -3.311829     160.33
 H      -5.156237    -0.645634    -2.538290      22.07
 C      -4.818977    -2.881208    -4.425871      91.61
 O      -6.309154    -3.037391    -3.920155     292.20
 H      -6.608063    -2.217005    -3.902509      35.44
 H      -4.698420    -3.683422    -5.106826      26.93
 H      -5.063006    -1.964948    -5.087261      25.64
55
name = lig-ACN-frame_789
 C       3.934163    -0.142969     0.234111      36.42
 H       2.950672    -0.271320    -0.415733      22.62
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 C       4.758630    -0.279382     2.510963      68.85
 H       4.932062     0.146820     3.557587      24.22
 C       5.867869    -0.960567     2.074298      11.08
 O       6.910574    -1.257895     3.093505     177.91
 C       6.486603    -1.486945     4.501588     114.97
 H       7.501090    -1.655655     5.030562      27.46
 H       5.876595    -2.393762     4.621389      27.58
 H       6.176182    -0.595080     5.176577      25.02
 C       6.102339    -1.332955     0.677662      13.65
 O       7.118761    -2.185043     0.283688     190.08
 H       7.739695    -2.193372     1.012199      21.02
 C       4.979652    -1.028201    -0.160497      44.37
 H       4.915357    -1.324261    -1.196537      25.49
 C       3.750227     0.141322     1.698461      24.42
 C       2.483871     0.842381     2.216218      90.53
 H       2.556935     1.749655     2.538325      28.10
 O       2.168680     0.214531     3.649638     161.39
 H       1.468603    -0.670031     3.588226      23.41
 C       1.213217     1.039122     1.251800      85.99
 H       1.686139     1.587467     0.264103      21.70
 C       0.024856     1.911723     1.735553      96.17
 O       0.241104     3.373778     1.974516     286.55
 H       0.839487     3.843714     1.434554      32.00
 H      -0.368064     1.293495     2.684437      23.84
 H      -0.540337     1.921375     0.815482      24.43
 C      -1.480313    -2.445071    -1.272764      59.92
 H      -1.885790    -3.410048    -1.141330      23.47
 C      -0.870609    -0.453451    -2.689241      52.66
 H      -0.986908     0.257341    -3.685785      20.33
 C      -0.257952     0.138384    -1.582105       1.99
 O       0.245361     1.396768    -1.598019     191.39
 C       0.327451     2.112067    -2.933484      89.83
 H      -0.687973     2.194764    -3.290782      25.60
 H       0.760542     3.161081    -2.756358      24.07
 H       0.727412     1.377390    -3.698996      26.15
 C      -0.090994    -0.587371    -0.261739      18.08
 O       0.810641    -0.261999     0.885627     158.49
 C      -0.501763    -1.821870    -0.308482      48.07
 H      -0.501238    -2.453890     0.675199      20.90
 C      -1.713148    -1.659764    -2.457455      13.32
 C      -2.433462    -2.212407    -3.714428      87.93
 H      -2.361565    -1.547609    -4.649513      26.37
 O      -2.221003    -3.624455    -4.064583     255.52
 H      -1.856580    -3.944705    -3.375360      35.30
 C      -3.844788    -2.155940    -3.387614      83.78
 H      -4.022383    -2.599917    -2.393041      25.59
 O      -4.226856    -0.635351    -3.392533     174.30
 H      -5.102915    -0.659587    -2.627073      22.05
 C      -4.908904    -2.778730    -4.359171      88.40
 O      -6.272959    -3.001419    -3.903972     290.71
 H      -6.654926    -2.105252    -3.797223      31.97
 H      -4.448488    -3.750490    -4.730606      26.15
 H      -4.792475    -2.000278    -5.192052      26.89
55
name = lig-ACN-frame_790
 C       3.904556    -0.241123     0.280116      63.65
 H       3.154479     0.189650    -0.511888      23.55
 C       4.719847    -0.270493     2.597239      63.60
 H       4.540781     0.088665     3.596897      26.12
 C       5.917905    -0.940633     2.171821      30.05
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 O       6.851651    -1.263186     3.070669     221.98
 C       6.580613    -1.502993     4.420992     128.61
 H       7.529630    -1.703816     4.892206      29.38
 H       5.932986    -2.447518     4.484169      27.09
 H       5.894384    -0.675269     4.794210      24.54
 C       6.062711    -1.259552     0.787466      34.96
 O       7.051289    -2.104466     0.232391     162.01
 H       7.909708    -2.115400     0.691228      18.73
 C       5.007074    -1.030428    -0.124859      54.67
 H       5.142293    -1.428231    -1.086957      25.90
 C       3.716441     0.047230     1.572297      26.98
 C       2.477428     0.814716     2.251745      97.29
 H       2.914248     1.682960     2.410163      28.48
 O       2.104827     0.216503     3.636049     168.53
 H       1.640473    -0.770337     3.249688      23.34
 C       1.323319     1.059731     1.312466      78.92
 H       1.814979     1.716014     0.405693      22.95
 C       0.050430     1.889215     1.667056     102.12
 O       0.238821     3.303517     2.037996     242.79
 H       1.089758     3.502360     1.451658      28.92
 H      -0.636714     1.651534     2.662718      23.32
 H      -0.719445     1.736996     0.983011      26.92
 C      -1.398251    -2.365690    -1.239552      65.85
 H      -1.801329    -3.253790    -1.073891      26.25
 C      -0.990473    -0.492306    -2.589919      51.66
 H      -1.398745     0.100957    -3.494102      20.57
 C      -0.286897     0.207970    -1.489863      15.32
 O       0.374907     1.477653    -1.682169     233.13
 C       0.279867     2.011985    -2.931127     100.15
 H      -0.688207     2.545980    -3.277290      24.28
 H       1.084760     2.884364    -2.794870      24.59
 H       0.913554     1.448328    -3.685791      26.05
 C       0.034935    -0.478542    -0.293640       4.22
 O       0.749255    -0.276954     0.844382     147.10
 C      -0.542671    -1.947824    -0.259811      40.72
 H      -0.073561    -2.632823     0.554726      21.11
 C      -1.547746    -1.724166    -2.510470      38.18
 C      -2.385643    -2.167953    -3.707796      65.77
 H      -1.917561    -1.556238    -4.515708      26.25
 O      -2.117967    -3.540824    -4.137176     196.44
 H      -1.427988    -4.109514    -3.504072      25.45
 C      -4.087120    -2.011799    -3.393158      82.68
 H      -4.215722    -2.542449    -2.442901      26.48
 O      -4.176500    -0.680763    -3.392008     317.14
 H      -4.855123    -0.304255    -2.848158      28.93
 C      -4.918032    -2.694692    -4.406348     105.72
 O      -6.195675    -2.943478    -3.867643     197.90
 H      -6.869816    -2.005649    -3.774832      27.31
 H      -4.555293    -3.776106    -4.288225      26.62
 H      -5.025257    -2.490442    -5.480041      26.72
55
name = lig-ACN-frame_791
 C       3.823866    -0.368158     0.239015      34.87
 H       3.296037     0.107861    -0.633302      22.19
 C       4.637491    -0.267500     2.579753      80.78
 H       4.310865    -0.361864     3.532018      26.65
 C       5.825852    -0.895842     2.218482      21.44
 O       6.973815    -1.309260     2.982363     198.70
 C       6.575416    -1.542959     4.400411     120.15
 H       7.408273    -1.565301     4.964505      31.54
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 H       5.994769    -2.579644     4.513520      26.49
 H       6.059839    -0.713122     4.909870      25.16
 C       6.008552    -1.320349     0.865409      10.32
 O       7.020300    -2.015501     0.226386     162.26
 H       7.936841    -1.689367     0.587001      23.67
 C       5.072343    -0.966573    -0.100407      33.43
 H       5.317346    -1.269980    -1.081140      22.93
 C       3.623383     0.019635     1.692331      15.88
 C       2.515183     0.794715     2.350583     114.16
 H       2.815784     1.702015     2.696601      27.98
 O       2.039103     0.238964     3.479579     272.31
 H       1.807658    -0.773455     3.426175      26.36
 C       1.313260     1.087926     1.265957      74.89
 H       1.807962     1.514055     0.276969      22.80
 C      -0.000396     1.886853     1.732552     104.34
 O       0.323228     3.217423     2.053846     283.22
 H       0.788273     3.746886     1.283724      28.26
 H      -0.270546     1.108851     2.643839      23.36
 H      -0.559519     1.865131     0.876743      26.63
 C      -1.313428    -2.462528    -1.273735      48.90
 H      -1.705673    -3.340767    -1.156292      24.88
 C      -1.069322    -0.313815    -2.418024      75.59
 H      -1.130872     0.258449    -3.304322      20.78
 C      -0.231145     0.226090    -1.460145      13.86
 O       0.425058     1.431710    -1.630133     196.76
 C       0.387997     2.083721    -3.059764      57.91
 H      -0.790561     2.351566    -3.137726      22.61
 H       1.075741     3.087125    -3.031016      22.50
 H       0.299377     1.275490    -3.888006      24.23
 C       0.036504    -0.657468    -0.355225      20.56
 O       0.754909    -0.227519     0.818081     167.92
 C      -0.508959    -1.835394    -0.179890      53.94
 H      -0.206147    -2.480782     0.674136      22.32
 C      -1.444054    -1.767352    -2.486814      20.68
 C      -2.406334    -2.237455    -3.634353      88.43
 H      -2.492746    -1.463571    -4.427941      25.52
 O      -2.024446    -3.502797    -4.209286     145.62
 H      -0.878965    -3.650325    -3.828171      21.46
 C      -4.005339    -1.985398    -3.435860      64.45
 H      -4.443793    -2.280535    -2.492515      25.84
 O      -4.173312    -0.455001    -3.368443     285.85
 H      -4.853097    -0.449272    -2.811713      29.96
 C      -4.902657    -2.828380    -4.480435      88.54
 O      -6.277477    -2.882986    -3.804364     199.72
 H      -6.658235    -1.884279    -4.046448      27.15
 H      -4.395175    -3.870737    -4.673632      26.26
 H      -4.842142    -2.286279    -5.433886      27.96
55
name = lig-ACN-frame_792
 C       3.766623    -0.352062     0.324321      68.12
 H       2.918285    -0.369956    -0.305443      23.66
 C       4.603548    -0.400670     2.651996      40.60
 H       4.540627    -0.056729     3.594736      23.53
 C       5.855001    -0.988399     2.164214       1.32
 O       7.008081    -1.328814     3.009317     179.48
 C       6.634895    -1.563317     4.389494     123.25
 H       7.432258    -1.699065     4.892424      33.00
 H       5.970324    -2.589691     4.409979      24.07
 H       5.994086    -0.785656     4.740585      23.70
 C       5.962264    -1.337883     0.802017      18.98
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 O       7.087346    -1.934759     0.292073     170.63
 H       7.956645    -1.849434     0.834079      23.80
 C       4.987925    -0.895282    -0.097379      55.85
 H       5.200236    -0.894453    -1.162101      23.13
 C       3.587706    -0.021751     1.625275      15.88
 C       2.382657     0.872664     2.183645      89.49
 H       2.717557     1.847085     2.410939      28.06
 O       1.918628     0.182577     3.498045     235.66
 H       1.595023    -0.605251     3.211050      31.49
 C       1.260646     1.091488     1.136754     102.96
 H       1.688598     1.817310     0.345699      23.38
 C       0.108461     1.796790     1.709115     110.67
 O       0.419584     3.211819     2.119789     302.49
 H       0.338237     3.582476     1.282282      31.74
 H      -0.515252     1.470877     2.727259      23.25
 H      -0.738227     1.757159     1.144790      27.22
 C      -1.171231    -2.563375    -1.278391      53.32
 H      -1.455680    -3.536555    -1.253497      23.28
 C      -1.127290    -0.294114    -2.450243      39.27
 H      -1.418089     0.288170    -3.200558      21.41
 C      -0.126418     0.181391    -1.465721       6.83
 O       0.510981     1.428418    -1.649782     184.90
 C       0.309796     2.066281    -3.021643      69.47
 H      -0.699022     2.817434    -3.116001      21.58
 H       1.259399     2.803028    -3.044279      24.19
 H       0.749604     1.332638    -3.896282      23.88
 C       0.115571    -0.551418    -0.247169      12.79
 O       0.824507    -0.235185     0.825372     185.66
 C      -0.568594    -1.950212    -0.195446      36.95
 H      -0.677187    -2.248630     0.816812      22.56
 C      -1.528273    -1.629034    -2.386585      23.96
 C      -2.395756    -2.130498    -3.620881      86.14
 H      -2.032248    -1.455971    -4.368328      25.67
 O      -1.946004    -3.481117    -4.237352     127.59
 H      -0.842206    -3.415162    -4.331036      25.12
 C      -3.883537    -2.081198    -3.392625      56.79
 H      -4.124020    -2.434631    -2.387227      25.74
 O      -4.192720    -0.334039    -3.389673     111.90
 H      -4.981370    -0.212636    -2.665392      22.76
 C      -4.898899    -2.782658    -4.430674      92.49
 O      -6.281087    -2.825770    -3.861008     279.08
 H      -6.651115    -2.096077    -4.125911      35.23
 H      -4.662567    -3.936068    -4.723109      26.41
 H      -5.052413    -2.276289    -5.324090      29.20
55
name = lig-ACN-frame_793
 C       3.680964    -0.345770     0.366422      35.86
 H       2.919225    -0.171343    -0.320502      24.10
 C       4.645100    -0.462036     2.608014      63.15
 H       4.603325     0.016661     3.535219      27.41
 C       5.820127    -1.102489     2.199399      17.34
 O       6.936336    -1.314112     2.989672     213.46
 C       6.661683    -1.600613     4.380174     123.28
 H       7.467371    -1.711462     4.888137      33.81
 H       5.963944    -2.608836     4.501096      25.51
 H       6.175376    -0.823714     4.889650      25.33
 C       6.000447    -1.276359     0.734477       4.47
 O       7.172336    -1.878545     0.313980     117.37
 H       7.669989    -2.090155     1.092920      20.51
 C       4.918634    -0.881700    -0.169025      36.53
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 H       5.060904    -1.134603    -1.265996      21.70
 C       3.571252    -0.025432     1.786735      21.41
 C       2.350443     0.817139     2.139030      95.99
 H       2.747178     1.811114     2.452715      27.17
 O       1.800187     0.235671     3.425257     253.64
 H       1.389087    -0.587017     3.310325      30.87
 C       1.242681     1.098923     1.088053      99.20
 H       1.558071     1.479504     0.120924      23.94
 C       0.024634     1.873853     1.800461     103.59
 O       0.479972     3.173375     2.139227     291.30
 H       0.575915     3.887003     1.449744      29.95
 H       0.107693     1.170301     2.824999      21.43
 H      -0.724831     1.809160     1.121961      27.70
 C      -1.111462    -2.482312    -1.365200      47.65
 H      -1.332106    -3.565432    -1.418889      22.35
 C      -1.068291    -0.324945    -2.414045      53.96
 H      -1.592732     0.277380    -3.030367      23.23
 C      -0.092629     0.170971    -1.492653       9.61
 O       0.556694     1.402826    -1.715848     203.88
 C       0.372773     2.068816    -2.887630      78.36
 H      -0.794889     2.645428    -3.046785      22.40
 H       1.199109     2.888832    -2.914158      23.65
 H       0.092249     1.308418    -3.864475      22.24
 C      -0.011091    -0.618938    -0.279180      13.87
 O       0.910253    -0.305963     0.819428     138.41
 C      -0.533111    -1.881836    -0.136027      54.20
 H      -0.371891    -2.542570     0.652027      23.69
 C      -1.645498    -1.666840    -2.328700      30.87
 C      -2.221522    -2.029370    -3.704388      83.86
 H      -2.165040    -1.266494    -4.434250      27.30
 O      -1.929875    -3.382993    -4.196399     250.68
 H      -1.066630    -3.496988    -4.275700      33.09
 C      -3.905791    -2.011004    -3.380813      67.30
 H      -4.014977    -2.375638    -2.349427      27.02
 O      -4.185417    -0.480540    -3.408151     203.15
 H      -5.052767    -0.344612    -2.608120      21.62
 C      -4.913004    -2.620846    -4.344188     107.77
 O      -6.241060    -2.796021    -3.928587     262.41
 H      -6.807024    -1.955414    -4.116744      29.43
 H      -4.453032    -3.765937    -4.371649      26.25
 H      -4.665786    -2.213700    -5.249171      29.64
55
name = lig-ACN-frame_794
 C       3.752939    -0.360309     0.374074      63.24
 H       3.098645     0.139534    -0.294738      25.14
 C       4.623950    -0.383536     2.640801      57.43
 H       4.587620    -0.513591     3.728435      25.55
 C       5.710470    -1.110778     2.085755      -0.60
 O       6.870919    -1.331518     2.970189     154.90
 C       6.641654    -1.617947     4.418560     118.62
 H       7.611065    -1.769915     4.790406      30.98
 H       6.007784    -2.653769     4.533807      25.54
 H       6.201329    -0.819496     4.936263      23.85
 C       5.982599    -1.237115     0.729766      28.32
 O       7.145923    -1.810191     0.272522     173.95
 H       7.868760    -2.011851     0.926182      20.00
 C       4.907564    -0.940130    -0.119202      57.30
 H       4.894720    -1.250800    -1.227720      23.42
 C       3.570448    -0.105217     1.724812      26.13
 C       2.431617     0.779431     2.306996      96.52
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 H       2.768150     1.826543     2.617073      26.42
 O       1.660056     0.355122     3.347607     242.91
 H       1.641764    -0.723528     3.199166      25.53
 C       1.222510     1.029252     1.096970      79.72
 H       1.639694     1.665896     0.373118      25.78
 C       0.075096     1.870953     1.804978     105.74
 O       0.525030     3.199684     2.214192     268.13
 H       1.032420     3.373419     1.275322      27.07
 H      -0.374851     1.405171     2.860192      23.75
 H      -0.903808     1.965919     1.460348      26.35
 C      -1.185293    -2.451299    -1.314938      58.15
 H      -1.257663    -3.636375    -1.330122      22.99
 C      -1.123773    -0.315971    -2.395021      57.59
 H      -1.129145     0.390732    -3.245656      20.51
 C      -0.146820     0.157768    -1.436253      14.05
 O       0.619250     1.264012    -1.637186     191.34
 C       0.303961     2.139652    -2.894848      65.36
 H      -0.683149     2.739161    -2.433183      22.52
 H       1.092734     2.860974    -3.123342      26.03
 H       0.415934     1.381658    -3.942316      22.46
 C       0.033562    -0.590869    -0.246371      19.33
 O       0.861942    -0.382282     0.728426     168.31
 C      -0.505096    -1.941989    -0.237591      48.20
 H       0.111724    -2.459204     0.417087      24.53
 C      -1.514728    -1.600377    -2.463091      33.89
 C      -2.349040    -2.009563    -3.703227      97.44
 H      -2.021891    -1.309839    -4.436065      28.69
 O      -1.934871    -3.277039    -4.161307     264.06
 H      -1.146980    -3.486941    -3.748069      31.65
 C      -3.848945    -1.878934    -3.358830     104.02
 H      -4.050303    -2.340866    -2.373692      26.90
 O      -4.177688    -0.612738    -3.378033     246.37
 H      -5.110648    -0.463697    -2.724615      21.70
 C      -4.735420    -2.592768    -4.335312      83.94
 O      -6.250023    -2.740019    -3.980026     162.82
 H      -6.606159    -1.637469    -4.147101      26.97
 H      -4.390173    -3.741448    -4.512327      25.78
 H      -4.855612    -2.133075    -5.246076      29.09
55
name = lig-ACN-frame_795
 C       3.795480    -0.284824     0.356497      36.89
 H       3.011319    -0.158094    -0.431686      26.74
 C       4.560853    -0.481493     2.656117      74.93
 H       4.154665    -0.231247     3.722457      25.63
 C       5.779025    -1.000671     2.186054      36.89
 O       6.787000    -1.393531     2.962735     210.66
 C       6.600191    -1.611315     4.360962     124.52
 H       7.625629    -1.688846     4.946280      27.31
 H       5.961095    -2.580609     4.562026      25.85
 H       6.052899    -0.818355     4.875237      24.10
 C       5.963712    -1.292645     0.758688      16.80
 O       7.096634    -1.757916     0.150905     138.00
 H       7.917725    -1.585146     0.769848      21.93
 C       4.916868    -1.031604    -0.141368      34.14
 H       5.198490    -1.096364    -1.257741      23.09
 C       3.542715    -0.055624     1.759924      11.31
 C       2.337740     0.836406     2.202398      94.44
 H       2.938155     1.781365     2.478435      25.96
 O       1.576502     0.341133     3.448339     174.23
 H       1.372060    -0.816624     3.394934      23.21
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 C       1.275699     1.018529     1.263610     102.56
 H       1.522395     1.456377     0.371236      25.64
 C       0.047436     1.835605     1.843869      96.03
 O       0.612177     3.187452     2.233240     280.48
 H       1.242540     3.688283     1.637485      30.13
 H      -0.273306     1.319567     2.843736      23.00
 H      -0.463604     1.885935     0.921353      26.18
 C      -1.305169    -2.463818    -1.372056      35.63
 H      -1.729062    -3.645679    -1.399978      21.34
 C      -1.080077    -0.192277    -2.456987      42.51
 H      -1.285052     0.301162    -3.536102      18.89
 C      -0.247499     0.210316    -1.391577       6.85
 O       0.719442     1.228362    -1.631329     165.94
 C       0.295562     2.143143    -2.767491      82.36
 H      -0.748949     2.826868    -2.925451      23.49
 H       1.131539     2.738353    -2.652346      26.68
 H       0.056568     1.567550    -3.931450      21.40
 C       0.000046    -0.665309    -0.301833      17.80
 O       0.910528    -0.306494     0.770398     136.17
 C      -0.381113    -1.990357    -0.350788      56.54
 H      -0.348854    -2.686993     0.470880      23.39
 C      -1.457691    -1.612848    -2.510832      14.53
 C      -2.354891    -1.930865    -3.642185      90.27
 H      -2.442985    -1.217648    -4.447351      27.41
 O      -1.950065    -3.293855    -4.160822     108.96
 H      -1.210844    -3.701781    -3.377478      24.44
 C      -3.832486    -2.080398    -3.307776      55.72
 H      -3.925541    -2.520946    -2.295069      26.23
 O      -4.218569    -0.413182    -3.314271     154.47
 H      -5.084362    -0.352881    -2.694180      22.44
 C      -4.738280    -2.708504    -4.465731      94.09
 O      -6.139223    -2.647641    -4.015674     249.41
 H      -6.490644    -1.683132    -4.139842      29.81
 H      -4.445851    -3.827855    -4.729777      25.75
 H      -4.442814    -2.080913    -5.290679      28.08
55
name = lig-ACN-frame_796
 C       3.756169    -0.301918     0.303831      65.00
 H       2.884056     0.012751    -0.376620      23.88
 C       4.422898    -0.512400     2.655034      38.69
 H       4.563575    -0.248903     3.821773      20.70
 C       5.761446    -0.955140     2.194720       1.46
 O       6.855592    -1.489585     3.002153     176.37
 C       6.490921    -1.578900     4.374193     115.52
 H       7.618345    -1.560809     4.928368      24.75
 H       5.996587    -2.602375     4.567905      24.94
 H       5.890249    -0.695665     4.712659      21.33
 C       5.903322    -1.294833     0.808346      15.11
 O       7.114883    -1.722974     0.067906     150.43
 H       7.923755    -1.755177     0.641651      22.72
 C       4.897893    -0.964911    -0.094255      65.11
 H       5.066437    -1.190755    -1.172704      24.11
 C       3.520547    -0.009055     1.682090      27.13
 C       2.317334     0.748494     2.283381      93.79
 H       2.401073     1.847637     2.665615      25.61
 O       1.634719     0.306460     3.575766     202.81
 H       1.216299    -0.673126     3.336443      26.12
 C       1.231558     1.093360     1.192624      94.44
 H       1.736312     1.727996     0.539695      26.77
 C       0.145667     1.916186     1.763799     124.03
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 O       0.633085     3.115754     2.310125     335.94
 H       0.828472     3.475401     1.496157      33.58
 H      -0.500638     1.447893     2.494420      26.95
 H      -0.763821     2.148892     1.129721      25.98
 C      -1.269922    -2.396642    -1.486528      51.56
 H      -2.057474    -3.390550    -1.352377      22.58
 C      -1.004947    -0.265338    -2.539807      55.67
 H      -1.426287     0.661689    -3.241155      20.70
 C      -0.217587     0.257128    -1.447145      -0.38
 O       0.659750     1.269719    -1.653462     203.13
 C       0.407796     2.180564    -2.650437     108.94
 H      -0.473664     2.542873    -2.361856      29.42
 H       1.002217     3.012331    -2.841799      27.16
 H       0.586217     1.469806    -3.747644      23.44
 C       0.068845    -0.682214    -0.275654     -17.42
 O       0.883632    -0.337202     0.816341     125.26
 C      -0.468024    -2.080917    -0.379784      44.75
 H      -0.310553    -2.648757     0.578455      23.12
 C      -1.569833    -1.479191    -2.477918      39.12
 C      -2.351657    -2.033796    -3.667698      91.50
 H      -2.123006    -1.309376    -4.462283      26.34
 O      -1.976979    -3.308442    -4.179005     126.07
 H      -1.069822    -3.882550    -3.622394      22.73
 C      -3.910045    -2.055209    -3.310144      57.06
 H      -4.363455    -2.471059    -2.375966      26.04
 O      -4.193702    -0.433098    -3.265198     239.95
 H      -4.893178    -0.298207    -2.601182      26.53
 C      -4.711594    -2.719269    -4.483269      98.58
 O      -6.027275    -2.580139    -4.092076     316.34
 H      -6.197896    -1.752933    -4.189521      36.73
 H      -4.534276    -3.829690    -4.594682      26.54
 H      -4.550060    -2.281263    -5.536520      26.82
55
name = lig-ACN-frame_797
 C       3.620085    -0.283546     0.342882      21.83
 H       3.094722     0.095760    -0.603374      23.21
 C       4.545342    -0.471676     2.594264      71.48
 H       3.977072    -0.371374     3.683922      24.86
 C       5.715985    -1.107133     2.141226      16.45
 O       6.841569    -1.503985     2.994403     148.28
 C       6.454812    -1.564365     4.450098     106.85
 H       7.452788    -1.569125     5.274697      25.21
 H       5.841393    -2.438066     4.690088      26.61
 H       5.774152    -0.668317     4.789004      21.92
 C       5.977374    -1.241560     0.737444      24.47
 O       7.077998    -1.676350     0.105922     151.24
 H       7.602701    -2.198373     0.699217      23.86
 C       4.859936    -0.874896    -0.089766      13.64
 H       4.929599    -1.245500    -1.092634      25.00
 C       3.482418    -0.010551     1.741292     -21.21
 C       2.219197     0.786435     2.417862      97.01
 H       2.962687     1.671978     2.661282      25.71
 O       1.766344     0.215173     3.614377     300.44
 H       1.366483    -0.589027     3.493807      32.60
 C       1.271399     1.024138     1.136823      80.88
 H       1.751604     1.309554     0.237467      26.21
 C      -0.005573     1.958782     1.689127      97.72
 O       0.653425     3.102292     2.382115     275.75
 H       0.934890     3.865756     1.879232      32.34
 H      -0.296062     1.326958     2.479927      27.57
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 H      -0.672449     2.326887     0.841655      25.86
 C      -1.266043    -2.342145    -1.444332      15.74
 H      -1.658927    -3.579014    -1.529420      21.31
 C      -0.975210    -0.199377    -2.537324      39.43
 H      -1.188553     0.496954    -3.529981      21.94
 C      -0.051808     0.084623    -1.464761      18.14
 O       0.689680     1.331207    -1.503745     174.12
 C       0.513135     2.260504    -2.703101      94.29
 H      -0.354789     2.685516    -2.947895      28.27
 H       1.335844     2.866037    -2.289346      25.16
 H       0.557865     1.766085    -3.917243      23.49
 C       0.093943    -0.696365    -0.351870      27.72
 O       0.771990    -0.357526     0.784129     142.50
 C      -0.560783    -1.904491    -0.304523      64.76
 H      -0.212829    -2.785468     0.323127      24.52
 C      -1.666358    -1.489969    -2.520244      13.39
 C      -2.439071    -2.072387    -3.664703      94.54
 H      -2.359130    -1.376735    -4.545374      27.80
 O      -1.989830    -3.405439    -4.206314     150.15
 H      -0.961379    -3.409259    -3.891795      25.13
 C      -3.885334    -1.873940    -3.459272     112.77
 H      -4.035868    -2.440517    -2.484387      27.52
 O      -4.099345    -0.610503    -3.276639     322.97
 H      -4.840919    -0.567348    -2.834417      31.30
 C      -4.621884    -2.674181    -4.467030      89.27
 O      -6.096704    -2.543484    -4.179240     249.96
 H      -6.288210    -1.484875    -4.153876      28.22
 H      -4.256897    -3.691906    -4.305263      25.10
 H      -4.405870    -2.358586    -5.566315      25.85
55
name = lig-ACN-frame_798
 C       3.656260    -0.247338     0.388140      67.32
 H       2.732756    -0.071910    -0.176360      26.10
 C       4.554043    -0.463779     2.552486      36.45
 H       4.573609    -0.608141     3.738703      23.14
 C       5.750578    -1.213577     2.139751      14.59
 O       6.738293    -1.503192     3.049658     178.23
 C       6.395735    -1.542526     4.472631     102.17
 H       7.617259    -1.696456     4.942403      23.53
 H       5.798378    -2.379269     4.688586      27.15
 H       5.962779    -0.468318     4.767321      21.83
 C       5.887293    -1.141186     0.712543      13.33
 O       7.096275    -1.687410     0.152340     162.15
 H       7.560107    -2.264730     0.857905      21.51
 C       4.804665    -0.827967    -0.135992      69.97
 H       4.977656    -0.814507    -1.157654      24.28
 C       3.438366    -0.063432     1.767088      35.97
 C       2.330431     0.759842     2.296484      91.61
 H       2.358272     1.926411     2.693048      23.40
 O       1.871267     0.144311     3.647945     242.46
 H       1.653524    -0.704734     3.443674      31.95
 C       1.167856     0.977154     1.249359      94.62
 H       1.770042     1.579489     0.504040      24.44
 C       0.073173     1.957184     1.627963     102.17
 O       0.605994     3.093835     2.478688     255.70
 H       1.103709     3.529608     1.593753      26.61
 H      -0.694691     1.587507     2.190184      28.27
 H      -0.598114     2.224543     0.700772      25.60
 C      -1.375380    -2.328320    -1.400789      59.28
 H      -1.321480    -3.579768    -1.493214      22.65
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 C      -0.976748    -0.250105    -2.522254      58.93
 H      -0.905299     0.408693    -3.476222      21.49
 C       0.059304     0.132906    -1.632992      -1.76
 O       0.655297     1.362605    -1.453970     185.66
 C       0.659658     2.317883    -2.696116      98.92
 H      -0.237975     2.795221    -2.750864      27.54
 H       1.386675     3.211821    -2.573599      26.54
 H       1.254107     1.632324    -3.453237      25.49
 C       0.085555    -0.652197    -0.357602      -1.04
 O       0.707735    -0.346724     0.846189     146.77
 C      -0.621636    -1.892635    -0.311746      43.73
 H      -0.457271    -2.439174     0.683170      23.10
 C      -1.534509    -1.524389    -2.527847      27.36
 C      -2.309171    -1.989871    -3.857287      81.73
 H      -2.067420    -1.246809    -4.663660      27.67
 O      -1.999352    -3.453739    -4.155009     205.01
 H      -1.158018    -3.553638    -4.269223      33.63
 C      -3.813758    -2.084136    -3.439170      77.20
 H      -4.045002    -2.564946    -2.453097      26.51
 O      -4.092941    -0.529375    -3.307147     258.39
 H      -4.879419    -0.356202    -2.795936      27.42
 C      -4.735481    -2.640734    -4.511615     100.12
 O      -6.124619    -2.541254    -4.272968     222.85
 H      -6.494677    -1.447515    -4.369242      25.94
 H      -4.642812    -3.693829    -4.483810      27.03
 H      -4.307817    -2.354801    -5.588064      25.37
55
name = lig-ACN-frame_799
 C       3.621727    -0.244701     0.389473      54.31
 H       2.881293    -0.063984    -0.335892      24.73
 C       4.506023    -0.556874     2.682287      78.56
 H       4.400417    -0.045264     3.661504      23.33
 C       5.648979    -1.084975     2.098542      15.72
 O       6.662173    -1.546082     3.033129     172.47
 C       6.400073    -1.500531     4.440097     101.26
 H       7.528160    -1.894848     5.027443      23.24
 H       5.649353    -2.140762     4.788336      25.51
 H       6.131945    -0.499313     5.028094      22.93
 C       5.910939    -1.227538     0.701622      27.95
 O       7.072403    -1.691985     0.186517     133.63
 H       7.781240    -1.829533     0.917928      21.89
 C       4.855588    -0.745657    -0.180885      19.34
 H       4.992904    -0.763033    -1.220972      23.96
 C       3.567866    -0.060228     1.776654      -5.64
 C       2.269220     0.669929     2.354057      94.14
 H       2.865388     1.779147     2.579040      25.84
 O       1.981586     0.140126     3.604267     237.72
 H       1.612261    -0.890550     3.594735      26.87
 C       1.180999     0.945821     1.365221      95.82
 H       1.639843     1.357390     0.406628      24.46
 C       0.024483     1.972110     1.707250     115.58
 O       0.529134     3.058524     2.439136     278.15
 H       1.268078     3.639614     1.990496      30.84
 H      -0.774240     1.546428     2.079827      30.46
 H       0.100563     2.504172     0.676059      22.00
 C      -1.381259    -2.406810    -1.399499      12.80
 H      -2.192146    -3.340297    -1.353906      22.57
 C      -0.829027    -0.268365    -2.643181      42.53
 H      -1.289450     0.371558    -3.409081      22.73
 C       0.045894     0.195198    -1.526897      11.65
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 O       0.647984     1.477528    -1.521659     227.64
 C       0.830530     2.287795    -2.580203     120.14
 H      -0.086255     2.521773    -2.964187      28.04
 H       1.399405     3.194959    -2.068742      25.29
 H       1.048470     1.886129    -3.663191      25.72
 C       0.022240    -0.590627    -0.375172      15.79
 O       0.653216    -0.317924     0.901685     139.28
 C      -0.647198    -1.856162    -0.303598      47.33
 H      -0.842023    -2.268089     0.691635      23.28
 C      -1.405789    -1.582101    -2.640506       4.91
 C      -2.127473    -2.073039    -3.835983      85.50
 H      -1.989152    -1.514463    -4.817169      25.95
 O      -2.019020    -3.426430    -4.136644     208.51
 H      -1.117073    -3.709833    -4.128366      29.78
 C      -3.805073    -2.051428    -3.450116      47.06
 H      -3.793765    -2.554990    -2.444090      25.74
 O      -4.107737    -0.517579    -3.347308     207.79
 H      -4.897566    -0.429381    -2.553444      22.76
 C      -4.808673    -2.729839    -4.599122      84.54
 O      -6.202153    -2.492518    -4.324157     309.35
 H      -6.443596    -1.633025    -4.686274      29.37
 H      -4.618331    -3.709356    -4.865115      26.41
 H      -4.637588    -1.941202    -5.505774      23.79
55
name = lig-ACN-frame_800
 C       3.727955    -0.281741     0.316732      68.05
 H       3.073434     0.225855    -0.297257      24.66
 C       4.413683    -0.480356     2.721684      63.79
 H       4.315543    -0.373497     3.748222      25.49
 C       5.663669    -1.032354     2.200491       7.01
 O       6.631120    -1.591454     2.944492     161.08
 C       6.406893    -1.480124     4.451945      89.58
 H       7.403800    -2.133093     4.999143      22.83
 H       5.483308    -1.936092     4.640890      25.42
 H       6.438613    -0.322507     4.569866      23.21
 C       5.848002    -1.246464     0.738730       8.02
 O       7.092097    -1.713893     0.204595     186.23
 H       7.748507    -1.552084     0.855054      23.40
 C       4.944268    -0.730067    -0.158118      55.71
 H       5.095357    -0.981409    -1.202825      25.95
 C       3.465590    -0.056159     1.727275      22.82
 C       2.372954     0.629627     2.391292      90.64
 H       2.752430     1.819605     2.740522      24.55
 O       2.019364     0.127945     3.689569     187.11
 H       1.384948    -0.847770     3.479039      23.79
 C       1.212750     0.928772     1.349093      84.49
 H       1.903841     1.396684     0.546194      24.03
 C       0.032708     2.007868     1.630555     104.33
 O       0.460321     3.095696     2.539994     319.64
 H       0.974417     3.516581     1.914666      33.50
 H      -0.676567     1.609635     2.199194      29.00
 H      -0.715335     2.194871     0.709775      24.69
 C      -1.340320    -2.313199    -1.470079      59.65
 H      -2.182318    -3.028135    -1.159827      22.71
 C      -0.622537    -0.318060    -2.701472      62.22
 H      -0.774649     0.359489    -3.470034      27.28
 C      -0.117867     0.264612    -1.534813      -4.81
 O       0.657600     1.424643    -1.434266     175.57
 C       0.857863     2.356991    -2.662008     111.33
 H       0.091079     2.963698    -3.025037      26.74
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 H       1.503441     3.235513    -2.196860      25.49
 H       1.728549     1.909939    -3.097245      26.89
 C      -0.017373    -0.592892    -0.265951       7.10
 O       0.547790    -0.359273     0.932148     153.89
 C      -0.761059    -1.792590    -0.323319      54.79
 H      -0.711473    -2.364059     0.567401      26.34
 C      -1.244737    -1.639281    -2.649819      21.81
 C      -2.269822    -2.113274    -3.787587      88.44
 H      -1.947713    -1.364968    -4.597683      27.49
 O      -1.972061    -3.547806    -4.153672     122.68
 H      -1.021943    -3.734278    -3.585643      23.98
 C      -3.746622    -1.897828    -3.576879      93.28
 H      -4.071512    -2.442023    -2.630184      25.98
 O      -4.120095    -0.633439    -3.375206     216.82
 H      -5.048232    -0.641882    -2.645355      21.01
 C      -4.762479    -2.608542    -4.647840      77.34
 O      -6.277387    -2.468469    -4.287408     295.09
 H      -6.606241    -1.881792    -4.888945      31.33
 H      -4.497975    -3.614013    -4.711662      26.91
 H      -4.415607    -2.117318    -5.736589      25.10
55
name = lig-ACN-frame_801
 C       3.752000    -0.159837     0.319493      44.52
 H       3.087357     0.083734    -0.473044      26.99
 C       4.459261    -0.458454     2.609052      74.10
 H       4.071855    -0.571847     3.495560      27.15
 C       5.642728    -1.074351     2.180916      30.84
 O       6.669609    -1.664015     2.978017     222.68
 C       6.438370    -1.439155     4.314836     116.46
 H       7.252989    -2.243389     4.941622      24.42
 H       5.433448    -1.651380     4.744438      25.86
 H       6.663203    -0.447387     4.822850      25.82
 C       5.931052    -1.175315     0.846308      25.42
 O       7.065625    -1.720429     0.267496     180.27
 H       7.785981    -1.962878     0.924312      23.55
 C       4.971879    -0.841262    -0.133829      36.08
 H       5.291885    -0.802909    -1.229534      22.05
 C       3.472497    -0.127212     1.693513      16.15
 C       2.258685     0.743897     2.365591      64.98
 H       2.617566     1.961185     2.670617      23.35
 O       1.988467     0.109279     3.796627     174.00
 H       1.451719    -0.889056     3.648122      23.77
 C       1.164930     1.005522     1.293694      83.16
 H       1.603623     1.373994     0.309049      22.50
 C       0.006933     1.895664     1.741766     100.23
 O       0.410876     3.143876     2.527414     273.96
 H       0.794780     3.867532     2.025967      32.13
 H      -0.536708     1.256654     2.340892      28.32
 H      -0.474308     2.428148     0.849223      23.97
 C      -1.375084    -2.223739    -1.463891      35.93
 H      -1.617308    -3.264706    -1.620461      23.90
 C      -0.495338    -0.398913    -2.750641      48.28
 H      -0.095126    -0.116491    -3.600415      27.77
 C      -0.098825     0.228624    -1.454848       6.07
 O       0.618805     1.426014    -1.401958     179.62
 C       0.987139     2.411880    -2.594507     101.83
 H       0.100850     2.343342    -3.187114      26.40
 H       1.344886     3.280168    -1.969194      24.83
 H       1.453295     1.893392    -3.391268      28.24
 C      -0.145635    -0.529030    -0.298336       4.63
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 O       0.517339    -0.330480     1.012849     109.54
 C      -0.797680    -1.782695    -0.239584      70.02
 H      -0.742894    -2.392486     0.602936      26.26
 C      -1.292488    -1.570374    -2.748250      17.72
 C      -2.221368    -2.087178    -3.841042      78.52
 H      -2.100808    -1.667995    -4.903434      27.14
 O      -1.948186    -3.621920    -4.144584      44.16
 H      -0.911226    -3.917174    -3.555487      21.77
 C      -3.865035    -2.034279    -3.584262      77.58
 H      -4.029599    -2.719351    -2.692038      26.67
 O      -4.149133    -0.549652    -3.372379     198.12
 H      -5.172582    -0.518291    -3.047301      24.05
 C      -4.728543    -2.497587    -4.675558     105.64
 O      -6.149305    -2.421000    -4.221450     212.15
 H      -6.818255    -2.329308    -5.119089      24.99
 H      -4.624211    -3.553756    -4.550192      25.45
 H      -4.739898    -2.281084    -5.830113      24.43
55
name = lig-ACN-frame_802
 C       3.782603    -0.136298     0.264256      65.88
 H       3.009473     0.127481    -0.483389      25.71
 C       4.458139    -0.554586     2.593461      53.17
 H       4.394483    -0.281512     3.559714      25.91
 C       5.722611    -1.156496     2.164032      15.55
 O       6.672368    -1.684833     2.973381     192.49
 C       6.515655    -1.446055     4.418364     105.20
 H       7.145929    -2.373916     5.001747      24.68
 H       5.382703    -1.593534     4.554334      23.61
 H       6.877155    -0.430490     4.559004      26.67
 C       6.000826    -1.145072     0.758345      26.79
 O       7.123406    -1.753081     0.331734     167.18
 H       7.493481    -2.392841     1.070061      20.58
 C       4.922764    -0.803390    -0.066923      49.50
 H       5.184637    -0.968198    -1.203406      19.56
 C       3.436456     0.030017     1.676927      -0.64
 C       2.196719     0.706781     2.355804      86.75
 H       2.804712     1.792070     2.727769      23.25
 O       1.922712     0.197400     3.735526     242.69
 H       1.660390    -0.768445     3.668486      28.00
 C       1.086524     1.003502     1.346214     103.28
 H       1.610362     1.468441     0.484223      23.48
 C      -0.003740     1.950407     1.894452     104.37
 O       0.347032     3.132150     2.527883     287.07
 H       0.681692     3.599282     1.585125      26.00
 H      -0.816222     1.528714     2.539182      25.51
 H      -0.670975     2.039074     0.966173      25.16
 C      -1.431031    -2.272896    -1.492818      41.86
 H      -1.734640    -3.245814    -1.438821      24.21
 C      -0.391027    -0.413563    -2.748480      68.37
 H      -0.057778     0.015246    -3.569286      28.24
 C       0.036903     0.178242    -1.556171     -17.36
 O       0.636437     1.478450    -1.414410     199.46
 C       0.912494     2.238916    -2.497488     139.54
 H       0.062287     2.742999    -3.027581      26.74
 H       1.198597     3.234198    -2.124229      27.12
 H       1.815839     2.097556    -2.957318      30.08
 C      -0.234672    -0.501175    -0.129298       3.79
 O       0.471982    -0.238705     0.981878     171.85
 C      -0.845500    -1.774800    -0.286490      58.71
 H      -0.858704    -2.383576     0.601276      24.53
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 C      -1.424303    -1.490527    -2.727563      11.79
 C      -2.159186    -2.218980    -3.985685      75.56
 H      -1.972187    -1.533944    -4.911776      26.95
 O      -1.974384    -3.598812    -4.086426     112.98
 H      -0.772039    -3.779457    -4.150992      20.85
 C      -3.835557    -1.966912    -3.536432      53.46
 H      -4.038888    -2.459876    -2.536399      25.96
 O      -4.153128    -0.537482    -3.349070     249.54
 H      -4.992741    -0.475431    -3.184214      31.79
 C      -4.773685    -2.655885    -4.684295      98.55
 O      -6.039832    -2.327290    -4.172100     219.95
 H      -6.734706    -2.755739    -5.002722      24.66
 H      -4.448461    -3.587854    -5.164209      25.36
 H      -4.420412    -1.819230    -5.387984      26.18
55
name = lig-ACN-frame_803
 C       3.680005    -0.124588     0.350157      34.02
 H       3.042607     0.296986    -0.493175      22.16
 C       4.455038    -0.551779     2.574965      72.78
 H       4.376478    -0.335359     3.637149      24.95
 C       5.652727    -1.105042     2.139375      15.04
 O       6.714188    -1.717205     2.988431     207.66
 C       6.563599    -1.482734     4.468323     111.40
 H       7.262057    -2.276366     5.078548      25.09
 H       5.494266    -1.518138     4.962319      24.59
 H       6.952679    -0.565747     4.819964      27.32
 C       5.948189    -1.221613     0.767883      11.11
 O       7.198113    -1.810232     0.294620     167.55
 H       7.694202    -2.204705     1.068108      21.02
 C       4.969411    -0.739862    -0.161550      31.60
 H       4.913117    -1.161772    -1.246679      25.08
 C       3.551133     0.049072     1.718056      39.23
 C       2.308728     0.691550     2.376084     103.63
 H       2.399119     1.965551     2.496515      23.74
 O       1.845221     0.283138     3.604028     328.48
 H       1.610234    -0.545913     3.604821      34.54
 C       1.033605     1.034630     1.498861      91.42
 H       1.452386     1.607583     0.708067      22.65
 C      -0.221731     1.903378     1.983626      94.04
 O       0.335609     3.205896     2.466010     269.75
 H       1.024617     3.752982     1.917930      29.49
 H      -0.453804     1.314981     2.946805      23.81
 H      -0.948558     2.161232     1.219757      25.07
 C      -1.494151    -2.249535    -1.513197      59.90
 H      -2.238419    -2.893305    -1.422400      25.28
 C      -0.451871    -0.418038    -2.736105      57.59
 H      -0.590821     0.227450    -3.519740      25.51
 C       0.110917     0.114863    -1.451706      10.42
 O       0.628066     1.353758    -1.335789     202.38
 C       0.872555     2.339180    -2.509605     106.75
 H       0.103798     2.110488    -3.304155      24.80
 H       1.109567     3.153763    -1.914756      25.93
 H       1.574153     1.775530    -3.038927      28.06
 C      -0.219167    -0.478262    -0.312649      16.71
 O       0.398831    -0.206164     0.977622     161.76
 C      -0.913998    -1.742096    -0.325994      41.63
 H      -0.972918    -2.391758     0.599211      23.65
 C      -1.354406    -1.568683    -2.694831      16.21
 C      -2.260824    -2.095106    -3.869229      88.62
 H      -2.010649    -1.643012    -4.899655      27.47
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 O      -1.993335    -3.581233    -4.075042     103.43
 H      -0.901950    -3.693950    -4.051609      24.25
 C      -3.678941    -1.980663    -3.551154      98.20
 H      -3.773844    -2.521052    -2.567952      26.13
 O      -4.086625    -0.603292    -3.387865     251.55
 H      -4.930052    -0.710160    -2.901261      26.80
 C      -4.600582    -2.540794    -4.639821      91.34
 O      -6.048439    -2.330283    -4.160007     282.36
 H      -6.804673    -2.535018    -4.706920      30.69
 H      -4.645492    -3.626739    -4.921338      25.33
 H      -4.546522    -1.922096    -5.561252      27.29
55
name = lig-ACN-frame_804
 C       3.793498    -0.147543     0.339312      67.80
 H       2.897831     0.254110    -0.219221      23.55
 C       4.529634    -0.470760     2.696558      53.51
 H       4.065867    -0.666600     3.737191      22.88
 C       5.736751    -1.145866     2.173515       8.00
 O       6.657128    -1.669778     3.033992     201.32
 C       6.657507    -1.531778     4.457236     113.32
 H       7.340439    -2.425842     4.770663      25.46
 H       5.569755    -1.834561     4.710371      25.68
 H       6.950432    -0.565174     4.775153      27.09
 C       5.932126    -1.313288     0.707052      17.69
 O       7.096349    -1.809171     0.230481     170.93
 H       7.780891    -1.802869     0.886287      26.05
 C       4.900809    -0.758569    -0.166020      53.77
 H       5.191605    -0.728380    -1.265549      22.25
 C       3.511574     0.022473     1.744001      -9.18
 C       2.230822     0.894635     2.292449      82.63
 H       2.967237     1.800382     2.692928      23.07
 O       1.813678     0.296316     3.624927     233.79
 H       1.492561    -0.624592     3.373024      26.83
 C       0.931887     1.087162     1.387189      87.02
 H       1.140827     1.584823     0.499349      21.51
 C      -0.187571     1.906000     2.159882      92.32
 O       0.294649     3.285285     2.447220     310.72
 H       0.853939     3.277517     1.736563      34.11
 H      -0.830270     1.535342     3.150784      23.56
 H      -1.000993     1.734556     1.498145      27.04
 C      -1.610761    -2.199662    -1.431756      27.76
 H      -2.177695    -3.076428    -1.387166      25.53
 C      -0.612068    -0.365730    -2.687320      66.96
 H      -0.689711     0.257274    -3.602575      22.47
 C       0.028744     0.096099    -1.597795      -0.34
 O       0.664306     1.335485    -1.303810     204.56
 C       0.854646     2.237357    -2.519642     119.83
 H      -0.222281     2.470258    -2.924011      24.77
 H       0.910066     3.233780    -2.316390      28.76
 H       1.757490     2.145909    -3.067387      28.77
 C      -0.084857    -0.656924    -0.270846       6.18
 O       0.300422    -0.257313     0.964137     145.07
 C      -0.960070    -1.718941    -0.305488      54.76
 H      -1.229573    -2.070189     0.779783      22.65
 C      -1.251642    -1.618655    -2.733287      44.36
 C      -2.137380    -1.998823    -3.798934      87.30
 H      -2.029772    -1.292984    -4.700393      27.58
 O      -2.008495    -3.516061    -4.072938     158.36
 H      -1.236961    -3.748476    -3.633627      31.05
 C      -3.702167    -2.023352    -3.536160      85.88
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 H      -3.992883    -2.738841    -2.719678      27.89
 O      -4.004424    -0.646725    -3.380374     202.54
 H      -4.917344    -0.453468    -2.681035      23.43
 C      -4.629077    -2.472529    -4.633370     117.25
 O      -6.000665    -2.324345    -4.107201     315.05
 H      -6.288108    -2.377571    -4.925312      32.67
 H      -4.211486    -3.513366    -4.608086      26.32
 H      -4.366658    -2.081105    -5.562623      28.24
55
name = lig-ACN-frame_805
 C       3.771075    -0.118852     0.400556      35.25
 H       3.229510     0.203642    -0.495724      27.17
 C       4.530184    -0.468064     2.668533      69.22
 H       4.556623    -0.391241     3.883548      23.13
 C       5.624788    -1.110851     2.206123      26.91
 O       6.705068    -1.639927     2.970163     215.14
 C       6.668479    -1.629295     4.430033     128.79
 H       7.551557    -2.149859     4.780067      28.41
 H       5.790865    -1.941695     5.056557      27.65
 H       6.836051    -0.610743     4.748778      28.30
 C       5.840431    -1.267357     0.795057      21.26
 O       6.991398    -1.803359     0.119612     151.22
 H       7.695918    -2.013381     0.855937      23.46
 C       4.958313    -0.828576    -0.113702      52.24
 H       5.196988    -0.701212    -1.150550      23.91
 C       3.478107     0.001896     1.778007      26.52
 C       2.217838     0.858297     2.276351      94.33
 H       2.304805     2.041064     2.364111      24.21
 O       1.820572     0.334606     3.588384     210.10
 H       1.397457    -0.739509     3.415010      22.42
 C       0.857642     1.112353     1.360320      84.03
 H       1.006793     1.733467     0.506055      20.74
 C      -0.174493     1.923528     2.246698      93.81
 O       0.241369     3.273976     2.372896     309.43
 H       0.634458     3.800286     1.703518      32.78
 H      -0.149838     1.419264     3.407798      21.83
 H      -1.053619     2.078695     1.747524      25.26
 C      -1.589703    -2.215179    -1.374928      58.42
 H      -2.194978    -3.155147    -1.375686      23.80
 C      -0.717205    -0.301068    -2.735120      54.17
 H      -0.491437     0.233482    -3.777245      20.37
 C       0.014162     0.123512    -1.459880      -2.34
 O       0.728437     1.349881    -1.435379     206.33
 C       0.755595     2.240632    -2.481486     120.82
 H      -0.116265     2.078839    -3.271514      23.83
 H       1.051628     3.004491    -1.872859      26.29
 H       1.459421     1.784200    -3.198808      28.04
 C      -0.004809    -0.708034    -0.327672      11.12
 O       0.294718    -0.265002     1.033999     152.49
 C      -1.038454    -1.746040    -0.189783      30.44
 H      -1.422278    -2.195892     0.838377      22.02
 C      -1.360754    -1.594228    -2.588129      21.73
 C      -2.138563    -2.115461    -3.867261      82.18
 H      -1.803127    -1.501779    -4.751962      27.04
 O      -1.978383    -3.431988    -4.101567     267.99
 H      -1.178245    -3.676770    -3.860863      32.92
 C      -3.733320    -1.923267    -3.468548      77.80
 H      -3.872106    -2.375423    -2.465091      26.35
 O      -3.943875    -0.547702    -3.260324     197.37
 H      -4.958227    -0.395701    -2.749870      22.71
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 C      -4.580760    -2.605372    -4.607224     105.06
 O      -5.914863    -2.336173    -4.174361     277.55
 H      -6.777056    -2.137437    -4.749544      28.59
 H      -4.636967    -3.601936    -5.056243      25.76
 H      -4.488284    -1.910565    -5.365139      28.13
55
name = lig-ACN-frame_806
 C       3.702227    -0.118351     0.387585      65.78
 H       2.986120     0.436050    -0.150693      21.32
 C       4.388247    -0.428478     2.679351      56.25
 H       4.342559     0.191258     3.745516      23.09
 C       5.649980    -1.145062     2.189958      15.09
 O       6.736869    -1.638154     2.919674     212.04
 C       6.718206    -1.623674     4.421456     124.21
 H       7.571727    -2.057698     4.671605      30.31
 H       5.879859    -2.251128     4.618458      29.03
 H       6.580718    -0.616936     4.900901      27.17
 C       5.881496    -1.278529     0.819870      27.12
 O       6.922408    -1.806153     0.129446     202.61
 H       7.480401    -2.514167     0.637642      23.34
 C       4.851945    -0.755733    -0.044178      53.58
 H       4.956463    -1.156629    -0.984022      25.44
 C       3.449482     0.084381     1.755209      12.59
 C       2.140779     0.767141     2.240879     119.64
 H       2.661302     1.800230     2.470629      24.54
 O       1.834273     0.384925     3.542714     236.40
 H       1.582708    -0.734306     3.598170      24.55
 C       0.865055     1.007599     1.406960     105.97
 H       1.277197     1.463724     0.475855      19.80
 C      -0.158582     1.917145     2.191266     101.08
 O       0.224275     3.352926     2.390172     279.51
 H       0.479711     3.495090     1.326881      26.00
 H       0.065137     1.530198     3.351291      21.64
 H      -1.095882     1.501441     2.146591      27.24
 C      -1.563309    -2.294214    -1.332732      35.60
 H      -2.364826    -3.148615    -1.179371      21.11
 C      -0.659425    -0.362338    -2.546738      57.11
 H      -0.628226     0.219654    -3.644271      22.05
 C      -0.037399     0.119905    -1.485050      17.77
 O       0.749737     1.209775    -1.452238     213.44
 C       0.715185     2.252506    -2.605775     104.65
 H      -0.402924     2.578814    -2.811156      24.08
 H       0.928806     3.265655    -2.417564      26.35
 H       1.493833     2.099308    -3.409809      26.08
 C      -0.173226    -0.599839    -0.167656       9.99
 O       0.340837    -0.242070     1.059525     195.43
 C      -0.991496    -1.744073    -0.150841      46.03
 H      -0.972321    -2.243358     0.902182      23.57
 C      -1.533568    -1.453062    -2.600776      34.11
 C      -2.247667    -2.033943    -3.770478      91.24
 H      -2.224044    -1.426610    -4.694640      28.15
 O      -1.908994    -3.551713    -4.162702     112.18
 H      -0.908809    -3.490923    -4.240449      26.21
 C      -3.613216    -1.934082    -3.425002      68.31
 H      -3.827952    -2.549216    -2.533521      27.03
 O      -3.942640    -0.407547    -3.166109     211.98
 H      -4.849458    -0.486005    -2.934222      27.95
 C      -4.614291    -2.536077    -4.684704      90.72
 O      -5.964685    -2.359750    -4.138948     239.82
 H      -6.382539    -2.114690    -5.203260      23.07
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 H      -4.189738    -3.578932    -4.721528      25.80
 H      -4.277343    -2.089197    -5.534277      29.15
55
name = lig-ACN-frame_807
 C       3.574479    -0.056442     0.335530      45.61
 H       2.919940     0.040295    -0.480101      25.73
 C       4.444120    -0.399678     2.661157      65.34
 H       4.150841    -0.403088     3.858852      22.66
 C       5.609901    -1.067103     2.252972       8.93
 O       6.758413    -1.583100     2.944029     203.33
 C       6.696480    -1.647565     4.338981     139.45
 H       7.575253    -1.820572     4.669600      32.70
 H       6.025588    -2.354364     4.760235      30.21
 H       6.355184    -0.634172     4.736758      26.85
 C       5.754367    -1.234440     0.770330       6.12
 O       6.915491    -1.877593     0.162480     178.98
 H       7.263432    -2.420230     0.857705      24.95
 C       4.741346    -0.783894    -0.068898      54.49
 H       4.821358    -0.896982    -1.098074      24.29
 C       3.386800     0.062688     1.743086      23.81
 C       2.219743     0.813201     2.283210     106.64
 H       2.478658     1.953897     2.369053      24.83
 O       1.827949     0.348234     3.636655     256.14
 H       1.768458    -0.637163     3.591006      27.88
 C       0.997681     1.031553     1.381717      85.58
 H       1.153131     1.673847     0.437383      18.44
 C      -0.075051     1.839943     2.289043      88.17
 O       0.146637     3.338197     2.284232     242.53
 H       0.654889     3.779838     1.465024      27.89
 H      -0.023853     1.560269     3.414570      22.71
 H      -0.971734     1.879907     1.729858      24.62
 C      -1.595807    -2.218066    -1.282880      57.54
 H      -2.015312    -3.362592    -1.329562      23.38
 C      -0.703386    -0.449199    -2.547040      42.66
 H      -0.578498     0.398175    -3.446042      20.28
 C      -0.061517     0.089465    -1.328162      -3.94
 O       0.853025     1.249444    -1.530383     176.19
 C       0.635661     2.275041    -2.662212      81.89
 H      -0.560258     2.261608    -2.846974      24.22
 H       1.215197     2.901149    -2.003606      23.69
 H       0.842108     1.886041    -3.694235      24.88
 C      -0.398079    -0.426085    -0.064783      18.99
 O       0.350425    -0.304133     1.087425     155.02
 C      -0.893960    -1.785692    -0.180757      38.74
 H      -0.889820    -2.462176     0.685515      21.09
 C      -1.552856    -1.567434    -2.454528      37.21
 C      -2.214332    -1.965153    -3.758892      67.33
 H      -1.865294    -1.272098    -4.507671      27.16
 O      -1.867698    -3.538186    -4.195149      65.34
 H      -0.709721    -3.727973    -3.994836      21.74
 C      -3.839411    -1.894607    -3.466508      97.13
 H      -4.162981    -2.458320    -2.581330      27.09
 O      -3.949437    -0.455041    -3.107313     262.03
 H      -4.794241    -0.282799    -2.906446      31.74
 C      -4.513636    -2.419567    -4.498304     104.31
 O      -6.003317    -2.376147    -4.230037     262.08
 H      -6.648405    -2.341999    -5.005546      28.37
 H      -4.378062    -3.554456    -4.524545      25.27
 H      -4.431334    -2.025668    -5.474862      27.69
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name = lig-ACN-frame_808
 C       3.518118    -0.120458     0.331347      43.15
 H       2.688514     0.313963    -0.227626      20.74
 C       4.431256    -0.418821     2.654113      60.98
 H       4.210501    -0.612927     3.791871      22.66
 C       5.634703    -1.006177     2.095271      21.07
 O       6.698327    -1.512653     2.881167     211.45
 C       6.650368    -1.607276     4.383806     128.61
 H       7.583866    -1.600485     4.637673      31.62
 H       6.123807    -2.415461     4.703466      30.88
 H       6.168917    -0.675275     4.855901      26.65
 C       5.696308    -1.221173     0.758335      25.87
 O       6.807478    -1.921580     0.269443     184.93
 H       7.487088    -1.989439     0.968990      24.85
 C       4.677746    -0.803116    -0.188439      51.12
 H       5.011697    -0.855188    -1.223780      22.75
 C       3.423982     0.033011     1.755518      26.16
 C       2.265980     0.894722     2.401603     107.29
 H       2.635958     1.929072     2.700579      26.45
 O       1.853667     0.308177     3.712721     325.05
 H       1.641288    -0.520091     3.571712      32.44
 C       0.990143     1.062488     1.494983     106.38
 H       1.284827     1.519558     0.473930      19.03
 C      -0.023930     1.895389     2.181149     108.07
 O       0.101340     3.306755     2.205080     349.25
 H       0.888645     3.400341     1.769682      33.91
 H      -0.186797     1.455563     3.181723      24.35
 H      -0.994885     1.476949     1.796728      25.76
 C      -1.640434    -2.325043    -1.216248      43.65
 H      -1.833465    -3.533291    -1.132772      23.02
 C      -0.729409    -0.390792    -2.439098      39.13
 H      -0.623164    -0.135346    -3.607111      19.76
 C      -0.089477     0.233533    -1.379212       9.01
 O       0.878482     1.186837    -1.602490     238.11
 C       0.519167     2.168098    -2.604116     107.44
 H      -0.469579     2.733604    -2.434365      24.55
 H       1.051690     3.163215    -2.783941      25.18
 H       0.906314     1.755488    -3.601279      24.23
 C      -0.386225    -0.456410    -0.039702       6.09
 O       0.384175    -0.272668     1.159673     151.05
 C      -0.913005    -1.774850    -0.067175      25.53
 H      -0.691616    -2.357003     0.773583      19.20
 C      -1.450196    -1.592526    -2.483393      12.30
 C      -2.206346    -2.093472    -3.693605      87.79
 H      -2.030646    -1.490495    -4.565552      27.42
 O      -1.872071    -3.356142    -4.183426     160.57
 H      -0.924747    -3.651676    -3.481580      21.36
 C      -3.798174    -1.803122    -3.296164      63.60
 H      -3.886102    -2.380246    -2.378290      27.27
 O      -3.991610    -0.459187    -3.084061     230.58
 H      -4.979733    -0.317391    -2.607665      24.11
 C      -4.726053    -2.467713    -4.606104      98.67
 O      -6.064458    -2.368892    -4.289245     341.22
 H      -6.353504    -2.619252    -5.058092      33.29
 H      -4.161749    -3.477364    -4.783313      26.14
 H      -4.279478    -1.812674    -5.311133      28.71
55
name = lig-ACN-frame_809
 C       3.525351    -0.195617     0.409249      62.15
 H       2.931823     0.421255    -0.333641      20.47
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 C       4.427689    -0.492234     2.618182      83.71
 H       4.342891    -0.076530     3.633922      26.64
 C       5.547099    -0.958418     2.117086      18.38
 O       6.635097    -1.448310     2.844358     216.86
 C       6.594712    -1.496222     4.353140     130.06
 H       7.574724    -1.546572     4.634761      29.94
 H       6.205391    -2.372329     4.574347      30.85
 H       6.012184    -0.699507     4.880449      26.71
 C       5.658430    -1.226141     0.620747      16.85
 O       6.742851    -1.965519     0.322964     175.21
 H       7.461246    -1.751707     1.044298      22.21
 C       4.690017    -0.787321    -0.223365      64.33
 H       4.640192    -1.044675    -1.340234      22.60
 C       3.419791     0.069568     1.780267      35.12
 C       2.271794     0.819516     2.523222     109.48
 H       2.793231     1.757796     2.733997      26.13
 O       1.902406     0.290597     3.759902     318.34
 H       1.461977    -0.598830     3.645321      28.34
 C       1.045141     1.067226     1.542648      98.16
 H       1.487145     1.576555     0.643489      20.31
 C      -0.201427     1.860040     2.122935     104.33
 O       0.113571     3.300598     2.117080     293.35
 H       0.997358     3.611455     1.812294      31.00
 H      -0.066799     1.660622     3.195071      23.68
 H      -1.209827     1.768024     1.603974      24.38
 C      -1.484282    -2.373511    -1.152291      44.85
 H      -2.222739    -3.309759    -1.114978      19.48
 C      -0.776941    -0.368934    -2.472036      37.53
 H      -0.428409     0.180438    -3.378633      18.23
 C      -0.178607     0.212382    -1.318397       6.79
 O       0.876870     1.168612    -1.593446     233.65
 C       0.470126     2.129279    -2.656994      94.65
 H      -0.628444     2.332390    -2.346191      24.63
 H       1.369560     2.827674    -2.409918      22.19
 H       0.081980     1.681414    -3.584349      23.15
 C      -0.131996    -0.505718    -0.095609      -0.67
 O       0.426190    -0.206287     1.216277     159.66
 C      -0.996237    -1.707679     0.025452      40.26
 H      -0.951861    -2.165817     0.955652      25.26
 C      -1.437708    -1.670386    -2.369705      26.13
 C      -2.282491    -1.971807    -3.628705      99.60
 H      -2.190766    -1.164120    -4.318682      27.33
 O      -1.900729    -3.300034    -4.134249     147.53
 H      -0.932045    -3.718307    -3.662947      23.42
 C      -3.728702    -2.042770    -3.272520      73.27
 H      -4.084365    -2.513254    -2.385593      26.57
 O      -4.069847    -0.358478    -3.053456      73.16
 H      -5.013596    -0.410202    -2.332938      21.75
 C      -4.636416    -2.379379    -4.559480      90.57
 O      -6.186856    -2.388910    -4.379377     267.84
 H      -6.739369    -2.700713    -5.152409      29.46
 H      -4.566895    -3.465889    -4.966849      24.38
 H      -4.634399    -1.742566    -5.401581      26.32
55
name = lig-ACN-frame_810
 C       3.527687    -0.121938     0.385621      43.11
 H       2.613740     0.035243    -0.298548      21.25
 C       4.342340    -0.368437     2.690101      47.00
 H       4.380961    -0.228132     3.697265      22.83
 C       5.517229    -1.035421     2.044306      18.06
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 O       6.621226    -1.367284     2.851338     259.66
 C       6.535834    -1.419493     4.233104     149.51
 H       7.538198    -1.219059     4.604304      29.92
 H       6.044572    -2.165749     4.677407      32.88
 H       6.045783    -0.524259     4.591469      29.92
 C       5.671145    -1.244041     0.719711      21.03
 O       6.782997    -2.027287     0.263560     191.23
 H       7.365429    -2.229392     1.049255      23.25
 C       4.611039    -0.799329    -0.183759      52.78
 H       4.644887    -1.036538    -1.357127      21.57
 C       3.351290     0.017040     1.801197      35.37
 C       2.241868     0.805799     2.491171     109.89
 H       2.452110     1.793526     2.711327      26.15
 O       1.929167     0.253374     3.864873     211.94
 H       1.727348    -0.875145     3.695589      21.29
 C       1.011197     1.091119     1.546570      82.00
 H       1.301631     1.601549     0.635902      20.37
 C      -0.181146     1.932417     2.149643      96.95
 O       0.086687     3.357296     2.042857     257.64
 H       1.007090     3.342487     1.405696      24.67
 H      -0.680111     1.568787     3.050806      24.42
 H      -1.039040     1.663049     1.397969      23.26
 C      -1.392722    -2.297107    -1.077209      34.78
 H      -2.061988    -3.163383    -0.867274      18.71
 C      -0.798961    -0.423647    -2.392823      51.30
 H      -1.045996     0.049504    -3.282680      22.29
 C      -0.035819     0.083808    -1.280196      15.50
 O       0.797027     1.127808    -1.567638     237.57
 C       0.364304     2.081509    -2.612475     117.01
 H      -0.259285     2.815879    -2.255196      26.22
 H       1.253965     2.885086    -2.871791      25.05
 H       0.534701     1.770204    -3.654912      24.74
 C      -0.027795    -0.604355    -0.009318      28.46
 O       0.481838    -0.223685     1.160164     197.75
 C      -0.942773    -1.627987     0.089871      53.13
 H      -1.430424    -1.917615     0.981292      23.93
 C      -1.452145    -1.581748    -2.323002      47.27
 C      -2.294223    -1.911603    -3.489073      84.37
 H      -2.080725    -1.223176    -4.276170      28.59
 O      -1.936988    -3.312129    -4.130300     179.21
 H      -0.951722    -3.273434    -4.084895      28.76
 C      -3.956058    -1.972329    -3.349270      80.55
 H      -4.095267    -2.696091    -2.572863      27.62
 O      -4.117977    -0.482338    -3.004503     185.86
 H      -5.080609    -0.279364    -2.479330      23.25
 C      -4.696010    -2.343281    -4.570358     101.46
 O      -6.239169    -2.386006    -4.361463     233.33
 H      -6.319645    -2.606479    -5.482229      22.88
 H      -4.166531    -3.323911    -4.899720      25.53
 H      -4.160697    -1.552608    -5.125956      26.80
55
name = lig-ACN-frame_811
 C       3.438173    -0.097589     0.403630      39.16
 H       2.543621     0.104229    -0.261919      22.05
 C       4.414953    -0.339911     2.662616      80.62
 H       4.082336    -0.355994     3.576513      26.62
 C       5.464940    -1.038572     2.165624      13.69
 O       6.650614    -1.343320     2.775403     214.95
 C       6.489613    -1.235623     4.254696     130.70
 H       7.547201    -1.480752     4.638735      28.04
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 H       5.983256    -2.068055     4.482157      31.61
 H       6.011924    -0.330680     4.536277      28.77
 C       5.672778    -1.338496     0.693365      12.74
 O       6.767737    -2.030436     0.186161     223.09
 H       7.117520    -2.590157     0.850924      26.70
 C       4.638149    -0.858726    -0.074092      58.45
 H       4.886039    -0.934362    -1.244399      22.93
 C       3.280034     0.050837     1.795028      12.71
 C       2.133240     0.853422     2.494164     107.46
 H       2.657222     1.681919     2.676601      25.96
 O       1.933512     0.240749     3.884772     196.07
 H       1.929194    -0.933451     3.743975      20.87
 C       0.927747     1.066736     1.602798     109.13
 H       1.330157     1.586128     0.779314      22.35
 C      -0.208306     1.973460     2.047263     100.24
 O       0.099998     3.381890     1.990794     277.59
 H       0.674820     3.652725     1.167335      28.30
 H      -0.528853     1.900957     3.058343      24.69
 H      -0.991057     1.746762     1.225863      23.92
 C      -1.500505    -2.274270    -0.956817      52.45
 H      -1.798867    -3.279312    -0.963840      24.54
 C      -0.781279    -0.370208    -2.304821      59.16
 H      -0.983568     0.373754    -2.887746      21.27
 C       0.147560    -0.050887    -1.366054      14.62
 O       0.773772     1.191389    -1.515103     247.65
 C       0.427327     2.085449    -2.593589     103.09
 H      -0.561625     2.364216    -2.460176      28.50
 H       1.380353     2.793170    -2.489287      22.84
 H       0.084378     1.438212    -3.386058      24.64
 C      -0.059506    -0.556144    -0.004122      21.33
 O       0.593259    -0.262645     1.198269     166.08
 C      -0.912976    -1.683596     0.139689      23.70
 H      -1.018159    -1.987290     1.222795      20.06
 C      -1.558327    -1.615568    -2.264932      20.19
 C      -2.409976    -2.072805    -3.543275      91.27
 H      -2.238970    -1.206609    -4.192615      26.27
 O      -1.981969    -3.251460    -4.091540     280.36
 H      -1.162088    -3.288848    -4.225621      34.01
 C      -4.001506    -1.870325    -3.253548      91.09
 H      -4.430443    -2.437077    -2.420127      26.59
 O      -4.205569    -0.601996    -2.917520     284.86
 H      -5.074027    -0.447154    -2.747443      30.05
 C      -4.744472    -2.268637    -4.628935      93.01
 O      -6.101600    -2.371755    -4.418444     243.28
 H      -6.857455    -2.574220    -5.221954      26.25
 H      -4.412651    -3.311408    -4.972529      24.57
 H      -4.851967    -1.653688    -5.539537      23.67
55
name = lig-ACN-frame_812
 C       3.473652    -0.214828     0.408785      76.40
 H       3.049743     0.390241    -0.378641      22.17
 C       4.316211    -0.366114     2.611943      58.26
 H       4.452577    -0.096965     3.578390      25.40
 C       5.555749    -1.046836     2.073904      13.77
 O       6.702536    -1.328647     2.847448     250.00
 C       6.504355    -1.160695     4.259372     119.91
 H       7.553552    -1.266909     4.862611      26.03
 H       5.692466    -1.679535     4.694065      29.09
 H       6.256634    -0.174403     4.562396      29.13
 C       5.558669    -1.394864     0.776853      26.11
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 O       6.690942    -1.992169     0.120516     205.46
 H       7.255999    -2.507099     0.812102      25.36
 C       4.570757    -0.820837    -0.072884      50.47
 H       4.623757    -0.960866    -1.213471      21.95
 C       3.297787     0.114713     1.802068      28.54
 C       2.195378     0.853077     2.610790     111.82
 H       2.385792     1.825401     2.777346      26.11
 O       1.911095     0.284249     3.835376     282.15
 H       1.483455    -0.722884     3.659591      23.05
 C       0.980636     1.078727     1.590279      97.23
 H       1.440025     1.505314     0.768021      21.44
 C      -0.316477     2.024227     1.942915     109.59
 O       0.149449     3.424134     1.943452     306.66
 H       0.327500     3.658060     1.104504      32.85
 H      -0.510364     1.774379     2.915840      26.08
 H      -1.416406     1.849225     1.556657      23.60
 C      -1.654913    -2.344709    -0.928195      38.35
 H      -2.071301    -3.286187    -0.771482      24.07
 C      -0.885356    -0.437683    -2.324241      47.08
 H      -1.014656    -0.025508    -3.231243      21.94
 C       0.180076    -0.009005    -1.297179      -3.50
 O       0.860431     1.251790    -1.383157     220.54
 C       0.420842     2.006984    -2.586276     115.64
 H      -0.421140     2.519077    -2.408894      27.71
 H       1.038687     3.023103    -2.701445      25.12
 H       0.844958     1.768223    -3.534330      25.01
 C      -0.064473    -0.550787     0.014546       6.08
 O       0.635392    -0.325890     1.216872     160.91
 C      -0.850006    -1.755148     0.178311      30.14
 H      -0.528721    -2.505892     0.996461      20.25
 C      -1.662754    -1.594856    -2.206769      25.18
 C      -2.499608    -1.965055    -3.448282      87.00
 H      -2.366296    -1.255026    -4.292685      25.64
 O      -2.073091    -3.315540    -4.096593     168.88
 H      -1.072825    -3.306270    -3.781956      25.96
 C      -4.001610    -2.073690    -3.355186      60.28
 H      -4.379576    -2.882578    -2.726844      26.37
 O      -4.275342    -0.485734    -2.809589     166.41
 H      -5.168802    -0.410842    -2.566622      26.60
 C      -4.715864    -2.268210    -4.755463      94.59
 O      -6.157444    -2.353866    -4.347033     285.88
 H      -6.500726    -2.633830    -5.199839      27.74
 H      -4.281612    -3.239385    -5.118393      25.66
 H      -4.159398    -1.442004    -5.318019      26.31
55
name = lig-ACN-frame_813
 C       3.423645    -0.101313     0.414992      35.51
 H       2.679586     0.311191    -0.197013      20.79
 C       4.458195    -0.431429     2.643358      75.71
 H       4.352192     0.038234     3.634102      25.40
 C       5.538188    -1.012283     2.121282      20.07
 O       6.704609    -1.323694     2.932922     221.86
 C       6.536597    -1.026556     4.349584     102.58
 H       7.554776    -1.608579     4.800167      25.29
 H       5.669575    -1.572668     4.749396      27.67
 H       6.542700     0.022304     4.396279      29.26
 C       5.552428    -1.432008     0.699502      22.13
 O       6.596965    -1.965715     0.083129     204.29
 H       7.387799    -2.016513     0.730622      24.32
 C       4.550472    -0.916676    -0.147040      51.83
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 H       4.726505    -1.052069    -1.218020      22.89
 C       3.362736     0.119891     1.827832      31.25
 C       2.182370     0.979618     2.533660     101.38
 H       2.723747     1.824955     2.817662      24.97
 O       1.824176     0.308220     3.843719     294.95
 H       1.547724    -0.561692     3.656153      28.80
 C       0.995142     1.073860     1.506167      94.96
 H       1.361999     1.552468     0.627445      20.36
 C      -0.269190     2.005733     2.006773      99.89
 O       0.141710     3.414895     1.900244     241.85
 H       0.394151     3.570576     0.892024      27.37
 H      -0.594974     1.925349     2.935137      26.05
 H      -0.972807     1.796086     1.046606      21.74
 C      -1.643021    -2.298332    -0.902028      58.00
 H      -2.122097    -3.313832    -0.896514      22.22
 C      -0.822379    -0.474176    -2.287234      40.85
 H      -0.607334    -0.088902    -3.269659      20.00
 C      -0.093663     0.122252    -1.208297      -6.47
 O       0.886736     1.221960    -1.363917     210.54
 C       0.527912     2.090469    -2.555231     103.10
 H      -0.432135     1.901719    -2.781075      28.31
 H       1.001872     3.018971    -2.152987      23.34
 H       0.790049     1.438838    -3.368026      25.48
 C      -0.044914    -0.701688     0.053412      13.59
 O       0.613854    -0.334594     1.196096     151.69
 C      -0.791266    -1.894386     0.027679      42.79
 H      -0.738536    -2.492237     1.031374      20.48
 C      -1.795948    -1.587250    -2.117663      20.34
 C      -2.524012    -1.929092    -3.408571      87.56
 H      -2.110253    -1.093702    -4.058946      25.23
 O      -2.124792    -3.327901    -4.046302      65.50
 H      -1.196006    -3.893417    -3.535324      23.41
 C      -4.034379    -2.029729    -3.385995      91.06
 H      -4.321966    -2.702109    -2.550455      26.70
 O      -4.284436    -0.602937    -2.808650     203.07
 H      -5.099428    -0.255297    -2.307963      24.30
 C      -4.632700    -2.261552    -4.702488     101.61
 O      -6.156767    -2.317458    -4.400279     306.07
 H      -6.672621    -2.656319    -5.013076      33.56
 H      -4.392920    -3.080010    -5.335934      27.12
 H      -4.698275    -1.309477    -5.354287      25.57
55
name = lig-ACN-frame_814
 C       3.466552    -0.071800     0.406105      44.63
 H       2.614843     0.112931    -0.183426      23.48
 C       4.455299    -0.291944     2.708163      41.03
 H       4.408863    -0.435487     3.872028      21.62
 C       5.582804    -1.081184     2.148141       8.75
 O       6.660609    -1.351746     2.929097     210.42
 C       6.616629    -0.952512     4.395875      94.77
 H       7.558313    -1.534689     4.982885      25.30
 H       5.587825    -1.232015     4.866185      26.51
 H       6.663440     0.082905     4.788161      27.79
 C       5.519413    -1.292138     0.708340       8.51
 O       6.636310    -2.005887     0.041083     208.53
 H       7.376026    -1.917747     0.604876      28.10
 C       4.416223    -0.922404    -0.123207      55.33
 H       4.560867    -1.087969    -1.130771      23.95
 C       3.402008     0.106969     1.840583      35.50
 C       2.250818     0.919389     2.431803     105.02
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 H       2.378360     1.993247     2.575837      25.33
 O       1.728198     0.386458     3.782451     297.19
 H       1.842691    -0.469804     3.682976      32.60
 C       1.005024     1.119316     1.533757      90.23
 H       1.304530     1.567443     0.554985      20.25
 C      -0.117343     1.947666     1.936260     107.29
 O       0.109407     3.375606     1.854647     238.71
 H       0.811224     3.635171     1.037030      26.47
 H      -0.536535     1.678275     2.827556      26.49
 H      -1.144639     1.684086     1.278774      23.21
 C      -1.672098    -2.319330    -1.033411      44.20
 H      -2.132784    -3.396363    -0.928614      23.57
 C      -0.795408    -0.483557    -2.209057      33.72
 H      -0.613567     0.010332    -3.238233      21.09
 C      -0.249986     0.144490    -1.083146      22.27
 O       0.744186     1.098265    -1.371125     248.57
 C       0.632103     2.026306    -2.495154     131.15
 H      -0.328500     2.227427    -2.772629      28.34
 H       0.768715     3.111527    -2.359365      26.59
 H       1.394396     2.071141    -3.244999      27.75
 C      -0.077105    -0.664215     0.010243      11.51
 O       0.573187    -0.320327     1.211678     147.44
 C      -0.691749    -1.992839     0.091579      28.14
 H      -0.765236    -2.521514     1.102667      18.54
 C      -1.737307    -1.477505    -2.144734      36.84
 C      -2.417297    -2.048320    -3.422941      92.17
 H      -2.305921    -1.347785    -4.362762      26.93
 O      -2.176497    -3.288467    -3.960728     150.60
 H      -1.236225    -3.652876    -3.326289      23.13
 C      -3.995686    -1.894745    -3.236833      64.34
 H      -4.480070    -2.741557    -2.677804      27.25
 O      -4.261776    -0.678854    -2.868262     206.05
 H      -5.373606    -0.861387    -2.626247      22.94
 C      -4.813580    -2.171745    -4.736471      90.73
 O      -6.129476    -2.302208    -4.443790     261.70
 H      -6.522535    -2.777455    -5.347807      23.00
 H      -4.292771    -3.052027    -4.991543      26.06
 H      -4.428109    -1.322278    -5.486988      26.19
55
name = lig-ACN-frame_815
 C       3.408562    -0.110308     0.499948      44.51
 H       2.770218     0.407853    -0.258375      21.44
 C       4.446848    -0.284764     2.673505      57.86
 H       4.201658    -0.028481     3.840268      21.62
 C       5.487579    -0.983313     2.133408      19.28
 O       6.678628    -1.382951     2.991332     195.99
 C       6.662208    -0.948947     4.381146      96.07
 H       7.610365    -1.571398     4.845569      25.84
 H       5.680230    -1.355592     5.011603      25.50
 H       6.879805     0.136016     4.236942      27.28
 C       5.656416    -1.266853     0.735417      20.93
 O       6.596369    -1.963067     0.069207     208.42
 H       7.339376    -2.284774     0.662346      24.75
 C       4.496233    -0.915427    -0.073007      48.02
 H       4.345976    -1.199602    -1.030995      24.69
 C       3.405678     0.196511     1.865689      29.24
 C       2.180455     0.902127     2.454333     124.88
 H       2.738536     1.836348     2.681402      23.31
 O       1.714269     0.482379     3.652450     317.97
 H       1.618054    -0.557171     3.787198      25.85
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 C       1.111543     0.999896     1.390251     110.75
 H       1.642041     1.420657     0.472508      18.90
 C      -0.157661     1.913825     1.917286      96.73
 O       0.113774     3.347910     1.830564     297.91
 H       0.965425     3.394460     1.440238      32.54
 H      -0.070347     1.785113     2.939674      23.99
 H      -1.130705     1.531054     1.282184      23.60
 C      -1.513397    -2.372649    -1.004194      52.39
 H      -2.256314    -3.269970    -1.015917      21.54
 C      -0.914993    -0.366449    -2.259004      52.85
 H      -0.857131     0.271779    -3.310646      20.57
 C      -0.206360     0.069833    -1.152599      15.02
 O       0.661130     1.074679    -1.356375     214.04
 C       0.653432     2.102036    -2.429728     126.50
 H      -0.082732     1.962262    -3.116291      27.35
 H       0.810253     2.786431    -1.683573      25.02
 H       1.470450     1.752168    -3.024214      27.78
 C      -0.191218    -0.691122     0.182819      16.32
 O       0.526236    -0.288990     1.241727     189.25
 C      -0.794758    -1.946979     0.056832      62.24
 H      -0.457188    -2.691637     0.774554      22.97
 C      -1.611865    -1.606314    -2.252613      30.28
 C      -2.471810    -1.940638    -3.488019      86.83
 H      -2.050110    -1.152548    -4.274413      25.08
 O      -2.119153    -3.386418    -3.842510     164.40
 H      -1.123940    -3.605001    -3.654700      26.59
 C      -3.975244    -2.029423    -3.402935      86.68
 H      -4.156816    -2.701879    -2.538975      25.79
 O      -4.340468    -0.532450    -2.811184      89.60
 H      -5.455584    -0.198856    -2.820760      21.57
 C      -4.657033    -2.175527    -4.653787      96.97
 O      -6.224424    -2.288382    -4.511850     175.44
 H      -6.704326    -2.715516    -5.515384      22.82
 H      -4.467467    -3.066405    -5.179190      25.93
 H      -4.399075    -1.276238    -5.386973      25.03
55
name = lig-ACN-frame_816
 C       3.491724    -0.185554     0.477034      55.27
 H       2.667267     0.172085    -0.264317      19.49
 C       4.401750    -0.267938     2.688391      70.32
 H       4.612713     0.173650     3.776357      24.20
 C       5.632160    -0.913102     2.211327      26.42
 O       6.599273    -1.444167     2.950889     251.34
 C       6.745407    -0.977056     4.285173     115.35
 H       7.701990    -1.417863     4.775495      25.76
 H       5.703141    -1.190572     4.976227      24.56
 H       6.788710     0.175043     4.559825      28.05
 C       5.610338    -1.257942     0.797623      13.14
 O       6.647914    -1.941276     0.127340     199.34
 H       7.077424    -2.566764     0.839747      25.75
 C       4.566308    -0.851453     0.004199      58.50
 H       4.806105    -1.161207    -0.967810      23.76
 C       3.351329     0.213491     1.868661      37.19
 C       2.222577     1.011997     2.383122      98.61
 H       2.297299     2.125599     2.589842      23.61
 O       1.688578     0.482851     3.714135     207.00
 H       1.289319    -0.537666     3.302203      20.57
 C       1.036887     1.047701     1.330606     109.38
 H       1.276334     1.400007     0.273190      15.32
 C      -0.044657     1.870010     1.941146      97.61
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 O       0.123310     3.319624     1.767719     285.17
 H       1.038516     3.532397     1.665707      32.29
 H      -0.435226     1.453136     2.908125      23.45
 H      -1.110140     1.763841     1.431347      23.66
 C      -1.465184    -2.431879    -1.150740      51.52
 H      -1.683385    -3.520193    -0.996368      24.51
 C      -1.067085    -0.368154    -2.298016      58.27
 H      -1.209800     0.459287    -3.233158      19.14
 C      -0.182908    -0.049562    -1.231909      11.23
 O       0.664561     1.108182    -1.268658     229.67
 C       0.674172     2.134656    -2.313817     131.46
 H      -0.196873     2.210898    -2.904767      26.80
 H       0.628211     3.190659    -2.151922      28.07
 H       1.631896     2.211183    -2.831231      27.43
 C      -0.275434    -0.607071     0.072979       3.49
 O       0.504921    -0.357409     1.288826     157.54
 C      -0.857985    -1.954719     0.116304      28.50
 H      -0.799921    -2.579854     0.968816      19.38
 C      -1.578708    -1.660167    -2.295702      50.11
 C      -2.374367    -1.956185    -3.518488      72.46
 H      -2.175702    -1.242499    -4.462471      24.94
 O      -2.042521    -3.464073    -3.790580     201.51
 H      -1.204226    -3.454086    -3.829982      33.45
 C      -4.001959    -1.868223    -3.312208      67.10
 H      -4.373183    -2.670702    -2.618294      26.45
 O      -4.339742    -0.508169    -2.816970     231.50
 H      -5.323295    -0.440028    -2.701666      26.73
 C      -4.716416    -2.286769    -4.764960      86.31
 O      -6.214710    -2.232520    -4.570237     249.72
 H      -6.593132    -2.682725    -5.511900      23.65
 H      -4.145527    -3.038985    -5.255924      25.68
 H      -4.554228    -1.247308    -5.257325      25.18
55
name = lig-ACN-frame_817
 C       3.451952    -0.156360     0.453843      61.01
 H       2.569964    -0.103620    -0.300017      20.62
 C       4.501890    -0.157161     2.738098      43.49
 H       4.300835     0.067924     3.829998      20.09
 C       5.564830    -0.870303     2.197100      31.38
 O       6.614174    -1.503432     2.943153     242.31
 C       6.789931    -0.983351     4.298714     107.39
 H       7.717701    -1.459927     4.603718      26.69
 H       5.913408    -1.570909     5.017330      24.95
 H       6.872852     0.190863     4.190915      27.65
 C       5.662083    -1.270025     0.880456      27.15
 O       6.705861    -1.938542     0.256804     225.46
 H       7.303960    -2.461874     0.804278      26.67
 C       4.684801    -0.834039    -0.038102      53.71
 H       4.695201    -0.872942    -1.149526      21.57
 C       3.428449     0.147457     1.845744      27.58
 C       2.151603     1.068363     2.320631      94.17
 H       2.661776     2.129480     2.581041      22.99
 O       1.687772     0.475305     3.710689     223.79
 H       1.288349    -0.528582     3.483878      22.58
 C       0.974977     1.045198     1.450132      98.89
 H       1.296232     1.498742     0.504763      19.30
 C      -0.169366     1.926000     1.937437      99.15
 O       0.134063     3.312585     1.743473     202.00
 H       1.222950     3.481899     1.826209      28.26
 H      -0.167329     1.837870     3.092314      21.55
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 H      -0.979101     1.606696     1.182971      23.53
 C      -1.395465    -2.548072    -1.154013      52.78
 H      -1.574505    -3.538239    -1.439404      18.70
 C      -1.046631    -0.361994    -2.259458      53.40
 H      -1.340893     0.330519    -3.239125      20.60
 C      -0.182827     0.102046    -1.234584      14.11
 O       0.675931     1.176103    -1.237901     223.53
 C       0.635433     2.228702    -2.253135     111.32
 H      -0.071664     1.836017    -2.970018      25.57
 H       0.455728     2.961731    -1.515707      25.63
 H       1.564197     2.204895    -2.840090      27.44
 C      -0.246109    -0.715010     0.013544      15.24
 O       0.435276    -0.390628     1.171288     155.51
 C      -0.954266    -1.920104     0.018390      49.51
 H      -1.136103    -2.276295     0.978710      24.70
 C      -1.635000    -1.614129    -2.296729      28.17
 C      -2.401670    -2.178828    -3.521851      95.92
 H      -2.061864    -1.563688    -4.492226      26.76
 O      -2.040265    -3.454678    -3.813817     258.37
 H      -1.184477    -3.656891    -3.571815      29.47
 C      -3.978444    -1.827893    -3.296058      70.17
 H      -4.327009    -2.520498    -2.476446      26.96
 O      -4.314235    -0.552708    -2.876450     298.98
 H      -5.039761    -0.585257    -2.414186      32.72
 C      -4.769911    -2.158545    -4.807016      92.96
 O      -6.135961    -2.238571    -4.644436     312.92
 H      -6.625113    -2.668702    -5.304715      31.05
 H      -4.589468    -3.223816    -4.863371      24.65
 H      -4.323233    -1.594497    -5.742185      25.59
55
name = lig-ACN-frame_819
 C       3.552025    -0.124646     0.424853      47.34
 H       2.851879     0.140430    -0.304632      24.32
 C       4.524605    -0.156552     2.686287      54.71
 H       4.585698     0.287646     3.571787      21.93
 C       5.540486    -0.951233     2.182958      17.42
 O       6.598427    -1.529466     2.977407     250.04
 C       6.916722    -1.011828     4.348759     106.08
 H       7.822563    -1.437926     4.524153      28.52
 H       6.160984    -1.731576     4.997887      25.77
 H       6.909863     0.153412     4.398835      27.63
 C       5.715668    -1.163556     0.861273      25.17
 O       6.840760    -1.934962     0.462423     155.42
 H       7.565041    -1.935579     1.232531      22.69
 C       4.750875    -0.799870    -0.102954      54.48
 H       4.678573    -0.939249    -1.262181      22.01
 C       3.466719     0.152206     1.846310      25.28
 C       2.065533     0.833047     2.338812      91.35
 H       2.315828     2.015469     2.581807      21.84
 O       1.792255     0.405484     3.835130     257.04
 H       1.785539    -0.493413     3.963623      28.88
 C       0.786132     0.998602     1.447575      97.28
 H       1.104616     1.519440     0.614760      20.69
 C      -0.336085     2.004623     1.989016      93.58
 O       0.109553     3.391775     1.684715     284.06
 H       0.988237     3.435367     1.569829      34.20
 H      -0.331512     1.909196     3.216109      21.48
 H      -1.138390     1.857650     1.310536      25.48
 C      -1.619122    -2.444533    -1.120116      46.75
 H      -2.108146    -3.311264    -1.224156      25.90
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 C      -0.992478    -0.396449    -2.365726      54.11
 H      -0.964560     0.181746    -3.255944      22.04
 C      -0.258922     0.134921    -1.240238      10.60
 O       0.671884     1.197129    -1.317009     221.49
 C       0.465541     2.452684    -2.121167      93.75
 H      -0.017576     1.864673    -2.986080      22.43
 H      -0.037343     3.100312    -1.407503      26.14
 H       1.465338     2.724958    -2.507357      26.12
 C      -0.238250    -0.684808    -0.014737      19.92
 O       0.434147    -0.342473     1.110513     185.81
 C      -0.789909    -1.963772    -0.042970      44.44
 H      -0.623596    -2.550731     0.922243      18.39
 C      -1.617509    -1.568721    -2.386143      30.49
 C      -2.416658    -2.066921    -3.565175      81.24
 H      -2.145198    -1.604816    -4.542865      26.53
 O      -2.216281    -3.611131    -3.864980      87.28
 H      -1.101561    -3.995185    -3.809356      23.22
 C      -3.952535    -2.004200    -3.359647      77.05
 H      -4.329336    -2.555403    -2.472652      25.68
 O      -4.165946    -0.618374    -3.010372     162.87
 H      -5.267495    -0.709890    -2.577310      22.32
 C      -4.624256    -2.347795    -4.849445      82.74
 O      -6.083610    -2.090155    -4.702865     276.02
 H      -6.776874    -2.409960    -5.417132      26.33
 H      -4.395230    -3.331684    -5.343491      25.22
 H      -4.270279    -1.465855    -5.330094      26.34
55
name = lig-ACN-frame_820
 C       3.614035    -0.083362     0.392417      51.75
 H       2.819276     0.107682    -0.206055      23.13
 C       4.477437    -0.223603     2.723470      40.46
 H       4.469928     0.092305     3.675514      22.78
 C       5.624832    -0.915410     2.245642      18.81
 O       6.591572    -1.483862     3.002192     256.63
 C       6.906068    -1.064736     4.327833     128.13
 H       7.964967    -1.271597     4.464130      27.11
 H       6.208790    -1.349119     5.271433      26.74
 H       6.854613     0.062442     4.485589      29.60
 C       5.758206    -1.245330     0.810130      12.00
 O       6.874303    -1.848900     0.456774     198.69
 H       7.348872    -2.436510     1.141048      24.47
 C       4.751365    -0.770335    -0.035339      76.65
 H       5.105471    -0.928393    -1.107860      23.91
 C       3.332304     0.151961     1.745125      42.22
 C       2.040914     0.956457     2.409137      80.71
 H       2.498025     2.084336     2.616663      21.29
 O       1.853818     0.311806     3.930369     168.80
 H       1.649557    -0.636311     3.474566      21.03
 C       0.826333     1.021389     1.480823     101.55
 H       1.179827     1.402030     0.555215      19.08
 C      -0.226126     1.987701     1.952119     102.87
 O       0.038478     3.390703     1.694601     249.52
 H       0.979596     3.427928     1.191396      27.37
 H      -0.587268     1.896950     3.154275      22.34
 H      -1.191220     1.722503     1.679037      25.85
 C      -1.699853    -2.231040    -1.102498      65.26
 H      -1.947240    -3.262601    -1.053671      26.09
 C      -0.889397    -0.356722    -2.480596      41.76
 H      -0.858452     0.128950    -3.326007      23.45
 C      -0.222200     0.092501    -1.318697       5.44
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 O       0.652210     1.178564    -1.375196     251.55
 C       0.335606     2.447370    -2.079027     109.23
 H      -0.343670     2.646965    -3.054808      23.41
 H      -0.250401     3.119107    -1.465474      27.35
 H       1.270500     3.057125    -2.107149      26.13
 C      -0.300335    -0.614468    -0.044685       0.72
 O       0.411644    -0.372091     1.168252     162.87
 C      -0.700878    -2.013788    -0.084522      25.24
 H      -0.598080    -2.688926     0.880847      19.02
 C      -1.679192    -1.668863    -2.338206       9.13
 C      -2.419342    -2.242971    -3.660637      96.32
 H      -2.150029    -1.554900    -4.459316      28.14
 O      -2.326678    -3.555885    -3.863983     159.44
 H      -1.103856    -3.602835    -3.878145      21.85
 C      -3.886585    -2.037785    -3.336860      79.68
 H      -4.075703    -2.791875    -2.546113      26.59
 O      -4.193647    -0.709457    -3.087175     254.21
 H      -5.168896    -0.415257    -3.228463      26.46
 C      -4.668826    -2.295570    -4.897316      86.57
 O      -5.976998    -2.027433    -4.685399     211.26
 H      -6.533752    -2.509913    -5.626764      21.08
 H      -4.550164    -3.418359    -5.157796      24.17
 H      -4.135689    -1.814193    -5.672100      26.63
55
name = lig-ACN-frame_821
 C       3.573822    -0.074247     0.380362      65.95
 H       3.085522     0.300328    -0.467736      21.68
 C       4.318732    -0.234243     2.677348      40.64
 H       4.022941    -0.345369     3.675469      23.41
 C       5.543659    -0.870259     2.286818      15.30
 O       6.632872    -1.480845     3.047815     250.10
 C       6.899378    -0.989846     4.351363     118.83
 H       7.962779    -1.349345     4.643388      26.27
 H       6.198803    -1.587540     5.066878      27.13
 H       6.778614     0.092974     4.332814      29.29
 C       5.714836    -1.209543     0.944939      12.50
 O       6.961618    -1.844757     0.316955     203.35
 H       7.224219    -2.439456     1.003524      27.39
 C       4.812590    -0.745518    -0.041584      35.64
 H       4.900332    -0.934634    -1.104355      23.85
 C       3.349244     0.196294     1.860193      24.63
 C       2.220790     0.880706     2.587508     102.53
 H       2.404494     2.062734     2.881164      22.14
 O       1.887512     0.295805     3.780778     269.03
 H       1.510436    -0.816276     3.813776      20.06
 C       0.977186     1.030332     1.502140      83.48
 H       1.449151     1.472392     0.601242      19.58
 C      -0.280202     1.948309     1.994936      92.74
 O       0.005421     3.380199     1.689251     223.90
 H       0.642297     3.404683     0.800193      25.57
 H      -0.110770     1.798895     3.209112      21.43
 H      -1.097563     1.703233     1.457989      26.20
 C      -1.630279    -2.334374    -1.131634      47.49
 H      -2.392747    -3.125235    -0.910615      18.91
 C      -0.868131    -0.489176    -2.519411      32.71
 H      -0.634677    -0.020471    -3.355228      22.45
 C      -0.197570     0.073566    -1.348749       6.93
 O       0.632936     1.191531    -1.480222     244.05
 C       0.148011     2.525066    -1.958306      93.01
 H      -0.073558     2.216048    -3.065599      21.31
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 H      -0.537073     2.929730    -1.282373      27.01
 H       1.179585     2.984878    -1.936996      24.53
 C      -0.177974    -0.644744    -0.076962      11.84
 O       0.353150    -0.327550     1.205029     159.58
 C      -0.824481    -1.847896    -0.109350      45.68
 H      -0.592423    -2.665778     0.702447      23.38
 C      -1.664329    -1.556046    -2.408105      42.50
 C      -2.419129    -2.112306    -3.534543      91.30
 H      -2.083236    -1.643822    -4.417363      30.20
 O      -2.292174    -3.643984    -3.920845      89.87
 H      -1.327055    -4.142706    -3.535364      23.63
 C      -3.957055    -2.088851    -3.619343      99.80
 H      -4.510625    -2.735859    -2.935247      27.39
 O      -4.253297    -0.678915    -3.107647     251.52
 H      -5.014250    -0.654815    -3.486533      34.12
 C      -4.500648    -2.416279    -4.794050      94.96
 O      -6.030488    -1.915364    -4.697135     188.95
 H      -6.548939    -2.468135    -5.546435      21.58
 H      -4.418392    -3.565920    -4.961227      24.46
 H      -4.117736    -1.831308    -5.542793      27.64
55
name = lig-ACN-frame_822
 C       3.611972    -0.011555     0.447303      62.38
 H       2.862007     0.495655    -0.174197      20.32
 C       4.355285    -0.398509     2.799527      61.02
 H       4.117688    -0.204734     3.900429      24.99
 C       5.551432    -0.964982     2.298647      16.66
 O       6.602504    -1.449531     3.036620     229.91
 C       6.842264    -0.917588     4.418798     117.04
 H       7.980249    -1.213609     4.663164      26.53
 H       6.127563    -1.367610     5.182899      28.46
 H       6.759492     0.117420     4.606927      30.99
 C       5.821705    -1.155861     0.841056       9.20
 O       6.856412    -1.791339     0.282957     225.28
 H       7.701254    -2.091899     0.738429      25.21
 C       4.745821    -0.707574     0.022587      70.61
 H       4.913276    -0.909351    -0.974350      24.84
 C       3.444383     0.213492     1.757828      43.63
 C       2.194417     0.827477     2.460368     107.04
 H       2.673384     1.895568     2.779107      21.03
 O       1.851792     0.250224     3.770465     225.75
 H       1.727423    -0.877256     3.483356      18.83
 C       1.036781     1.051152     1.570340      91.64
 H       1.435996     1.484679     0.573536      17.85
 C      -0.144064     1.921045     1.983504      99.69
 O      -0.014801     3.334711     1.694877     298.64
 H       0.167120     3.385525     0.802733      31.83
 H      -0.593492     1.936662     3.122919      22.83
 H      -1.000247     1.474949     1.669846      26.71
 C      -1.623504    -2.370634    -1.212220      48.12
 H      -2.385909    -3.276000    -1.140557      20.38
 C      -0.742292    -0.489681    -2.472897      38.00
 H      -0.772069    -0.042851    -3.442609      23.11
 C      -0.126276     0.091269    -1.350841      12.14
 O       0.655308     1.196687    -1.542453     288.13
 C       0.025404     2.481650    -1.881802     100.08
 H      -0.585482     2.600357    -2.888303      23.31
 H      -0.756625     2.712704    -1.250075      28.52
 H       0.651741     3.436857    -1.862243      25.16
 C      -0.049471    -0.617069    -0.102585      -3.48
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 O       0.358833    -0.235885     1.172830     165.99
 C      -0.949815    -1.832023    -0.061549      30.59
 H      -1.009240    -2.220368     1.029273      22.69
 C      -1.688545    -1.650655    -2.353660      27.27
 C      -2.428809    -2.147142    -3.613478      83.32
 H      -2.088633    -1.549471    -4.388017      29.86
 O      -2.205161    -3.704364    -3.935949     148.49
 H      -1.362159    -3.831698    -3.427609      27.67
 C      -3.952209    -1.951726    -3.423469      83.50
 H      -4.217444    -2.670673    -2.645993      26.45
 O      -4.338760    -0.681260    -3.179747     251.25
 H      -5.328609    -0.428142    -3.284656      25.74
 C      -4.616053    -2.477906    -5.017532      80.33
 O      -5.984989    -1.892389    -4.763077     308.71
 H      -6.609473    -2.272611    -5.318614      29.26
 H      -4.618768    -3.661909    -5.119225      23.86
 H      -4.100832    -2.080479    -5.837357      27.00
55
name = lig-ACN-frame_823
 C       3.682618     0.073326     0.488651      35.50
 H       2.892303     0.281068    -0.332782      21.11
 C       4.452565    -0.493457     2.750814      51.33
 H       4.539168    -0.204610     3.913895      21.13
 C       5.600585    -1.078137     2.251246      22.65
 O       6.635146    -1.403653     3.128593     269.13
 C       6.749675    -0.872532     4.453905     106.40
 H       7.891994    -1.159359     4.706895      25.52
 H       6.110686    -1.341085     5.196817      28.55
 H       6.603755     0.152112     4.334600      31.06
 C       5.737284    -1.062854     0.860367      15.96
 O       6.814656    -1.749992     0.210069     173.55
 H       7.439792    -1.534782     1.001350      27.21
 C       4.750618    -0.680299    -0.046056      47.91
 H       4.919510    -0.800229    -1.050774      22.67
 C       3.492242     0.086316     1.973820      39.32
 C       2.246659     0.842963     2.370285      84.12
 H       2.414169     2.023227     2.596475      22.61
 O       1.806337     0.201477     3.740346     230.88
 H       1.661964    -0.878518     3.637312      22.23
 C       0.987313     1.070114     1.448190      86.95
 H       1.378730     1.713827     0.543446      17.87
 C      -0.143053     1.926845     2.031157      95.40
 O      -0.028011     3.306369     1.706663     262.74
 H      -0.107652     3.426088     0.741120      29.05
 H      -0.093389     1.764566     3.217285      22.00
 H      -0.898889     1.605172     1.439763      26.65
 C      -1.642911    -2.346891    -1.077266      32.38
 H      -1.937758    -3.496944    -0.838764      26.65
 C      -0.788383    -0.544951    -2.451883      50.45
 H      -0.679711     0.213930    -3.316697      19.30
 C       0.001572     0.036676    -1.366705     -11.95
 O       0.746331     1.303219    -1.604683     226.71
 C      -0.225758     2.462831    -1.809478      80.12
 H      -0.599240     2.423787    -2.897742      23.16
 H      -0.850468     2.499946    -1.044139      30.59
 H       0.675526     3.134625    -1.604393      23.11
 C      -0.161376    -0.652806    -0.091041      13.18
 O       0.421753    -0.221686     1.114680     173.92
 C      -0.978512    -1.780115     0.010391      43.67
 H      -1.390358    -2.137918     0.950096      19.18
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 C      -1.522421    -1.701527    -2.443095      33.94
 C      -2.400845    -2.216378    -3.688200      98.04
 H      -2.207636    -1.699167    -4.576793      29.14
 O      -2.141738    -3.569739    -3.915895     236.66
 H      -1.230386    -3.744830    -3.816128      29.06
 C      -3.924271    -2.043432    -3.439432      58.65
 H      -4.341626    -2.616657    -2.611909      26.68
 O      -4.400724    -0.568237    -3.208261     151.67
 H      -5.453655    -1.053235    -3.083294      23.36
 C      -4.771753    -2.475745    -5.018443      89.50
 O      -5.959369    -1.882447    -4.888571     311.45
 H      -6.505029    -2.255306    -5.476629      31.00
 H      -4.868048    -3.638792    -5.035691      24.36
 H      -4.163277    -2.050904    -5.787236      26.17
55
name = lig-ACN-frame_824
 C       3.663558     0.031301     0.586676      56.91
 H       2.873081     0.688716     0.027224      20.30
 C       4.492500    -0.455192     2.791225      65.79
 H       4.198441    -0.532046     3.990990      20.22
 C       5.645418    -1.081716     2.255483       4.48
 O       6.731281    -1.463100     3.127371     233.03
 C       6.668995    -0.793894     4.457817     103.09
 H       7.707236    -0.926020     4.977451      27.21
 H       5.935580    -1.281792     5.063303      29.99
 H       6.470197     0.232295     4.522935      32.68
 C       5.740072    -1.173152     0.788179      20.92
 O       6.849703    -1.661532     0.222595     224.73
 H       7.637657    -1.932040     0.656927      25.23
 C       4.768899    -0.564375    -0.082382      68.18
 H       4.840785    -0.644751    -1.163110      25.32
 C       3.441296     0.043173     1.889572      40.89
 C       2.217752     0.805587     2.523298      92.86
 H       2.643390     1.832716     2.906417      24.29
 O       1.756764     0.267011     3.642188     339.49
 H       1.590772    -0.647824     3.477724      29.25
 C       1.031981     1.055640     1.277679      81.59
 H       1.374046     1.440661     0.231291      16.59
 C      -0.185529     1.888073     2.021463      95.37
 O      -0.018058     3.361357     1.770567     199.56
 H      -0.200591     3.380713     0.677526      25.39
 H      -0.102052     1.799566     3.161873      23.69
 H      -1.188703     1.520092     2.084598      25.36
 C      -1.582176    -2.304986    -1.107921      33.76
 H      -2.290507    -3.276117    -1.013420      23.24
 C      -0.747239    -0.495016    -2.462502      33.52
 H      -0.792985    -0.063088    -3.591744      20.36
 C       0.057554    -0.043403    -1.405212       6.63
 O       0.712611     1.267345    -1.635930     252.67
 C      -0.292638     2.405657    -1.716277      82.97
 H      -0.885750     2.317583    -2.670739      25.80
 H      -0.965209     2.302113    -1.016498      31.76
 H       0.021393     3.525986    -1.721063      25.07
 C      -0.215499    -0.509417    -0.057291      -4.07
 O       0.487250    -0.300507     1.048041     139.86
 C      -1.052669    -1.714854     0.080228      42.40
 H      -0.827454    -2.188865     0.977036      23.49
 C      -1.454599    -1.779514    -2.401629      38.08
 C      -2.328001    -2.113355    -3.624802      77.13
 H      -2.040197    -1.401054    -4.363059      28.20
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 O      -2.123377    -3.538474    -3.951784     218.93
 H      -1.303962    -3.670829    -3.715452      32.73
 C      -3.994455    -2.075964    -3.643936      88.72
 H      -4.265377    -2.718684    -2.814266      26.79
 O      -4.413389    -0.652204    -3.218979     171.93
 H      -5.453768    -0.457667    -2.933175      24.73
 C      -4.626741    -2.511394    -4.794027      99.73
 O      -6.127690    -1.782481    -5.010631     173.52
 H      -6.542490    -2.474635    -5.772033      20.55
 H      -4.682254    -3.617736    -4.981011      25.01
 H      -4.059447    -2.159963    -5.645666      25.52
55
name = lig-ACN-frame_825
 C       3.608858     0.028301     0.481688      55.18
 H       3.083957     0.738547    -0.259845      18.92
 C       4.412484    -0.468564     2.789219      35.07
 H       4.156244    -0.476358     3.973790      20.28
 C       5.655619    -1.019585     2.264601       7.56
 O       6.779530    -1.463683     3.064892     214.29
 C       6.595261    -0.783857     4.472013     110.59
 H       7.578075    -0.883617     4.954347      27.41
 H       5.870801    -1.251491     4.983044      33.27
 H       6.265391     0.207195     4.180135      32.38
 C       5.785013    -1.211665     0.829739       9.99
 O       6.982569    -1.647912     0.145225     211.17
 H       7.260414    -2.222680     0.879948      27.26
 C       4.810499    -0.534463     0.030143      37.49
 H       5.060471    -0.412441    -1.092249      22.51
 C       3.429274     0.045110     1.981644      21.10
 C       2.239075     0.853310     2.379629      89.67
 H       2.570007     1.924765     2.567873      22.31
 O       1.613278     0.263400     3.672121     325.48
 H       1.439453    -0.574831     3.564367      30.57
 C       1.014786     1.045484     1.411038     101.98
 H       1.384066     1.621406     0.531182      18.90
 C      -0.097626     1.904495     2.033295     102.77
 O      -0.050009     3.340647     1.814709     266.97
 H      -0.052288     3.647200     0.894634      30.89
 H       0.238721     1.846044     3.060509      22.17
 H      -1.063355     1.532125     1.672527      24.80
 C      -1.587137    -2.301054    -1.086316      49.74
 H      -2.379711    -3.114214    -0.933321      19.76
 C      -0.649184    -0.584435    -2.520304      38.95
 H      -0.523734     0.102018    -3.514866      21.26
 C      -0.047634     0.090002    -1.453188      -1.55
 O       0.644447     1.227673    -1.651464     252.72
 C      -0.393256     2.283117    -1.669300      72.02
 H      -1.052007     2.043137    -2.521430      24.70
 H      -0.852192     2.285443    -0.770613      28.66
 H       0.342626     3.183783    -1.688480      22.48
 C      -0.228315    -0.532269    -0.122102       5.23
 O       0.595330    -0.329041     1.041218     162.60
 C      -1.010647    -1.675258     0.019299      52.07
 H      -1.047131    -2.190283     0.890767      25.63
 C      -1.537818    -1.630575    -2.313721      40.18
 C      -2.346576    -2.040350    -3.569161      77.72
 H      -2.018846    -1.455422    -4.430787      29.26
 O      -2.118343    -3.513254    -4.028161     199.65
 H      -1.404729    -3.873299    -3.668014      32.51
 C      -3.981282    -1.961653    -3.438169      86.19
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 H      -4.228594    -2.702480    -2.667441      27.41
 O      -4.346769    -0.732560    -3.217992     306.11
 H      -5.210211    -0.780365    -3.164871      34.91
 C      -4.691545    -2.469710    -4.914128      75.90
 O      -6.115232    -1.782489    -5.066641     198.85
 H      -6.615293    -2.505491    -5.889566      19.36
 H      -4.810252    -3.497450    -4.690592      25.09
 H      -4.044964    -2.225275    -5.821786      24.12
55
name = lig-ACN-frame_826
 C       3.679666     0.044334     0.507549      58.98
 H       2.948108     0.329017    -0.241287      22.43
 C       4.396650    -0.539499     2.740273      65.20
 H       4.351886    -0.271208     3.834092      23.27
 C       5.648462    -1.033215     2.250519      21.24
 O       6.696244    -1.374282     3.068102     260.74
 C       6.568215    -0.841460     4.360144     149.64
 H       7.507624    -0.826073     4.800300      28.29
 H       5.941771    -1.308935     4.963544      33.22
 H       6.348423     0.258277     4.352921      31.75
 C       5.854012    -1.099387     0.882781      11.36
 O       7.027138    -1.670549     0.193230     199.66
 H       7.641127    -2.393711     0.602923      25.50
 C       4.876434    -0.582669     0.075895      54.81
 H       5.153277    -0.656107    -1.094845      21.73
 C       3.391748     0.088881     1.809611      43.52
 C       2.146031     0.846137     2.403004     110.94
 H       2.431041     1.844116     2.704231      23.56
 O       1.518807     0.326481     3.687307     285.70
 H       1.492010    -0.678915     3.549350      24.35
 C       1.082959     1.051226     1.454569     107.15
 H       1.420138     1.530225     0.568666      21.73
 C      -0.042624     1.915431     2.098012     102.93
 O      -0.053214     3.348440     1.864360     318.86
 H       0.224040     3.386041     1.000326      33.12
 H      -0.407089     1.745678     3.055142      24.80
 H      -0.950255     1.471250     1.592996      25.16
 C      -1.728497    -2.234568    -1.081899      35.00
 H      -2.192433    -3.188431    -0.870483      24.70
 C      -0.621083    -0.574553    -2.551249      25.49
 H      -0.451917    -0.187224    -3.638403      22.50
 C      -0.140058     0.050475    -1.376703       8.58
 O       0.588551     1.215667    -1.657129     262.23
 C      -0.391536     2.256519    -1.632117      91.51
 H      -1.178600     2.201394    -2.424483      25.24
 H      -0.855873     2.340248    -0.739725      28.87
 H       0.085788     3.310561    -1.895313      23.66
 C      -0.087068    -0.578097    -0.122189      15.31
 O       0.641662    -0.285766     0.988475     178.34
 C      -0.915207    -1.742493    -0.012681      41.47
 H      -1.184173    -1.918861     0.967766      21.78
 C      -1.656033    -1.568543    -2.402970      15.77
 C      -2.413728    -2.139509    -3.582697     102.15
 H      -2.298222    -1.339143    -4.380253      28.15
 O      -2.154969    -3.434655    -4.074921     200.09
 H      -1.152776    -3.564674    -3.766581      26.06
 C      -3.867527    -2.087715    -3.409025      65.16
 H      -4.303356    -2.615212    -2.589334      26.00
 O      -4.341502    -0.584783    -3.122144     213.08
 H      -5.283763    -0.577342    -3.410459      28.43
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 C      -4.795988    -2.449558    -4.920912      82.58
 O      -5.955682    -1.808234    -5.067423     202.98
 H      -6.698313    -2.410400    -5.794896      19.68
 H      -4.942446    -3.470813    -5.088041      25.46
 H      -4.032886    -2.150313    -5.781941      23.61
55
name = lig-ACN-frame_827
 C       3.743928    -0.000092     0.416007      35.12
 H       3.041670     0.258622    -0.297304      23.42
 C       4.352826    -0.463660     2.648507      42.53
 H       4.144298    -0.429857     3.678396      22.77
 C       5.575421    -1.031949     2.241298      30.92
 O       6.616710    -1.312107     3.057660     274.35
 C       6.630697    -0.857750     4.416964     131.80
 H       7.558559    -1.023186     4.704657      29.87
 H       6.006302    -1.392919     4.936465      34.50
 H       6.217900     0.207862     4.527494      30.55
 C       5.990940    -1.082814     0.845351      29.97
 O       7.012794    -1.667654     0.273040     193.98
 H       7.519942    -2.046056     1.025807      25.07
 C       4.946342    -0.658632    -0.047127      39.44
 H       4.846323    -1.059803    -1.192724      20.71
 C       3.403637     0.065123     1.898752      31.91
 C       2.189427     0.809051     2.571814     105.80
 H       2.611377     1.696637     2.832133      24.75
 O       1.510382     0.342230     3.664388     292.19
 H       1.402843    -0.810896     3.741830      21.80
 C       1.074169     1.142923     1.366915      76.96
 H       1.467566     1.690987     0.595294      23.11
 C      -0.238883     1.850707     2.068145      96.52
 O       0.006910     3.337232     1.912251     219.63
 H       0.649545     3.560597     1.065705      28.01
 H      -0.197685     1.655421     3.061691      24.92
 H      -1.175901     1.616114     1.483609      24.66
 C      -1.769295    -2.125438    -1.118849      47.58
 H      -2.481416    -2.869558    -1.026062      29.20
 C      -0.796301    -0.581879    -2.520149      50.59
 H      -0.518593    -0.055254    -3.430744      23.40
 C      -0.038166    -0.052562    -1.436946       2.46
 O       0.559516     1.226562    -1.630265     230.34
 C      -0.415537     2.412172    -1.652341      68.91
 H      -1.175127     1.928351    -2.324877      25.66
 H      -0.892299     2.484591    -0.687724      26.89
 H       0.177355     3.374535    -1.907662      23.24
 C      -0.030344    -0.656714    -0.141520      -3.03
 O       0.661566    -0.243504     0.996750     157.70
 C      -0.908484    -1.796825    -0.009712      48.83
 H      -0.774086    -2.464856     0.848981      22.09
 C      -1.663943    -1.693640    -2.409590      38.76
 C      -2.495649    -2.062381    -3.668152      72.47
 H      -2.140043    -1.400011    -4.539947      26.64
 O      -2.113497    -3.438668    -4.106494     111.61
 H      -0.948717    -3.682793    -3.980811      22.95
 C      -4.141375    -2.041284    -3.507857     101.05
 H      -4.285816    -2.733259    -2.682467      27.38
 O      -4.301323    -0.568595    -3.042788     146.27
 H      -5.257242    -0.167317    -3.578963      23.83
 C      -4.572139    -2.538637    -4.818531      92.01
 O      -5.939229    -1.720970    -5.019883     210.08
 H      -6.480544    -2.393263    -5.720315      21.51
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 H      -4.601419    -3.557367    -4.894337      26.39
 H      -3.852277    -2.013764    -5.600191      23.13
55
name = lig-ACN-frame_828
 C       3.711294    -0.091753     0.395180      63.73
 H       3.132615     0.363909    -0.315749      23.32
 C       4.398329    -0.451108     2.766249      34.35
 H       4.240518    -0.618954     3.733752      19.66
 C       5.580236    -0.926931     2.157785       2.73
 O       6.635644    -1.318366     3.067880     204.14
 C       6.651490    -0.908219     4.549501     123.78
 H       7.593636    -0.930983     4.818589      30.16
 H       6.128339    -1.460958     5.149808      32.49
 H       6.431609     0.219932     4.549770      31.07
 C       5.809600    -1.056623     0.771577       2.78
 O       7.118261    -1.722755     0.396366     198.61
 H       7.719169    -1.734301     1.136967      29.94
 C       4.853274    -0.722143    -0.119520      64.16
 H       5.198653    -0.881212    -1.245691      18.09
 C       3.382471     0.064782     1.753716      36.33
 C       2.195999     0.888028     2.406635     104.53
 H       2.515080     1.728310     2.763217      27.09
 O       1.537820     0.257881     3.738092     207.93
 H       1.340854    -0.852903     3.426558      19.95
 C       0.973141     1.155126     1.432748      99.25
 H       1.364885     1.618459     0.550332      21.69
 C      -0.239281     1.881547     1.911946     121.35
 O       0.049439     3.302703     1.980779     255.69
 H       0.903775     3.389591     1.344136      28.99
 H      -0.385220     1.564923     2.860867      25.37
 H      -1.302752     1.562333     1.612988      24.69
 C      -1.817523    -2.230570    -1.062233      23.86
 H      -2.565799    -2.841572    -0.702272      26.81
 C      -0.850663    -0.525025    -2.524660      49.13
 H      -1.031289     0.052815    -3.312095      24.09
 C       0.026542    -0.041162    -1.483951      -2.37
 O       0.573529     1.254119    -1.589775     226.29
 C      -0.436497     2.431266    -1.680097      72.25
 H      -1.259636     2.432661    -2.531257      24.18
 H      -0.760693     2.825116    -0.721610      26.60
 H       0.343478     3.181820    -2.060614      23.33
 C      -0.033688    -0.702388    -0.169267      -7.53
 O       0.672935    -0.257683     0.984378     144.25
 C      -0.882877    -1.849860    -0.069976      41.90
 H      -0.845037    -2.645933     0.782073      21.33
 C      -1.680476    -1.651750    -2.456869      23.63
 C      -2.510953    -2.056634    -3.642572      77.82
 H      -2.429471    -1.260985    -4.508346      25.61
 O      -2.101386    -3.470899    -4.156202      81.40
 H      -1.004041    -3.620730    -3.629210      21.09
 C      -4.072893    -1.904626    -3.417849     106.67
 H      -4.775704    -2.517675    -2.776463      27.37
 O      -4.300242    -0.659158    -3.039155     251.04
 H      -5.166465    -0.230953    -3.568191      25.66
 C      -4.545993    -2.399119    -4.841050      90.94
 O      -5.879330    -1.764999    -4.991402     311.19
 H      -6.349600    -2.039095    -5.696822      30.20
 H      -4.625199    -3.428093    -4.625667      26.33
 H      -3.827922    -2.302306    -5.799039      23.59
55
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name = lig-ACN-frame_829
 C       3.543750    -0.119431     0.340444      31.51
 H       2.806798     0.339786    -0.291621      21.03
 C       4.347429    -0.418813     2.684039      61.99
 H       4.129979    -0.182191     3.645736      24.65
 C       5.659029    -0.841521     2.302474      13.52
 O       6.675231    -1.338293     3.104721     253.02
 C       6.686804    -0.932528     4.529325     133.53
 H       7.653919    -1.057959     4.776605      27.63
 H       6.055679    -1.523259     5.024129      32.72
 H       6.252418     0.089519     4.757138      30.32
 C       5.897518    -1.195371     0.816933      -1.88
 O       7.076119    -1.697921     0.507911     163.37
 H       7.648522    -1.508602     1.345748      21.59
 C       4.797478    -0.782960    -0.173261      41.28
 H       4.871595    -0.586296    -1.276928      21.25
 C       3.413222     0.057543     1.780018      23.12
 C       2.082632     0.866103     2.323799      95.86
 H       2.381413     1.806468     2.530486      26.25
 O       1.670950     0.207889     3.641545     279.73
 H       1.359793    -0.731455     3.424456      25.17
 C       0.960304     1.004880     1.337136      97.91
 H       1.256099     1.637607     0.457258      20.43
 C      -0.264127     1.881117     1.944003      97.71
 O       0.101470     3.286812     2.020945     309.98
 H       0.826540     3.503185     1.553402      35.38
 H      -0.710394     1.608064     2.775407      26.41
 H      -0.741611     1.898333     0.873654      21.88
 C      -1.766894    -2.324032    -1.124791      53.62
 H      -2.333155    -3.229978    -1.087384      26.27
 C      -0.835703    -0.444923    -2.523944      39.13
 H      -0.823386     0.136454    -3.361697      22.21
 C      -0.087029     0.019886    -1.435967       6.22
 O       0.529699     1.291567    -1.566603     246.84
 C      -0.289113     2.465699    -1.771724      69.19
 H      -1.238140     2.157273    -2.480713      22.57
 H      -0.744983     2.714516    -0.721252      24.27
 H       0.360994     3.325682    -2.075461      23.49
 C      -0.019454    -0.681509    -0.224387      -2.10
 O       0.620020    -0.369105     0.939234     164.85
 C      -0.842169    -1.903801    -0.116999      34.92
 H      -0.985700    -1.948500     1.069576      18.28
 C      -1.734335    -1.619888    -2.303492      21.00
 C      -2.469022    -2.153716    -3.525158      98.49
 H      -2.102198    -1.410828    -4.375783      25.83
 O      -2.122763    -3.403315    -4.140793     185.17
 H      -1.258002    -3.783121    -3.557705      24.71
 C      -3.936931    -2.023869    -3.429379      78.72
 H      -4.132899    -2.817254    -2.586116      26.00
 O      -4.334395    -0.538841    -3.033996     237.49
 H      -5.127548    -0.551434    -3.434335      31.24
 C      -4.632919    -2.344151    -4.847361      93.23
 O      -5.867318    -1.765309    -4.990659     300.98
 H      -6.208518    -2.129896    -5.772120      28.94
 H      -4.737851    -3.435168    -4.993403      25.54
 H      -3.920462    -1.939661    -5.739499      23.92
55
name = lig-ACN-frame_830
 C       3.574326    -0.207531     0.368873      65.56
 H       2.878571    -0.047065    -0.503161      21.02
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 C       4.378789    -0.290271     2.651676      47.50
 H       4.246846    -0.004789     3.687571      21.34
 C       5.608371    -0.899003     2.251915       9.26
 O       6.706585    -1.299517     3.127752     267.07
 C       6.681886    -0.999863     4.504331     137.99
 H       7.659034    -1.056053     4.923181      26.40
 H       6.128891    -1.678721     5.008321      31.28
 H       6.396350     0.068243     4.596302      30.23
 C       5.735191    -1.131925     0.937912      13.48
 O       7.057737    -1.670442     0.550209     204.31
 H       7.634586    -1.798381     1.362371      23.90
 C       4.764913    -0.769654    -0.007072      70.92
 H       4.996257    -1.196650    -0.945534      24.98
 C       3.301164     0.085749     1.698839      34.46
 C       2.137964     0.718771     2.308926     134.60
 H       2.328841     1.700338     2.588670      24.99
 O       1.787000     0.220232     3.499592     350.95
 H       1.632834    -0.618494     3.435631      32.57
 C       0.953749     0.886975     1.296224      99.43
 H       1.472107     1.357586     0.351513      19.48
 C      -0.276922     1.855476     1.746792      98.51
 O       0.168915     3.288269     2.121070     263.44
 H       0.819253     3.414921     1.371595      30.35
 H      -0.766855     1.486105     2.583280      26.18
 H      -1.290026     1.841422     1.095446      23.69
 C      -1.554698    -2.390466    -1.105765      42.00
 H      -2.087572    -3.390113    -0.981574      20.78
 C      -0.924506    -0.461508    -2.455700      34.95
 H      -0.719238    -0.139725    -3.485773      22.26
 C      -0.213151     0.176248    -1.407485      12.18
 O       0.569377     1.286912    -1.548447     241.45
 C      -0.216792     2.485143    -1.832801      80.86
 H      -1.043180     2.252805    -2.775443      21.77
 H      -0.769027     2.960953    -0.927832      24.97
 H       0.511735     3.252354    -2.262004      23.59
 C      -0.120957    -0.742080    -0.256251      19.78
 O       0.546019    -0.463560     0.919152     182.18
 C      -0.865282    -1.842847    -0.064295      46.25
 H      -0.948635    -2.519041     0.949673      21.98
 C      -1.675722    -1.573571    -2.316527      44.64
 C      -2.313580    -2.038060    -3.561178      79.83
 H      -2.038798    -1.247743    -4.374818      26.58
 O      -2.124751    -3.432479    -4.051205     232.62
 H      -1.370940    -3.812188    -3.804425      32.26
 C      -3.948736    -2.065204    -3.456592      67.13
 H      -4.428719    -2.667968    -2.547765      25.25
 O      -4.339856    -0.585038    -3.069550     215.98
 H      -5.265069    -0.478878    -3.132977      29.96
 C      -4.518109    -2.402298    -4.805971      80.90
 O      -6.012742    -1.682448    -4.995198     161.72
 H      -6.623609    -2.268815    -5.765837      22.78
 H      -4.400518    -3.441861    -5.230190      25.34
 H      -3.833108    -1.653401    -5.429051      24.83
55
name = lig-ACN-frame_831
 C       3.581456    -0.297322     0.341637      46.28
 H       2.702357    -0.153878    -0.425404      21.19
 C       4.395679    -0.118572     2.676382      63.32
 H       4.164417     0.113643     3.798029      20.75
 C       5.500042    -0.913822     2.388423      27.08
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 O       6.680026    -1.254430     3.036254     255.97
 C       6.653250    -1.017501     4.552441     124.22
 H       7.738136    -1.155712     4.750509      27.31
 H       5.961305    -1.608196     5.086251      31.49
 H       6.309737    -0.041988     4.815632      32.62
 C       5.864554    -1.133537     0.999644      18.88
 O       6.945032    -1.630801     0.528022     216.56
 H       7.323811    -2.098438     1.255220      24.68
 C       4.829886    -0.911636     0.040523      55.93
 H       4.942728    -1.306697    -0.877432      23.25
 C       3.408178     0.038681     1.692453      31.11
 C       2.114272     0.796270     2.179032      93.68
 H       2.515982     1.779003     2.289023      24.45
 O       1.813434     0.152002     3.557784     252.57
 H       1.708787    -0.828145     3.480188      26.77
 C       0.946611     0.886639     1.217916     101.79
 H       1.421856     1.319784     0.221646      18.28
 C      -0.232209     1.810146     1.666405      96.30
 O       0.225816     3.143995     2.124841     208.24
 H       0.773245     3.712533     1.331254      27.10
 H      -0.435157     1.358924     2.616529      24.10
 H      -1.079602     1.913328     0.873970      23.60
 C      -1.499732    -2.453014    -1.188606      46.10
 H      -2.018493    -3.490291    -1.068481      21.51
 C      -0.946143    -0.359559    -2.434918      31.48
 H      -1.051633     0.289551    -3.426272      19.42
 C      -0.286987     0.136100    -1.313919      15.44
 O       0.603932     1.290530    -1.540999     210.20
 C      -0.143723     2.545269    -1.987970      72.61
 H      -0.995776     2.406264    -2.897215      21.53
 H      -0.620390     3.022017    -0.981962      23.84
 H       0.768638     3.252173    -2.266955      23.05
 C      -0.242015    -0.597441    -0.142742       1.86
 O       0.514159    -0.477855     0.973835     166.58
 C      -0.917140    -1.940852    -0.019251      30.87
 H      -0.368842    -2.580997     0.821218      20.13
 C      -1.560517    -1.720525    -2.365452      32.04
 C      -2.404367    -2.047288    -3.619318      84.96
 H      -2.166084    -1.411705    -4.502661      26.22
 O      -2.085048    -3.478404    -3.956907     249.20
 H      -1.218679    -3.528645    -3.778375      31.47
 C      -3.977078    -1.930886    -3.417984      86.10
 H      -4.309998    -2.856004    -2.682449      25.57
 O      -4.299677    -0.707503    -3.130016     222.92
 H      -5.436247    -0.713929    -2.905130      23.44
 C      -4.554151    -2.232162    -4.894332      78.95
 O      -6.026988    -1.711123    -4.957014     211.80
 H      -6.500092    -2.585483    -5.566951      22.42
 H      -4.601781    -3.410181    -4.967673      24.28
 H      -4.022296    -1.749281    -5.815156      24.97
55
name = lig-ACN-frame_832
 C       3.644673    -0.425726     0.380440      51.49
 H       2.825819    -0.237430    -0.433781      22.41
 C       4.401151    -0.073350     2.754607      42.62
 H       4.060647     0.476295     3.786002      18.40
 C       5.563068    -0.821701     2.371052      16.97
 O       6.631485    -1.194681     3.173258     263.09
 C       6.630085    -1.028133     4.526817     127.47
 H       7.688314    -1.315433     4.969686      25.83
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 H       6.027494    -1.847600     4.894984      28.45
 H       6.441281    -0.049765     4.801313      31.31
 C       5.713444    -1.121416     0.988992      10.85
 O       6.997995    -1.696983     0.485199     196.94
 H       7.625035    -2.256942     1.052054      24.81
 C       4.809579    -1.049298    -0.053536      61.96
 H       5.162323    -1.149075    -0.990101      21.14
 C       3.408379     0.101209     1.711353      21.83
 C       2.180671     0.799055     2.201063      97.56
 H       2.254625     1.836917     2.632827      22.26
 O       1.796417     0.190306     3.543662     159.15
 H       1.450600    -0.874097     3.283344      21.51
 C       1.035756     0.946167     1.165910     102.26
 H       1.346272     1.412338     0.142115      18.06
 C      -0.097637     1.743339     1.718494     111.55
 O       0.281186     3.009867     2.082605     282.85
 H       0.562046     3.487558     1.259367      30.33
 H      -0.911683     1.339476     2.393536      24.50
 H      -0.840469     1.794053     0.850805      23.62
 C      -1.503561    -2.507231    -1.248919      42.23
 H      -1.724511    -3.596114    -1.431171      22.25
 C      -1.011761    -0.398933    -2.384061      50.60
 H      -1.242064     0.459371    -3.219481      19.46
 C      -0.274804     0.140334    -1.292417      -6.78
 O       0.510904     1.295997    -1.566277     206.47
 C       0.025431     2.575361    -2.070010      84.47
 H      -0.723319     2.249981    -3.067768      20.02
 H      -0.713101     3.137078    -1.266786      24.77
 H       0.928605     3.263472    -2.448241      23.49
 C      -0.413378    -0.663914     0.013780       7.64
 O       0.492675    -0.392525     1.061689     148.59
 C      -0.836770    -1.966393    -0.127692      50.67
 H      -0.817879    -2.544477     0.859895      21.39
 C      -1.538341    -1.650862    -2.477564      26.33
 C      -2.423460    -2.191652    -3.614246     105.31
 H      -2.121110    -1.548186    -4.435576      26.14
 O      -2.074834    -3.514798    -3.879856     241.30
 H      -1.023976    -3.698794    -3.678343      24.84
 C      -3.931138    -2.034399    -3.651272      74.31
 H      -4.375193    -2.780131    -2.775093      24.76
 O      -4.319961    -0.602814    -3.046214     153.29
 H      -5.437410    -0.728312    -2.910408      24.86
 C      -4.694996    -2.160833    -4.931961     109.35
 O      -5.983173    -1.791676    -4.896657     293.27
 H      -6.524621    -2.333282    -5.503718      27.86
 H      -4.635260    -3.353136    -5.173539      24.73
 H      -3.997876    -1.712893    -5.732287      25.83
55
name = lig-ACN-frame_833
 C       3.557776    -0.437366     0.437160      57.27
 H       2.772763    -0.207556    -0.320279      21.39
 C       4.436595    -0.089683     2.701495      51.49
 H       4.537612     0.258568     3.860178      20.65
 C       5.615718    -0.681881     2.319187       6.79
 O       6.656435    -1.144638     3.176344     240.67
 C       6.573715    -1.064638     4.676552     110.13
 H       7.728092    -1.266912     4.948661      25.00
 H       5.774762    -1.594738     5.219106      28.69
 H       6.320656    -0.136602     5.025375      30.72
 C       5.840475    -1.306247     0.932746       2.02
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 O       7.018634    -1.747221     0.451300     177.16
 H       7.496398    -1.967891     1.340459      22.19
 C       4.783740    -1.063855    -0.036603      47.98
 H       4.878169    -1.441502    -1.059210      22.88
 C       3.476086     0.132813     1.713182      33.58
 C       2.208738     0.810489     2.306530     100.03
 H       2.690462     1.898823     2.446838      22.44
 O       1.724363     0.254513     3.448510     263.13
 H       1.231716    -0.801368     3.312817      22.00
 C       1.127802     0.901850     1.296294      98.86
 H       1.635751     1.214359     0.358281      21.71
 C      -0.161748     1.682976     1.664671      98.51
 O       0.338685     3.042856     2.080490     282.62
 H       0.711056     3.375546     1.320114      33.51
 H      -0.358895     1.088415     2.683923      21.68
 H      -0.834130     1.787718     0.825694      24.52
 C      -1.403558    -2.467366    -1.385122      58.65
 H      -1.661016    -3.491612    -1.298974      21.99
 C      -1.088585    -0.360260    -2.356771      52.10
 H      -1.023922     0.133684    -3.450152      19.92
 C      -0.360974     0.115250    -1.265987      22.02
 O       0.456004     1.262086    -1.521070     226.45
 C       0.073031     2.512008    -2.185284      82.61
 H      -0.576089     2.526574    -3.241851      21.62
 H      -0.460270     3.342422    -1.420207      23.65
 H       1.206677     2.995991    -2.444634      22.45
 C      -0.286646    -0.611190    -0.070573       7.76
 O       0.409396    -0.385102     1.085758     159.49
 C      -0.880370    -2.042613    -0.160231      48.33
 H      -1.031787    -2.714287     0.649380      20.67
 C      -1.711108    -1.656425    -2.405893      42.91
 C      -2.264960    -2.158309    -3.726790      71.92
 H      -1.948674    -1.656549    -4.595425      26.63
 O      -2.092748    -3.676747    -3.849386     127.98
 H      -0.972881    -3.903159    -3.453053      21.48
 C      -4.005118    -2.018824    -3.620647      52.15
 H      -4.596554    -2.847258    -2.931651      24.45
 O      -4.305461    -0.584682    -2.990902     213.74
 H      -5.193022    -0.499679    -2.983458      30.84
 C      -4.573481    -2.268154    -5.065725      82.02
 O      -6.117595    -1.802501    -4.821116     277.82
 H      -6.484131    -2.025985    -5.557813      32.97
 H      -4.380820    -3.355271    -5.609209      24.54
 H      -4.311319    -1.451362    -5.717716      26.22
55
name = lig-ACN-frame_834
 C       3.560697    -0.385584     0.451705      57.52
 H       2.743393    -0.307278    -0.195603      23.71
 C       4.603524    -0.110395     2.613209      50.24
 H       4.233441     0.209275     3.680803      18.82
 C       5.780745    -0.800644     2.203556      25.47
 O       6.703551    -1.091471     3.175080     178.21
 C       6.490650    -1.002655     4.793708      77.68
 H       7.533129    -1.505370     5.173541      24.95
 H       5.771888    -1.875902     4.953885      25.22
 H       6.419459    -0.013631     5.046619      26.98
 C       5.823255    -1.273936     0.905511      20.82
 O       7.077664    -1.837947     0.487884     186.64
 H       7.788743    -1.886960     1.111208      24.02
 C       4.725256    -1.077554     0.088992      64.96
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 H       4.675708    -1.694700    -0.880517      22.44
 C       3.469116     0.087210     1.789687      21.18
 C       2.249307     0.820074     2.264418      95.74
 H       2.395554     2.000355     2.617334      23.38
 O       1.632503     0.277719     3.529112     237.09
 H       1.455756    -0.689165     3.192025      25.43
 C       1.050981     0.889678     1.251032     100.57
 H       1.359655     1.276256     0.316889      22.52
 C      -0.044551     1.774828     1.731646     107.18
 O       0.310754     3.102303     2.054896     242.57
 H       1.094457     3.421508     1.383811      28.45
 H      -0.684867     1.447448     2.767457      23.27
 H      -0.905276     1.637048     1.151125      26.62
 C      -1.430953    -2.532471    -1.322444      51.00
 H      -1.878374    -3.439394    -1.422449      21.58
 C      -1.168838    -0.352714    -2.441520      53.31
 H      -0.983085     0.335460    -3.327055      20.30
 C      -0.453531     0.160046    -1.316716      10.03
 O       0.420056     1.222022    -1.441462     204.43
 C       0.149194     2.458413    -2.265786      75.40
 H      -0.605934     2.042636    -3.181996      20.24
 H      -0.417129     3.230179    -1.488387      23.58
 H       1.291029     2.814889    -2.560120      22.71
 C      -0.182689    -0.771923    -0.178438       9.48
 O       0.393618    -0.467286     1.085078     170.45
 C      -0.854019    -1.933448    -0.149657      55.39
 H      -0.475777    -2.448075     0.637764      22.97
 C      -1.749079    -1.609698    -2.471632      15.90
 C      -2.379227    -2.251679    -3.718639      89.32
 H      -1.995532    -1.768543    -4.557016      27.19
 O      -2.122703    -3.739905    -3.841169     146.97
 H      -0.963764    -4.011653    -3.472156      20.33
 C      -3.942651    -1.934061    -3.628686      83.02
 H      -4.087330    -2.823466    -2.824345      24.55
 O      -4.231278    -0.720567    -3.036661     282.15
 H      -5.144230    -0.566690    -3.219186      29.56
 C      -4.613952    -2.103620    -5.077735      84.42
 O      -6.148109    -1.898745    -4.794636     250.18
 H      -6.731381    -2.008202    -5.672339      26.79
 H      -4.542344    -3.300969    -5.359920      24.37
 H      -4.091911    -1.527874    -5.813260      26.94
55
name = lig-ACN-frame_835
 C       3.591114    -0.376577     0.488732      49.74
 H       2.805202    -0.327324    -0.176278      23.08
 C       4.648901    -0.109767     2.607928      53.66
 H       4.793829     0.207183     3.643728      19.93
 C       5.772753    -0.852283     2.326787       9.14
 O       6.870808    -1.062233     3.272165     258.83
 C       6.435906    -1.013276     4.636945     110.26
 H       7.374154    -1.377927     5.261283      25.20
 H       5.360060    -1.483508     4.930425      26.01
 H       6.153287    -0.055193     5.064050      28.37
 C       5.953186    -1.222553     0.920642      -6.02
 O       7.050169    -1.933336     0.441647     181.00
 H       7.610697    -1.946412     1.254897      24.08
 C       4.711518    -1.167748     0.103006      38.67
 H       4.892312    -1.552435    -1.031062      19.74
 C       3.468803     0.079052     1.809886      30.71
 C       2.127655     0.772366     2.263039      80.08
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 H       2.483210     1.964910     2.557407      21.83
 O       1.617777     0.270218     3.592202     285.43
 H       1.463602    -0.584703     3.615297      32.09
 C       0.990928     0.869030     1.215086      99.49
 H       1.288133     1.235592     0.309624      22.21
 C      -0.112842     1.852603     1.859855      93.02
 O       0.321585     3.249451     2.003463     208.13
 H       1.046019     3.383412     1.155757      25.91
 H      -0.435226     1.330485     2.978987      21.37
 H      -0.777585     1.944683     1.089750      25.46
 C      -1.623880    -2.427637    -1.273958      52.43
 H      -1.851731    -3.452717    -1.124496      21.44
 C      -1.174797    -0.338195    -2.517057      63.05
 H      -1.590531     0.213379    -3.277830      21.20
 C      -0.417528     0.100081    -1.370762      12.35
 O       0.413806     1.247862    -1.383428     233.77
 C       0.188572     2.297709    -2.266624     103.81
 H      -0.548834     2.037860    -3.276630      21.98
 H      -0.408065     3.260339    -1.801123      24.44
 H       1.116460     2.822919    -2.862064      23.88
 C      -0.209895    -0.705160    -0.222549       8.06
 O       0.460021    -0.487317     1.006643     170.32
 C      -0.761182    -2.046674    -0.202670      44.75
 H      -0.759786    -2.682294     0.602108      21.84
 C      -1.644072    -1.728962    -2.459850      24.53
 C      -2.422517    -2.320572    -3.683924     103.77
 H      -2.054327    -1.806705    -4.540278      25.17
 O      -2.214241    -3.708912    -3.834394     214.49
 H      -1.029858    -3.736707    -3.629552      21.12
 C      -3.900021    -2.068814    -3.720895      85.79
 H      -4.605760    -2.862249    -3.194242      24.61
 O      -4.153217    -0.766661    -3.069734     185.80
 H      -5.256361    -0.653324    -3.385942      24.47
 C      -4.731106    -2.041433    -4.933707     100.95
 O      -6.084156    -1.938091    -4.783039     189.14
 H      -6.466384    -2.466471    -5.787871      21.58
 H      -4.441032    -3.178021    -5.393172      23.74
 H      -4.462781    -1.302720    -5.672537      25.90
55
name = lig-ACN-frame_836
 C       3.649562    -0.495694     0.501210      46.33
 H       2.887457    -0.291267    -0.237853      22.15
 C       4.586428    -0.069341     2.782119      46.12
 H       4.427465     0.528860     3.590834      17.94
 C       5.859549    -0.849736     2.343362       5.26
 O       6.939180    -1.033104     3.248275     238.21
 C       6.364129    -0.972269     4.587514      94.54
 H       7.078544    -1.484406     5.327168      24.43
 H       5.427737    -1.783294     4.519034      24.02
 H       6.309411     0.106962     4.727011      27.25
 C       5.942024    -1.289678     0.983721      18.80
 O       6.980181    -1.980938     0.418688     168.27
 H       7.688293    -2.529717     0.963436      24.50
 C       4.884162    -1.129418     0.111794      45.74
 H       4.909822    -1.466567    -1.058638      20.65
 C       3.481229     0.071781     1.818933      -0.78
 C       2.096221     0.668156     2.353893      97.46
 H       2.363276     1.924386     2.476922      21.97
 O       1.653155     0.283323     3.622885     288.40
 H       1.508401    -0.631209     3.421253      28.59
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 C       0.974060     0.906407     1.340544      94.28
 H       1.512858     1.425808     0.600402      22.23
 C      -0.197991     1.893549     1.821302      87.47
 O       0.367579     3.353993     1.959212     238.63
 H       0.736060     3.566834     1.034666      27.91
 H      -0.446152     1.623424     3.062981      22.28
 H      -1.120048     1.733128     1.462530      26.58
 C      -1.665703    -2.447741    -1.223232      54.80
 H      -2.375093    -3.308212    -1.266797      21.77
 C      -1.158320    -0.465011    -2.486825      70.63
 H      -1.351938     0.145619    -3.275596      23.15
 C      -0.307422     0.037388    -1.438699       1.35
 O       0.394917     1.249645    -1.341881     213.58
 C       0.140086     2.282393    -2.391758      83.34
 H      -0.504644     1.693803    -3.358449      19.74
 H      -0.361456     3.169486    -1.793702      23.64
 H       1.255843     2.479372    -2.499784      23.64
 C      -0.291803    -0.752933    -0.184868       5.74
 O       0.528991    -0.418960     0.864895     182.76
 C      -0.784998    -2.086663    -0.238640      60.93
 H      -0.682170    -2.605916     0.716813      22.24
 C      -1.701067    -1.756052    -2.475662      31.80
 C      -2.379258    -2.279996    -3.706872      84.05
 H      -2.060123    -1.719043    -4.596548      24.52
 O      -2.269854    -3.727043    -3.831380     257.69
 H      -1.325928    -4.147444    -3.742614      27.35
 C      -4.068057    -2.150526    -3.590243      67.79
 H      -4.284608    -2.981907    -2.855773      25.03
 O      -4.120177    -0.779481    -3.079166     149.82
 H      -5.155481    -0.288844    -2.972169      23.79
 C      -4.619284    -2.112134    -5.089765      70.33
 O      -6.149834    -1.976421    -4.742778     217.75
 H      -6.759619    -2.701527    -5.426264      23.94
 H      -4.362498    -2.911441    -5.960279      24.00
 H      -4.193800    -1.109926    -5.348215      26.07
55
name = lig-ACN-frame_837
 C       3.717061    -0.548152     0.549277      53.88
 H       2.889887    -0.570466    -0.234575      21.98
 C       4.583183    -0.098388     2.759374      58.66
 H       4.466824     0.158597     3.698108      22.97
 C       5.798403    -0.683137     2.368036       5.28
 O       6.912255    -1.018325     3.148800     225.20
 C       6.382465    -0.970944     4.589784      86.60
 H       7.116147    -1.396097     5.231443      27.02
 H       5.213520    -1.476484     4.662860      24.90
 H       6.009319     0.003130     5.105830      25.96
 C       5.893787    -1.394771     1.106370      -5.25
 O       6.990792    -2.056817     0.394337     193.69
 H       7.484708    -2.596731     1.080508      23.78
 C       4.943888    -0.993976     0.123616      34.54
 H       5.212878    -1.553665    -0.885480      20.68
 C       3.505782    -0.054279     1.864327      28.02
 C       2.179094     0.749215     2.384783      69.52
 H       2.542349     1.901717     2.788627      22.44
 O       1.705898     0.191908     3.684576     209.85
 H       1.300537    -0.846922     3.691316      23.26
 C       0.971452     0.999140     1.372697      73.63
 H       1.338918     1.514301     0.470326      21.53
 C      -0.122931     1.962125     1.883489     100.25
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 O       0.289506     3.310151     1.874984     292.16
 H       0.707285     3.533328     1.109767      33.59
 H      -0.428535     1.789736     3.084252      22.38
 H      -0.797454     1.857798     1.078178      25.63
 C      -1.706192    -2.580167    -1.300447      48.28
 H      -2.326282    -3.503798    -0.971247      21.46
 C      -1.021265    -0.507576    -2.491964      64.25
 H      -0.791458    -0.094713    -3.449955      23.04
 C      -0.304661    -0.044660    -1.404901      18.02
 O       0.305794     1.200114    -1.348368     218.53
 C       0.175193     2.249980    -2.423384     103.39
 H      -0.337908     1.842457    -3.573283      21.63
 H      -0.633844     3.015877    -2.177705      26.12
 H       0.992309     2.906809    -2.825434      25.33
 C      -0.246292    -0.788458    -0.243527      17.02
 O       0.590921    -0.366306     0.799797     185.66
 C      -0.923513    -2.025243    -0.113562      36.68
 H      -0.595254    -2.679195     0.785888      20.82
 C      -1.794272    -1.716972    -2.432024      28.38
 C      -2.526453    -2.319570    -3.671771      88.42
 H      -2.171286    -1.724066    -4.573596      25.18
 O      -2.312622    -3.791015    -3.865667     254.94
 H      -1.485266    -3.860579    -3.614704      32.18
 C      -3.949823    -2.116832    -3.549425      85.92
 H      -4.513049    -2.764638    -2.891560      27.06
 O      -4.146093    -0.783960    -3.052576     262.81
 H      -5.033449    -0.754066    -2.768420      30.18
 C      -4.671850    -2.121143    -5.069461      69.94
 O      -6.148420    -2.025835    -4.747062     267.13
 H      -6.644019    -2.495441    -5.524079      26.60
 H      -4.439411    -3.020848    -5.773855      24.81
 H      -4.282067    -1.141838    -5.602839      26.00
55
name = lig-ACN-frame_838
 C       3.662668    -0.482769     0.568104      44.44
 H       2.706012    -0.406170    -0.118736      20.67
 C       4.586939    -0.151231     2.731339      40.87
 H       4.516109     0.159780     3.730932      21.64
 C       5.831658    -0.731671     2.290135      14.33
 O       6.777242    -0.931217     3.249856     256.86
 C       6.449449    -0.991101     4.606965     102.24
 H       7.279294    -1.445707     5.037887      26.65
 H       5.581675    -1.876329     4.809907      25.18
 H       6.471457     0.155348     4.883980      24.77
 C       5.964364    -1.347403     1.013907      29.17
 O       6.957726    -2.116213     0.541011     206.69
 H       7.667041    -2.309643     1.143372      23.74
 C       4.945650    -1.031165     0.137923      59.50
 H       4.997994    -1.222272    -0.950302      24.25
 C       3.419931    -0.079593     1.888858      21.86
 C       2.242199     0.702524     2.408802      81.99
 H       2.792666     1.794942     2.680502      22.52
 O       1.760921     0.109492     3.740761     169.83
 H       1.480917    -0.885456     3.154184      20.88
 C       1.118998     1.047582     1.335495      69.28
 H       1.609213     1.606475     0.446259      21.32
 C      -0.091624     1.895015     1.848797     101.16
 O       0.215077     3.345374     1.846818     281.83
 H       0.902565     3.318907     1.150611      28.90
 H      -0.629656     1.423331     2.811456      23.34
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 H      -1.011135     1.702430     1.275965      24.89
 C      -1.679404    -2.513882    -1.150055      55.32
 H      -2.059573    -3.599752    -1.304952      21.23
 C      -0.926588    -0.663235    -2.613767      55.59
 H      -0.970833    -0.094171    -3.618748      21.00
 C      -0.362954    -0.016239    -1.434759      -6.50
 O       0.280801     1.236917    -1.435906     204.21
 C       0.116782     2.223546    -2.460260      95.25
 H      -0.207190     1.540847    -3.549815      19.75
 H      -0.567799     2.989056    -2.078159      25.65
 H       1.134295     2.506154    -2.299513      24.68
 C      -0.193942    -0.789588    -0.171885       6.73
 O       0.652831    -0.360488     0.867391     172.03
 C      -1.052791    -1.999431    -0.100659      45.46
 H      -1.147954    -2.663747     0.907214      20.80
 C      -1.793099    -1.821001    -2.392939      26.66
 C      -2.501842    -2.398405    -3.623921      89.91
 H      -2.073837    -1.853277    -4.555231      24.09
 O      -2.315378    -3.787004    -3.883427     302.85
 H      -1.520852    -4.056797    -3.628777      32.91
 C      -4.062459    -2.020497    -3.695844      97.44
 H      -4.425718    -2.884574    -3.151176      26.40
 O      -4.224726    -0.750438    -2.983865     276.98
 H      -5.079332    -0.756409    -2.634249      30.55
 C      -4.750316    -2.126278    -4.883781     113.61
 O      -6.107384    -2.045768    -4.765016     307.70
 H      -6.473172    -2.251498    -5.526306      33.76
 H      -4.447863    -3.232588    -5.149725      25.41
 H      -4.456566    -1.482657    -5.806006      25.19
55
name = lig-ACN-frame_840
 C       3.590868    -0.366078     0.438021      54.67
 H       2.658954    -0.147353    -0.133663      19.76
 C       4.511675    -0.210997     2.762256      41.19
 H       4.479621     0.102101     3.926372      20.25
 C       5.707613    -0.862237     2.374443       7.38
 O       6.875787    -0.887490     3.227157     197.62
 C       6.661367    -1.031880     4.821471     102.68
 H       7.612900    -1.444284     5.105138      26.31
 H       5.967499    -1.957041     4.910500      24.35
 H       6.603379     0.131102     5.150210      25.37
 C       5.857744    -1.253393     0.967218      -1.51
 O       6.931465    -2.158345     0.766163     108.69
 H       7.549914    -2.133571     1.598020      22.15
 C       4.818727    -1.070545     0.019891      60.05
 H       4.844923    -1.602915    -0.876555      22.17
 C       3.481367     0.040097     1.778985      21.69
 C       2.241138     0.691164     2.408817      85.61
 H       2.615959     1.810006     2.749288      22.71
 O       1.788253     0.000304     3.643393     231.37
 H       1.613801    -0.963753     3.229869      24.04
 C       1.159412     0.851323     1.318590      99.66
 H       1.633783     1.385570     0.377516      20.99
 C       0.075489     1.814539     1.756041     108.49
 O       0.080888     3.198823     1.880400     269.98
 H       0.248977     3.493675     0.872613      26.81
 H      -0.494971     1.329064     2.558815      25.13
 H      -0.832588     1.644328     1.026033      23.03
 C      -1.713633    -2.452640    -0.954058      61.05
 H      -2.578752    -3.053713    -0.780675      21.22
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 C      -0.993114    -0.651936    -2.504367      53.38
 H      -0.785869    -0.017306    -3.520987      17.70
 C      -0.286454    -0.073835    -1.409148      12.75
 O       0.265004     1.160327    -1.499951     226.74
 C       0.041687     2.264011    -2.534636      96.22
 H      -0.594653     1.575316    -3.338030      20.20
 H      -0.522781     2.917426    -1.964030      28.05
 H       1.058229     2.536017    -2.581086      26.05
 C      -0.248820    -0.608470    -0.100770      26.52
 O       0.621266    -0.430235     0.939714     199.83
 C      -1.045079    -1.789427     0.021401      40.54
 H      -0.928991    -2.343750     1.100578      20.54
 C      -1.540713    -2.013812    -2.381887      24.24
 C      -2.497273    -2.360412    -3.610556      82.76
 H      -2.344907    -1.805685    -4.637028      22.72
 O      -2.381940    -3.806654    -3.879893     171.53
 H      -1.269621    -4.194636    -3.670857      21.87
 C      -3.979502    -2.068329    -3.367238      69.19
 H      -4.333968    -2.795560    -2.758760      27.23
 O      -4.315587    -0.612906    -2.872433     172.84
 H      -5.463279    -0.787569    -3.055909      23.44
 C      -4.729519    -2.325717    -4.904807      86.64
 O      -6.220776    -1.937275    -4.710156     236.74
 H      -6.845064    -2.583659    -5.399043      26.35
 H      -4.690174    -3.267322    -5.406767      26.60
 H      -4.582013    -1.542349    -5.690843      25.58
55
name = lig-ACN-frame_841
 C       3.705873    -0.353371     0.412938      45.33
 H       3.008166    -0.405790    -0.378715      22.59
 C       4.486879    -0.213926     2.771502      48.89
 H       3.992351     0.036319     3.862148      20.12
 C       5.723348    -0.761916     2.442915      13.56
 O       6.913657    -0.949204     3.229176     253.94
 C       6.780592    -1.063521     4.669720     109.53
 H       7.822979    -1.261601     5.120638      25.59
 H       5.935005    -1.630402     5.112627      28.07
 H       6.332895    -0.040559     5.184967      25.96
 C       5.717591    -1.419467     1.162224       7.25
 O       6.866608    -2.063661     0.754154     182.61
 H       7.277202    -2.408792     1.546606      24.54
 C       4.845093    -1.081961     0.082230      48.79
 H       5.015448    -1.514357    -0.896126      22.84
 C       3.526682     0.095712     1.798571      32.73
 C       2.244513     0.691409     2.293936      89.34
 H       2.391256     1.833227     2.684109      23.01
 O       1.766671    -0.034539     3.585566     226.16
 H       1.477901    -0.930770     3.385782      26.30
 C       1.158049     0.899007     1.299206      84.34
 H       1.645618     1.310034     0.332631      20.76
 C      -0.121061     1.689849     1.746294      96.52
 O       0.110676     3.150613     1.874898     310.63
 H       0.176052     3.544905     1.074549      32.41
 H      -0.479972     1.392842     2.678705      24.97
 H      -0.713431     1.500661     0.778180      22.12
 C      -1.730100    -2.418503    -1.016268      57.56
 H      -2.138210    -3.353253    -0.804966      23.06
 C      -0.922376    -0.678482    -2.402386      44.23
 H      -0.886739    -0.434831    -3.569382      21.37
 C      -0.272812     0.031696    -1.375952      17.64
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 O       0.407257     1.261831    -1.526258     231.29
 C      -0.065446     2.188188    -2.490792     131.29
 H      -0.583749     2.098540    -3.577145      24.03
 H      -0.489814     3.074273    -2.105481      28.44
 H       0.770017     2.624907    -3.021521      26.90
 C      -0.251382    -0.699580    -0.108746      20.84
 O       0.576096    -0.445704     0.971221     154.64
 C      -1.077503    -1.783124     0.099619      44.25
 H      -1.181346    -2.234549     1.165391      19.54
 C      -1.655576    -1.834758    -2.261754      34.84
 C      -2.483869    -2.410419    -3.449173      68.85
 H      -1.915298    -1.717214    -4.203956      23.65
 O      -2.434049    -3.779505    -3.899650     171.03
 H      -1.323096    -4.039140    -3.445269      20.97
 C      -4.054779    -2.115370    -3.408650      95.39
 H      -4.371307    -2.699276    -2.643681      27.96
 O      -4.296590    -0.736254    -2.929698     261.91
 H      -5.206501    -0.476773    -3.176662      28.68
 C      -4.828321    -2.239969    -4.648677     122.20
 O      -6.177486    -1.920041    -4.684893     236.82
 H      -6.651215    -2.454107    -5.630075      24.62
 H      -4.628562    -3.238069    -4.817692      28.38
 H      -4.085029    -1.687713    -5.266350      27.87
55
name = lig-ACN-frame_842
 C       3.772630    -0.325195     0.444849      71.94
 H       3.145981     0.106976    -0.247000      23.54
 C       4.473928    -0.151085     2.820281      63.42
 H       4.353303     0.213694     3.956724      21.71
 C       5.712681    -0.763167     2.522602      16.63
 O       6.863637    -1.033013     3.184495     265.55
 C       6.814431    -1.009797     4.592768     106.87
 H       7.945367    -1.257915     4.911981      24.99
 H       6.326554    -1.922933     4.802109      27.68
 H       6.523420     0.098512     4.990689      25.70
 C       5.745504    -1.437856     1.279642      12.00
 O       6.874557    -2.081323     0.739473     204.75
 H       7.499039    -2.428845     1.401961      24.36
 C       4.870567    -1.134531     0.228743      45.81
 H       5.206385    -1.455537    -0.838383      21.53
 C       3.531331     0.059458     1.739987      26.76
 C       2.181399     0.677709     2.338698      93.75
 H       2.491496     1.719122     2.799961      22.66
 O       1.753817     0.011558     3.468408     299.01
 H       1.577050    -0.787446     3.200070      32.07
 C       1.039574     0.918437     1.237795      94.96
 H       1.453911     1.501117     0.381218      21.62
 C      -0.267015     1.638162     1.655788     110.48
 O       0.143221     3.104371     1.905677     262.82
 H       0.463440     3.442203     1.010354      28.93
 H      -0.475721     1.286305     2.565291      26.99
 H      -1.308720     1.466535     1.227398      23.92
 C      -1.775164    -2.456212    -0.933728      52.30
 H      -2.147687    -3.422862    -0.944719      23.36
 C      -0.864266    -0.663144    -2.429494      34.56
 H      -0.894320     0.014174    -3.355184      21.20
 C      -0.266509     0.053568    -1.325352     -10.17
 O       0.532883     1.294361    -1.555853     196.67
 C      -0.120697     2.276729    -2.575001      74.43
 H      -0.831106     1.528942    -2.827860      24.59
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 H      -0.699332     2.840606    -1.877047      26.67
 H       0.744093     2.773194    -3.095663      23.45
 C      -0.233246    -0.690251    -0.088366       4.58
 O       0.579659    -0.450545     1.017770     170.57
 C      -1.110654    -1.855299     0.135354      41.28
 H      -1.145696    -2.198949     1.153886      21.81
 C      -1.850091    -1.750180    -2.163834      27.41
 C      -2.458426    -2.308522    -3.432228      62.94
 H      -2.265847    -1.787334    -4.421024      23.15
 O      -2.410967    -3.766755    -3.826903     185.55
 H      -1.467520    -4.357926    -3.701867      24.37
 C      -4.174654    -2.095381    -3.180527      95.42
 H      -4.543370    -2.824814    -2.552897      28.01
 O      -4.216311    -0.766842    -2.938466     299.92
 H      -5.014082    -0.441454    -3.126177      31.33
 C      -4.713516    -2.355405    -4.632632     101.94
 O      -6.199251    -1.863198    -4.640916     271.46
 H      -6.382031    -2.152392    -5.599682      29.81
 H      -4.761118    -3.335557    -4.852183      28.33
 H      -4.331900    -1.788071    -5.457714      27.42
55
name = lig-ACN-frame_843
 C       3.762354    -0.250204     0.498587      38.80
 H       3.275339     0.056874    -0.387563      23.25
 C       4.522130    -0.082406     2.855769      49.61
 H       4.377159     0.528125     3.794963      21.43
 C       5.632640    -0.908048     2.482199      19.37
 O       6.865528    -1.059412     3.150056     252.04
 C       6.893987    -1.015049     4.609321     109.17
 H       8.082728    -0.961225     4.908548      24.42
 H       6.330330    -1.683783     5.151372      28.86
 H       6.372307    -0.038200     5.026679      26.73
 C       5.859079    -1.398890     1.178863      18.93
 O       6.949438    -2.177706     0.765994     170.29
 H       7.666352    -2.125584     1.520471      22.68
 C       4.885308    -1.164442     0.273617      42.58
 H       5.134766    -1.595391    -0.850133      20.88
 C       3.440089     0.092096     1.908696      15.82
 C       2.168274     0.829405     2.274897      91.05
 H       2.417173     1.907142     2.573454      23.93
 O       1.688076     0.005448     3.427951     240.78
 H       1.531016    -0.881750     3.199421      28.55
 C       0.912541     0.901655     1.220201      95.12
 H       1.288978     1.237034     0.290281      22.38
 C      -0.269190     1.733728     1.770577     119.32
 O       0.122825     3.016562     1.895595     266.97
 H       0.795305     3.265912     1.056848      26.84
 H      -0.588915     1.372065     2.622054      27.78
 H      -0.953319     1.697733     0.863565      23.37
 C      -1.844920    -2.438820    -0.909873      48.48
 H      -2.611927    -3.129672    -0.623008      20.95
 C      -0.998266    -0.567127    -2.354507      46.27
 H      -0.966420    -0.320956    -3.414986      20.34
 C      -0.164344     0.034313    -1.313693       3.57
 O       0.593815     1.198716    -1.583372     195.01
 C      -0.229989     2.233681    -2.477571      98.67
 H      -0.865158     1.983035    -3.276149      25.40
 H      -0.572697     3.166676    -1.933185      25.21
 H       0.453330     2.690224    -3.302164      24.19
 C      -0.262493    -0.682793    -0.031105      15.85
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 O       0.586929    -0.467927     0.990067     193.37
 C      -1.044839    -1.870932     0.128431      40.80
 H      -0.839733    -2.412198     0.952954      22.01
 C      -1.750977    -1.736376    -2.211985      21.16
 C      -2.666613    -2.316903    -3.406770      82.51
 H      -2.409988    -1.558149    -4.192812      25.55
 O      -2.374609    -3.736662    -3.710226     233.83
 H      -1.412157    -3.783131    -3.597393      28.63
 C      -4.040739    -2.203137    -3.222319      84.48
 H      -4.372054    -2.679961    -2.332755      27.15
 O      -4.167249    -0.610580    -2.834563     155.13
 H      -5.268739    -0.505026    -2.960230      24.93
 C      -4.789045    -2.497929    -4.667278      97.64
 O      -6.148180    -1.830867    -4.608101     332.50
 H      -6.696693    -1.910869    -5.254552      36.31
 H      -4.681902    -3.489068    -4.919848      29.19
 H      -4.088681    -1.981406    -5.244820      31.04
55
name = lig-ACN-frame_844
 C       3.767866    -0.298813     0.627068      65.10
 H       2.881593    -0.227849    -0.010654      23.88
 C       4.544000    -0.092547     2.806405      55.13
 H       4.614923     0.242310     3.803447      23.39
 C       5.647055    -0.957516     2.473109      -1.15
 O       6.874336    -1.087148     3.232736     221.12
 C       6.929116    -0.950282     4.662969     114.91
 H       8.121303    -0.930262     4.949338      24.37
 H       6.587681    -1.807381     5.031459      28.28
 H       6.471388     0.064353     4.958114      26.43
 C       5.885623    -1.417808     1.079227      -4.82
 O       7.049221    -2.255252     0.831138     147.03
 H       7.629490    -2.114472     1.628951      21.83
 C       4.804469    -1.063027     0.149739      51.01
 H       4.661350    -1.483604    -1.021940      20.65
 C       3.495578     0.203227     1.863457      35.78
 C       2.097165     0.879577     2.247473     100.87
 H       2.100634     1.822684     2.740466      25.59
 O       1.599016     0.077600     3.453681     170.63
 H       1.452334    -0.914024     3.005817      23.75
 C       1.008156     0.880745     1.289710     105.19
 H       1.207293     1.451970     0.459906      24.89
 C      -0.272884     1.668420     1.764241     102.89
 O       0.165056     3.141133     1.920062     258.28
 H       0.814068     3.345413     1.201016      30.78
 H      -0.780565     1.474083     2.609296      27.71
 H      -1.103347     1.554193     1.031776      25.73
 C      -1.860602    -2.267354    -0.937153      57.32
 H      -2.461002    -3.245645    -0.797632      21.81
 C      -1.103524    -0.554940    -2.315787      44.47
 H      -0.990719     0.004822    -3.182555      22.10
 C      -0.210958    -0.066964    -1.367610      10.98
 O       0.505483     1.106945    -1.696598     239.27
 C      -0.203489     2.189100    -2.417331      79.69
 H      -1.039268     1.787560    -2.727078      28.41
 H      -0.494201     2.781688    -1.433902      23.49
 H       0.760596     2.609259    -2.911877      22.27
 C      -0.246480    -0.713429    -0.109906      15.71
 O       0.598153    -0.494761     1.010637     182.00
 C      -0.951605    -1.912811     0.072829      54.84
 H      -0.938624    -2.335164     0.965002      23.60
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 C      -1.755248    -1.831986    -2.194454      41.98
 C      -2.515123    -2.284531    -3.361115      93.90
 H      -2.215784    -1.827984    -4.306157      25.81
 O      -2.305187    -3.656526    -3.596317     310.25
 H      -1.523759    -3.929379    -3.443157      35.47
 C      -4.178044    -2.063894    -3.278709      75.41
 H      -4.542063    -2.795819    -2.481877      26.24
 O      -4.189641    -0.635348    -2.804337     194.25
 H      -5.287235    -0.237618    -2.482573      22.78
 C      -4.845277    -2.498575    -4.576931     117.52
 O      -6.058105    -1.819848    -4.535284     272.71
 H      -6.427128    -2.356621    -5.365471      27.74
 H      -5.146827    -3.513631    -4.617483      26.85
 H      -4.395849    -2.206165    -5.475414      27.93
55
name = lig-ACN-frame_845
 C       3.597983    -0.371897     0.591549       8.63
 H       2.699839    -0.386248    -0.123641      21.26
 C       4.627101    -0.154464     2.820683      59.58
 H       4.438735     0.126448     3.766056      24.17
 C       5.763368    -0.877928     2.387862      11.58
 O       6.838760    -1.121802     3.245281     224.44
 C       6.936895    -0.900911     4.718686     110.88
 H       8.102300    -0.779407     4.857834      25.14
 H       6.589962    -1.670568     5.249858      29.83
 H       6.399885    -0.034819     5.171614      28.19
 C       5.873841    -1.473246     1.049423       8.49
 O       7.013028    -2.229879     0.870829     190.94
 H       7.465350    -2.357120     1.693283      23.03
 C       4.865403    -1.038231     0.100335      38.06
 H       4.893725    -1.493348    -1.072433      21.41
 C       3.598970     0.330562     1.913001       8.01
 C       2.155504     0.802444     2.458960      96.76
 H       2.378177     1.781903     2.661166      26.02
 O       1.534604     0.153472     3.481806     217.18
 H       1.271762    -0.981540     3.208843      20.95
 C       0.988520     0.931976     1.255419      93.75
 H       1.480889     1.225282     0.437549      25.51
 C      -0.236351     1.735729     1.747934     113.28
 O       0.178340     3.216093     1.943778     290.73
 H       0.534606     3.457535     1.153785      33.66
 H      -0.324937     1.327410     2.730716      25.38
 H      -1.029035     1.655340     1.074311      26.67
 C      -1.830999    -2.383184    -0.894800      49.95
 H      -2.347790    -3.439308    -0.779527      20.80
 C      -1.099603    -0.563540    -2.432436      47.25
 H      -1.428656    -0.118108    -3.288339      22.48
 C      -0.340793    -0.091382    -1.376906      17.67
 O       0.476256     0.935482    -1.763997     262.79
 C      -0.144282     2.159304    -2.205250     126.12
 H      -0.917736     2.029426    -2.828420      28.34
 H      -0.490662     3.048288    -1.487604      25.86
 H       0.195770     2.725573    -3.134474      25.57
 C      -0.078305    -0.778327    -0.118944      18.52
 O       0.632971    -0.480577     0.990541     194.43
 C      -0.963576    -1.903344     0.059955      47.86
 H      -0.979597    -2.295251     1.027976      23.05
 C      -1.844526    -1.679416    -2.214522      21.38
 C      -2.442619    -2.249958    -3.432802      78.19
 H      -2.149350    -1.603933    -4.228713      26.09
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 O      -2.288050    -3.710613    -3.520268     254.94
 H      -1.365555    -3.928395    -3.324295      28.69
 C      -4.110285    -1.949661    -3.209937      78.66
 H      -4.597938    -2.590575    -2.342396      24.27
 O      -4.268130    -0.683960    -2.831145     235.47
 H      -5.194982    -0.488470    -2.282069      23.62
 C      -4.822127    -2.480602    -4.499417     106.66
 O      -6.149919    -1.783425    -4.541691     228.28
 H      -6.993075    -2.095651    -5.266278      27.07
 H      -4.718777    -3.465858    -4.130309      28.30
 H      -4.257584    -2.532585    -5.360236      29.55
55
name = lig-ACN-frame_846
 C       3.692322    -0.406282     0.549173      48.45
 H       2.914481    -0.174753    -0.278627      22.66
 C       4.637849    -0.102800     2.806080      59.67
 H       4.695483     0.138645     3.778311      22.41
 C       5.799485    -0.762709     2.401790      10.28
 O       6.844469    -1.182873     3.256391     229.06
 C       6.895742    -0.864072     4.719560     116.00
 H       8.000596    -0.666929     4.927276      26.44
 H       6.578397    -1.675959     5.246594      29.39
 H       6.351262     0.040253     4.833669      29.91
 C       5.840376    -1.367002     1.120133      11.49
 O       6.920227    -2.208992     0.813792     160.20
 H       7.337395    -2.395564     1.718198      22.57
 C       4.839348    -1.076841     0.198255      54.53
 H       5.094278    -1.491899    -0.914315      21.52
 C       3.550910     0.100156     1.883940      26.38
 C       2.235000     0.856690     2.427093      87.81
 H       2.347992     1.682231     2.940577      26.42
 O       1.504258     0.140632     3.623426     145.23
 H       1.360168    -0.941591     3.260773      22.25
 C       1.158824     0.980637     1.231356      88.77
 H       1.440325     1.492945     0.386948      25.25
 C      -0.088974     1.878580     1.768214     116.54
 O       0.176434     3.201180     1.942110     249.33
 H       0.238459     3.682106     0.999098      28.05
 H      -0.513461     1.558881     2.760145      24.64
 H      -0.948306     1.761846     1.233504      27.12
 C      -1.739722    -2.490410    -0.999401      55.69
 H      -2.530591    -3.286630    -0.694532      21.37
 C      -1.175989    -0.562736    -2.455076      25.42
 H      -0.928477    -0.015400    -3.346176      21.55
 C      -0.313260    -0.070088    -1.371894      -8.06
 O       0.577397     0.932090    -1.789577     215.87
 C      -0.197478     2.206331    -2.157592      64.72
 H      -1.136387     2.009060    -2.360077      28.58
 H      -0.103059     2.690357    -1.087250      23.19
 H       0.743487     2.546249    -2.566234      22.22
 C      -0.138050    -0.855467    -0.191976       9.63
 O       0.692654    -0.412306     0.972741     158.27
 C      -0.989598    -1.916844     0.112685      42.27
 H      -0.773824    -2.501030     1.044649      21.68
 C      -1.905092    -1.730314    -2.156052      19.52
 C      -2.618193    -2.278999    -3.415536     105.69
 H      -2.251615    -1.967101    -4.313090      26.92
 O      -2.319322    -3.727410    -3.511628     151.86
 H      -1.180891    -3.855737    -3.380014      23.56
 C      -3.982539    -2.054933    -3.204465      85.23
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 H      -3.981946    -2.735257    -2.215229      23.56
 O      -4.327863    -0.541011    -2.845172     251.17
 H      -5.188483    -0.570736    -2.652944      30.56
 C      -4.868839    -2.507228    -4.404831     107.57
 O      -6.220944    -1.766115    -4.539786     239.14
 H      -6.639330    -2.368213    -5.294395      29.49
 H      -5.250335    -3.502284    -4.565209      26.27
 H      -4.386802    -2.108529    -5.240645      28.23
55
name = lig-ACN-frame_847
 C       3.759421    -0.329198     0.572878      32.36
 H       3.031581    -0.040719    -0.250579      22.42
 C       4.591817    -0.024492     2.809166      59.30
 H       4.273412     0.508203     3.692385      24.43
 C       5.794564    -0.762030     2.501947      20.89
 O       6.877527    -1.229224     3.274995     244.66
 C       6.835784    -0.810600     4.631332     134.44
 H       7.847882    -0.639396     4.955158      27.26
 H       6.456624    -1.607037     5.217781      28.25
 H       6.293092     0.056407     4.894139      29.20
 C       5.903074    -1.274142     1.188622      19.39
 O       6.811593    -2.192758     0.754889     186.59
 H       7.619947    -2.349412     1.379002      22.70
 C       4.885088    -1.172211     0.233119      46.26
 H       4.910485    -1.545826    -0.847723      22.27
 C       3.431423    -0.093701     1.936134      26.64
 C       2.249173     0.775935     2.357557      96.40
 H       2.626414     1.662593     2.518251      28.44
 O       1.606086     0.124088     3.620626     222.16
 H       1.433609    -0.794379     3.332334      28.59
 C       1.214988     1.081374     1.302742      77.47
 H       1.772262     1.489777     0.491202      24.82
 C      -0.016523     1.816427     1.762252     103.78
 O       0.239937     3.338420     1.934263     186.46
 H       0.202789     3.730810     0.919373      27.20
 H      -0.280801     1.406943     2.839988      24.01
 H      -0.658239     1.615762     1.039893      28.47
 C      -1.728680    -2.474166    -0.975702      48.24
 H      -2.236962    -3.482080    -0.944198      21.85
 C      -1.144731    -0.565250    -2.301321      47.34
 H      -1.222419    -0.251642    -3.395803      21.47
 C      -0.218678    -0.139676    -1.429340      15.03
 O       0.630812     0.944417    -1.773231     246.26
 C      -0.044380     2.249921    -1.979810      94.75
 H      -0.866976     2.063005    -2.564987      26.79
 H      -0.357472     2.801496    -1.027402      26.86
 H       0.107727     2.993668    -2.722689      24.30
 C      -0.193615    -0.690185    -0.095666      -5.01
 O       0.722004    -0.367254     0.871695     116.93
 C      -0.936787    -2.023897     0.045925      38.56
 H      -0.916459    -2.576962     1.105102      21.36
 C      -1.828832    -1.793876    -2.257455      25.37
 C      -2.539431    -2.351923    -3.403760      80.72
 H      -2.372310    -1.685615    -4.161391      27.58
 O      -2.421720    -3.741395    -3.530384     168.21
 H      -1.270549    -4.195791    -3.470511      22.13
 C      -4.233082    -2.095015    -3.125981      68.94
 H      -4.840766    -2.650562    -2.244938      24.56
 O      -4.282605    -0.591903    -2.928350     267.65
 H      -5.123013    -0.288681    -2.873972      30.55
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 C      -4.989963    -2.433924    -4.415625     108.66
 O      -6.253237    -1.805733    -4.513561     326.73
 H      -6.666713    -2.096505    -5.240136      34.61
 H      -4.844931    -3.572023    -4.456661      26.86
 H      -4.302869    -2.163373    -5.199509      28.82
55
name = lig-ACN-frame_848
 C       3.720924    -0.395004     0.571139      66.44
 H       2.945593    -0.310230    -0.173838      23.71
 C       4.524294    -0.096465     2.895532      66.27
 H       4.548330     0.419226     3.933743      22.15
 C       5.723732    -0.828761     2.533045      -0.22
 O       6.861717    -1.178098     3.274425     215.05
 C       6.803061    -0.778633     4.686905     126.66
 H       7.792543    -0.672906     4.984955      26.68
 H       6.225768    -1.522726     5.281826      26.82
 H       6.273833     0.107265     4.658468      29.03
 C       5.884555    -1.316763     1.165678      11.41
 O       6.848148    -2.224839     0.714347     172.66
 H       7.624977    -2.136310     1.262851      26.16
 C       4.862753    -1.063994     0.249170      53.98
 H       5.107197    -1.602798    -0.633094      22.53
 C       3.506497    -0.060802     1.911540      33.67
 C       2.258453     0.653486     2.387478     122.34
 H       2.552650     1.522966     2.753926      28.58
 O       1.771752     0.160196     3.520907     315.21
 H       1.566408    -0.650974     3.398803      35.73
 C       1.241227     1.018346     1.283488      86.88
 H       1.673429     1.617595     0.423522      23.39
 C       0.034773     1.889058     1.750439     106.52
 O       0.298823     3.370314     1.891551     272.25
 H       0.500927     3.627251     1.025555      32.80
 H      -0.350339     1.465080     2.838836      24.39
 H      -0.822498     1.803450     1.237323      28.05
 C      -1.702419    -2.523785    -0.971751      53.85
 H      -1.980579    -3.537560    -0.856969      21.90
 C      -1.095590    -0.622441    -2.398177      39.12
 H      -1.371706     0.215081    -3.165890      19.53
 C      -0.150679    -0.091795    -1.354192     -24.87
 O       0.720977     1.013124    -1.736273     219.95
 C      -0.049129     2.274785    -1.907449      83.08
 H      -1.022150     2.079942    -2.295513      25.75
 H      -0.294824     2.736535    -0.919734      26.51
 H       0.841800     2.703882    -2.252503      23.87
 C      -0.232097    -0.668600    -0.059536      19.77
 O       0.769962    -0.298338     0.836935     187.74
 C      -0.826578    -1.912812     0.009352      39.59
 H      -0.733906    -2.519859     1.078877      21.26
 C      -1.711439    -1.861757    -2.193908      25.15
 C      -2.692233    -2.370961    -3.317327      66.24
 H      -2.482416    -1.983978    -4.237585      25.85
 O      -2.532512    -3.823365    -3.613109     147.93
 H      -1.358994    -4.065244    -3.428868      23.97
 C      -4.430676    -1.986022    -3.134670      69.10
 H      -4.854025    -2.470770    -2.115081      23.93
 O      -4.186345    -0.695547    -3.021530     232.90
 H      -5.126196    -0.280743    -2.627668      23.36
 C      -4.943076    -2.436206    -4.497922      99.24
 O      -6.348118    -1.862085    -4.468990     265.04
 H      -6.807342    -1.755262    -5.415465      30.57
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 H      -5.209214    -3.546840    -4.431244      25.04
 H      -4.401068    -2.049110    -5.383331      26.63
55
name = lig-ACN-frame_849
 C       3.600228    -0.519141     0.592591      31.74
 H       2.787821    -0.485620    -0.046378      21.79
 C       4.592682    -0.305183     2.909707      56.54
 H       4.369221     0.044220     4.057896      20.50
 C       5.716605    -0.942796     2.482626      25.41
 O       6.811369    -1.092926     3.311321     234.07
 C       6.759533    -0.726124     4.739962     127.53
 H       7.675413    -0.798648     5.080671      28.59
 H       6.175167    -1.527459     5.330369      27.05
 H       6.523827     0.286104     5.025006      29.10
 C       5.823541    -1.417138     1.160083      18.15
 O       6.931470    -2.207886     0.723524     214.50
 H       7.577612    -2.291265     1.450724      24.04
 C       4.934782    -1.019591     0.155020      51.10
 H       4.950885    -1.252970    -0.823328      23.97
 C       3.611225     0.110223     1.893563      14.52
 C       2.356500     0.833222     2.306212      88.57
 H       2.557373     1.758487     2.530006      28.09
 O       1.817678     0.067308     3.594601     181.49
 H       1.655545    -0.835454     3.320340      27.10
 C       1.194944     1.000574     1.217045      83.05
 H       1.759594     1.486268     0.312056      21.83
 C       0.007025     2.000692     1.801401      98.06
 O       0.399989     3.321887     1.834423     299.41
 H       0.917853     3.604763     1.098670      31.89
 H      -0.236098     1.821404     3.001877      22.32
 H      -0.764945     1.771915     1.162492      26.36
 C      -1.477932    -2.553203    -0.921959      35.60
 H      -2.085045    -3.328131    -0.627845      23.12
 C      -0.974881    -0.609851    -2.400343      31.29
 H      -1.084996    -0.115857    -3.471263      21.49
 C      -0.217294    -0.007170    -1.433797      25.50
 O       0.696530     0.980042    -1.631428     272.53
 C       0.029189     2.309213    -1.814940     103.94
 H      -0.667626     2.470023    -2.627262      24.16
 H      -0.222714     2.586885    -0.840901      27.77
 H       0.520226     3.107329    -2.301466      24.67
 C      -0.082974    -0.620058    -0.191123       0.01
 O       0.783590    -0.318039     0.888878     161.25
 C      -0.825235    -1.875137     0.118038      31.89
 H      -0.362316    -2.417812     1.117329      20.06
 C      -1.799383    -1.878466    -2.233048      -5.19
 C      -2.864998    -2.475955    -3.264566      99.88
 H      -2.598637    -1.782627    -4.020599      24.32
 O      -2.636136    -3.877372    -3.664546     223.60
 H      -1.640773    -4.119429    -3.424705      25.51
 C      -4.219164    -2.111525    -3.241569      82.15
 H      -4.886984    -2.614146    -2.414800      23.84
 O      -4.177233    -0.524787    -3.060613     144.60
 H      -5.190883    -0.133156    -2.507956      20.75
 C      -5.110657    -2.486620    -4.523933      83.15
 O      -6.453985    -1.883279    -4.446166     231.50
 H      -6.517577    -1.952224    -5.587320      26.29
 H      -4.980072    -3.594299    -4.914693      24.39
 H      -4.503226    -1.942507    -5.340555      26.06
55
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name = lig-ACN-frame_850
 C       3.714202    -0.507691     0.636877      61.61
 H       2.975438    -0.305889    -0.077386      23.44
 C       4.526669    -0.367368     2.796954      48.55
 H       4.317110    -0.149001     3.991514      20.10
 C       5.727129    -1.059820     2.481263      10.19
 O       6.827658    -1.036838     3.382698     234.65
 C       6.747958    -0.727468     4.797448     114.00
 H       7.625524    -1.024390     5.056757      27.61
 H       5.834651    -1.327250     5.324073      25.63
 H       6.456307     0.323229     4.903452      28.36
 C       5.895537    -1.511737     1.055064      -2.81
 O       7.006563    -2.149705     0.754175     150.08
 H       7.506754    -2.528948     1.578955      22.41
 C       4.850671    -1.095044     0.090887      62.03
 H       5.122092    -1.237512    -0.835888      23.41
 C       3.592964     0.109159     1.887349      37.72
 C       2.356102     0.956682     2.333760      90.09
 H       2.595226     1.817072     2.717590      27.09
 O       1.874183     0.080206     3.595220     109.95
 H       1.686178    -0.914510     3.105787      21.66
 C       1.197431     1.086224     1.310304      80.25
 H       1.482825     1.582526     0.254799      19.25
 C       0.048733     1.914783     1.781220     101.82
 O       0.548219     3.393890     1.785068     175.92
 H       1.053578     3.398529     0.799826      25.26
 H      -0.214678     1.475738     2.900105      22.78
 H      -0.902330     1.918718     1.314110      25.19
 C      -1.443077    -2.481100    -0.912154      58.23
 H      -1.878791    -3.407274    -0.724357      24.02
 C      -1.058998    -0.751404    -2.510391      29.30
 H      -0.838285    -0.486022    -3.587763      22.08
 C      -0.242401    -0.058234    -1.452148     -14.79
 O       0.666690     1.067142    -1.637475     218.55
 C       0.092440     2.409010    -1.788958      99.95
 H      -0.653191     2.057415    -2.455970      24.91
 H      -0.527743     2.751530    -1.055587      28.01
 H       1.009278     2.870064    -1.996598      25.70
 C      -0.004542    -0.723165    -0.149717      18.05
 O       0.737810    -0.349750     0.920572     149.71
 C      -0.666739    -1.832899     0.106851      52.85
 H      -0.696387    -2.315347     1.177750      21.71
 C      -1.790767    -1.864881    -2.096978      35.85
 C      -2.638079    -2.460715    -3.368833      65.48
 H      -2.275310    -2.056783    -4.280120      24.62
 O      -2.715104    -3.888968    -3.686282     279.61
 H      -1.956662    -4.230381    -3.516030      33.67
 C      -4.325972    -2.116709    -3.251570      67.04
 H      -4.665760    -2.392478    -2.230709      23.43
 O      -4.208199    -0.460934    -3.103526     148.41
 H      -5.349759    -0.484391    -2.805190      21.30
 C      -5.124480    -2.413303    -4.565314      94.31
 O      -6.503162    -1.959761    -4.494872     298.89
 H      -7.160217    -1.988965    -5.200037      32.50
 H      -5.192310    -3.597327    -4.567889      23.94
 H      -4.619968    -1.887724    -5.479083      25.52
55
name = lig-ACN-frame_851
 C       3.793010    -0.321738     0.476996      30.78
 H       3.143510     0.013249    -0.355395      21.15
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 C       4.524708    -0.357934     2.808348      46.99
 H       4.512583     0.120547     3.903558      19.64
 C       5.671343    -1.047896     2.447520      15.46
 O       6.847762    -1.084646     3.344333     215.56
 C       6.666611    -0.747557     4.809256     114.19
 H       7.451356    -0.966838     5.374751      26.83
 H       5.773429    -1.386757     5.345295      24.39
 H       6.635264     0.351425     4.999868      26.85
 C       5.902831    -1.467570     1.138856      19.62
 O       7.109250    -2.143104     0.687271     195.05
 H       7.706827    -2.315657     1.484674      22.80
 C       4.924035    -1.292968     0.191071      53.62
 H       4.863924    -1.589734    -0.778389      24.05
 C       3.508891    -0.002882     1.850653      12.33
 C       2.345186     0.826150     2.450046     106.48
 H       2.636109     1.759032     2.756182      26.17
 O       1.907096     0.213367     3.508459     225.60
 H       1.555924    -0.919274     3.363521      21.18
 C       1.222219     1.062408     1.296262      77.86
 H       1.822506     1.573622     0.363595      20.69
 C       0.086935     1.971386     1.826912      91.64
 O       0.649862     3.339173     1.765293     211.79
 H       0.816107     3.712251     0.744816      24.47
 H      -0.136276     1.943218     2.988562      22.17
 H      -0.788273     1.790297     1.111106      23.26
 C      -1.604101    -2.516494    -0.863359      42.70
 H      -1.892564    -3.553790    -0.617868      23.18
 C      -0.979901    -0.729784    -2.437322      44.82
 H      -1.185082    -0.218556    -3.371851      21.96
 C      -0.151239    -0.136083    -1.453072      15.49
 O       0.626271     1.049248    -1.632664     246.42
 C       0.034838     2.403300    -1.897271     123.34
 H      -0.429693     2.872619    -2.709094      24.68
 H      -0.186867     2.809116    -1.017255      30.08
 H       0.828774     3.086041    -2.159857      26.22
 C      -0.009068    -0.669408    -0.171529      -4.14
 O       0.770664    -0.259675     1.023076     135.04
 C      -0.622429    -2.005103     0.068805      30.52
 H      -0.541330    -2.406824     1.090544      19.82
 C      -1.746719    -1.933822    -2.218799      16.35
 C      -2.579781    -2.433191    -3.431641      63.69
 H      -2.075613    -1.862568    -4.245054      24.16
 O      -2.734827    -3.894955    -3.652347     273.71
 H      -1.890274    -4.281029    -3.625515      30.75
 C      -4.268699    -1.849637    -3.302503      82.96
 H      -4.664742    -2.504764    -2.544080      24.52
 O      -4.303859    -0.575766    -3.154532     293.37
 H      -5.114169    -0.048615    -2.976731      26.21
 C      -5.113633    -2.398054    -4.562455      78.42
 O      -6.573747    -1.987376    -4.461735     305.37
 H      -6.698216    -2.461864    -5.190353      33.64
 H      -5.059666    -3.589981    -4.685695      24.81
 H      -4.539441    -2.076732    -5.560067      25.55
55
name = lig-ACN-frame_852
 C       3.898099    -0.317446     0.403670      65.03
 H       3.232466    -0.089299    -0.502073      20.66
 C       4.514940    -0.310971     2.818040      56.61
 H       4.306589     0.215425     3.780830      20.72
 C       5.787363    -0.936268     2.533224      12.80
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 O       6.818164    -1.157284     3.342317     228.51
 C       6.601238    -0.788975     4.757819     106.30
 H       7.440258    -1.201251     5.128450      26.59
 H       5.577643    -1.394028     5.070039      25.86
 H       6.295403     0.309810     4.882119      27.18
 C       5.996845    -1.526796     1.170873       1.75
 O       7.086742    -2.087945     0.636045     231.76
 H       7.874023    -2.143635     1.153433      26.23
 C       4.869624    -1.285132     0.227842      48.64
 H       5.137859    -1.975714    -0.572216      21.93
 C       3.576535    -0.064960     1.769583      32.95
 C       2.397713     0.767197     2.255849      95.43
 H       2.821972     1.686933     2.474781      24.96
 O       1.806617     0.247940     3.658504     158.65
 H       1.573767    -0.818334     3.332572      21.54
 C       1.295514     1.030660     1.359856      74.59
 H       1.742178     1.567837     0.344732      19.25
 C       0.184438     2.081198     1.805031     105.95
 O       0.709752     3.340248     1.776128     317.92
 H       0.634944     3.710561     0.926515      30.03
 H      -0.182635     1.764763     2.850928      22.79
 H      -0.836722     1.975746     1.235706      23.05
 C      -1.659011    -2.605527    -0.971629      38.75
 H      -2.472690    -3.388108    -0.686081      19.28
 C      -0.944494    -0.695156    -2.340490      35.81
 H      -1.173284    -0.006728    -3.075048      20.10
 C      -0.064043    -0.113125    -1.392819       5.32
 O       0.559573     1.053192    -1.730651     261.69
 C       0.054128     2.454689    -1.994356      84.23
 H      -0.741810     2.134842    -2.641754      23.81
 H      -0.515955     2.705978    -1.197110      28.26
 H       1.074008     2.824523    -2.157387      23.38
 C      -0.003150    -0.766464    -0.040744       2.96
 O       0.710702    -0.268281     0.988540     167.66
 C      -0.653401    -2.025808     0.040283      54.44
 H      -0.241538    -2.661624     0.732270      22.75
 C      -1.664776    -1.986944    -2.245399      16.43
 C      -2.713942    -2.367916    -3.418713      90.67
 H      -2.361736    -1.970867    -4.432954      22.92
 O      -2.703410    -3.808514    -3.614502     193.59
 H      -1.616536    -4.108914    -3.482065      23.67
 C      -4.152964    -1.996037    -3.427292      96.97
 H      -4.532371    -2.361172    -2.505262      24.85
 O      -4.317694    -0.433793    -3.189171     258.66
 H      -5.136166    -0.543788    -2.843481      26.41
 C      -5.039699    -2.394093    -4.538802      93.37
 O      -6.523698    -2.055533    -4.474800     237.07
 H      -7.192715    -2.437344    -5.195546      31.22
 H      -4.873134    -3.567219    -4.486578      24.44
 H      -4.856302    -1.818855    -5.539421      24.15
55
name = lig-ACN-frame_853
 C       3.884322    -0.513804     0.435594      36.19
 H       3.054421    -0.309821    -0.357795      20.01
 C       4.606729    -0.289882     2.755186      53.06
 H       4.272021    -0.145875     3.711941      21.20
 C       5.826584    -0.870296     2.438664      21.73
 O       6.844147    -1.198359     3.399059     272.99
 C       6.512335    -0.892000     4.694018     116.30
 H       7.287956    -1.026312     5.454623      25.89
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 H       5.610730    -1.522686     5.181091      26.52
 H       6.467616     0.250226     4.832379      27.51
 C       5.909148    -1.434097     1.206618      38.82
 O       7.066990    -2.051914     0.578395     197.59
 H       7.655603    -2.360885     1.322946      23.77
 C       5.047517    -1.321387     0.209343      49.03
 H       5.081250    -1.543474    -0.916544      20.73
 C       3.667276    -0.021649     1.738145      28.41
 C       2.454685     0.765747     2.240921      72.73
 H       2.710496     1.735704     2.645019      23.56
 O       1.763012     0.285650     3.678815     190.64
 H       1.545206    -0.660428     3.625333      25.54
 C       1.228930     1.032613     1.210683      73.93
 H       1.657966     1.412392     0.150971      17.90
 C       0.229052     1.978826     1.814076      93.75
 O       0.765279     3.461844     1.851547     263.65
 H       1.021383     3.764471     0.993790      28.59
 H       0.031648     1.799311     2.847119      22.79
 H      -0.691784     2.012212     1.034411      20.54
 C      -1.527132    -2.560354    -1.042043      91.56
 H      -2.190819    -3.553953    -0.838729      17.77
 C      -0.971765    -0.714437    -2.319576      39.20
 H      -0.951099    -0.305530    -3.249113      22.08
 C      -0.175604    -0.130415    -1.287190      20.20
 O       0.648397     1.047660    -1.766406     218.89
 C      -0.050792     2.312505    -2.076454     130.74
 H      -0.566960     2.439813    -3.070454      23.50
 H      -0.418374     2.960523    -1.371639      26.99
 H       0.571207     3.152323    -2.513687      25.04
 C      -0.025854    -0.827085    -0.126850      19.00
 O       0.647975    -0.389246     1.034741     134.81
 C      -0.753209    -2.122365    -0.014270      34.87
 H      -0.730317    -2.656500     0.835782      23.94
 C      -1.727360    -1.830674    -2.243525      46.09
 C      -2.648897    -2.310450    -3.464431      55.01
 H      -2.188533    -1.676507    -4.357485      22.30
 O      -2.632537    -3.747839    -3.569549     133.92
 H      -1.517549    -4.143741    -3.182618      21.09
 C      -4.234500    -1.943918    -3.288796      72.03
 H      -4.605776    -2.457532    -2.492172      24.47
 O      -4.289158    -0.398297    -3.229401     298.40
 H      -4.981141    -0.060862    -2.827110      29.92
 C      -5.044568    -2.454740    -4.681372      74.91
 O      -6.416757    -2.126319    -4.387624     216.37
 H      -6.783914    -2.394854    -5.427559      28.36
 H      -5.015784    -3.582693    -5.013372      25.02
 H      -4.352112    -1.973866    -5.520935      25.44
55
name = lig-ACN-frame_854
 C       3.766566    -0.693059     0.503668      52.48
 H       2.999095    -0.615433    -0.346917      21.38
 C       4.668248    -0.235266     2.758103      53.48
 H       4.543201     0.021364     3.703552      21.84
 C       5.904544    -0.927566     2.433845       8.60
 O       6.873697    -1.254550     3.338584     214.65
 C       6.464006    -0.909027     4.837002      82.07
 H       7.396416    -1.292751     5.350345      24.39
 H       5.534405    -1.583245     5.013857      26.57
 H       5.994756     0.147893     4.888312      24.71
 C       6.068807    -1.406383     1.025572       3.11
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 O       7.110491    -2.059393     0.631344     160.88
 H       7.768396    -2.530489     1.279642      22.86
 C       4.974772    -1.206217     0.045351      47.07
 H       5.470791    -1.590746    -0.942186      19.05
 C       3.643869     0.021388     1.796997      22.64
 C       2.339091     0.783232     2.315279      99.14
 H       2.740159     1.842772     2.441405      23.16
 O       1.811218     0.328217     3.529324     316.97
 H       1.660483    -0.488701     3.372458      32.95
 C       1.273099     0.883275     1.143322      77.77
 H       1.567192     1.192232     0.081077      18.19
 C       0.274746     2.062356     1.761732      99.52
 O       0.764978     3.420280     1.977069     263.70
 H       1.279744     3.745779     1.098764      25.63
 H       0.034149     1.715257     2.700098      24.88
 H      -0.854126     2.005344     1.274688      22.42
 C      -1.539646    -2.582543    -1.118229      63.61
 H      -1.739695    -3.780509    -1.109262      19.53
 C      -0.961814    -0.575171    -2.450005      30.32
 H      -0.783748    -0.111819    -3.379843      20.43
 C      -0.242483    -0.045383    -1.395648       1.34
 O       0.682695     0.995748    -1.723243     196.42
 C      -0.132319     2.263844    -2.253961      68.00
 H      -1.018024     1.930662    -2.898349      22.68
 H      -0.649608     2.332638    -1.342434      24.48
 H       0.851122     2.727261    -2.380883      22.33
 C      -0.085029    -0.871380    -0.096756       0.73
 O       0.592938    -0.480095     1.087360     146.94
 C      -0.747892    -2.096573     0.017414      46.10
 H      -0.897007    -2.430556     0.975458      21.23
 C      -1.857713    -1.768442    -2.240992      30.99
 C      -2.575441    -2.244847    -3.366343      62.87
 H      -2.331579    -1.749276    -4.423434      21.81
 O      -2.544408    -3.690294    -3.543357     134.03
 H      -1.431658    -4.126336    -3.189277      19.79
 C      -4.285419    -1.850498    -3.299917      76.68
 H      -4.746466    -2.175555    -2.481972      25.79
 O      -4.201008    -0.486488    -3.276335     237.01
 H      -5.214421    -0.265438    -2.968932      22.15
 C      -4.903892    -2.465902    -4.645991      90.94
 O      -6.319565    -2.184089    -4.416250     289.53
 H      -6.910240    -2.124809    -5.204970      33.43
 H      -4.602586    -3.578116    -4.739199      25.95
 H      -4.778124    -1.741161    -5.533915      24.83
55
name = lig-ACN-frame_855
 C       3.677791    -0.694589     0.564751      38.67
 H       2.743089    -0.768686     0.001953      20.56
 C       4.740263    -0.184713     2.719011      41.28
 H       4.715841     0.477653     3.498766      19.95
 C       5.864799    -0.979178     2.331276       3.07
 O       6.884618    -1.260677     3.377131     203.24
 C       6.422937    -1.019319     4.784323     103.37
 H       7.432197    -1.217600     5.488306      24.54
 H       5.694287    -1.773036     5.073854      27.22
 H       6.318099     0.068204     5.132247      26.11
 C       6.073145    -1.298217     0.973836      12.52
 O       7.275063    -2.151446     0.590453     193.24
 H       7.869700    -2.024960     1.372588      23.83
 C       4.995833    -1.114983     0.074036      52.01
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 H       4.769036    -1.606119    -0.914792      19.86
 C       3.587652    -0.108190     1.822143      10.91
 C       2.381695     0.784772     2.147829      97.94
 H       2.576336     1.917941     2.363530      21.64
 O       1.852573     0.322749     3.417691     299.97
 H       1.636395    -0.609131     3.365569      27.48
 C       1.222715     0.833432     1.228353      96.98
 H       1.787016     0.992047     0.330007      21.46
 C       0.242920     2.015538     1.725432      98.89
 O       0.787535     3.301652     2.061606     224.20
 H       0.912519     3.922442     1.129241      23.61
 H      -0.064400     1.645271     2.634483      23.89
 H      -0.677443     2.266337     0.941490      20.68
 C      -1.540394    -2.543403    -1.102312      62.77
 H      -2.208388    -3.538450    -1.145877      14.46
 C      -1.064471    -0.518623    -2.472411      45.84
 H      -1.275607    -0.047533    -3.456463      17.51
 C      -0.148680    -0.115165    -1.411822      13.90
 O       0.633618     0.961999    -1.700832     256.49
 C      -0.138255     2.076786    -2.243569     105.61
 H      -0.483715     1.750275    -3.273153      20.51
 H      -0.767600     2.780020    -1.642917      23.59
 H       0.237268     3.013706    -2.739688      25.17
 C      -0.172171    -0.740362    -0.110484      17.81
 O       0.539696    -0.461416     1.082204     183.59
 C      -0.819563    -2.029152    -0.036018      53.99
 H      -0.409223    -2.739074     0.670307      23.32
 C      -1.728492    -1.674770    -2.208886      19.43
 C      -2.739506    -2.292359    -3.360251      70.58
 H      -2.228747    -1.658305    -4.268576      21.47
 O      -2.472816    -3.661093    -3.528937     187.07
 H      -1.324172    -3.893044    -3.425646      23.75
 C      -4.079705    -1.945423    -3.385421     113.22
 H      -4.564936    -2.409133    -2.661533      25.52
 O      -4.179155    -0.432041    -3.321191     157.47
 H      -5.334375    -0.248434    -3.061281      20.65
 C      -4.822101    -2.362675    -4.568183      92.39
 O      -6.303340    -2.273904    -4.418761     325.76
 H      -6.533272    -2.161813    -5.292886      34.04
 H      -4.600335    -3.488513    -4.627281      27.07
 H      -4.221344    -1.993996    -5.460612      27.60
55
name = lig-ACN-frame_856
 C       3.717556    -0.690690     0.569771      68.52
 H       2.937557    -0.856854    -0.090192      22.22
 C       4.732595    -0.109261     2.596610      58.16
 H       4.806337     0.360365     3.614030      20.27
 C       5.890949    -0.935937     2.357691      13.80
 O       6.819861    -1.224359     3.337607     257.87
 C       6.504440    -1.149898     4.709482      98.85
 H       7.515250    -1.573104     5.320497      23.46
 H       5.656984    -1.740233     4.958483      30.32
 H       6.097122    -0.105455     4.878771      26.74
 C       6.142861    -1.375061     0.957552       4.56
 O       7.229453    -2.070850     0.549906     213.24
 H       8.017218    -2.021611     1.073555      25.97
 C       4.928822    -1.169590     0.123646      52.17
 H       5.144185    -1.508209    -0.868489      23.23
 C       3.601991    -0.149710     1.849010      42.12
 C       2.425578     0.683976     2.143122      90.17
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 H       3.002017     1.729517     2.219870      21.05
 O       1.867799     0.312275     3.450868     212.97
 H       1.774555    -0.795111     3.309926      22.15
 C       1.196303     0.923063     1.139145      88.32
 H       1.292036     1.341642     0.214296      19.45
 C       0.140171     1.880959     1.711086      84.45
 O       0.846364     3.196960     2.074320     283.45
 H       0.659004     3.812258     1.343489      28.21
 H      -0.607702     1.621360     2.381332      24.24
 H      -0.494209     1.968298     0.627932      19.46
 C      -1.633426    -2.414576    -1.069551      54.61
 H      -2.144941    -3.391917    -0.784004      21.27
 C      -1.113333    -0.519203    -2.344067      66.43
 H      -1.367037     0.265099    -3.167720      15.88
 C      -0.145843    -0.137028    -1.452369      14.91
 O       0.648048     1.057537    -1.652849     235.90
 C      -0.135330     2.047568    -2.389295      87.45
 H      -0.746345     1.687775    -3.244694      20.37
 H      -0.957382     2.166661    -1.574692      23.25
 H       0.836097     2.581937    -2.397405      22.16
 C      -0.226163    -0.711336    -0.130797      25.14
 O       0.478056    -0.376887     1.034413     155.84
 C      -0.779315    -1.993938    -0.066632      45.26
 H      -0.459575    -2.690554     0.809773      15.88
 C      -1.812576    -1.789858    -2.295450      37.51
 C      -2.461907    -2.223353    -3.421454      73.28
 H      -2.175605    -1.750921    -4.482107      20.62
 O      -2.454606    -3.703026    -3.546297     214.96
 H      -1.463468    -4.004559    -3.264261      23.64
 C      -4.125287    -1.896615    -3.282623      69.78
 H      -4.447889    -2.267313    -2.433944      27.03
 O      -4.181947    -0.411538    -3.332673     196.92
 H      -5.237191    -0.135375    -2.849457      21.56
 C      -4.773102    -2.482413    -4.618049      97.08
 O      -6.228768    -2.296465    -4.465244     236.75
 H      -6.730437    -2.469178    -5.441984      30.72
 H      -4.573092    -3.581789    -4.835905      25.60
 H      -4.592831    -1.806340    -5.485618      25.13
55
name = lig-ACN-frame_857
 C       3.778810    -0.777772     0.453917      42.50
 H       3.027511    -0.585982    -0.225424      23.17
 C       4.803923    -0.118947     2.651485      50.72
 H       4.441274     0.241021     3.723433      17.12
 C       5.904153    -0.842327     2.315634      34.28
 O       6.871792    -1.219913     3.204842     241.23
 C       6.481115    -1.238563     4.651086     108.76
 H       7.583022    -1.695946     5.183897      24.74
 H       5.791374    -1.989364     4.781540      30.16
 H       6.407578    -0.295970     5.237801      26.95
 C       6.031893    -1.415267     1.068393      18.20
 O       7.168809    -1.966452     0.456223     201.71
 H       7.789877    -2.190441     1.250647      25.66
 C       5.074137    -1.348128     0.105323      48.25
 H       5.249368    -1.566474    -0.860063      22.16
 C       3.606857    -0.135563     1.716570      -0.25
 C       2.344244     0.695528     2.224912      81.06
 H       2.642643     1.853508     2.512288      20.79
 O       1.883679     0.307562     3.497876     219.72
 H       1.675084    -0.880941     3.584421      19.84
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 C       1.205598     0.958204     1.138459      90.45
 H       1.755560     1.241881     0.342381      23.57
 C       0.070113     1.902548     1.626982     100.98
 O       0.803604     3.020776     2.062632     303.35
 H       0.856975     3.639507     1.400314      31.46
 H      -0.366096     1.414076     2.509804      23.52
 H      -0.767053     2.359464     0.824101      21.14
 C      -1.746037    -2.478303    -0.993291      58.65
 H      -2.059472    -3.499818    -1.030898      23.72
 C      -1.130192    -0.518713    -2.317638      41.48
 H      -1.268117    -0.029283    -3.401190      17.26
 C      -0.190164    -0.040331    -1.357536      18.10
 O       0.626043     1.005519    -1.638738     230.96
 C      -0.056112     2.129883    -2.453843      91.62
 H      -0.202311     1.810559    -3.472336      23.27
 H      -0.969765     2.685533    -1.867981      22.48
 H       0.329251     3.167414    -2.692223      24.39
 C      -0.081879    -0.743833    -0.157350      22.96
 O       0.457114    -0.275348     0.968049     198.62
 C      -0.781442    -1.980491    -0.031340      46.23
 H      -1.009741    -2.282178     1.109492      17.40
 C      -1.759697    -1.720710    -2.213322      15.53
 C      -2.509909    -2.303702    -3.558242      62.44
 H      -1.990664    -1.709209    -4.427678      21.99
 O      -2.463268    -3.727130    -3.602743     310.25
 H      -1.737770    -4.062453    -3.214089      31.11
 C      -4.070272    -1.852166    -3.371303      89.61
 H      -4.435695    -2.241828    -2.527159      26.97
 O      -4.213954    -0.438802    -3.310807     274.89
 H      -5.069414    -0.283868    -2.747945      24.99
 C      -4.784592    -2.538900    -4.613037      89.38
 O      -6.201717    -2.315432    -4.528600     242.85
 H      -6.840388    -2.905240    -5.279147      28.85
 H      -4.289290    -3.508337    -4.794385      27.04
 H      -4.286979    -1.868650    -5.380996      26.59
55
name = lig-ACN-frame_858
 C       3.818249    -0.751468     0.364469      59.32
 H       3.136669    -0.776058    -0.463484      21.30
 C       4.579529    -0.178866     2.654616      64.39
 H       4.599173     0.297358     3.756963      19.97
 C       5.904974    -0.808105     2.327118     -16.86
 O       7.000869    -1.182347     3.189601     277.69
 C       6.573538    -1.386142     4.567234      79.94
 H       7.588612    -1.978592     5.112102      23.85
 H       5.673107    -1.931596     4.729994      30.79
 H       6.321023    -0.401638     4.941482      27.32
 C       6.007558    -1.460533     0.978642       9.80
 O       7.208702    -1.911491     0.479157     182.52
 H       7.877643    -2.301094     1.142445      24.49
 C       4.978591    -1.449338     0.030212      39.75
 H       5.125351    -2.031734    -0.810055      21.47
 C       3.674327    -0.055164     1.639579      21.65
 C       2.277648     0.749261     2.252305      68.78
 H       2.733099     1.907569     2.421098      19.50
 O       1.865304     0.269973     3.610816     200.13
 H       1.667504    -0.909286     3.327886      17.86
 C       1.212040     0.924034     1.149781      96.02
 H       1.680025     1.218265     0.303030      21.95
 C       0.117802     1.911398     1.556980     102.33
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 O       0.751029     3.054526     2.124810     228.68
 H       1.301353     3.523676     1.303102      25.62
 H      -0.307964     1.415522     2.485045      22.71
 H      -0.915162     1.905381     0.884456      20.99
 C      -1.655800    -2.531072    -0.994642      53.07
 H      -2.294425    -3.299947    -0.801859      18.22
 C      -1.086307    -0.514665    -2.389762      29.77
 H      -0.978827    -0.004285    -3.435869      18.42
 C      -0.309514     0.031572    -1.386108       4.65
 O       0.610990     1.138904    -1.686953     222.58
 C       0.052959     2.251574    -2.514673      92.91
 H      -0.001107     1.882134    -3.518536      24.29
 H      -1.072383     2.316826    -2.302975      23.86
 H       0.905753     2.868738    -2.226574      22.99
 C      -0.031397    -0.826818    -0.192393       7.75
 O       0.528869    -0.292217     0.979016     182.51
 C      -0.940604    -1.966248     0.056838      37.10
 H      -0.758224    -2.480711     1.161136      22.27
 C      -1.802998    -1.773989    -2.202088      31.95
 C      -2.610983    -2.280065    -3.404267      84.94
 H      -2.127827    -1.842163    -4.355260      23.57
 O      -2.510894    -3.746014    -3.686403     256.05
 H      -1.611832    -3.988826    -3.606353      30.12
 C      -4.013605    -1.965759    -3.490627     103.64
 H      -4.372225    -2.498185    -2.701060      25.47
 O      -4.246445    -0.456283    -3.302930     296.96
 H      -5.006774    -0.426163    -2.918781      30.65
 C      -4.726615    -2.455935    -4.657464     114.56
 O      -6.209675    -2.369082    -4.560453     279.36
 H      -6.355338    -2.921204    -5.321197      32.68
 H      -4.751483    -3.503797    -4.509039      25.41
 H      -4.399462    -2.187356    -5.722058      26.31
55
name = lig-ACN-frame_859
 C       3.743349    -0.640908     0.332427      33.89
 H       2.764225    -0.679149    -0.215342      18.52
 C       4.638977    -0.308168     2.604691      25.48
 H       4.295735     0.212352     3.571786      19.03
 C       5.862433    -0.942201     2.262330      10.67
 O       7.026875    -1.108444     3.125047     266.20
 C       6.651686    -1.464821     4.490330     102.79
 H       7.559724    -2.088494     5.170077      24.17
 H       5.838334    -2.183993     4.378839      29.28
 H       6.521655    -0.632602     5.159004      28.59
 C       6.070193    -1.416907     0.942091       8.04
 O       7.302227    -1.926751     0.529447     206.78
 H       7.832667    -1.985231     1.321927      23.10
 C       4.891421    -1.506867     0.056210      57.72
 H       4.851444    -2.176779    -0.821380      22.55
 C       3.536120     0.001797     1.632090       5.86
 C       2.380526     0.729041     2.212348      77.37
 H       2.760430     1.903821     2.604400      19.22
 O       1.861829     0.270983     3.568639     170.81
 H       1.754458    -0.922587     3.592988      19.54
 C       1.229792     0.913352     1.132579      85.65
 H       1.551513     1.266514     0.223017      20.91
 C       0.156136     1.831826     1.655978      88.24
 O       0.684286     3.231664     2.141239     182.71
 H       1.376742     3.589714     1.370878      26.25
 H      -0.628655     1.476874     2.482861      21.30
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 H      -0.298359     2.234064     0.646273      19.44
 C      -1.642632    -2.481949    -1.007933      59.55
 H      -2.152562    -3.344527    -0.844609      16.30
 C      -1.058327    -0.600294    -2.454162      42.91
 H      -1.298566    -0.042650    -3.405221      20.37
 C      -0.246746     0.016882    -1.454646       6.51
 O       0.515829     1.163071    -1.669987     239.06
 C       0.220221     2.266241    -2.581264     120.45
 H       0.510575     2.318120    -3.594776      25.87
 H      -0.759096     2.696378    -2.374703      24.98
 H       0.620026     3.253629    -2.217305      24.96
 C      -0.185671    -0.733591    -0.126601      19.02
 O       0.613795    -0.507999     0.971211     148.54
 C      -0.898429    -1.909600     0.072783      45.95
 H      -0.636666    -2.690575     0.938744      23.46
 C      -1.795068    -1.806020    -2.212669      35.76
 C      -2.521293    -2.297640    -3.422507      62.75
 H      -2.104019    -1.629184    -4.222573      25.74
 O      -2.542811    -3.735854    -3.722937     194.46
 H      -1.515512    -4.200915    -3.673102      25.61
 C      -4.154543    -1.922736    -3.411307      82.00
 H      -4.765454    -2.357185    -2.693283      24.40
 O      -4.253591    -0.550449    -3.296302     275.90
 H      -5.173333    -0.324661    -3.062412      25.70
 C      -4.772622    -2.600416    -4.799278      92.37
 O      -6.207992    -2.371012    -4.596104     338.88
 H      -6.733674    -2.396424    -5.299677      36.55
 H      -4.273803    -3.510697    -4.819806      28.98
 H      -4.412633    -2.101953    -5.782541      27.94
55
name = lig-ACN-frame_860
 C       3.656081    -0.648292     0.423568      54.86
 H       2.906784    -0.651289    -0.455126      18.59
 C       4.678578    -0.351497     2.539100      57.78
 H       4.709143    -0.242360     3.594666      21.07
 C       5.854643    -1.031895     2.193900       9.07
 O       6.971861    -1.022950     3.036714     257.45
 C       6.714401    -1.555155     4.442290      87.82
 H       7.834937    -2.143451     4.477984      22.67
 H       5.850538    -2.288193     4.569517      28.36
 H       6.480862    -0.769968     5.110054      28.54
 C       6.029570    -1.437537     0.854536       7.55
 O       7.340249    -1.950432     0.597266     199.78
 H       7.874537    -1.721777     1.386637      23.06
 C       4.822277    -1.404067     0.141646      58.01
 H       4.911542    -1.895384    -0.916618      21.36
 C       3.634082    -0.142872     1.692894      39.29
 C       2.397897     0.702443     2.181702      86.59
 H       2.747428     1.972067     2.330570      20.77
 O       1.895007     0.288665     3.442553     270.44
 H       1.872424    -0.786590     3.352744      23.53
 C       1.271974     0.802499     1.264632      90.02
 H       1.716697     1.133633     0.342047      21.73
 C       0.171495     2.012815     1.665086      89.17
 O       0.619013     3.291131     2.150875     289.73
 H       0.968932     3.706818     1.409720      30.92
 H      -0.571543     1.482773     2.514364      21.69
 H      -0.606460     2.101910     0.788916      22.06
 C      -1.698490    -2.481966    -0.980263      60.85
 H      -1.822278    -3.518494    -1.021599      23.66
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 C      -1.051058    -0.621089    -2.458208      50.04
 H      -1.210040    -0.075688    -3.361274      19.54
 C      -0.217565    -0.074024    -1.449410       4.59
 O       0.479777     1.151783    -1.626254     197.57
 C       0.297063     2.400007    -2.588183      93.02
 H       0.830248     1.976650    -3.402617      24.93
 H      -0.653618     2.376169    -2.952425      25.27
 H       0.868261     3.109794    -1.976746      23.72
 C      -0.299235    -0.581050    -0.124054      14.58
 O       0.759613    -0.552421     0.957335     122.04
 C      -0.837330    -1.923837    -0.045035      24.68
 H      -0.675417    -2.319159     1.005535      17.69
 C      -1.704908    -1.806633    -2.258848      12.40
 C      -2.656199    -2.325583    -3.499831      72.34
 H      -2.278726    -1.859002    -4.445373      22.48
 O      -2.520416    -3.727081    -3.740517     193.21
 H      -1.456219    -3.918914    -3.221626      20.57
 C      -4.196207    -2.060556    -3.453071      68.81
 H      -4.544726    -2.548585    -2.566898      25.28
 O      -4.269320    -0.554098    -3.313045     183.84
 H      -5.381049    -0.304046    -3.002328      21.43
 C      -4.809689    -2.620313    -4.863637     103.21
 O      -6.219740    -2.397644    -4.610994     301.68
 H      -6.516519    -2.099683    -5.587313      29.35
 H      -4.815130    -3.611641    -5.217772      26.17
 H      -4.366762    -1.843688    -5.479111      27.53
55
name = lig-ACN-frame_861
 C       3.707526    -0.790853     0.475670      43.75
 H       2.867127    -0.450456    -0.236992      21.47
 C       4.711865    -0.407229     2.672245      42.45
 H       4.647868     0.110105     3.511074      20.93
 C       5.859517    -0.980980     2.178480      18.66
 O       6.892587    -0.986329     3.016107     299.41
 C       6.856320    -1.628367     4.304170      86.81
 H       7.901271    -2.134867     4.735770      23.79
 H       5.985502    -2.458207     4.300100      27.63
 H       6.764038    -0.846245     5.037960      27.19
 C       6.025634    -1.524842     0.846800       8.99
 O       7.270806    -1.979440     0.572504     181.83
 H       7.883079    -1.703450     1.369900      22.08
 C       4.904528    -1.343760    -0.043025      61.74
 H       4.946211    -1.600893    -1.219315      20.26
 C       3.579562    -0.193710     1.787420      14.11
 C       2.459314     0.684040     2.195941      87.23
 H       3.038158     1.877181     2.308716      19.81
 O       1.946719     0.269593     3.443543     295.42
 H       1.782242    -0.613998     3.370396      29.29
 C       1.269665     0.877188     1.189298      91.37
 H       1.691170     1.366422     0.275821      20.46
 C       0.125412     1.995034     1.674260      85.03
 O       0.594839     3.314847     2.119574     280.64
 H       0.640424     3.991231     1.467539      29.84
 H      -0.286316     1.626105     2.784436      20.55
 H      -0.606064     2.091721     0.833268      21.73
 C      -1.625513    -2.530723    -1.117896      57.09
 H      -2.205355    -3.409323    -0.723857      15.54
 C      -1.021238    -0.559704    -2.477899      37.38
 H      -0.898932    -0.116681    -3.411730      20.97
 C      -0.262694     0.053923    -1.427272       4.63
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 O       0.498972     1.172697    -1.552188     220.93
 C       0.368550     2.275700    -2.560916     116.99
 H       1.052395     2.430983    -3.450536      25.27
 H      -0.557972     2.602603    -2.753394      27.07
 H       0.548927     3.184183    -1.940179      24.52
 C      -0.162179    -0.656063    -0.096803      16.90
 O       0.762807    -0.434520     0.886020     182.86
 C      -0.870531    -1.891671    -0.041183      45.39
 H      -0.680214    -2.494002     0.812412      24.64
 C      -1.843660    -1.881742    -2.392065      29.26
 C      -2.660862    -2.305430    -3.525622      84.21
 H      -2.394279    -1.674133    -4.371417      26.14
 O      -2.447755    -3.775766    -3.712940     132.16
 H      -1.421699    -4.221722    -3.336115      23.79
 C      -4.142104    -2.203128    -3.505196      89.39
 H      -4.708945    -2.743829    -2.662161      23.65
 O      -4.330903    -0.631400    -3.367173     141.72
 H      -5.347981    -0.686781    -2.740242      20.31
 C      -4.860099    -2.492447    -4.795512     108.12
 O      -6.286986    -2.370417    -4.659305     246.62
 H      -6.851248    -2.295594    -5.655244      28.27
 H      -4.432032    -3.501406    -4.900949      27.99
 H      -4.542627    -1.953061    -5.625000      29.48
55
name = lig-ACN-frame_862
 C       3.788916    -0.837115     0.481797      44.66
 H       2.888657    -0.825079    -0.160401      21.10
 C       4.603397    -0.351764     2.757691      43.53
 H       4.684836     0.109379     3.642570      21.29
 C       5.761904    -0.957146     2.243017     -13.64
 O       7.047871    -0.974385     3.000751     277.07
 C       6.964602    -1.675431     4.248349      91.94
 H       8.039648    -2.242449     4.197820      24.11
 H       6.120917    -2.565676     4.220080      27.70
 H       6.676117    -1.098901     5.143970      28.04
 C       5.949254    -1.523955     0.838582       3.56
 O       7.227981    -2.040824     0.470920     194.16
 H       7.798185    -1.953808     1.278014      22.92
 C       5.017216    -1.315758    -0.149437      52.48
 H       5.121626    -1.629656    -1.273146      20.11
 C       3.584580    -0.326982     1.762180      30.72
 C       2.459606     0.698073     2.161712      62.45
 H       2.931502     1.825807     2.625474      19.11
 O       1.959698     0.250360     3.570806     237.74
 H       1.825847    -0.622739     3.546115      27.69
 C       1.302206     1.155166     1.085535      59.68
 H       1.724777     1.589620     0.063964      17.25
 C       0.145291     1.897247     1.739242      95.11
 O       0.611125     3.328574     2.077509     208.44
 H       0.583004     3.738506     1.033661      23.58
 H      -0.448179     1.250562     2.591686      21.33
 H      -0.675668     2.000638     1.047779      22.73
 C      -1.590005    -2.463070    -1.188834      49.53
 H      -2.327489    -3.395443    -1.126526      17.80
 C      -1.048693    -0.595522    -2.500782      55.41
 H      -1.078399    -0.075537    -3.424644      21.58
 C      -0.370469     0.043773    -1.379636       1.23
 O       0.575529     1.225379    -1.510913     216.36
 C       0.363196     2.267922    -2.442779     104.07
 H       1.009234     1.884634    -3.349231      23.71
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 H      -0.563073     2.051390    -2.795247      25.63
 H       0.691640     3.175877    -1.939557      24.01
 C      -0.060807    -0.759116    -0.274665       4.52
 O       0.701233    -0.285840     0.844636     115.81
 C      -0.897669    -1.955540    -0.080257      49.79
 H      -0.771207    -2.560838     0.717697      24.70
 C      -1.776620    -1.690615    -2.321344      36.84
 C      -2.524587    -2.419725    -3.594028      62.21
 H      -2.147318    -1.906164    -4.479811      24.99
 O      -2.362802    -3.829623    -3.735487     248.03
 H      -1.329355    -3.931555    -3.698153      26.58
 C      -4.246464    -2.053580    -3.508808      84.16
 H      -4.613797    -2.766960    -2.633400      23.06
 O      -4.424349    -0.785112    -3.349315     271.41
 H      -5.164762    -0.431084    -2.722303      24.16
 C      -4.872072    -2.514264    -4.826620     102.68
 O      -6.371828    -2.332791    -4.663619     274.67
 H      -6.695502    -2.782502    -5.529740      29.61
 H      -4.774058    -3.575028    -5.187240      25.99
 H      -4.466351    -1.850074    -5.495854      29.20
55
name = lig-ACN-frame_863
 C       3.739157    -0.824913     0.342589      42.73
 H       2.960291    -0.916504    -0.354196      20.58
 C       4.649575    -0.378610     2.685576      34.96
 H       4.310833    -0.153902     3.712837      17.08
 C       5.882756    -1.012536     2.250236      19.75
 O       7.091990    -0.949288     2.911659     267.86
 C       7.095590    -1.809628     4.207652      89.28
 H       8.160846    -2.180664     4.442455      24.18
 H       6.292582    -2.731312     4.054007      24.25
 H       6.918497    -1.090055     5.074325      27.29
 C       6.044914    -1.433692     0.939613      20.75
 O       7.150995    -2.079060     0.421500     222.23
 H       7.798063    -2.197946     1.097436      27.85
 C       4.987588    -1.307425    -0.019468      54.86
 H       5.118503    -1.771772    -0.997623      21.27
 C       3.530841    -0.290837     1.736133      11.71
 C       2.374952     0.682348     2.220150      87.00
 H       3.163644     1.704206     2.266640      21.87
 O       1.948368     0.276089     3.591567     228.41
 H       1.906584    -0.765301     3.451797      25.46
 C       1.344197     1.132933     1.184451      48.70
 H       1.838016     1.777316     0.234135      19.07
 C       0.172930     1.934696     1.730159     105.91
 O       0.580065     3.241431     2.018203     239.40
 H       0.933701     3.762408     1.099855      25.23
 H       0.132203     1.536055     2.843466      21.43
 H      -0.663097     1.830873     1.107699      24.96
 C      -1.696167    -2.410051    -1.151073      49.96
 H      -1.813104    -3.627608    -1.203825      21.86
 C      -1.031885    -0.353415    -2.542836      48.20
 H      -1.239500     0.218935    -3.483852      19.43
 C      -0.241808     0.052755    -1.479649       7.85
 O       0.575640     1.111652    -1.380714     211.21
 C       0.309572     2.194672    -2.450654     106.07
 H       1.041058     2.098488    -3.376200      24.06
 H      -0.713662     2.502266    -2.720645      24.18
 H       0.504675     3.188382    -2.047047      25.89
 C      -0.099982    -0.751381    -0.287212       2.57
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 O       0.627837    -0.183242     0.756323     130.04
 C      -0.760723    -2.004146    -0.130307      59.30
 H      -0.726714    -2.367694     0.817991      20.71
 C      -1.758689    -1.746437    -2.422115      25.86
 C      -2.535377    -2.353934    -3.600367      85.84
 H      -2.226189    -1.873162    -4.493234      25.86
 O      -2.270188    -3.862548    -3.744515     240.47
 H      -1.426012    -4.087868    -3.739361      31.31
 C      -4.137761    -2.235598    -3.541468      62.25
 H      -4.555392    -2.744883    -2.511937      23.54
 O      -4.503518    -0.669488    -3.278441     241.96
 H      -5.234703    -0.715969    -2.818736      28.64
 C      -4.977123    -2.553570    -4.900454     101.72
 O      -6.381246    -2.319822    -4.674765     326.54
 H      -6.866529    -2.647762    -5.311977      36.16
 H      -4.694246    -3.625760    -5.251826      26.77
 H      -4.641571    -1.859239    -5.583764      29.77
55
name = lig-ACN-frame_864
 C       3.625645    -0.721805     0.371963      49.96
 H       2.912636    -0.537127    -0.345952      22.76
 C       4.662638    -0.519772     2.494177      50.21
 H       4.651307    -0.115522     3.605514      21.33
 C       5.948247    -0.946704     2.230397      10.15
 O       7.173112    -1.020507     2.987502     308.91
 C       7.252450    -1.835978     4.124599     101.33
 H       8.262342    -2.201252     4.201333      25.25
 H       6.487643    -2.796126     4.059934      27.04
 H       6.772133    -1.271852     5.048276      26.04
 C       6.069964    -1.380695     0.903114      14.12
 O       7.133399    -2.126835     0.397342     189.21
 H       7.878841    -2.118630     1.099563      24.24
 C       4.925413    -1.361307     0.116680      54.72
 H       5.106974    -1.818845    -0.780699      23.17
 C       3.549331    -0.234821     1.646550      32.56
 C       2.445352     0.617348     2.258194      86.16
 H       2.742141     1.829892     2.584586      20.55
 O       1.932045     0.305965     3.511676     213.05
 H       1.727011    -0.859456     3.662865      21.01
 C       1.276507     0.921302     1.247444      75.16
 H       2.024374     1.440609     0.372804      19.91
 C       0.233673     1.912099     1.805146     105.18
 O       0.569340     3.316597     1.956709     321.08
 H       1.089419     3.722855     1.305574      30.72
 H      -0.180337     1.558973     2.832484      23.23
 H      -0.632414     1.824863     1.238316      26.20
 C      -1.593327    -2.406552    -1.217773      31.85
 H      -2.270586    -3.425222    -0.940125      19.77
 C      -1.133789    -0.354481    -2.565815      85.40
 H      -1.108842     0.322328    -3.509714      19.51
 C      -0.123372    -0.068188    -1.575666       5.95
 O       0.543774     1.183106    -1.420487     197.69
 C       0.299417     2.190150    -2.387532      84.89
 H       0.767141     1.967597    -3.448789      23.85
 H      -0.836837     2.075129    -2.539445      21.50
 H       0.817773     2.970383    -1.801665      23.18
 C      -0.157997    -0.644853    -0.273496      15.96
 O       0.613094    -0.195649     0.756687     192.25
 C      -0.692221    -1.926078    -0.167012      47.69
 H      -0.513071    -2.604845     0.648076      20.54
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 C      -1.726385    -1.689810    -2.457379      22.29
 C      -2.578029    -2.297705    -3.642425      86.77
 H      -2.349827    -1.669078    -4.452105      25.67
 O      -2.254744    -3.815252    -3.753125     219.43
 H      -1.359942    -3.904307    -3.471947      28.75
 C      -4.095753    -2.239312    -3.595782      63.20
 H      -4.520853    -3.096441    -2.786405      22.98
 O      -4.484012    -0.695447    -3.238354     214.84
 H      -5.378209    -0.665486    -2.967766      26.35
 C      -4.962824    -2.558909    -4.906447      94.93
 O      -6.392815    -2.330007    -4.616960     268.02
 H      -6.763324    -2.332684    -5.571578      29.22
 H      -4.810578    -3.694470    -5.172626      25.74
 H      -4.595409    -1.981085    -5.715233      27.87
55
name = lig-ACN-frame_865
 C       3.697122    -0.655469     0.380471      52.84
 H       2.942738    -0.572399    -0.381780      20.94
 C       4.710359    -0.483668     2.596332      40.47
 H       4.560931     0.085904     3.691702      19.05
 C       6.019516    -0.922593     2.127244      -3.42
 O       7.211941    -1.009413     2.982636     281.10
 C       7.331292    -1.928357     4.146025     106.10
 H       8.348102    -2.056108     4.208612      26.14
 H       6.861722    -2.987508     3.908022      28.70
 H       7.130462    -1.497762     5.245393      26.39
 C       6.020734    -1.466339     0.788015       4.53
 O       7.171527    -2.149186     0.389905     189.92
 H       7.891948    -1.891357     1.062503      24.03
 C       4.796642    -1.424856     0.004767      50.93
 H       4.778596    -1.865223    -0.899521      23.41
 C       3.622697    -0.185695     1.730987      25.97
 C       2.408809     0.618785     2.223993      86.45
 H       3.002243     1.760268     2.273948      20.14
 O       1.907785     0.235256     3.558255     179.50
 H       1.751776    -0.992480     3.466339      18.91
 C       1.297948     0.897026     1.240858      77.40
 H       1.526104     1.456889     0.167687      17.10
 C       0.191821     1.894475     1.843429      95.27
 O       0.601783     3.407236     1.963795     263.16
 H       0.852660     3.551482     1.045178      28.17
 H      -0.124673     1.575454     2.820065      23.66
 H      -0.546993     1.885859     1.097133      24.08
 C      -1.439976    -2.368240    -1.309173      73.02
 H      -2.266994    -3.257240    -1.152857      19.48
 C      -1.047970    -0.488783    -2.567451      52.42
 H      -1.205151    -0.015218    -3.588618      21.41
 C      -0.177952     0.015701    -1.569730      19.39
 O       0.568056     1.158047    -1.504357     254.02
 C       0.254792     2.245633    -2.370630     110.27
 H       0.621140     1.933255    -3.428209      23.80
 H      -0.860911     2.733889    -2.467141      22.92
 H       0.643456     3.261845    -2.203443      25.18
 C      -0.103947    -0.633397    -0.319224       8.92
 O       0.607098    -0.391694     0.878129     141.19
 C      -0.765540    -1.907803    -0.234857      47.70
 H      -0.457702    -2.507744     0.699806      21.63
 C      -1.811365    -1.656559    -2.429998      30.34
 C      -2.561061    -2.275763    -3.677039      75.38
 H      -2.172849    -1.923928    -4.588335      26.00
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 O      -2.275881    -3.631690    -3.785838     198.51
 H      -1.230537    -3.978987    -3.504019      24.04
 C      -4.226205    -2.089370    -3.611710      79.92
 H      -4.540792    -2.783967    -2.607288      22.28
 O      -4.378922    -0.875254    -3.224342     194.10
 H      -5.497219    -0.691539    -3.022555      21.27
 C      -4.883177    -2.568879    -4.875591      95.87
 O      -6.357723    -2.346897    -4.580908     229.06
 H      -6.883120    -2.016181    -5.551186      26.92
 H      -4.765979    -3.748162    -5.049190      25.32
 H      -4.585657    -1.970535    -5.714201      27.21
55
name = lig-ACN-frame_866
 C       3.783700    -0.659488     0.432196      33.21
 H       2.759050    -0.531613    -0.067685      17.49
 C       4.840465    -0.298490     2.708340      35.96
 H       4.814488    -0.186305     3.969065      20.75
 C       5.946269    -0.968087     2.150275       4.12
 O       7.166504    -0.954635     2.868539     223.24
 C       7.464199    -2.036873     4.140058      76.61
 H       8.457543    -2.094397     4.200184      26.76
 H       6.893508    -3.011799     4.008770      27.37
 H       6.782031    -1.454090     4.912183      24.84
 C       5.971395    -1.598286     0.749198      -6.77
 O       7.197706    -2.137379     0.357029     211.39
 H       7.813612    -1.894905     1.036044      25.87
 C       4.852834    -1.473366    -0.164601      49.99
 H       4.798181    -1.973565    -1.091751      21.52
 C       3.684193    -0.205515     1.799326      21.92
 C       2.432143     0.663287     2.208640      76.32
 H       2.750133     1.807073     2.660766      22.06
 O       1.916532     0.142906     3.559961     185.92
 H       1.948472    -0.994509     3.449622      23.28
 C       1.220113     0.972281     1.235302      60.77
 H       1.830258     1.354226     0.256009      18.78
 C       0.155664     1.979008     1.803487     114.45
 O       0.635932     3.298697     1.959094     289.24
 H       0.635229     4.104019     1.230938      25.00
 H      -0.071074     1.716865     2.780484      24.98
 H      -0.777851     1.868222     1.290028      24.71
 C      -1.576784    -2.505806    -1.333604      33.34
 H      -1.508308    -3.670620    -1.265020      19.39
 C      -0.919790    -0.465190    -2.650495      41.84
 H      -0.955955     0.208543    -3.504280      21.63
 C      -0.288924     0.124787    -1.454824      -3.00
 O       0.625254     1.204060    -1.599635     160.98
 C       0.180291     2.417255    -2.533931      67.99
 H       0.277427     2.251441    -3.640743      24.31
 H      -1.013402     2.523774    -2.174432      22.05
 H       1.005050     2.927493    -1.995911      22.48
 C      -0.040984    -0.761358    -0.263165      14.15
 O       0.603121    -0.552544     0.979796      93.90
 C      -0.752545    -1.894337    -0.260807      35.55
 H      -0.886916    -2.487045     0.757166      20.52
 C      -1.804077    -1.649508    -2.502730       9.69
 C      -2.576273    -2.179438    -3.670040     100.45
 H      -2.443854    -1.436196    -4.338816      27.57
 O      -2.321382    -3.618031    -3.825080     143.32
 H      -1.124900    -3.651881    -3.832097      23.21
 C      -4.068611    -2.238510    -3.559591      68.42
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 H      -4.556253    -3.072679    -2.776349      24.04
 O      -4.351360    -0.752464    -3.177585     135.74
 H      -5.538658    -0.702742    -2.944756      21.77
 C      -4.936398    -2.558280    -4.857326      96.62
 O      -6.289175    -2.359186    -4.568802     284.04
 H      -6.788326    -2.078186    -5.401464      29.13
 H      -4.525258    -3.675643    -5.105754      25.35
 H      -4.540152    -1.956803    -5.712318      27.46
55
name = lig-ACN-frame_867
 C       3.825233    -0.758882     0.526156      45.94
 H       2.936734    -0.608672    -0.270355      23.12
 C       4.877693    -0.253735     2.633439      35.69
 H       5.013252     0.294565     3.756435      19.77
 C       5.905553    -1.086707     2.127669      24.52
 O       7.168024    -1.030340     2.792115     244.30
 C       7.427989    -1.970461     3.982427     103.72
 H       8.496035    -1.970037     4.033783      26.00
 H       7.071337    -2.906796     3.758893      28.88
 H       7.085128    -1.536296     5.032392      26.72
 C       5.961053    -1.611919     0.821806      10.71
 O       7.187279    -2.121499     0.332144     206.61
 H       7.796732    -2.040640     1.101352      24.07
 C       4.922644    -1.414604    -0.065643      54.40
 H       5.002162    -1.762336    -1.139394      20.42
 C       3.747169    -0.107159     1.808317      20.90
 C       2.424541     0.647987     2.348333      94.19
 H       2.851188     1.822938     2.542026      21.56
 O       1.950072     0.065722     3.504569     269.42
 H       1.928382    -0.924058     3.481302      26.05
 C       1.231918     0.868694     1.267704      77.00
 H       1.491784     1.211327     0.185469      20.20
 C       0.125479     1.940972     1.776284     112.03
 O       0.691280     3.256762     1.989840     272.58
 H       0.619503     3.655474     0.993741      24.88
 H      -0.151204     1.555750     2.675523      26.30
 H      -0.760814     2.003914     1.087842      23.91
 C      -1.588890    -2.498973    -1.360089      50.84
 H      -2.098751    -3.477513    -1.495241      21.18
 C      -0.950913    -0.422249    -2.515579      37.98
 H      -0.849148     0.049132    -3.445550      20.31
 C      -0.197889     0.077150    -1.405120       7.80
 O       0.605482     1.267254    -1.771768     214.46
 C       0.172426     2.457580    -2.512073      97.41
 H       0.149000     2.270859    -3.597199      24.48
 H      -0.986466     2.929145    -2.133307      23.02
 H       0.689288     3.435524    -2.288244      25.19
 C      -0.101160    -0.734054    -0.219836      -5.22
 O       0.634842    -0.480138     1.005590     109.09
 C      -0.877147    -2.085930    -0.270651      41.02
 H      -0.637140    -2.745603     0.673362      21.76
 C      -1.608618    -1.658997    -2.505143      31.79
 C      -2.563429    -2.116997    -3.692591      88.24
 H      -2.376037    -1.785465    -4.611518      27.75
 O      -2.279752    -3.616410    -3.942847     173.71
 H      -1.269454    -3.905375    -4.150852      26.42
 C      -4.106030    -2.187358    -3.487295      75.60
 H      -4.194811    -2.872425    -2.489983      24.13
 O      -4.370068    -0.691125    -3.127071     197.95
 H      -5.375353    -0.657969    -2.766630      24.57
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 C      -4.794921    -2.552875    -4.832213      95.81
 O      -6.275704    -2.376566    -4.538353     291.10
 H      -6.651937    -2.395881    -5.325338      34.60
 H      -4.912481    -3.614329    -5.314771      24.07
 H      -4.527859    -1.721978    -5.559323      26.33
55
name = lig-ACN-frame_868
 C       3.735007    -0.772893     0.539635      43.75
 H       2.845918    -0.666204    -0.257658      22.80
 C       4.898169    -0.276798     2.523607      43.63
 H       5.116190     0.554897     3.331327      20.19
 C       5.967276    -1.117172     2.187508      30.36
 O       7.193030    -1.130623     2.749899     283.02
 C       7.437756    -1.871971     3.829371     114.32
 H       8.561865    -1.977338     3.873325      24.87
 H       7.012775    -2.783952     3.692235      31.40
 H       6.927410    -1.456377     4.774384      27.56
 C       6.070462    -1.603738     0.877493      10.61
 O       7.170711    -2.125645     0.339629     188.36
 H       7.963235    -2.122522     1.008866      22.74
 C       4.932536    -1.349457     0.118749      56.91
 H       4.988010    -1.561474    -1.042458      21.47
 C       3.692094    -0.050706     1.740795      23.84
 C       2.468353     0.630295     2.260351      92.09
 H       2.702612     1.764955     2.673611      21.55
 O       1.965455     0.000587     3.534239     241.75
 H       1.894362    -0.863010     3.417352      30.07
 C       1.261817     0.802782     1.270604      84.79
 H       1.806210     1.314915     0.423468      21.97
 C       0.159751     1.767136     1.797620     100.94
 O       0.712689     3.205206     1.984552     288.14
 H       1.172755     3.557146     1.261039      30.79
 H      -0.447235     1.587059     2.571520      26.59
 H      -0.446603     1.860043     0.815862      22.63
 C      -1.599101    -2.475528    -1.398983      35.67
 H      -2.377886    -3.111642    -1.233266      21.89
 C      -0.980256    -0.415951    -2.430057      50.50
 H      -1.081744     0.269685    -3.243793      21.65
 C      -0.079493     0.081849    -1.462511       0.64
 O       0.620571     1.262240    -1.806182     208.21
 C       0.057386     2.483287    -2.458593      68.88
 H       0.227578     2.336755    -3.561631      22.56
 H      -1.186620     2.665125    -2.215227      22.35
 H       0.886915     3.165851    -2.076470      23.72
 C      -0.201704    -0.744703    -0.151797       4.07
 O       0.583663    -0.431947     0.948366     149.25
 C      -0.806217    -2.056817    -0.178528      43.61
 H      -0.571806    -2.898420     0.533749      21.48
 C      -1.583603    -1.680075    -2.576577      26.44
 C      -2.373835    -2.222452    -3.763895      86.68
 H      -2.185126    -1.459128    -4.448222      26.87
 O      -2.264614    -3.610229    -4.054561     294.46
 H      -1.407210    -3.732370    -4.048062      34.05
 C      -4.071636    -1.977810    -3.418902      73.20
 H      -4.560513    -2.714895    -2.603670      24.96
 O      -4.413604    -0.728964    -3.091425     303.15
 H      -5.147075    -0.698540    -2.696121      34.06
 C      -4.808727    -2.487772    -4.727943      86.60
 O      -6.241664    -2.382954    -4.512061     247.79
 H      -6.840441    -2.694909    -5.342069      27.34
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 H      -4.089935    -3.386732    -4.925823      25.20
 H      -4.391801    -1.757570    -5.554447      26.84
55
name = lig-ACN-frame_869
 C       3.662131    -0.737462     0.471267      45.61
 H       2.709542    -0.823325    -0.161884      20.40
 C       4.893339    -0.179407     2.518362      52.59
 H       4.951947     0.224764     3.539824      23.89
 C       5.987372    -1.040847     2.169458      13.39
 O       7.317447    -1.045864     2.643583     268.21
 C       7.461945    -1.950142     3.936145     104.74
 H       8.613331    -2.068724     4.182078      25.41
 H       6.972066    -2.843487     3.964815      29.97
 H       7.101100    -1.316021     4.739444      27.57
 C       6.006816    -1.574359     0.868489       3.00
 O       7.232140    -2.177647     0.313916     202.40
 H       7.901339    -1.963851     1.010403      23.17
 C       4.879358    -1.372841     0.066951      43.54
 H       4.986776    -1.925148    -0.992774      19.88
 C       3.688264    -0.133815     1.728535      28.83
 C       2.419771     0.568703     2.273474      97.91
 H       2.711927     1.739434     2.500357      23.07
 O       2.006374     0.000318     3.543413     256.31
 H       2.005845    -0.988192     3.528999      26.85
 C       1.323919     0.830488     1.279695      85.57
 H       1.656574     1.180311     0.308543      22.23
 C       0.248458     1.805482     1.664187     119.15
 O       0.698670     3.047472     2.039743     311.81
 H       1.231879     3.364389     1.325008      31.24
 H      -0.095295     1.347748     2.555014      26.29
 H      -0.684813     1.757808     0.945839      23.93
 C      -1.552509    -2.421299    -1.251266      68.87
 H      -1.735490    -3.415030    -1.201617      25.22
 C      -0.978422    -0.396431    -2.570703      43.57
 H      -1.230231     0.322661    -3.385055      19.87
 C      -0.185177     0.023053    -1.463098       8.93
 O       0.655553     1.169692    -1.681695     206.31
 C       0.019819     2.424240    -2.408542      71.81
 H       0.110268     2.521606    -3.554718      22.54
 H      -1.164941     2.498861    -1.997130      23.14
 H       0.358367     3.358620    -1.762729      23.26
 C      -0.107888    -0.667942    -0.255376      18.51
 O       0.557894    -0.477711     0.952086     135.70
 C      -0.774416    -1.931358    -0.252355      49.37
 H      -0.813407    -2.351093     0.717249      22.36
 C      -1.613889    -1.727313    -2.485059      31.02
 C      -2.440087    -2.126486    -3.725893      90.79
 H      -2.162475    -1.719347    -4.667835      26.16
 O      -2.210427    -3.584922    -4.158356     248.42
 H      -1.448511    -3.962324    -3.821803      30.33
 C      -3.969113    -2.018846    -3.474492      80.67
 H      -4.033196    -2.798468    -2.603331      24.81
 O      -4.417817    -0.578907    -3.016594     235.42
 H      -5.289491    -0.746525    -2.574307      27.26
 C      -4.742901    -2.352707    -4.657268     106.63
 O      -6.190363    -2.436861    -4.470942     177.36
 H      -6.443358    -2.875269    -5.492853      25.68
 H      -4.728007    -3.504864    -4.886538      22.26
 H      -4.641273    -1.794758    -5.648318      24.39
55
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name = lig-ACN-frame_870
 C       3.737288    -0.788350     0.403817      47.27
 H       2.836876    -0.796523    -0.183916      22.37
 C       4.876198    -0.167359     2.606879      34.75
 H       4.700485     0.178061     3.550460      22.23
 C       6.068891    -0.866601     2.027912     -13.64
 O       7.436189    -1.023579     2.727560     221.04
 C       7.475217    -1.878317     4.042878      89.47
 H       8.627374    -2.216147     3.909663      25.18
 H       6.865020    -2.721776     3.779692      29.02
 H       7.180967    -1.373856     4.921213      28.09
 C       6.000922    -1.570109     0.725089       0.73
 O       7.152527    -2.164285     0.343585     181.28
 H       7.825971    -1.946953     0.978195      20.06
 C       4.799394    -1.513938    -0.130141      46.61
 H       4.701923    -2.120419    -1.125402      20.07
 C       3.686890    -0.205153     1.769370      12.76
 C       2.457410     0.528758     2.306280      91.56
 H       2.901674     1.580062     2.598052      24.12
 O       2.029576     0.044204     3.574244     191.66
 H       2.135384    -1.114712     3.559528      22.87
 C       1.318136     0.757570     1.098655      95.05
 H       1.907767     1.020962     0.317053      25.87
 C       0.204646     1.710970     1.659884      99.78
 O       0.736498     3.003612     2.096001     241.93
 H       0.890417     3.702852     1.252702      25.78
 H      -0.219637     1.283011     2.564615      25.93
 H      -0.676711     1.939300     0.907211      23.18
 C      -1.468211    -2.455480    -1.259381      52.46
 H      -1.715113    -3.480287    -1.217193      22.60
 C      -1.024385    -0.471880    -2.620583      38.42
 H      -0.948374    -0.089002    -3.707814      22.10
 C      -0.249043     0.132622    -1.584751       4.26
 O       0.629747     1.163366    -1.586398     238.22
 C      -0.013379     2.309996    -2.181565      89.11
 H       0.375197     2.239243    -3.335931      22.68
 H      -1.163532     2.028879    -2.297495      24.03
 H       0.309947     3.339812    -1.781192      24.22
 C      -0.013559    -0.671472    -0.323551      -2.35
 O       0.610817    -0.462574     0.964269     138.01
 C      -0.785988    -1.780427    -0.160142      43.31
 H      -0.743744    -2.223384     0.755292      24.31
 C      -1.669749    -1.644339    -2.467242      26.90
 C      -2.423916    -2.083901    -3.706737      75.48
 H      -2.147016    -1.252105    -4.440853      25.46
 O      -2.202981    -3.538772    -4.209466     159.97
 H      -1.282645    -3.767344    -3.593691      22.82
 C      -3.932369    -1.959247    -3.426926      68.70
 H      -4.237287    -2.618803    -2.574997      25.67
 O      -4.331343    -0.526460    -2.954487     146.67
 H      -5.450950    -0.658522    -2.577615      23.08
 C      -4.754318    -2.426696    -4.751593      90.09
 O      -6.194288    -2.458718    -4.411549     277.44
 H      -6.724263    -2.673064    -5.212883      29.29
 H      -4.097468    -3.312194    -5.177640      24.95
 H      -4.364599    -1.520145    -5.316211      26.86
55
name = lig-ACN-frame_871
 C       3.760675    -0.852926     0.445262      51.66
 H       2.958053    -0.672277    -0.143835      24.11
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 C       4.943520    -0.338825     2.539213      49.81
 H       5.110414     0.162638     3.349683      19.04
 C       6.116130    -0.736078     1.974443     -12.46
 O       7.384884    -0.970096     2.794782     261.84
 C       7.459022    -1.784635     3.957551     102.74
 H       8.557300    -2.240723     4.149140      25.14
 H       6.655418    -2.629538     4.101364      27.68
 H       7.300960    -1.184380     4.811422      27.48
 C       5.989153    -1.451607     0.664932       2.10
 O       7.094565    -2.184543     0.318205     141.77
 H       7.746781    -2.055302     1.083590      20.94
 C       4.853450    -1.614708    -0.129974      56.98
 H       4.815710    -2.105023    -1.114525      21.02
 C       3.756230    -0.284106     1.709606      35.26
 C       2.515136     0.555817     2.203200      83.76
 H       2.670111     1.667082     2.369798      24.03
 O       2.036904     0.049833     3.606258     127.53
 H       1.929534    -1.166079     3.744054      20.62
 C       1.378956     0.761094     1.195204      97.55
 H       1.694859     1.199516     0.374541      25.65
 C       0.224280     1.696380     1.652667      92.60
 O       0.772898     3.014160     2.138194     246.19
 H       0.546952     3.650270     1.311575      25.92
 H      -0.435263     1.206795     2.490718      23.99
 H      -0.464567     1.765364     0.750613      23.48
 C      -1.436831    -2.418302    -1.299258      64.11
 H      -2.192275    -3.169987    -1.019681      21.58
 C      -0.932812    -0.398240    -2.599596      29.49
 H      -0.823485     0.187555    -3.609528      20.15
 C      -0.145148     0.032717    -1.493132      10.42
 O       0.597717     1.217606    -1.508901     253.70
 C      -0.008377     2.278352    -2.173714      92.47
 H       0.481861     2.599642    -3.260072      22.68
 H      -1.132318     2.273117    -2.256028      26.19
 H       0.137514     3.115886    -1.384569      24.27
 C      -0.102119    -0.673611    -0.304099      19.61
 O       0.685272    -0.459347     0.799156     161.42
 C      -0.864440    -1.872651    -0.140242      51.46
 H      -0.669423    -2.495606     0.658809      24.27
 C      -1.657149    -1.726074    -2.446275      27.76
 C      -2.432731    -2.110675    -3.676393      76.15
 H      -2.231924    -1.397834    -4.592330      24.42
 O      -2.193981    -3.373951    -4.163081     177.89
 H      -1.099477    -3.873136    -4.109858      22.31
 C      -4.090781    -1.925092    -3.383570      84.11
 H      -4.379007    -2.627553    -2.612118      26.85
 O      -4.200358    -0.596672    -2.959662     189.90
 H      -5.359439    -0.433616    -2.682254      23.13
 C      -4.711234    -2.312886    -4.740169     103.26
 O      -6.140470    -2.512463    -4.369168     304.29
 H      -6.644583    -2.312117    -5.073943      34.07
 H      -4.398990    -3.281223    -5.287591      25.84
 H      -4.888815    -1.561509    -5.567225      25.62
55
name = lig-ACN-frame_872
 C       3.722940    -0.941169     0.401240      63.65
 H       2.862570    -0.937654    -0.167549      23.44
 C       4.974859    -0.353931     2.493691      48.35
 H       4.836107    -0.051795     3.423814      22.95
 C       6.176888    -0.888095     1.943099      36.32
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 O       7.280137    -0.851934     2.668962     256.31
 C       7.355390    -1.689558     3.978164      79.35
 H       8.379573    -2.200837     3.730018      24.20
 H       6.494306    -2.526696     4.011035      25.48
 H       7.422254    -0.968672     4.789908      25.76
 C       6.141811    -1.428250     0.708296      20.11
 O       7.136281    -2.229405     0.260602     129.24
 H       7.919340    -2.233219     0.944655      18.39
 C       4.911205    -1.520935     0.016502      68.16
 H       5.030706    -2.117098    -0.820491      23.21
 C       3.766399    -0.273932     1.702578      11.09
 C       2.565836     0.484907     2.225008     102.09
 H       3.060355     1.400441     2.461487      27.03
 O       2.090398     0.092692     3.547627     188.32
 H       2.034113    -1.050031     3.331904      23.85
 C       1.372707     0.846076     1.238199      78.81
 H       1.904479     1.295366     0.549891      27.34
 C       0.282109     1.755629     1.702742     111.93
 O       0.736242     2.984235     2.133541     327.97
 H       0.828595     3.578902     1.477500      33.85
 H      -0.397618     1.277545     2.592066      24.38
 H      -0.342897     1.943666     0.815625      24.64
 C      -1.644659    -2.416967    -1.259598      36.13
 H      -2.157270    -3.493332    -1.328046      21.72
 C      -0.816057    -0.442079    -2.509184      64.91
 H      -1.131392     0.324798    -3.278885      22.27
 C      -0.069667    -0.052630    -1.451492       4.37
 O       0.599030     1.182713    -1.440515     180.57
 C      -0.037295     2.495688    -2.183834      73.99
 H       0.557327     2.719458    -3.264638      22.62
 H      -1.031358     2.165707    -2.507541      25.46
 H      -0.015397     3.376272    -1.523626      25.36
 C      -0.209870    -0.760714    -0.166536       4.89
 O       0.823390    -0.517017     0.705273     121.53
 C      -0.838598    -2.029243    -0.190012      51.65
 H      -0.905299    -2.494005     0.805143      22.92
 C      -1.504999    -1.584794    -2.541191      23.43
 C      -2.538261    -2.039013    -3.622962      83.16
 H      -2.357360    -1.178271    -4.437320      24.45
 O      -2.200878    -3.376573    -4.145732     181.45
 H      -1.091283    -3.313285    -4.103502      24.55
 C      -3.989664    -2.000533    -3.471882      95.54
 H      -4.403303    -2.724085    -2.826616      27.73
 O      -4.131780    -0.616162    -2.967334     248.20
 H      -5.084466    -0.410176    -2.760800      28.19
 C      -4.833347    -2.185219    -4.714998      97.62
 O      -6.147553    -2.560337    -4.318120     244.83
 H      -6.829819    -2.231399    -5.145953      25.75
 H      -4.258332    -3.104370    -5.041816      26.37
 H      -4.437508    -1.385746    -5.483708      26.25
55
name = lig-ACN-frame_873
 C       3.748493    -0.950910     0.452074      53.49
 H       2.841848    -1.259800    -0.101933      22.32
 C       4.865918    -0.308095     2.440790      65.39
 H       4.925098    -0.031375     3.455176      23.00
 C       6.049392    -0.952041     2.040950       4.70
 O       7.321687    -0.797374     2.664634     264.26
 C       7.317265    -1.548148     3.882602      89.95
 H       8.186517    -2.277326     3.922480      24.47
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 H       6.220788    -2.146095     3.961818      24.16
 H       7.327055    -0.945248     4.845705      27.10
 C       6.220531    -1.551850     0.696548       8.26
 O       7.291108    -2.300708     0.164594     207.13
 H       8.105390    -2.198080     0.677725      24.93
 C       5.006712    -1.490528    -0.017149      50.49
 H       4.914664    -2.060446    -0.850587      22.88
 C       3.716424    -0.329938     1.660328      40.81
 C       2.610929     0.540914     2.266897     105.15
 H       2.915600     1.523798     2.447302      28.14
 O       2.150588     0.033893     3.497101     264.04
 H       2.014234    -0.898571     3.672334      28.20
 C       1.474768     0.800593     1.168036      77.69
 H       1.815405     1.250124     0.340668      25.75
 C       0.220089     1.753940     1.705354      90.19
 O       0.748110     3.074388     2.190874     277.63
 H       1.282180     3.348758     1.409256      30.29
 H      -0.281350     1.245747     2.728156      24.29
 H      -0.596599     1.802510     0.997663      25.72
 C      -1.718519    -2.384032    -1.343924      51.33
 H      -2.233773    -3.498463    -1.474368      23.18
 C      -0.800628    -0.428483    -2.539862      40.74
 H      -0.748142     0.191300    -3.460627      21.03
 C      -0.084762     0.058680    -1.356405     -10.66
 O       0.601458     1.261708    -1.413499     188.00
 C      -0.056017     2.510380    -2.192725      80.13
 H       0.877771     2.492039    -2.968044      21.66
 H      -0.988754     2.308745    -2.543482      27.98
 H      -0.087869     3.310897    -1.482578      26.40
 C      -0.080772    -0.824637    -0.185784     -13.52
 O       0.976414    -0.558812     0.801840     106.45
 C      -0.896262    -2.102440    -0.164904      41.23
 H      -0.967461    -2.831671     0.750555      22.21
 C      -1.649417    -1.681283    -2.462508      33.58
 C      -2.412970    -1.953607    -3.733578      74.12
 H      -2.200348    -1.159301    -4.604539      24.56
 O      -2.184825    -3.367094    -4.134416     249.81
 H      -1.287981    -3.704158    -3.960517      27.12
 C      -3.973211    -1.954932    -3.401302      90.27
 H      -4.130375    -2.618983    -2.643310      28.14
 O      -4.138048    -0.595236    -2.933958     293.17
 H      -4.938387    -0.599087    -2.687736      33.86
 C      -4.772601    -2.238419    -4.738760      83.28
 O      -6.220941    -2.521400    -4.316157     209.27
 H      -7.047388    -2.475498    -5.081285      27.35
 H      -4.477987    -2.936125    -5.508897      26.21
 H      -5.114835    -1.153377    -5.133554      22.63
55
name = lig-ACN-frame_874
 C       3.884766    -1.029632     0.419206      41.85
 H       2.935866    -0.957905    -0.287911      22.58
 C       4.908656    -0.331354     2.482354      25.38
 H       4.926130     0.549627     3.194412      19.95
 C       6.104290    -0.966882     1.942473      -2.06
 O       7.333629    -0.761204     2.688503     258.34
 C       7.283285    -1.479775     3.939561      80.01
 H       8.011856    -2.303636     3.973798      25.91
 H       6.153299    -2.027592     4.034903      23.14
 H       7.458886    -0.639441     4.747626      23.26
 C       6.166031    -1.675512     0.715060      -0.10
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 O       7.396240    -2.295027     0.119137     186.94
 H       8.107461    -2.054388     0.728038      23.89
 C       5.033643    -1.596538    -0.158246      50.14
 H       5.118608    -1.917684    -1.159992      21.69
 C       3.679082    -0.296518     1.705150      -9.89
 C       2.561972     0.605226     2.138904      91.21
 H       2.974338     1.475384     2.405223      27.75
 O       2.158480    -0.042196     3.576274     169.11
 H       2.246938    -0.849446     3.369189      32.85
 C       1.412576     0.772453     1.158687      88.74
 H       1.870248     1.195945     0.293252      24.57
 C       0.290194     1.704448     1.759378      93.42
 O       0.746790     3.098519     2.180296     223.16
 H       1.495006     3.549495     1.479862      25.99
 H      -0.056576     1.153336     2.831501      23.70
 H      -0.506891     1.864915     1.082324      25.62
 C      -1.652801    -2.430482    -1.264626      41.49
 H      -2.530219    -3.232168    -0.951977      19.11
 C      -0.835493    -0.456778    -2.477887      54.83
 H      -0.477926    -0.170554    -3.423091      23.07
 C      -0.212930     0.056558    -1.328679      -3.15
 O       0.539006     1.346182    -1.387628     189.50
 C       0.015291     2.377346    -2.154848     121.61
 H       0.561474     2.810030    -3.084307      25.73
 H      -0.867141     2.163188    -2.583091      28.63
 H      -0.030921     3.197716    -1.480510      27.08
 C       0.104486    -0.873486    -0.241861      -0.09
 O       0.981518    -0.658474     0.897408     100.67
 C      -0.888376    -1.958561    -0.203648      37.73
 H      -0.595766    -2.792217     0.614069      23.00
 C      -1.680829    -1.487221    -2.514247      20.96
 C      -2.309081    -2.039904    -3.802080      81.83
 H      -1.889853    -1.406847    -4.745056      24.04
 O      -2.186455    -3.368699    -4.181940     298.42
 H      -1.502262    -3.633666    -3.716329      32.60
 C      -3.885236    -1.891271    -3.440636      76.69
 H      -4.041627    -2.616796    -2.778862      27.91
 O      -4.234538    -0.565614    -2.899165     250.35
 H      -5.127913    -0.510190    -2.355007      26.21
 C      -4.906447    -2.167279    -4.711844      79.85
 O      -6.269479    -2.533767    -4.277033     298.58
 H      -6.535982    -2.584389    -5.160452      30.79
 H      -4.473159    -2.883490    -5.344291      27.44
 H      -4.740988    -1.121343    -5.398817      24.64
55
name = lig-ACN-frame_875
 C       3.881288    -1.009320     0.337422      42.31
 H       3.107713    -0.696786    -0.510566      21.87
 C       5.023096    -0.320429     2.382560      34.96
 H       5.298564     0.343339     3.349023      19.30
 C       6.186827    -0.940376     1.886657      -2.24
 O       7.286084    -0.761774     2.635275     221.53
 C       7.273365    -1.434566     4.089129      60.43
 H       8.037497    -2.145202     3.966649      26.02
 H       6.115649    -1.908198     4.406717      23.60
 H       7.598561    -0.642148     4.934167      23.93
 C       6.225823    -1.782370     0.647791       6.87
 O       7.357112    -2.183587     0.179611     115.49
 H       8.132601    -2.256464     0.865878      20.66
 C       5.059347    -1.699361    -0.158019      49.95
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 H       5.110845    -1.978373    -1.246419      20.83
 C       3.869272    -0.375689     1.599692      23.95
 C       2.568897     0.516387     2.196734      89.41
 H       2.843027     1.467231     2.323738      28.18
 O       2.166532    -0.023481     3.514197     220.95
 H       2.169384    -1.050111     3.673751      25.45
 C       1.377793     0.718558     1.228276      80.71
 H       1.715069     1.146263     0.220253      22.23
 C       0.381545     1.728258     1.819318     109.43
 O       0.761799     3.020561     2.158618     284.21
 H       1.008392     3.493052     1.221901      26.34
 H      -0.098720     1.298070     2.869671      23.95
 H      -0.498831     1.697935     1.184192      25.55
 C      -1.636300    -2.211495    -1.239863      58.98
 H      -2.246797    -3.232025    -1.134882      24.31
 C      -0.810953    -0.383515    -2.476387      56.16
 H      -0.776262     0.306873    -3.257871      20.75
 C      -0.101821     0.095817    -1.289897      17.83
 O       0.485386     1.235423    -1.328243     227.42
 C      -0.050633     2.364730    -2.187703     103.92
 H       0.723786     2.345072    -2.974628      24.57
 H      -0.988319     2.158890    -2.540796      27.83
 H      -0.201331     3.279490    -1.642807      26.72
 C       0.115403    -0.802899    -0.246563      31.83
 O       0.851296    -0.702036     0.890619     133.46
 C      -0.668202    -1.899730    -0.231345      50.22
 H      -0.792416    -2.368091     0.869035      21.56
 C      -1.653906    -1.638911    -2.441250      36.71
 C      -2.414240    -1.968170    -3.784953      64.64
 H      -2.065723    -1.128754    -4.601501      24.30
 O      -2.177487    -3.457260    -4.206649     213.33
 H      -1.269249    -3.875521    -4.000812      24.56
 C      -3.960787    -1.815277    -3.588242     103.98
 H      -4.089990    -2.556930    -2.945251      27.74
 O      -4.296626    -0.529631    -2.867762     184.05
 H      -5.257470    -1.037455    -2.354096      22.38
 C      -4.881041    -2.114337    -4.633950     108.74
 O      -6.253540    -2.503938    -4.285815     298.91
 H      -6.860464    -2.774113    -4.919289      33.31
 H      -4.471638    -3.018701    -4.937004      27.83
 H      -5.058691    -1.345443    -5.585511      24.50
55
name = lig-ACN-frame_876
 C       3.942081    -0.951508     0.228279      44.82
 H       2.961898    -0.974342    -0.385564      20.93
 C       5.080793    -0.311138     2.219990      42.26
 H       4.890797    -0.041470     3.410304      23.16
 C       6.217916    -1.018977     1.858865      36.44
 O       7.363598    -0.838319     2.729211     241.46
 C       7.325415    -1.353262     4.089328      83.40
 H       7.917326    -2.216355     4.275833      25.55
 H       6.120725    -1.764060     4.399853      21.90
 H       7.654903    -0.434302     4.820076      23.47
 C       6.175530    -1.654353     0.693607      14.51
 O       7.434254    -2.175391     0.177102     166.94
 H       8.051710    -2.339896     0.969968      21.53
 C       5.030519    -1.729558    -0.116478      52.20
 H       5.083074    -2.441082    -1.049373      20.01
 C       3.871597    -0.329814     1.523539      23.58
 C       2.709881     0.317541     2.193166     116.27
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 H       3.089220     1.226425     2.377741      28.56
 O       2.179917     0.024007     3.478251     193.76
 H       2.047901    -1.153731     3.489026      23.04
 C       1.477853     0.586191     1.317355      76.66
 H       1.966105     1.196313     0.366897      21.60
 C       0.256007     1.612057     1.894848      81.39
 O       0.837163     2.995746     2.075137     298.48
 H       0.655136     3.515184     1.371463      30.86
 H      -0.019980     1.212840     2.980262      23.37
 H      -0.587897     1.669543     1.187425      23.85
 C      -1.595827    -2.223269    -1.187924      47.33
 H      -2.144335    -3.198114    -1.076415      23.54
 C      -0.883945    -0.363597    -2.481924      62.97
 H      -1.231712     0.307618    -3.211506      22.51
 C      -0.030856    -0.020398    -1.440285      14.10
 O       0.502992     1.366481    -1.265300     222.34
 C      -0.105549     2.303437    -2.243073     117.21
 H       0.482934     2.416766    -3.125665      27.14
 H      -1.086631     2.178988    -2.589208      28.18
 H       0.159399     3.206900    -1.672057      25.54
 C       0.050952    -0.739524    -0.216424       9.55
 O       0.773832    -0.565082     0.962651     152.29
 C      -0.665158    -1.990330    -0.200729      41.19
 H      -0.814636    -2.548499     0.815842      21.18
 C      -1.521993    -1.530915    -2.519496      27.72
 C      -2.479167    -1.952584    -3.704159      68.68
 H      -2.050210    -1.362640    -4.692876      21.59
 O      -2.248038    -3.420710    -4.220383     149.38
 H      -1.121104    -3.346270    -4.018332      21.16
 C      -4.048225    -1.781320    -3.466544      77.67
 H      -4.320721    -2.508140    -2.851624      27.47
 O      -4.349312    -0.557596    -2.866629     206.17
 H      -5.410818    -0.468080    -2.294854      21.52
 C      -4.898780    -2.250213    -4.857867      80.07
 O      -6.251346    -2.436044    -4.171275     242.00
 H      -6.631367    -2.626651    -5.211262      25.81
 H      -4.467378    -3.013543    -5.412626      27.91
 H      -4.959193    -1.329094    -5.646370      25.57
55
name = lig-ACN-frame_877
 C       3.885924    -0.971593     0.172644      52.98
 H       2.980711    -1.210596    -0.343233      21.85
 C       5.018429    -0.351586     2.281572      47.57
 H       4.914628     0.328974     3.328504      20.80
 C       6.266762    -0.985850     2.016156       6.56
 O       7.470495    -0.970422     2.735363     236.83
 C       7.330868    -1.280231     4.112002      91.29
 H       7.978238    -2.145538     4.295848      26.37
 H       6.097278    -1.427792     4.443597      23.06
 H       7.734809    -0.325598     4.756778      25.20
 C       6.359861    -1.626877     0.606951      -4.14
 O       7.423016    -2.216270     0.155089     178.69
 H       8.172237    -2.234289     0.742251      21.00
 C       5.070163    -1.734291    -0.117389      46.31
 H       5.010059    -2.552769    -0.983597      20.28
 C       3.885610    -0.350429     1.413976      41.24
 C       2.699074     0.404971     2.132949      92.27
 H       3.040731     1.347057     2.322014      28.11
 O       2.251406    -0.074424     3.549379     138.38
 H       1.912703    -1.221850     3.574383      21.78
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 C       1.471256     0.725782     1.332222      70.43
 H       1.852863     1.209705     0.224520      20.04
 C       0.376573     1.551815     1.949909     102.32
 O       0.852373     2.901676     2.049666     312.92
 H       0.821563     3.295434     1.131714      27.91
 H      -0.040786     1.272989     2.936272      24.83
 H      -0.526828     1.383366     1.256772      23.83
 C      -1.513810    -2.415655    -1.333161      54.90
 H      -2.284658    -3.109483    -1.254803      18.59
 C      -0.895674    -0.267484    -2.552506      33.37
 H      -0.807793     0.355092    -3.475137      20.02
 C       0.054895     0.083425    -1.432089     -14.81
 O       0.450180     1.423565    -1.315750     195.78
 C      -0.032186     2.345360    -2.277036     105.46
 H       0.290743     2.158086    -3.251959      26.47
 H      -1.129403     2.157233    -2.188718      26.15
 H      -0.043485     3.402207    -1.946218      25.82
 C       0.011554    -0.817356    -0.198357      -2.43
 O       0.706150    -0.528147     1.004870     102.44
 C      -0.778517    -1.985403    -0.141782      60.09
 H      -0.433858    -2.742781     0.575550      24.12
 C      -1.640272    -1.598539    -2.459678      19.92
 C      -2.513732    -1.976840    -3.649678      69.02
 H      -2.417529    -1.040423    -4.464020      23.50
 O      -2.341966    -3.235125    -4.169243     171.68
 H      -1.344806    -3.853618    -3.865637      23.09
 C      -4.093717    -1.959991    -3.429879      72.62
 H      -4.391791    -2.654094    -2.768510      27.45
 O      -4.383001    -0.514865    -2.906235     221.41
 H      -5.386065    -0.517641    -2.531051      24.06
 C      -4.888931    -2.238501    -4.827140      84.98
 O      -6.211645    -2.402103    -4.240120     259.78
 H      -7.260259    -2.449715    -4.586634      28.94
 H      -4.665183    -3.164013    -5.241365      27.51
 H      -4.889914    -1.317045    -5.531645      26.03
55
name = lig-ACN-frame_878
 C       3.915533    -1.136497     0.220493      45.07
 H       3.151876    -1.066881    -0.447494      23.67
 C       5.043424    -0.391097     2.369569      37.18
 H       5.106847     0.436814     3.264805      18.94
 C       6.275808    -0.964732     1.903182      -4.14
 O       7.502631    -1.080321     2.654345     237.56
 C       7.368044    -1.197684     4.221935      73.53
 H       7.890560    -2.163418     4.543823      25.49
 H       6.157191    -1.490320     4.522365      22.93
 H       7.809303    -0.270839     4.836044      24.38
 C       6.300856    -1.556212     0.691186      11.64
 O       7.447565    -2.295180     0.064098     179.90
 H       8.235231    -2.295229     0.660592      22.76
 C       5.193604    -1.688687    -0.127848      47.58
 H       5.371382    -2.242702    -1.146089      19.48
 C       3.867006    -0.330671     1.500947     -16.10
 C       2.632029     0.518665     2.169072      84.77
 H       2.918674     1.449040     2.548248      25.54
 O       2.383564    -0.145266     3.534899     155.53
 H       2.291017    -1.215821     3.414492      23.64
 C       1.403355     0.730269     1.233438      63.86
 H       1.643438     1.399262     0.146211      16.70
 C       0.436774     1.569774     1.983265     111.10
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 O       0.838764     2.890023     2.062547     268.05
 H       1.394690     3.239085     1.159681      24.75
 H       0.434122     1.167697     2.955802      25.03
 H      -0.579528     1.578699     1.435875      22.98
 C      -1.505349    -2.489768    -1.389079      65.22
 H      -1.792148    -3.460198    -1.395432      20.83
 C      -0.803122    -0.394213    -2.463515      47.99
 H      -0.800455     0.070607    -3.511956      17.46
 C      -0.151816     0.133848    -1.383639      15.93
 O       0.500581     1.420402    -1.330227     216.76
 C      -0.093964     2.391843    -2.345848     106.07
 H       0.219667     2.122901    -3.263257      26.76
 H      -1.219523     2.481582    -2.429192      24.97
 H       0.509628     3.317571    -2.131918      24.82
 C       0.007894    -0.760838    -0.230945       6.29
 O       0.662750    -0.599867     0.982430     118.42
 C      -0.787150    -2.012805    -0.259742      37.95
 H      -0.779556    -2.583199     0.628061      23.16
 C      -1.677632    -1.498936    -2.412289      37.57
 C      -2.655166    -1.871780    -3.574857      77.37
 H      -2.338256    -1.080135    -4.471701      22.88
 O      -2.366103    -3.198192    -4.183519     169.37
 H      -1.540397    -3.617709    -3.572507      24.14
 C      -4.109300    -1.942694    -3.419943     106.04
 H      -4.346708    -2.650074    -2.693969      27.90
 O      -4.414404    -0.603365    -3.005416     300.25
 H      -5.197876    -0.640006    -2.684829      31.20
 C      -4.921349    -2.224799    -4.640591     105.03
 O      -6.273386    -2.379318    -4.233912     323.18
 H      -6.647053    -2.074790    -5.072874      31.20
 H      -4.461514    -3.049762    -5.169141      28.93
 H      -4.716436    -1.434993    -5.398066      28.82
55
name = lig-ACN-frame_879
 C       4.002548    -1.117983     0.426285      63.98
 H       3.232772    -1.109797    -0.237877      22.42
 C       5.094329    -0.340020     2.327167      57.22
 H       5.054259     0.020957     3.429500      20.76
 C       6.320180    -0.971095     1.931421       7.83
 O       7.467853    -1.157445     2.712499     277.17
 C       7.384676    -1.168107     4.171299      92.23
 H       8.127989    -2.041225     4.560244      26.34
 H       6.211696    -1.145042     4.496500      24.58
 H       7.818977    -0.119076     4.469029      27.07
 C       6.385078    -1.698015     0.601358       0.29
 O       7.390729    -2.286503     0.043570     152.30
 H       8.132593    -2.520911     0.747219      21.54
 C       5.186801    -1.591031    -0.181961      51.76
 H       5.310938    -1.968863    -1.240333      19.86
 C       3.879774    -0.354449     1.611059      36.90
 C       2.714901     0.405364     2.168023     102.42
 H       3.008119     1.425843     2.179623      25.64
 O       2.476523    -0.140801     3.431555     269.15
 H       2.481760    -1.015105     3.391157      31.07
 C       1.345223     0.586128     1.202718      71.69
 H       1.987312     0.931083     0.103812      18.51
 C       0.350859     1.572851     2.028239      96.77
 O       0.881489     3.034084     2.140674     267.76
 H       1.380302     3.299880     1.247705      25.15
 H       0.355724     1.261483     2.991355      25.91
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 H      -0.784396     1.456358     1.842430      23.52
 C      -1.511172    -2.429957    -1.343833      56.09
 H      -1.893360    -3.376667    -1.415964      21.67
 C      -0.855263    -0.460888    -2.456546      53.96
 H      -0.953787     0.343441    -3.278422      17.31
 C      -0.249998     0.164107    -1.266154      13.24
 O       0.437921     1.395292    -1.421782     204.27
 C       0.013456     2.389508    -2.434272     107.29
 H       0.122854     2.118157    -3.390573      26.36
 H      -1.123201     2.790750    -2.206341      24.01
 H       0.481311     3.308065    -2.046459      24.53
 C      -0.120559    -0.781731    -0.212455      23.54
 O       0.693265    -0.617028     0.920036     152.89
 C      -0.675870    -2.017026    -0.338697      64.36
 H      -0.759133    -2.512557     0.543460      23.18
 C      -1.737925    -1.569599    -2.461233      40.12
 C      -2.565637    -1.834522    -3.652382      71.39
 H      -2.490940    -0.984084    -4.536199      24.41
 O      -2.311729    -3.208809    -4.173479     235.99
 H      -1.447125    -3.431859    -3.964412      30.41
 C      -4.121824    -1.890448    -3.281054      99.88
 H      -4.295990    -2.570240    -2.481969      26.61
 O      -4.509192    -0.555311    -3.028471     270.73
 H      -5.318545    -0.528705    -2.486086      26.33
 C      -4.834381    -2.297635    -4.551239      92.12
 O      -6.404049    -2.322767    -4.294964     278.17
 H      -6.886995    -2.220331    -5.096077      33.90
 H      -4.612208    -3.272953    -5.030134      26.78
 H      -4.808044    -1.384650    -5.149015      27.39
55
name = lig-ACN-frame_880
 C       3.984476    -1.011652     0.395873      50.86
 H       3.006879    -1.222422     0.063019      21.39
 C       5.248324    -0.322376     2.378381      62.73
 H       5.236139     0.115191     3.346071      24.14
 C       6.325790    -1.100511     1.915319      38.08
 O       7.427612    -1.248131     2.718737     247.39
 C       7.407929    -1.040147     4.096376     104.75
 H       8.139166    -1.941945     4.551839      24.69
 H       6.420636    -1.394819     4.654821      25.01
 H       7.797173    -0.058576     4.516954      25.56
 C       6.305356    -1.654706     0.615338      16.86
 O       7.463674    -2.346109     0.025191     211.86
 H       8.227484    -2.551605     0.682485      24.03
 C       5.163982    -1.520154    -0.161579      58.44
 H       4.922185    -1.966427    -1.082153      21.29
 C       4.038499    -0.432159     1.647569      24.23
 C       2.713657     0.274044     2.021597     109.21
 H       3.019940     1.278885     2.242006      25.85
 O       2.490096    -0.082662     3.436076     260.29
 H       2.275681    -0.933102     3.536312      30.78
 C       1.417972     0.545618     1.327367      72.23
 H       1.559767     1.309051     0.248511      16.99
 C       0.441747     1.656197     2.077305      98.33
 O       0.871254     3.038911     2.213350     299.17
 H       0.803214     3.428772     1.397252      30.88
 H       0.329776     1.331414     3.017123      25.65
 H      -0.459599     1.709279     1.357202      21.87
 C      -1.603748    -2.428212    -1.381880      61.34
 H      -2.295565    -3.205785    -1.108390      21.12
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 C      -1.061263    -0.284197    -2.439988      63.74
 H      -1.066114     0.291096    -3.412000      21.01
 C      -0.293461     0.136535    -1.388344      13.52
 O       0.354877     1.342667    -1.476442     235.07
 C       0.114091     2.400997    -2.422260      93.10
 H       0.322346     2.032641    -3.440999      24.27
 H      -1.088507     2.592768    -2.314246      23.34
 H       0.837339     3.197794    -2.318127      25.81
 C      -0.141690    -0.700679    -0.162035       8.35
 O       0.722584    -0.692087     0.912865     148.35
 C      -0.660116    -2.106176    -0.245518      28.82
 H      -0.154067    -2.847159     0.280108      22.06
 C      -1.631947    -1.583341    -2.491708      21.20
 C      -2.542349    -1.936214    -3.714450      63.75
 H      -2.320035    -1.038544    -4.497466      22.69
 O      -2.244090    -3.221349    -4.181725     245.03
 H      -1.317776    -3.296091    -4.344817      28.68
 C      -4.107115    -1.906700    -3.242564      58.95
 H      -4.165180    -2.481471    -2.262759      24.26
 O      -4.578455    -0.377648    -2.969203     177.29
 H      -5.500972    -0.470413    -2.314353      23.02
 C      -4.995184    -2.361825    -4.535503      89.68
 O      -6.434334    -2.267062    -4.327525     232.53
 H      -6.935222    -2.725733    -5.244114      27.85
 H      -4.578783    -3.414564    -4.798846      26.75
 H      -4.544341    -1.791651    -5.363924      28.05
55
name = lig-ACN-frame_881
 C       3.948439    -0.968009     0.324235      58.05
 H       3.004105    -1.039086    -0.313759      20.43
 C       5.282193    -0.359450     2.427879      64.83
 H       5.468846     0.336072     3.117362      24.06
 C       6.323969    -1.161519     1.931452      16.33
 O       7.494969    -1.363148     2.637768     203.97
 C       7.434451    -1.011037     4.166375      85.75
 H       8.472007    -1.583875     4.593360      23.50
 H       6.407203    -1.220907     4.492008      26.57
 H       7.574474     0.094581     4.242314      26.92
 C       6.355983    -1.653308     0.568536       1.30
 O       7.444145    -2.367977     0.034467     221.48
 H       8.128190    -2.346762     0.701436      25.44
 C       5.144982    -1.593135    -0.220241      52.37
 H       5.390989    -2.100373    -1.068624      20.17
 C       4.038566    -0.380078     1.624527      22.17
 C       2.809894     0.322431     2.147221     100.36
 H       3.143114     1.342592     2.127194      25.98
 O       2.422240    -0.033363     3.512615     223.91
 H       2.093877    -1.049484     3.463164      24.51
 C       1.483644     0.651270     1.331562      56.46
 H       1.907173     1.183661     0.182420      18.03
 C       0.505683     1.644546     2.076011     107.23
 O       0.904027     3.000917     2.282228     310.16
 H       0.584008     3.566334     1.515958      27.98
 H       0.012588     1.310919     2.948628      24.94
 H      -0.404366     1.552191     1.416365      23.04
 C      -1.581486    -2.398719    -1.274639      57.97
 H      -2.022165    -3.440735    -1.553188      23.52
 C      -1.244959    -0.213503    -2.499995      49.68
 H      -1.301753     0.406693    -3.385395      20.62
 C      -0.330556     0.115424    -1.399416      -3.90
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 O       0.383585     1.326915    -1.397401     192.30
 C       0.165157     2.312955    -2.473137     101.45
 H       0.458699     1.958947    -3.511312      24.49
 H      -0.789283     3.099494    -2.606295      24.04
 H       0.800401     3.028510    -1.990065      25.06
 C      -0.158390    -0.825139    -0.277398       7.41
 O       0.779399    -0.667360     0.968598      75.05
 C      -0.737718    -2.058158    -0.321230      56.95
 H      -0.394075    -2.791185     0.419046      20.25
 C      -1.678069    -1.552765    -2.485248      36.18
 C      -2.589830    -1.914910    -3.624412      76.41
 H      -2.460545    -1.279754    -4.586039      21.27
 O      -2.232555    -3.301064    -4.266439     151.34
 H      -1.118598    -3.292758    -3.959232      20.36
 C      -4.178292    -1.728968    -3.372847      72.47
 H      -4.469060    -2.478656    -2.472924      23.56
 O      -4.487082    -0.392458    -2.964370     245.42
 H      -5.428236    -0.261538    -2.294551      22.22
 C      -5.019751    -2.436699    -4.444294      93.89
 O      -6.446025    -2.240933    -4.364112     198.08
 H      -6.725309    -2.834448    -5.295201      27.45
 H      -4.939245    -3.591632    -4.353366      24.58
 H      -4.808277    -2.029750    -5.483172      24.70
55
name = lig-ACN-frame_882
 C       4.052474    -0.991208     0.287180      37.36
 H       3.130345    -0.680411    -0.393923      20.49
 C       5.181885    -0.423023     2.309020      47.70
 H       5.153823     0.041799     3.203415      22.38
 C       6.378455    -1.155180     1.911430      39.38
 O       7.601812    -1.457917     2.683780     301.62
 C       7.468748    -0.969822     4.028085     134.73
 H       8.471513    -1.317690     4.736502      24.65
 H       6.732303    -1.492509     4.583302      27.98
 H       7.373540     0.097482     4.089076      29.04
 C       6.332775    -1.711801     0.560764      29.74
 O       7.398992    -2.349074     0.071709     183.38
 H       8.160002    -2.456389     0.676436      21.53
 C       5.211586    -1.674541    -0.254008      43.52
 H       5.023770    -1.949468    -1.217449      19.08
 C       3.978349    -0.341991     1.552640      19.12
 C       2.830708     0.546767     2.330278      84.95
 H       3.208063     1.485299     2.740901      22.92
 O       2.356703     0.003463     3.588226     176.80
 H       2.185887    -1.175707     3.456578      20.53
 C       1.582663     0.678282     1.292425      58.80
 H       2.054085     1.205503     0.184173      18.92
 C       0.440126     1.544718     1.974176      96.98
 O       0.963965     2.968174     2.365084     211.00
 H       0.885229     3.467314     1.363723      24.85
 H       0.537172     1.023406     2.960652      21.64
 H      -0.467705     1.687866     1.420811      23.24
 C      -1.609562    -2.419450    -1.490647      51.81
 H      -1.660793    -3.620577    -1.440857      19.21
 C      -1.222386    -0.240413    -2.416417      60.48
 H      -1.569042     0.516410    -3.041525      20.41
 C      -0.371507     0.135237    -1.380641      10.00
 O       0.346160     1.294534    -1.314723     219.42
 C       0.311054     2.299651    -2.460279      74.25
 H       0.656442     1.723336    -3.464271      23.40
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 H      -0.908003     2.329942    -2.479054      21.16
 H       0.997450     3.127289    -2.357516      25.18
 C       0.018461    -0.774118    -0.284712      -0.18
 O       0.762968    -0.568156     0.899701     135.97
 C      -0.743199    -2.033062    -0.254133      33.41
 H      -0.979322    -2.536202     0.745483      20.00
 C      -1.935107    -1.513251    -2.430556      32.73
 C      -2.706816    -1.926260    -3.693749      64.77
 H      -2.397300    -1.082866    -4.350686      26.14
 O      -2.245452    -3.283029    -4.265507     149.15
 H      -1.549885    -3.984117    -3.617083      22.70
 C      -4.247031    -1.771424    -3.357195      73.21
 H      -4.450576    -2.303910    -2.284866      22.74
 O      -4.330717    -0.375080    -3.032292     170.40
 H      -5.437016    -0.485311    -2.505090      20.60
 C      -5.001850    -2.480284    -4.495044      83.55
 O      -6.511955    -2.226938    -4.373184     292.17
 H      -7.021215    -2.436488    -5.153342      32.03
 H      -4.518813    -3.530052    -4.202300      26.41
 H      -4.542866    -2.375068    -5.493262      27.73
55
name = lig-ACN-frame_883
 C       4.038707    -0.889678     0.241615      55.76
 H       3.201351    -0.971560    -0.615490      19.69
 C       5.202500    -0.525119     2.319230      51.93
 H       5.088968    -0.407695     3.364444      20.74
 C       6.382557    -1.162597     1.857816      23.46
 O       7.552936    -1.478184     2.643406     299.89
 C       7.519352    -0.957640     3.978254     106.94
 H       8.726334    -0.970984     4.264877      24.40
 H       6.844293    -1.515211     4.551719      28.84
 H       7.165522     0.047061     3.988383      29.58
 C       6.342285    -1.797450     0.630603      -5.05
 O       7.467028    -2.399385     0.055060     190.52
 H       8.131576    -2.595323     0.837713      25.10
 C       5.136603    -1.633555    -0.210040      52.66
 H       5.370689    -2.125002    -1.149028      18.49
 C       3.995533    -0.281248     1.566518      24.51
 C       2.766043     0.552063     2.285950      82.16
 H       3.093929     1.651013     2.390677      23.34
 O       2.309086     0.008149     3.633076     152.28
 H       2.197903    -1.202439     3.560847      19.86
 C       1.568654     0.815231     1.249786      61.76
 H       1.990988     1.401295     0.193105      18.48
 C       0.542993     1.570715     1.950785     113.35
 O       0.971375     2.847066     2.363674     292.70
 H       1.521037     3.316217     1.684317      29.97
 H       0.051913     1.052571     2.910090      23.08
 H      -0.356968     1.523406     1.436599      25.62
 C      -1.479037    -2.451363    -1.421890      53.65
 H      -2.286398    -3.375680    -1.405977      20.48
 C      -1.291078    -0.266079    -2.288944      38.31
 H      -1.429758     0.416678    -3.081980      20.82
 C      -0.269939     0.093038    -1.299568       5.51
 O       0.375881     1.371789    -1.259144     220.86
 C       0.357748     2.112899    -2.431937      91.06
 H       0.891603     1.496672    -3.368001      22.65
 H      -0.631469     2.726899    -2.896777      22.46
 H       0.878570     3.040163    -2.063750      24.07
 C       0.016984    -0.796303    -0.257707      19.71
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 O       0.826504    -0.471014     0.839983     151.32
 C      -0.799826    -1.933525    -0.323151      51.03
 H      -0.628688    -2.675967     0.586354      22.15
 C      -1.994446    -1.475851    -2.426952      22.28
 C      -2.731796    -1.956380    -3.732200      91.99
 H      -2.739271    -1.418463    -4.661238      25.55
 O      -2.339106    -3.196544    -4.225238     214.58
 H      -2.029281    -3.620038    -3.334081      27.71
 C      -4.190195    -1.923491    -3.348350      63.19
 H      -4.485609    -2.587913    -2.340862      23.45
 O      -4.282177    -0.349027    -3.134645     148.55
 H      -5.242549     0.194704    -2.703401      22.57
 C      -5.077730    -2.509331    -4.522484      91.80
 O      -6.471851    -2.226920    -4.370592     291.05
 H      -6.706636    -2.343056    -5.240382      33.09
 H      -5.174249    -3.694650    -4.612152      24.28
 H      -4.738680    -2.068095    -5.504820      26.79
55
name = lig-ACN-frame_884
 C       3.972011    -0.762886     0.248266      31.36
 H       2.911341    -0.626942    -0.236877      19.08
 C       5.188272    -0.608860     2.437465      47.84
 H       5.312082    -0.142074     3.498198      17.99
 C       6.321570    -1.240729     1.883297      33.35
 O       7.445991    -1.451678     2.544049     253.39
 C       7.573569    -0.919503     3.956844     111.12
 H       8.761252    -0.829469     4.197128      25.64
 H       7.242204    -1.528156     4.691622      30.08
 H       7.151940     0.045224     4.012339      31.17
 C       6.377479    -1.834411     0.546923       4.57
 O       7.490758    -2.476173     0.061064     177.23
 H       8.206495    -2.620240     0.768205      21.69
 C       5.226919    -1.624270    -0.140819      59.46
 H       5.005981    -2.107796    -1.144857      21.19
 C       4.014514    -0.287187     1.557914      13.75
 C       2.738664     0.378539     2.100902      98.31
 H       3.193164     1.400934     2.503333      22.25
 O       2.310515     0.051852     3.534348     199.13
 H       2.066216    -1.047064     3.440435      22.33
 C       1.542760     0.773160     1.235245      74.39
 H       1.956687     1.491040     0.278178      19.44
 C       0.431175     1.629797     1.930330     100.05
 O       1.023292     2.844731     2.406133     308.22
 H       1.645668     3.046462     1.786000      33.97
 H       0.101511     0.991792     2.918012      21.56
 H      -0.199071     1.916371     1.164876      24.69
 C      -1.614271    -2.356118    -1.360232      48.52
 H      -2.073540    -3.412310    -0.998468      21.25
 C      -1.270618    -0.163544    -2.253974      73.79
 H      -1.331304     0.527987    -3.096384      21.09
 C      -0.266242     0.130708    -1.319420      14.71
 O       0.328498     1.334670    -1.194876     224.81
 C       0.465957     2.092162    -2.476990      77.26
 H       1.100286     1.410874    -3.363681      23.39
 H      -0.659236     2.343949    -2.841242      21.70
 H       1.227381     2.933250    -2.311605      24.32
 C      -0.043781    -0.722050    -0.208482       8.01
 O       0.943650    -0.480239     0.810828     163.25
 C      -0.684345    -2.013591    -0.276188      38.15
 H      -0.314496    -2.896205     0.414984      20.11
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 C      -1.745344    -1.516843    -2.436220      29.37
 C      -2.759525    -1.877309    -3.663424      75.71
 H      -2.496494    -1.065385    -4.280895      24.84
 O      -2.396494    -3.222734    -4.156337     277.63
 H      -1.958814    -3.725996    -3.632781      34.00
 C      -4.278596    -1.924827    -3.396891      78.67
 H      -4.481626    -2.388401    -2.247578      23.30
 O      -4.284594    -0.434303    -3.271593     257.16
 H      -5.221346    -0.399373    -2.901844      25.72
 C      -5.105978    -2.474941    -4.550936      84.85
 O      -6.509295    -2.188085    -4.349835     243.19
 H      -7.081035    -2.436557    -5.260253      27.79
 H      -4.632860    -3.551001    -4.858060      24.49
 H      -4.688862    -1.860165    -5.371432      27.17
55
name = lig-ACN-frame_885
 C       4.157273    -0.815969     0.305362      67.63
 H       3.367905    -0.692417    -0.452778      21.24
 C       5.078919    -0.609531     2.420413      48.34
 H       5.139526     0.035433     3.456398      19.51
 C       6.198472    -1.330210     1.903778       8.82
 O       7.466470    -1.418477     2.610728     290.00
 C       7.667135    -0.890847     3.884877     116.94
 H       8.800422    -0.763440     3.886984      25.45
 H       7.350579    -1.632337     4.535963      28.21
 H       7.176248     0.016087     4.148156      31.16
 C       6.319241    -1.769574     0.540387      -9.07
 O       7.465733    -2.552911     0.064984     229.07
 H       8.135363    -2.544900     0.744412      26.90
 C       5.063748    -1.552486    -0.269682      52.72
 H       5.057419    -2.020472    -1.352296      20.49
 C       3.998958    -0.400902     1.657471      46.82
 C       2.795012     0.411746     2.131484      95.14
 H       3.172802     1.576266     2.144166      21.67
 O       2.323641     0.017756     3.358115     307.48
 H       2.015397    -0.830096     3.439978      29.83
 C       1.495742     0.665468     1.213919      76.11
 H       1.909983     1.263056     0.227463      19.01
 C       0.383065     1.660813     1.849242      87.59
 O       1.098052     2.909642     2.496054     210.30
 H       1.649569     3.360050     1.676957      26.86
 H      -0.252595     1.122215     2.725510      23.29
 H      -0.467879     1.881927     1.283308      24.38
 C      -1.601134    -2.313245    -1.174008      39.93
 H      -1.934111    -3.352193    -1.595142      22.33
 C      -1.154662    -0.183436    -2.401022      35.32
 H      -1.577313     0.597400    -3.105163      19.17
 C      -0.381246     0.181175    -1.245101      -6.31
 O       0.341309     1.389330    -1.221113     193.35
 C       0.603564     2.054924    -2.491801      71.87
 H       0.932075     1.114589    -3.321631      22.46
 H      -0.383709     2.474405    -2.922537      23.24
 H       1.165113     3.057588    -2.299367      23.88
 C      -0.049001    -0.747327    -0.139590      14.30
 O       1.000334    -0.604188     0.720234     165.95
 C      -0.523557    -2.059808    -0.222322      44.06
 H      -0.340862    -2.730455     0.691499      20.02
 C      -1.715408    -1.491397    -2.398798      19.08
 C      -2.607477    -1.934108    -3.506295      92.28
 H      -2.509924    -1.377353    -4.374755      24.99
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 O      -2.423158    -3.277176    -4.155486     205.91
 H      -1.430905    -3.464445    -3.818602      25.60
 C      -4.214959    -1.801452    -3.392076      74.25
 H      -4.724658    -2.426258    -2.416984      22.57
 O      -4.494726    -0.472985    -3.362526     304.04
 H      -5.178408    -0.210499    -3.015520      33.61
 C      -5.014316    -2.329243    -4.651730      80.07
 O      -6.573946    -2.184437    -4.303033     182.99
 H      -6.929343    -2.736206    -5.221600      27.53
 H      -4.978362    -3.541803    -4.605177      23.31
 H      -4.757103    -1.840777    -5.601985      26.21
55
name = lig-ACN-frame_886
 C       4.031221    -0.850091     0.242610      33.08
 H       3.258852    -0.492156    -0.342359      22.37
 C       5.124434    -0.637999     2.460581      59.81
 H       5.093572    -0.376582     3.664573      21.11
 C       6.219281    -1.330986     1.955831      20.21
 O       7.441675    -1.412965     2.542469     267.59
 C       7.749895    -0.891557     3.917625     124.23
 H       8.799175    -0.717508     3.975074      26.67
 H       7.436744    -1.487679     4.698287      29.56
 H       7.251808     0.065495     3.998792      31.14
 C       6.243552    -1.840467     0.539572      32.93
 O       7.303875    -2.525084     0.102777     188.74
 H       7.992608    -2.525381     0.811981      22.28
 C       5.274108    -1.598012    -0.357329      54.90
 H       5.277488    -1.721121    -1.518571      18.92
 C       3.894104    -0.460746     1.587733      20.10
 C       2.745121     0.545313     2.063396      93.28
 H       3.213117     1.649987     2.403638      20.73
 O       2.318238    -0.030818     3.370617     273.94
 H       2.209162    -0.870950     3.153179      31.12
 C       1.519386     0.678793     1.136977      81.06
 H       1.841184     1.213515     0.155734      19.67
 C       0.481603     1.716814     1.853129      99.67
 O       1.097303     2.861179     2.470094     235.86
 H       1.247523     3.582048     1.683684      27.01
 H       0.002678     1.294016     2.795868      22.30
 H      -0.049106     2.082856     1.006136      22.59
 C      -1.407688    -2.370506    -1.225668      54.97
 H      -1.939751    -3.325939    -0.970878      21.07
 C      -1.085792    -0.259575    -2.383613      62.97
 H      -1.176751     0.391920    -3.339411      19.52
 C      -0.400422     0.223183    -1.213641       2.93
 O       0.339405     1.460334    -1.236190     236.40
 C       0.632313     2.026184    -2.514512      87.65
 H       1.305237     1.284474    -3.359994      23.00
 H      -0.102175     2.627458    -3.008313      24.12
 H       1.633190     2.537163    -2.213694      24.15
 C      -0.013764    -0.762365    -0.244177       7.19
 O       1.041439    -0.707363     0.710291     148.32
 C      -0.591955    -2.046882    -0.170612      45.52
 H      -0.241796    -2.754043     0.562058      22.17
 C      -1.792610    -1.479944    -2.222959      31.24
 C      -2.604394    -1.986531    -3.581986      77.14
 H      -2.227422    -1.216498    -4.170280      27.01
 O      -2.354095    -3.346121    -4.035111     144.07
 H      -1.338466    -3.515822    -4.585233      24.68
 C      -4.188607    -1.815126    -3.445466      68.68
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 H      -4.578125    -2.446573    -2.432842      22.82
 O      -4.681501    -0.267135    -3.400471     176.72
 H      -5.463084    -0.529429    -2.793004      23.60
 C      -5.011625    -2.320920    -4.629708      90.72
 O      -6.514720    -2.187270    -4.311744     270.65
 H      -6.889722    -2.759354    -4.977174      32.40
 H      -4.786211    -3.450989    -4.966478      24.59
 H      -4.928449    -1.694011    -5.509989      26.94
55
name = lig-ACN-frame_887
 C       3.978362    -0.910742     0.097510      61.92
 H       3.272488    -0.729673    -0.578349      22.88
 C       5.011222    -0.720183     2.419906      43.29
 H       4.990957    -0.386827     3.570709      19.63
 C       6.216526    -1.287898     1.915797      13.65
 O       7.493141    -1.455303     2.533747     280.22
 C       7.755117    -0.860865     3.886748     121.30
 H       8.762976    -0.939746     3.897832      26.95
 H       7.407840    -1.572405     4.620121      29.88
 H       7.335049     0.134938     4.043874      31.84
 C       6.157708    -1.851099     0.663516       3.58
 O       7.287061    -2.556759     0.131430     208.54
 H       8.067278    -2.669284     0.811705      22.15
 C       5.158955    -1.448733    -0.295801      60.20
 H       5.519623    -1.802303    -1.291147      19.23
 C       3.959613    -0.405838     1.490023      18.96
 C       2.770328     0.440031     2.040386      79.30
 H       3.212552     1.596288     2.304878      20.47
 O       2.301542    -0.053895     3.402597     238.49
 H       2.033893    -1.038609     3.417942      23.70
 C       1.617974     0.768576     1.104297      86.55
 H       1.971175     1.252633     0.182326      21.06
 C       0.562941     1.682050     1.771334     111.34
 O       1.137448     2.857321     2.402783     321.31
 H       0.989428     3.522125     1.825988      32.47
 H      -0.068381     1.035691     2.365419      24.51
 H      -0.308792     1.955965     1.123852      23.09
 C      -1.426080    -2.541962    -1.251766      33.86
 H      -1.998241    -3.431184    -1.153588      20.95
 C      -1.117481    -0.323438    -2.235148      47.30
 H      -0.939350     0.145147    -3.258466      20.35
 C      -0.248336     0.208771    -1.275464      10.72
 O       0.254668     1.453053    -1.257965     248.75
 C       0.842852     2.054340    -2.549245      77.74
 H       0.699454     1.025275    -3.298702      20.49
 H       0.059396     2.614777    -2.888604      25.53
 H       1.646002     2.829017    -2.409876      23.70
 C       0.109709    -0.738378    -0.228612       8.25
 O       1.054686    -0.616986     0.753407     158.85
 C      -0.596497    -1.979087    -0.183982      50.24
 H      -0.246576    -2.618078     0.553029      23.22
 C      -1.848613    -1.582700    -2.293227      20.85
 C      -2.608001    -1.888601    -3.590854      83.64
 H      -2.279616    -1.452492    -4.488026      25.80
 O      -2.292092    -3.394607    -3.895961     142.64
 H      -1.536294    -3.199029    -4.588784      25.98
 C      -4.223384    -1.712250    -3.530943      66.48
 H      -4.424647    -2.078490    -2.391282      22.12
 O      -4.760268    -0.232807    -3.370310     125.15
 H      -5.708802    -0.204175    -2.602080      20.87
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 C      -5.038844    -2.326143    -4.654676     103.18
 O      -6.400380    -2.241384    -4.311054     325.87
 H      -6.875232    -2.625673    -4.964646      34.04
 H      -4.575522    -3.351510    -4.889698      25.11
 H      -4.724236    -1.623585    -5.434199      27.23
55
name = lig-ACN-frame_888
 C       3.937062    -0.810413     0.103045      59.68
 H       3.193585    -0.788874    -0.608904      22.05
 C       4.950664    -0.733907     2.324744      53.78
 H       4.743907    -0.155140     3.266279      20.10
 C       6.217740    -1.280100     1.981186      19.80
 O       7.468097    -1.461814     2.562364     336.71
 C       7.743554    -0.920306     3.819159     123.19
 H       8.762037    -0.894692     3.986440      25.57
 H       7.052880    -1.382836     4.567167      30.05
 H       7.446858     0.146466     3.868152      31.77
 C       6.208046    -1.820673     0.627696       3.92
 O       7.280001    -2.604204     0.145836     223.50
 H       7.915704    -2.570215     0.902941      23.61
 C       5.157634    -1.497819    -0.262059      54.39
 H       5.101694    -1.892944    -1.233162      21.52
 C       3.917573    -0.404122     1.397879      31.82
 C       2.825562     0.310354     2.130944      97.52
 H       3.380470     1.403679     2.421782      19.97
 O       2.304459    -0.038359     3.392469     267.58
 H       1.932050    -1.072512     3.149868      20.88
 C       1.716090     0.771744     1.075376      92.93
 H       2.126462     1.162208     0.233805      23.52
 C       0.536244     1.590132     1.668294      99.43
 O       1.161757     2.845753     2.339986     262.86
 H       1.007849     3.626116     1.711578      28.54
 H       0.323477     1.148174     2.536004      23.89
 H      -0.190421     1.852078     0.815811      20.64
 C      -1.544832    -2.501570    -1.240725      52.10
 H      -1.632836    -3.461426    -1.375988      25.59
 C      -1.179477    -0.379305    -2.263236      33.03
 H      -1.641021     0.432037    -2.894131      20.46
 C      -0.120965     0.049083    -1.301218      -4.28
 O       0.264584     1.523609    -1.332753     219.09
 C       0.822077     2.035933    -2.553553      95.21
 H       1.357767     1.262736    -3.488998      22.92
 H       0.310905     2.786532    -3.009215      25.94
 H       1.846339     2.290574    -2.222636      24.42
 C       0.144207    -0.737775    -0.199076      12.17
 O       1.052029    -0.433314     0.812224     191.70
 C      -0.552168    -2.044012    -0.283426      44.62
 H      -0.503876    -2.568211     0.616796      21.94
 C      -1.713182    -1.631580    -2.351096      23.82
 C      -2.648830    -1.876505    -3.585625      82.75
 H      -2.278756    -1.192523    -4.327300      25.69
 O      -2.308892    -3.342866    -3.776777     237.46
 H      -1.557984    -3.470260    -4.160949      32.38
 C      -4.267078    -1.550802    -3.415992      74.07
 H      -4.734098    -2.332989    -2.643166      22.67
 O      -4.714679    -0.276939    -3.359661     196.99
 H      -5.598629    -0.269762    -2.467008      18.88
 C      -4.891429    -2.272553    -4.705541      99.77
 O      -6.365316    -2.320888    -4.290313     233.22
 H      -6.713178    -2.602230    -5.291133      27.89
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 H      -4.681724    -3.360076    -4.738456      25.02
 H      -4.927898    -1.994796    -5.731981      25.54
55
name = lig-ACN-frame_889
 C       4.015633    -0.792669     0.058707      37.16
 H       3.124568    -0.483415    -0.540219      20.24
 C       5.040681    -0.629677     2.338186      53.23
 H       5.057030    -0.389613     3.361377      21.52
 C       6.180353    -1.333568     1.878492       5.67
 O       7.382795    -1.498065     2.542525     276.03
 C       7.661512    -0.878321     3.859780     104.86
 H       8.682741    -1.255312     4.078359      25.56
 H       7.094722    -1.297842     4.770460      28.74
 H       7.528601     0.195114     3.719109      31.31
 C       6.250339    -1.764678     0.532829      12.13
 O       7.274740    -2.634681     0.182408     227.72
 H       8.031932    -2.666264     0.737768      24.80
 C       5.138442    -1.636624    -0.336717      58.93
 H       5.266860    -2.077521    -1.252833      22.45
 C       3.838789    -0.495971     1.534880      19.65
 C       2.811525     0.507411     2.104034      82.61
 H       3.396065     1.528853     2.476140      19.53
 O       2.304800    -0.103561     3.370977     206.43
 H       1.903170    -1.230555     3.327602      19.47
 C       1.737704     0.803550     1.111064      92.03
 H       2.098074     1.199094     0.315199      24.90
 C       0.692134     1.666707     1.713118     119.94
 O       1.115335     2.833859     2.218485     268.32
 H       1.304430     3.548212     1.394797      25.67
 H       0.085032     1.137316     2.278710      26.57
 H      -0.186904     1.834471     0.954210      21.85
 C      -1.407573    -2.397323    -1.256424      53.16
 H      -1.969655    -3.223499    -1.125499      24.28
 C      -1.137388    -0.225830    -2.287893      26.95
 H      -1.674555     0.598483    -2.722764      21.30
 C      -0.149733     0.113555    -1.446515      11.86
 O       0.218114     1.411616    -1.428008     219.78
 C       0.969790     2.027331    -2.557940      71.71
 H       0.884251     1.034622    -3.425882      21.53
 H       0.386227     2.830336    -2.947936      24.74
 H       1.843569     2.528019    -2.205058      25.07
 C       0.141069    -0.806864    -0.258698       0.59
 O       0.958994    -0.505407     0.815291     115.81
 C      -0.512075    -2.086926    -0.215393      49.81
 H      -0.277708    -2.895959     0.480980      20.30
 C      -1.697528    -1.553596    -2.366757      36.78
 C      -2.620034    -1.880096    -3.439443     100.45
 H      -2.344723    -1.371126    -4.388783      24.77
 O      -2.457251    -3.283105    -3.744134     184.84
 H      -1.452256    -3.380147    -3.490354      25.75
 C      -4.225284    -1.718828    -3.473995      70.36
 H      -4.604309    -2.209553    -2.475898      23.34
 O      -4.615085    -0.232978    -3.279754     185.30
 H      -5.510655    -0.271752    -2.522094      21.62
 C      -4.861666    -2.334065    -4.670441      99.34
 O      -6.331411    -2.376874    -4.327679     227.25
 H      -6.919407    -2.953371    -5.108625      26.62
 H      -4.234792    -3.194294    -4.726282      25.61
 H      -4.530974    -1.671741    -5.433179      27.63
55
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name = lig-ACN-frame_890
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name = lig-ACN-frame_891
 C       4.026515    -0.943849     0.248065      38.03
 H       2.931275    -0.710519    -0.188202      18.21
 C       5.100378    -0.594888     2.372217      55.59
 H       5.168819    -0.120849     3.258691      19.03
 C       6.275138    -1.259905     1.816961       6.66
 O       7.294219    -1.614731     2.612514     283.01
 C       7.482840    -0.892142     3.812504      88.63
 H       8.417328    -1.371638     4.461137      23.61
 H       6.607799    -1.025280     4.649291      28.03
 H       7.499009     0.137277     3.435928      29.06
 C       6.218804    -1.975284     0.449497      11.57
 O       7.338295    -2.669212     0.086669     207.17
 H       8.126721    -2.711495     0.760569      24.14
 C       5.170999    -1.655448    -0.361395      64.24
 H       4.947357    -1.956289    -1.402907      21.29
 C       4.081659    -0.256451     1.444040      22.03
 C       2.794328     0.389207     2.042851      88.42
 H       3.240813     1.403155     2.393401      20.33
 O       2.334366    -0.107669     3.296125     261.22
 H       1.849795    -1.042698     3.549726      22.69
 C       1.568350     0.633494     1.074533     103.46
 H       1.951063     1.005359     0.277122      23.10
 C       0.474017     1.799951     1.638489      87.93
 O       1.185980     3.148206     2.076013     299.80
 H       1.513167     3.556658     1.319493      30.88
 H      -0.011539     1.466282     2.579983      23.75
 H      -0.520248     1.902489     1.128012      22.50
 C      -1.410609    -2.300720    -1.271611      51.92
 H      -1.519594    -3.407791    -1.237397      23.85
 C      -1.105218    -0.159303    -2.407554      40.13
 H      -1.119503     0.454832    -3.272239      21.25
 C      -0.211858     0.253463    -1.420456       1.02
 O       0.408458     1.497298    -1.388704     226.14
 C       0.981757     1.971994    -2.632558      80.20
 H       1.220004     0.941903    -3.435751      22.24
 H       0.526298     2.873526    -3.237509      22.34
 H       1.833440     2.438813    -2.217971      25.01
 C       0.208040    -0.724252    -0.323233      14.80
 O       0.989484    -0.565888     0.801552     187.24
 C      -0.396012    -1.981190    -0.369541      49.63
 H      -0.434335    -2.760950     0.524278      18.86
 C      -1.860006    -1.423477    -2.290745      37.59
 C      -2.619236    -1.919695    -3.416482      88.47
 H      -2.441184    -1.432177    -4.460824      25.73
 O      -2.581774    -3.378549    -3.719190     177.26
 H      -1.988327    -3.800871    -2.976546      27.20
 C      -4.168142    -1.727570    -3.227509      82.47
 H      -4.515154    -2.236404    -2.315526      25.63
 O      -4.349345    -0.379627    -3.105699     287.06
 H      -5.150834    -0.251509    -2.950851      33.67
 C      -4.832826    -2.374639    -4.603942      79.86
 O      -6.329489    -2.564628    -4.396213     322.94
 H      -6.688166    -2.974031    -5.103217      33.66
 H      -4.224755    -3.144156    -4.481803      27.05
 H      -4.416057    -1.700722    -5.370402      28.15
55
name = lig-ACN-frame_892
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 C       3.992426    -0.946609     0.163666      55.16
 H       3.094212    -1.282457    -0.538351      19.42
 C       5.216862    -0.477621     2.231801      23.25
 H       5.193068    -0.091275     3.247312      12.64
 C       6.220997    -1.371286     1.837129       4.35
 O       7.367644    -1.741872     2.627906     303.67
 C       7.389887    -0.880417     3.822488      86.57
 H       8.490452    -1.229259     4.341677      24.57
 H       6.339795    -0.999734     4.449070      27.09
 H       7.635737     0.219486     3.741059      29.60
 C       6.271197    -1.918958     0.601501     -15.67
 O       7.381675    -2.687231    -0.000778     293.04
 H       8.025030    -2.736751     0.740834      30.48
 C       5.086582    -1.635971    -0.266911      63.72
 H       5.299769    -2.296029    -1.185207      19.72
 C       4.009688    -0.262505     1.450362      35.70
 C       2.740476     0.438119     2.004030     111.60
 H       2.965668     1.534786     2.228593      22.34
 O       2.364573    -0.120362     3.341464     259.50
 H       2.036996    -0.935662     2.925428      25.49
 C       1.578455     0.836239     1.111030      82.66
 H       1.960772     1.240553     0.305959      23.01
 C       0.558072     1.918918     1.722700     103.61
 O       1.138268     3.123201     1.950939     304.38
 H       1.233463     3.634379     1.040213      26.02
 H       0.195249     1.515681     2.747113      21.91
 H      -0.094363     2.103411     0.883915      20.58
 C      -1.490517    -2.293137    -1.285678      55.65
 H      -2.050801    -3.354134    -1.350880      22.13
 C      -1.070181    -0.244988    -2.382979      53.88
 H      -1.590039     0.440908    -3.059599      20.69
 C      -0.148709     0.298285    -1.323342       9.13
 O       0.508595     1.570526    -1.360866     241.64
 C       1.052932     2.012016    -2.678801      68.78
 H       1.260441     0.895564    -3.333470      23.80
 H       0.054035     2.388959    -3.189996      21.45
 H       2.021959     2.548233    -2.741089      24.53
 C       0.093769    -0.618348    -0.325719      15.37
 O       0.989389    -0.566504     0.760953     141.27
 C      -0.462843    -1.929059    -0.445854      48.63
 H       0.187363    -2.685531     0.225725      18.80
 C      -1.735008    -1.468718    -2.373318      25.40
 C      -2.728746    -2.068566    -3.465502      91.22
 H      -2.241727    -1.444673    -4.369826      25.01
 O      -2.502055    -3.465997    -3.670375     255.90
 H      -1.858319    -3.759395    -3.206958      33.65
 C      -4.215395    -1.802230    -3.278926     102.82
 H      -4.557693    -2.414121    -2.505239      26.87
 O      -4.280771    -0.316574    -3.008042     238.93
 H      -5.275227    -0.146628    -2.688429      24.69
 C      -4.834338    -2.375901    -4.430820     115.40
 O      -6.314638    -2.606162    -4.363810     272.30
 H      -6.400728    -2.912471    -5.301370      29.18
 H      -4.645742    -3.315492    -4.787852      24.13
 H      -4.778349    -1.858684    -5.423082      24.80
55
name = lig-ACN-frame_893
 C       3.973558    -0.964021     0.122734      42.92
 H       3.088877    -0.751858    -0.569198      19.59
 C       5.217626    -0.369842     2.097156      47.98
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 H       5.226315     0.259244     3.095524      17.31
 C       6.260719    -1.448435     1.931330      -5.29
 O       7.354064    -1.747428     2.685813     280.47
 C       7.427742    -0.909382     3.876237      67.64
 H       8.280947    -1.378185     4.702626      22.65
 H       6.403190    -1.150736     4.549949      27.65
 H       7.380654     0.150592     3.446005      29.29
 C       6.323905    -1.893748     0.500287      16.58
 O       7.302730    -2.631731     0.003640     210.53
 H       8.095497    -2.657620     0.520101      25.12
 C       5.187869    -1.786385    -0.188027      60.33
 H       4.949054    -2.200413    -1.222864      21.08
 C       3.913760    -0.379568     1.369670      12.18
 C       2.822305     0.662112     2.111479      78.93
 H       3.410183     1.498239     2.474374      21.33
 O       2.362094    -0.161452     3.286150     273.71
 H       2.144075    -0.971086     3.156959      30.78
 C       1.636754     0.932154     1.129680      80.82
 H       1.956698     1.385052     0.256543      19.99
 C       0.589810     1.826970     1.692415      99.83
 O       1.147925     3.196270     1.904224     266.97
 H       1.403740     3.686767     0.890111      22.62
 H       0.060409     1.565987     2.746269      21.60
 H      -0.337126     1.742236     1.165054      23.08
 C      -1.460792    -2.375495    -1.317268      43.97
 H      -2.219413    -3.241226    -0.883724      18.54
 C      -1.079978    -0.130734    -2.368828      39.88
 H      -1.267837     0.669160    -3.165532      19.61
 C      -0.188527     0.268480    -1.402396      -5.13
 O       0.611675     1.626825    -1.372987     181.44
 C       0.997357     1.929629    -2.756752      90.11
 H       1.599307     1.002790    -3.386526      22.97
 H       0.197183     2.510982    -3.466691      22.45
 H       1.612087     2.879921    -2.493142      23.61
 C       0.034624    -0.617381    -0.260489      16.68
 O       0.950376    -0.422320     0.702977     148.01
 C      -0.496785    -1.920505    -0.350680      55.83
 H       0.033124    -2.709179     0.345897      19.08
 C      -1.668050    -1.510140    -2.418992      25.60
 C      -2.644566    -2.076148    -3.529259      69.66
 H      -2.623732    -1.634350    -4.675662      23.28
 O      -2.420401    -3.601881    -3.624682     139.33
 H      -1.365491    -3.552335    -3.614092      25.36
 C      -4.179533    -1.810644    -3.180102      69.55
 H      -4.499232    -2.215189    -2.314260      26.59
 O      -4.278151    -0.322038    -2.938054     176.80
 H      -5.313684    -0.288076    -2.334142      21.78
 C      -4.987099    -2.439542    -4.555212      85.13
 O      -6.333317    -2.586884    -4.295627     235.80
 H      -6.873640    -3.308403    -5.017302      26.48
 H      -4.304798    -3.198346    -4.599411      27.15
 H      -4.713370    -1.556963    -5.180539      27.13
55
name = lig-ACN-frame_894
 C       3.997797    -1.035613     0.117226      58.44
 H       3.294613    -0.827000    -0.650878      20.98
 C       5.177722    -0.463390     2.102916      21.20
 H       5.385332     0.396328     2.930519      14.46
 C       6.244389    -1.301318     1.822778       4.28
 O       7.307088    -1.714814     2.758570     319.64
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 C       7.406519    -0.977095     3.965932      96.04
 H       8.575069    -1.187274     4.432240      23.95
 H       6.417621    -1.016264     4.701947      26.85
 H       7.637035     0.195326     3.864807      27.42
 C       6.254968    -1.907430     0.579685     -15.30
 O       7.333001    -2.634095    -0.014941     238.17
 H       8.148433    -2.505638     0.590536      28.24
 C       5.020113    -1.821144    -0.320775      54.40
 H       5.321503    -2.269761    -1.279999      21.47
 C       4.036482    -0.274153     1.414997      47.07
 C       2.952683     0.507853     2.096883     103.73
 H       3.260844     1.411871     2.492466      23.09
 O       2.356894    -0.111251     3.246368     251.43
 H       2.094151    -0.939547     2.751004      24.78
 C       1.678457     0.963685     1.097498      77.52
 H       2.189017     1.441209     0.254055      20.99
 C       0.514263     1.843812     1.711554     101.53
 O       1.102210     3.211527     1.921690     262.42
 H       1.564284     3.479662     0.953280      24.18
 H       0.624082     1.406064     2.821158      20.09
 H      -0.336737     1.880199     1.119043      23.70
 C      -1.327934    -2.286387    -1.301020      37.62
 H      -1.634252    -3.473755    -1.470283      20.00
 C      -1.121695    -0.120626    -2.460948      45.75
 H      -1.093113     0.373308    -3.505697      18.91
 C      -0.184840     0.331528    -1.391031       6.11
 O       0.554801     1.455494    -1.491786     235.11
 C       0.983555     2.001602    -2.774134      88.08
 H       1.808975     1.139227    -3.197444      23.45
 H       0.094036     2.014787    -3.507065      21.63
 H       1.711071     2.959136    -2.655304      23.14
 C       0.069040    -0.585820    -0.294890       3.24
 O       1.006869    -0.239796     0.764432     172.01
 C      -0.545111    -1.949592    -0.189883      46.66
 H      -0.731510    -2.454364     0.775353      18.67
 C      -1.658789    -1.474883    -2.450547      28.66
 C      -2.573286    -2.084012    -3.493052      70.86
 H      -2.201904    -1.652083    -4.573854      23.15
 O      -2.324079    -3.615878    -3.586728      87.05
 H      -1.324244    -3.837925    -4.170226      23.74
 C      -4.132205    -1.815013    -3.168943      85.82
 H      -4.311385    -2.468563    -2.408129      26.71
 O      -4.309268    -0.425939    -2.900731     196.35
 H      -5.452275    -0.217514    -2.400513      20.14
 C      -4.920875    -2.336899    -4.502697      89.62
 O      -6.459885    -2.589607    -4.220954     225.37
 H      -6.771470    -3.500742    -4.804168      28.24
 H      -4.668380    -3.278794    -4.968313      24.75
 H      -4.911742    -1.716569    -5.436277      25.91
55
name = lig-ACN-frame_895
 C       3.941708    -1.002708     0.129392      43.85
 H       3.027880    -1.040892    -0.289923      20.01
 C       5.251445    -0.452727     2.282348      45.10
 H       5.265244    -0.023715     3.440537      16.00
 C       6.318766    -1.242020     1.784719      28.75
 O       7.195596    -1.634947     2.722210     255.78
 C       7.457189    -0.933127     4.070978      59.09
 H       8.346186    -1.680276     4.448377      22.44
 H       6.637592    -1.339288     4.870592      25.50
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 H       7.513357     0.259165     3.916452      26.08
 C       6.166116    -2.019695     0.480823      23.44
 O       7.325199    -2.601199     0.032112     174.27
 H       8.072409    -2.580677     0.755440      26.23
 C       5.107214    -1.813011    -0.331888      65.91
 H       4.932169    -2.242092    -1.269161      23.00
 C       4.107208    -0.275028     1.291967       9.14
 C       2.871011     0.522351     1.948254      89.04
 H       3.356199     1.357127     2.261791      23.37
 O       2.359328    -0.142902     3.185868     185.15
 H       1.605605    -0.987906     3.080564      19.87
 C       1.745568     1.003356     1.065608      79.63
 H       2.037229     1.563413     0.121885      19.04
 C       0.697006     1.916765     1.786342     107.29
 O       1.020255     3.213410     1.986617     340.07
 H       1.297139     3.595271     1.176545      30.38
 H       0.096209     1.510280     2.732810      22.19
 H      -0.170818     1.828446     1.197910      23.69
 C      -1.210348    -2.247832    -1.311118      54.74
 H      -1.457572    -3.390380    -1.495634      19.34
 C      -1.042624    -0.200401    -2.515239      63.95
 H      -1.310514     0.457401    -3.377168      20.55
 C      -0.245185     0.184165    -1.483470      10.48
 O       0.508816     1.377428    -1.575439     248.53
 C       1.014191     1.948253    -2.794681      93.25
 H       1.929142     1.322834    -3.328565      23.73
 H       0.246772     2.109069    -3.548828      23.80
 H       1.187197     3.128400    -2.476748      23.06
 C       0.124060    -0.529257    -0.249869       8.86
 O       1.001888    -0.246496     0.759381     190.90
 C      -0.609038    -1.704091    -0.104269      46.55
 H      -0.404537    -2.261516     0.767033      20.73
 C      -1.583482    -1.447141    -2.335708      43.76
 C      -2.458837    -2.124524    -3.480419      84.28
 H      -2.215302    -1.512801    -4.492749      25.44
 O      -2.284344    -3.529490    -3.566155     219.70
 H      -1.463752    -3.769590    -4.183635      26.86
 C      -4.043671    -1.949900    -3.337161      92.62
 H      -4.376454    -2.537193    -2.539248      26.15
 O      -4.331523    -0.541776    -2.869918     131.58
 H      -5.554232    -0.614724    -2.757852      20.93
 C      -5.008812    -2.279988    -4.436249      93.64
 O      -6.473143    -2.570189    -4.133810     288.57
 H      -6.543962    -3.161043    -4.852820      31.50
 H      -4.446750    -3.203904    -4.736895      25.75
 H      -4.966132    -1.355043    -5.069606      27.75
55
name = lig-ACN-frame_896
 C       4.004161    -0.997966     0.149738      52.93
 H       3.089203    -1.065123    -0.277757      21.66
 C       5.183174    -0.403436     2.182911      15.57
 H       4.935143    -0.267160     3.326814      10.32
 C       6.186970    -1.250322     1.833007      24.71
 O       7.262822    -1.597285     2.716747     325.17
 C       7.448374    -1.053967     4.055081      86.24
 H       8.542645    -1.276873     4.420110      25.38
 H       6.511029    -1.171792     4.750863      30.89
 H       7.602563     0.172321     4.015332      30.14
 C       6.237515    -1.903095     0.536108     -20.80
 O       7.328502    -2.639237     0.075418     259.11
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 H       8.029206    -2.696425     0.752308      28.65
 C       5.037428    -1.779515    -0.339439      61.49
 H       5.039604    -2.408429    -1.137401      22.49
 C       4.060144    -0.263792     1.413936      48.16
 C       2.931386     0.552906     1.878597     114.08
 H       3.202529     1.409761     2.329136      24.14
 O       2.369535    -0.158310     3.119657     171.98
 H       1.678392    -0.931963     2.661882      18.83
 C       1.699723     1.003609     1.057478      87.64
 H       2.049070     1.511435     0.032314      18.68
 C       0.688057     1.851024     1.762497      90.85
 O       1.017050     3.375543     2.101662     262.12
 H       1.027848     3.837782     1.284749      29.55
 H       0.597208     1.416598     2.820736      21.17
 H      -0.103358     1.892369     1.061608      22.43
 C      -1.186710    -2.292083    -1.142464      64.90
 H      -1.616198    -3.221672    -0.741884      20.95
 C      -1.002768    -0.264536    -2.511776      25.13
 H      -1.290981     0.519468    -3.150669      18.86
 C      -0.046421     0.196199    -1.520958      18.66
 O       0.506569     1.379258    -1.607749     248.51
 C       0.972463     1.951975    -2.836795     111.89
 H       2.100400     1.489874    -3.053769      23.81
 H       0.381400     1.948923    -3.677943      25.82
 H       1.382453     3.035318    -2.419243      22.37
 C       0.048682    -0.397357    -0.288094      28.94
 O       1.001388    -0.277401     0.720118     179.23
 C      -0.613108    -1.641191    -0.100813      55.59
 H      -0.167923    -2.261376     0.560819      20.64
 C      -1.609764    -1.579856    -2.401629      23.80
 C      -2.443690    -2.060369    -3.522282      88.94
 H      -2.079318    -1.640286    -4.552347      25.22
 O      -2.247915    -3.498196    -3.590810     259.03
 H      -1.401456    -3.635469    -3.690356      34.23
 C      -4.044463    -1.997772    -3.232015      78.82
 H      -4.048263    -2.826417    -2.450636      24.50
 O      -4.294801    -0.689301    -2.876581     219.29
 H      -5.368435    -0.511953    -2.452569      21.04
 C      -5.027278    -2.264168    -4.515782      92.22
 O      -6.357262    -2.569245    -4.048506     297.88
 H      -7.026903    -2.709065    -4.724785      33.35
 H      -4.772492    -3.034972    -5.380828      25.06
 H      -5.029696    -1.366418    -5.149573      28.00
55
name = lig-ACN-frame_897
 C       3.974543    -0.971714     0.157662      58.40
 H       3.244859    -0.766905    -0.621234      20.74
 C       5.123149    -0.410794     2.226219      43.07
 H       5.257713     0.340072     3.077055      15.25
 C       6.210378    -1.299516     1.914470      15.35
 O       7.363455    -1.614836     2.666390     290.30
 C       7.421163    -1.050134     3.974452     105.24
 H       8.313884    -1.582153     4.399228      25.02
 H       6.650395    -1.534697     4.681359      30.41
 H       7.377155     0.176643     3.929513      27.45
 C       6.268851    -1.745929     0.572118       5.19
 O       7.291928    -2.685381     0.141277     198.79
 H       8.085598    -2.561829     0.658806      22.51
 C       5.137876    -1.783636    -0.193195      58.29
 H       5.131291    -2.281312    -1.106153      22.52
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 C       3.937357    -0.263563     1.306673      20.75
 C       2.886704     0.650150     2.021010      96.52
 H       3.409619     1.496215     2.275039      21.75
 O       2.349322    -0.171838     3.024986     235.95
 H       2.128860    -1.011884     2.607787      24.99
 C       1.720655     0.968832     0.956187      78.76
 H       2.197940     1.541628    -0.052195      18.34
 C       0.635470     2.000464     1.793041      92.51
 O       1.028165     3.389811     2.180731     234.76
 H       0.979233     3.952829     1.234047      24.98
 H       0.524274     1.448396     2.739810      23.11
 H      -0.437725     1.950213     1.564474      22.88
 C      -1.433322    -2.333247    -1.098085      42.28
 H      -1.830766    -3.273914    -1.051866      22.14
 C      -0.950288    -0.366836    -2.438191      55.81
 H      -1.145879    -0.009060    -3.397630      20.77
 C       0.005324     0.203669    -1.581356       7.20
 O       0.551663     1.557943    -1.631052     233.10
 C       1.088018     2.010296    -2.870516     102.13
 H       2.021510     1.305877    -3.195371      24.21
 H       0.366734     1.758140    -3.589325      25.09
 H       1.173316     3.163669    -2.972854      24.30
 C       0.037298    -0.419826    -0.259575      17.73
 O       1.035290    -0.221012     0.702990     177.96
 C      -0.500324    -1.719448    -0.099215      49.75
 H      -0.565389    -1.995996     0.898663      19.92
 C      -1.529405    -1.616738    -2.331253      13.35
 C      -2.524620    -2.128629    -3.542905      76.03
 H      -2.350719    -1.390559    -4.413509      23.74
 O      -2.185322    -3.557604    -3.686189     235.80
 H      -1.392267    -3.682713    -3.143507      27.65
 C      -3.994714    -2.076451    -3.278000      63.99
 H      -4.508691    -2.806267    -2.493588      23.50
 O      -4.259551    -0.708894    -2.783515     232.90
 H      -5.254016    -0.677231    -2.480848      21.75
 C      -4.963345    -2.309644    -4.658601      75.39
 O      -6.256674    -2.562126    -3.915381     206.89
 H      -6.887257    -2.336731    -4.821806      28.50
 H      -4.768228    -3.190252    -5.436936      23.98
 H      -4.989424    -1.274361    -4.958686      27.92
55
name = lig-ACN-frame_898
 C       3.965470    -0.955692     0.056699      48.09
 H       3.173885    -0.864787    -0.796164      18.02
 C       5.166355    -0.425229     2.303645      53.55
 H       5.283952     0.387222     2.974684      22.13
 C       6.287338    -1.214775     1.923198      32.60
 O       7.396840    -1.599549     2.584721     312.09
 C       7.416291    -1.114930     3.974131     106.43
 H       8.374769    -1.257003     4.394477      23.48
 H       6.480052    -1.475638     4.437950      32.82
 H       7.322834     0.109370     4.050453      29.06
 C       6.299652    -1.845301     0.646135      -5.56
 O       7.236881    -2.679886     0.229109     143.78
 H       8.169017    -2.533576     0.633543      22.20
 C       5.146312    -1.686492    -0.148450      56.69
 H       5.275858    -2.165613    -1.134925      21.70
 C       3.994589    -0.213292     1.346307      43.98
 C       2.800887     0.658141     1.898783     103.90
 H       3.044886     1.453833     2.544128      23.98
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 O       2.290908    -0.174882     3.049409     205.38
 H       2.224179    -1.007673     2.743390      28.45
 C       1.660615     1.189009     1.051248      55.87
 H       2.019982     1.668935    -0.116239      15.19
 C       0.626799     2.067331     1.878646     105.62
 O       1.055070     3.351388     2.178130     267.72
 H       1.173862     3.945266     1.310490      27.43
 H       0.539811     1.596353     2.823563      23.73
 H      -0.215275     2.094706     1.118064      21.38
 C      -1.529114    -2.305237    -1.022028      24.21
 H      -2.049249    -3.123484    -0.816633      22.16
 C      -0.819804    -0.382475    -2.551324      68.46
 H      -0.773979     0.108446    -3.502676      17.04
 C      -0.054379     0.286355    -1.490217      -1.00
 O       0.579286     1.678304    -1.623839     203.55
 C       1.118389     1.981807    -3.031133     101.07
 H       2.269876     1.650850    -3.215616      24.26
 H       0.473062     1.782264    -3.901368      24.10
 H       1.251826     3.031591    -2.852145      25.56
 C       0.193077    -0.569151    -0.316151      25.80
 O       1.036483    -0.171094     0.699513     136.58
 C      -0.615867    -1.812404    -0.106893      24.25
 H      -0.534148    -2.303979     0.888164      19.43
 C      -1.619989    -1.661831    -2.296080      29.33
 C      -2.446852    -2.244832    -3.410439      84.74
 H      -2.112411    -1.741913    -4.357935      26.24
 O      -2.144417    -3.614986    -3.833223     146.04
 H      -1.126165    -3.927824    -3.306945      21.81
 C      -4.053543    -2.103272    -3.392865      73.20
 H      -4.342721    -2.994278    -2.555526      22.44
 O      -4.228558    -0.750898    -2.687665     256.67
 H      -5.087679    -0.577850    -2.755376      29.86
 C      -4.873078    -2.278020    -4.539300     108.91
 O      -6.155797    -2.552641    -3.917516     268.11
 H      -7.079518    -2.415703    -4.307684      30.83
 H      -4.381854    -3.226241    -5.131490      25.88
 H      -4.882982    -1.561987    -5.352775      27.93
55
name = lig-ACN-frame_899
 C       4.088911    -0.827638     0.172520      44.33
 H       3.015563    -0.845222    -0.407578      16.53
 C       5.171021    -0.332415     2.243402      57.19
 H       5.013652    -0.192703     3.236802      17.55
 C       6.285753    -1.125417     1.855944      -1.76
 O       7.464666    -1.517983     2.633915     305.62
 C       7.416571    -1.123639     3.990601     119.60
 H       8.272667    -1.458819     4.406358      23.64
 H       6.703838    -1.648554     4.619184      31.31
 H       7.267886     0.073691     3.975824      28.00
 C       6.127572    -1.906550     0.695890       9.13
 O       7.271772    -2.739780     0.256823     195.57
 H       8.048388    -2.639124     0.943783      23.62
 C       5.144347    -1.634405    -0.300227      53.22
 H       5.216228    -2.284946    -1.257871      20.79
 C       4.066911    -0.167476     1.378674      21.77
 C       2.842603     0.621152     1.919154      87.14
 H       3.421305     1.497001     2.193360      21.56
 O       2.212034    -0.158016     3.091350     163.85
 H       1.701813    -1.018098     2.646096      19.45
 C       1.604929     1.227216     1.110895      56.74
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 H       1.908904     2.172761     0.208641      16.00
 C       0.583002     2.001086     1.855534     103.86
 O       1.139951     3.423917     2.172743     267.17
 H       1.319865     3.710851     1.345153      32.50
 H       0.129770     1.530859     2.669086      24.74
 H      -0.381096     2.160528     1.245259      21.31
 C      -1.540159    -2.212922    -1.013599      40.13
 H      -2.081847    -3.113812    -0.715830      20.53
 C      -0.754074    -0.462776    -2.555931      64.23
 H      -0.914451     0.016691    -3.545992      20.78
 C      -0.091625     0.270406    -1.474937       3.18
 O       0.547650     1.561599    -1.713369     240.24
 C       1.128056     2.018388    -3.041966      96.83
 H       2.111147     1.377584    -3.127317      24.28
 H       0.466649     1.623922    -3.907981      22.31
 H       1.217333     3.025493    -3.118051      26.44
 C       0.255109    -0.579964    -0.386144      14.89
 O       0.991679    -0.155021     0.716120     148.20
 C      -0.612197    -1.744786    -0.038518      43.88
 H      -0.161911    -2.498890     0.739140      20.06
 C      -1.624291    -1.527972    -2.302592      24.83
 C      -2.340954    -2.271483    -3.527357      72.42
 H      -2.046958    -1.612940    -4.363811      26.31
 O      -2.124549    -3.722810    -3.898685     135.65
 H      -0.949880    -3.870518    -4.132691      22.07
 C      -3.880623    -2.012412    -3.194397      77.63
 H      -4.312271    -2.988128    -2.546240      23.58
 O      -4.191671    -0.823569    -2.655540     298.91
 H      -5.046767    -0.716865    -2.481167      29.19
 C      -4.820126    -2.333572    -4.544525      87.22
 O      -6.121529    -2.557045    -3.922851     305.08
 H      -6.552408    -2.465136    -4.680674      34.59
 H      -4.524981    -3.471962    -4.849380      24.89
 H      -4.852635    -1.542593    -5.289891      27.91
55
name = lig-ACN-frame_900
 C       4.124707    -0.746408     0.138703      40.92
 H       3.137006    -0.572178    -0.586761      20.24
 C       5.222474    -0.280899     2.303057      36.87
 H       5.115640    -0.020319     3.305681      12.37
 C       6.277112    -1.158167     1.869713      41.98
 O       7.395237    -1.401448     2.606516     276.87
 C       7.452206    -1.114017     4.092389     129.90
 H       8.383580    -1.357185     4.325444      27.07
 H       6.661557    -1.658630     4.486651      34.99
 H       7.321943     0.003886     4.445561      31.49
 C       6.227720    -1.937660     0.518000       3.39
 O       7.190558    -2.770982     0.308958     134.63
 H       7.846683    -2.748145     1.012714      23.67
 C       5.152034    -1.647791    -0.313541      59.41
 H       4.827279    -2.096498    -1.351273      20.38
 C       4.069745    -0.114815     1.423395      32.66
 C       2.858556     0.663159     2.076705      94.50
 H       3.157458     1.488280     2.790434      20.40
 O       2.196466    -0.091174     3.090627     193.57
 H       1.396806    -0.712967     2.503163      18.28
 C       1.664085     1.043791     1.108709      65.60
 H       2.171352     1.427403    -0.077001      17.64
 C       0.481256     2.086857     1.872178      86.63
 O       1.185729     3.371388     2.151787     252.78
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 H       1.471504     3.835511     1.311447      28.57
 H       0.359407     1.795761     2.885432      23.71
 H      -0.368449     2.200391     1.125486      22.05
 C      -1.476059    -2.093675    -1.010314      61.50
 H      -1.922129    -3.160790    -1.095198      21.93
 C      -0.812866    -0.425428    -2.550277      48.77
 H      -0.804042     0.020301    -3.601059      19.59
 C       0.013065     0.172587    -1.655616      23.77
 O       0.492335     1.412912    -1.780722     252.40
 C       1.053934     1.867799    -2.991901     117.14
 H       2.151583     1.460084    -3.252895      25.46
 H       0.323503     1.709565    -3.915970      23.08
 H       1.157033     2.862833    -2.798051      28.05
 C       0.136018    -0.423093    -0.311928      25.66
 O       0.978766    -0.108947     0.730473     179.44
 C      -0.486884    -1.635866    -0.135186      49.97
 H      -0.400606    -2.145456     0.967648      18.33
 C      -1.497412    -1.610716    -2.318902      27.63
 C      -2.296645    -2.148139    -3.606720      82.64
 H      -2.213467    -1.739619    -4.590333      25.62
 O      -2.136923    -3.716915    -3.925667     132.77
 H      -1.050272    -3.741428    -4.020761      23.74
 C      -3.763926    -2.194845    -3.233905      79.40
 H      -3.720542    -2.824701    -2.197200      22.64
 O      -4.127688    -0.768760    -2.579884     175.07
 H      -5.154379    -0.982899    -2.377157      23.45
 C      -4.659316    -2.462875    -4.372089      93.79
 O      -6.138583    -2.520198    -4.012964     245.78
 H      -6.791203    -2.962058    -4.730727      28.54
 H      -4.265745    -3.245282    -5.243553      24.30
 H      -4.536177    -1.556882    -4.966768      27.22
55
name = lig-ACN-frame_901
 C       4.082022    -0.663694     0.119813      45.80
 H       3.381433    -0.406542    -0.817058      19.76
 C       5.228769    -0.341003     2.303858      27.93
 H       5.589067     0.426749     2.958919      15.22
 C       6.191918    -1.189732     1.823588       8.60
 O       7.366974    -1.292339     2.611310     290.30
 C       7.453672    -1.129554     4.124422     116.90
 H       8.412789    -1.426170     4.380000      25.13
 H       6.842812    -1.713022     4.682490      33.82
 H       7.281874    -0.048968     4.295373      30.21
 C       6.256502    -1.727133     0.582987     -19.59
 O       7.183504    -2.896825     0.295245     205.20
 H       7.995574    -2.700175     0.787970      25.04
 C       5.073272    -1.588550    -0.257318      41.63
 H       5.289036    -2.149794    -1.262109      21.80
 C       4.092346    -0.046533     1.502630      15.23
 C       2.803305     0.693684     2.137458      89.23
 H       3.152515     1.820847     2.318853      20.75
 O       2.161506    -0.101838     3.165351     211.31
 H       1.664294    -0.906980     2.642590      20.28
 C       1.681434     1.074163     1.115515      65.85
 H       2.214831     1.758023     0.091487      18.33
 C       0.671864     2.131426     1.787716     107.89
 O       1.212689     3.338178     2.109422     246.95
 H       1.383431     3.849720     1.115069      24.23
 H       0.279274     1.592490     2.649509      23.99
 H      -0.305575     2.235073     1.250133      22.72
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 C      -1.343028    -2.204316    -1.128318      45.28
 H      -1.859674    -3.031552    -0.442983      20.39
 C      -0.831252    -0.394602    -2.711236      40.38
 H      -0.907480     0.203132    -3.693133      18.12
 C       0.101374     0.065471    -1.631935      24.02
 O       0.512010     1.361547    -1.790745     236.85
 C       0.982395     1.805366    -3.024103     111.45
 H       2.011555     1.231350    -3.284307      24.87
 H       0.264771     1.803268    -3.967977      22.54
 H       1.268076     2.828150    -2.862953      27.08
 C       0.063296    -0.295968    -0.299620      28.45
 O       0.957593    -0.153766     0.789277     175.90
 C      -0.547734    -1.564903    -0.149116      24.04
 H      -0.554791    -1.948765     0.994804      17.72
 C      -1.400091    -1.671833    -2.524539      22.82
 C      -2.266515    -2.200030    -3.571241      97.25
 H      -1.993214    -1.461634    -4.274277      25.65
 O      -2.104834    -3.576533    -3.932377     278.55
 H      -1.367675    -3.910695    -3.546369      32.66
 C      -3.740727    -2.231176    -3.069040      63.76
 H      -3.866216    -3.277727    -2.381068      23.30
 O      -4.047548    -0.834815    -2.569859     158.51
 H      -5.232672    -0.581190    -2.563985      20.85
 C      -4.647551    -2.480582    -4.323359      84.93
 O      -6.085029    -2.515696    -4.123237     257.45
 H      -6.200940    -3.511981    -4.594739      25.02
 H      -4.315228    -3.558994    -4.841154      24.00
 H      -4.443160    -1.586993    -4.908818      27.36
55
name = lig-ACN-frame_902
 C       4.046341    -0.579497     0.213441      47.90
 H       3.096126    -0.336299    -0.333179      20.26
 C       5.148096    -0.248566     2.247795      35.85
 H       5.228484     0.292762     3.274237      16.04
 C       6.287943    -1.132819     1.960053      52.06
 O       7.411082    -1.268704     2.658540     326.28
 C       7.431355    -1.116255     4.054309     155.09
 H       8.457887    -1.396197     4.229634      26.00
 H       6.723734    -1.728331     4.459623      35.70
 H       7.317659    -0.104195     4.438029      33.59
 C       6.241781    -1.844487     0.611339       7.53
 O       7.096084    -2.854272     0.266467     136.38
 H       8.089284    -2.682113     0.503710      21.20
 C       5.161591    -1.466541    -0.178130      54.94
 H       4.972961    -1.916376    -1.189081      21.11
 C       3.987343    -0.059975     1.428805      33.23
 C       2.799926     0.710998     2.008848      77.89
 H       3.251289     1.471131     2.816938      18.53
 O       2.171949    -0.115422     3.256366     168.28
 H       2.144915    -0.946297     2.953535      27.87
 C       1.705134     1.172180     1.103609      73.72
 H       2.136327     1.675533    -0.032714      16.79
 C       0.711203     2.001520     1.695427      99.83
 O       1.304431     3.431589     2.066874     225.01
 H       1.332621     3.954139     1.159464      26.66
 H       0.377690     1.659591     2.725161      22.75
 H       0.022214     2.141664     0.887030      22.30
 C      -1.171717    -2.294924    -1.246767      47.36
 H      -1.987133    -3.178705    -1.349412      19.93
 C      -0.667478    -0.489736    -2.703286      56.31
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 H      -1.010154     0.100040    -3.582328      20.78
 C      -0.015634     0.168799    -1.694713      -0.57
 O       0.593249     1.421846    -1.762199     236.75
 C       1.001971     1.837584    -3.143600      94.98
 H       1.763910     1.083403    -3.488148      25.88
 H       0.084993     1.750167    -3.792386      23.34
 H       1.477304     2.888785    -3.183933      25.09
 C       0.117700    -0.462311    -0.296913       2.76
 O       0.933914    -0.128050     0.800106     122.35
 C      -0.764288    -1.543622    -0.106362      52.76
 H      -0.646241    -2.159103     0.850766      21.43
 C      -1.296116    -1.703772    -2.461392      38.88
 C      -2.340490    -2.222574    -3.527007      93.69
 H      -2.547574    -1.768106    -4.399038      28.86
 O      -2.027035    -3.542167    -3.952849     270.31
 H      -1.170473    -3.807054    -3.690048      30.20
 C      -3.838629    -2.150092    -3.013031      76.25
 H      -4.153546    -2.785390    -1.981368      21.71
 O      -3.989467    -0.932761    -2.528114     195.60
 H      -5.093954    -0.604792    -2.696623      22.24
 C      -4.600249    -2.451517    -4.320857     102.02
 O      -6.036552    -2.589907    -4.221733     339.32
 H      -6.387630    -3.421373    -4.320168      33.23
 H      -4.136272    -3.513951    -4.622252      24.52
 H      -4.340865    -1.913901    -5.266824      26.27
55
name = lig-ACN-frame_903
 C       4.029943    -0.641320     0.155681      49.33
 H       3.319808    -0.825635    -0.580520      20.92
 C       5.169743    -0.186465     2.318524      44.36
 H       4.838312    -0.060064     3.454252      15.33
 C       6.238499    -1.034543     1.913788       6.07
 O       7.488360    -1.273589     2.627662     317.04
 C       7.436526    -1.095069     4.092025     109.21
 H       8.376261    -1.405332     4.666322      24.33
 H       6.708064    -1.724495     4.532442      33.53
 H       7.179874    -0.134345     4.323452      33.63
 C       6.124680    -1.826880     0.774547      16.04
 O       7.034171    -2.786043     0.205267     239.89
 H       7.929083    -2.656651     0.676309      25.17
 C       5.142875    -1.343412    -0.183256      44.43
 H       5.150892    -1.864518    -1.119038      21.86
 C       3.995292    -0.063346     1.534836      22.89
 C       2.839891     0.629551     2.097578      89.40
 H       3.169727     1.811591     2.406626      20.78
 O       2.238989    -0.090318     3.239775     218.78
 H       2.048292    -0.997815     2.977447      26.03
 C       1.751608     1.059448     1.008930      60.76
 H       2.231030     1.521940    -0.061428      17.81
 C       0.663248     2.212435     1.669885      92.90
 O       1.334970     3.422978     1.998987     327.15
 H       1.425586     3.852688     1.213689      32.07
 H       0.246439     1.670906     2.642293      22.94
 H      -0.263550     2.285180     1.142364      23.51
 C      -1.219508    -2.405406    -1.255227      21.97
 H      -1.452840    -3.544267    -1.027054      18.49
 C      -0.548412    -0.470342    -2.704611      56.00
 H      -0.640376    -0.029522    -3.689099      21.02
 C      -0.002361     0.290325    -1.527419       8.29
 O       0.711190     1.528142    -1.795021     232.45
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 C       0.960318     1.812195    -3.215855      96.50
 H       1.567161     1.173525    -3.689606      28.33
 H       0.078506     2.059802    -3.820518      24.64
 H       1.567981     2.843877    -3.003099      23.72
 C       0.136299    -0.524657    -0.398244       6.65
 O       0.894616    -0.099526     0.741308     155.04
 C      -0.813328    -1.723010    -0.108550      30.92
 H      -0.924405    -2.029464     0.922565      21.28
 C      -1.276995    -1.695588    -2.549817      26.30
 C      -2.371598    -2.196844    -3.466819      94.48
 H      -2.175610    -1.445881    -4.071926      27.37
 O      -1.956612    -3.654349    -3.969589     146.49
 H      -0.931656    -3.411791    -4.043233      26.07
 C      -3.878457    -2.220467    -3.057889      61.20
 H      -4.099282    -3.275598    -2.427182      23.50
 O      -4.021695    -0.751359    -2.429379     203.40
 H      -5.013311    -0.571316    -2.370889      25.03
 C      -4.571735    -2.621119    -4.367660      88.82
 O      -6.046104    -2.600919    -4.283138     296.74
 H      -6.247373    -3.537930    -4.469698      29.95
 H      -4.120048    -3.622404    -4.706197      25.73
 H      -4.337194    -1.677414    -4.959552      26.27
55
name = lig-ACN-frame_904
 C       3.981962    -0.666475     0.198245      58.86
 H       3.208318    -0.286213    -0.307599      21.55
 C       5.165333    -0.270355     2.428218      72.29
 H       5.448679     0.377974     3.425030      20.67
 C       6.302645    -1.002805     1.993575      -2.12
 O       7.485809    -1.272479     2.610503     289.96
 C       7.380207    -1.068621     4.148912      81.92
 H       8.513742    -1.275831     4.366008      24.61
 H       6.587609    -1.712300     4.583093      29.28
 H       7.229438    -0.101289     4.330405      31.07
 C       6.085655    -1.687637     0.717168      17.12
 O       6.981687    -2.658476     0.233188     234.26
 H       7.669486    -2.810128     0.857699      27.06
 C       5.159744    -1.442176    -0.226959      60.29
 H       5.405567    -1.801003    -1.147774      22.39
 C       4.071162    -0.126862     1.483990      16.92
 C       2.722149     0.653959     2.085142      78.75
 H       3.179048     1.721988     2.557319      20.99
 O       2.306365    -0.053758     3.225321     214.14
 H       1.662796    -0.791039     2.663927      21.19
 C       1.571383     1.024187     1.030878      89.41
 H       2.279940     1.421770     0.116490      19.36
 C       0.680912     2.232307     1.613843     101.57
 O       1.356866     3.435041     1.950862     308.50
 H       1.738927     3.881439     1.179358      30.83
 H       0.384212     1.848531     2.708015      22.32
 H      -0.103022     2.509795     0.963898      23.84
 C      -1.286788    -2.430733    -1.198683      45.36
 H      -1.804355    -3.405265    -1.045149      22.47
 C      -0.570258    -0.421534    -2.627288      52.76
 H      -0.392817    -0.016241    -3.569082      20.39
 C       0.088073     0.236303    -1.626579      12.81
 O       0.772780     1.504746    -1.808661     226.07
 C       0.913135     1.910785    -3.192452     110.81
 H       1.285786     1.149044    -3.674871      30.11
 H      -0.029558     2.152154    -3.625401      27.42
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 H       1.723979     2.822054    -3.378795      24.14
 C       0.038212    -0.462187    -0.313502      26.90
 O       0.828085    -0.170043     0.698858     200.34
 C      -0.563877    -1.731679    -0.192904      52.51
 H      -0.651056    -2.115794     0.741842      21.51
 C      -1.258751    -1.739378    -2.430689      38.44
 C      -2.222081    -2.211344    -3.545337      94.28
 H      -2.368198    -1.792628    -4.408142      28.09
 O      -1.990492    -3.616202    -3.982916     121.67
 H      -0.803495    -3.871038    -3.980659      20.86
 C      -3.768023    -2.252532    -3.060282      50.76
 H      -3.938602    -2.690027    -1.917539      20.87
 O      -4.113218    -0.744407    -2.414221     249.04
 H      -4.950413    -0.645984    -2.227741      30.92
 C      -4.623347    -2.589401    -4.419614      92.83
 O      -6.043020    -2.660332    -4.325726     232.89
 H      -6.489641    -3.497919    -4.954909      25.49
 H      -4.259840    -3.525796    -4.881027      24.36
 H      -4.289470    -1.914084    -5.336578      24.21
55
name = lig-ACN-frame_905
 C       4.023183    -0.638024     0.252345      47.12
 H       3.335422    -0.406708    -0.491415      23.28
 C       5.174338    -0.308110     2.425743      35.03
 H       5.134597     0.615404     3.143360      14.27
 C       6.256053    -1.059298     1.972775      15.90
 O       7.433455    -1.268141     2.716949     317.91
 C       7.416943    -1.011776     4.072642     103.07
 H       8.430345    -1.395066     4.602750      23.52
 H       6.650393    -1.748572     4.575231      30.72
 H       7.207861    -0.127385     4.374771      37.49
 C       6.191611    -1.595267     0.640884      -4.59
 O       7.040919    -2.583105     0.296502     151.40
 H       7.774934    -2.716168     0.977083      19.96
 C       5.010336    -1.452203    -0.267050      55.32
 H       4.851399    -1.893015    -1.202952      22.85
 C       3.987801    -0.085090     1.577176      48.45
 C       2.778253     0.688564     1.954875      84.35
 H       3.041514     1.774070     2.461557      20.56
 O       2.259044    -0.068379     3.225380     125.70
 H       1.557098    -0.976325     3.078671      20.12
 C       1.541627     1.079607     1.096811      92.64
 H       1.790615     1.499666     0.014340      17.76
 C       0.640118     2.148886     1.586701      90.96
 O       1.427908     3.461943     1.965875     253.15
 H       1.615161     3.741505     0.904729      24.28
 H      -0.094512     1.914995     2.471210      23.14
 H      -0.065375     2.223362     0.780470      23.16
 C      -1.263257    -2.293164    -1.166879      58.29
 H      -2.041855    -2.951929    -0.976459      24.22
 C      -0.661289    -0.521527    -2.640330      63.51
 H      -0.946133    -0.177537    -3.601864      22.94
 C       0.175649     0.176119    -1.659438      21.66
 O       0.802263     1.394072    -1.779791     226.82
 C       0.840449     1.952120    -3.196671     105.96
 H       1.034427     1.305611    -3.867045      30.23
 H      -0.077204     2.428403    -3.379104      27.32
 H       1.716474     2.812914    -3.133218      24.16
 C       0.012689    -0.370022    -0.378637      11.45
 O       0.827855    -0.191562     0.853236     136.69
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 C      -0.398724    -1.760472    -0.200901      33.61
 H       0.057279    -2.194250     0.571788      20.11
 C      -1.293855    -1.682991    -2.443140      22.62
 C      -2.192013    -2.244032    -3.622294      89.69
 H      -1.922980    -1.542068    -4.294554      28.68
 O      -2.007483    -3.602184    -3.981404     166.24
 H      -1.018288    -4.031593    -3.500231      22.11
 C      -3.718797    -2.073261    -3.093792      63.26
 H      -3.859322    -3.192597    -2.438607      23.85
 O      -4.131160    -0.879702    -2.510937     248.52
 H      -5.113732    -0.930326    -2.691979      26.16
 C      -4.590216    -2.567424    -4.419313      79.54
 O      -6.090064    -2.732217    -4.334763     236.17
 H      -6.302518    -3.023318    -5.331277      26.34
 H      -4.160831    -3.516418    -4.561917      25.46
 H      -4.338808    -1.676626    -5.162590      24.48
55
name = lig-ACN-frame_906
 C       3.956261    -0.562843     0.248357      65.25
 H       2.971579    -0.608734    -0.235524      21.65
 C       5.072885    -0.193388     2.353003      48.33
 H       5.170456    -0.145571     3.447819      13.01
 C       6.147848    -1.035448     1.916646      11.12
 O       7.377798    -1.286337     2.666030     272.59
 C       7.409752    -0.997997     4.172876      96.12
 H       8.547278    -1.251663     4.430993      25.38
 H       6.530785    -1.577773     4.745993      29.85
 H       7.304751    -0.035366     4.267519      37.57
 C       6.171477    -1.617716     0.592375     -12.67
 O       7.229606    -2.600853     0.296013     161.60
 H       7.998676    -2.284157     0.915012      24.74
 C       5.039433    -1.413773    -0.123523      59.03
 H       5.052152    -2.080104    -1.040789      19.47
 C       3.947401    -0.072263     1.518821      31.53
 C       2.754034     0.711892     2.086558      94.15
 H       3.237045     1.761292     2.370005      20.32
 O       2.183830    -0.018334     3.228088     227.27
 H       2.058313    -0.902943     2.662794      22.37
 C       1.641725     1.031422     1.069616      83.49
 H       2.157069     1.453925     0.129438      19.74
 C       0.568087     2.232708     1.628860      92.74
 O       1.377078     3.320939     1.956700     258.29
 H       1.568567     4.016666     1.092908      25.33
 H       0.031668     1.922177     2.593433      22.28
 H      -0.084496     2.626823     0.845438      20.87
 C      -1.289435    -2.251931    -1.137316      57.64
 H      -1.534112    -3.182498    -0.802079      25.48
 C      -0.635684    -0.447724    -2.753626      62.56
 H      -0.748259     0.310238    -3.535129      19.26
 C       0.088424     0.121933    -1.650959       0.36
 O       0.835562     1.286038    -1.867619     210.10
 C       0.747505     2.004677    -3.106720     121.90
 H       0.910279     1.456694    -3.868542      29.94
 H      -0.135589     2.585139    -3.212343      27.32
 H       1.648262     2.741265    -3.011522      24.58
 C       0.273879    -0.498981    -0.280004      20.45
 O       0.779702    -0.114276     0.924873     178.51
 C      -0.325967    -1.704962    -0.229042      48.27
 H      -0.273933    -2.397859     0.638944      20.68
 C      -1.424533    -1.705007    -2.439286      38.82
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 C      -2.236638    -2.118844    -3.576372     102.44
 H      -2.071791    -1.713772    -4.508760      29.09
 O      -1.997907    -3.629348    -3.948964     161.47
 H      -1.071061    -3.717648    -3.565631      27.21
 C      -3.750587    -2.164214    -3.320922      80.21
 H      -3.773950    -3.007331    -2.297234      22.00
 O      -4.153342    -0.997760    -2.613634     184.46
 H      -5.152496    -0.428187    -2.775500      22.48
 C      -4.541862    -2.516009    -4.406677     112.85
 O      -6.051805    -2.757803    -4.326598     294.10
 H      -6.258692    -2.832565    -5.169102      34.12
 H      -4.129273    -3.321030    -4.868268      27.20
 H      -4.473458    -1.790786    -5.333981      25.41
55
name = lig-ACN-frame_907
 C       3.881534    -0.628430     0.217560      37.53
 H       2.963151    -0.678272    -0.539623      19.88
 C       5.069025    -0.233052     2.353390      40.14
 H       4.821382    -0.012893     3.316274      17.41
 C       6.218705    -0.974744     1.924932      24.18
 O       7.233848    -1.309810     2.630663     252.52
 C       7.392963    -0.930964     4.154755      95.72
 H       8.409164    -1.409909     4.367567      23.55
 H       6.649697    -1.553157     4.893472      27.18
 H       7.321556     0.063479     4.330048      30.79
 C       6.248769    -1.722803     0.711098      25.33
 O       7.307602    -2.490140     0.284123     223.07
 H       8.157499    -2.292565     0.667459      28.04
 C       5.096454    -1.460287    -0.147525      37.91
 H       5.026265    -1.900129    -1.243070      21.39
 C       3.903897     0.049900     1.522805      19.31
 C       2.708408     0.780369     2.201872      98.22
 H       3.019208     1.698559     2.791876      23.43
 O       2.123344     0.015035     3.221318     290.36
 H       1.946860    -0.834566     3.086741      30.00
 C       1.606713     1.158056     1.107315      98.48
 H       2.090508     1.285450     0.165161      22.63
 C       0.636296     2.193922     1.555351     110.82
 O       1.371801     3.331501     2.039083     329.79
 H       1.486960     3.836246     1.213304      30.03
 H       0.223072     1.698710     2.482178      24.66
 H      -0.287291     2.258769     0.950004      24.84
 C      -1.233775    -2.287585    -1.218439      51.57
 H      -1.670776    -3.234172    -1.283023      25.41
 C      -0.671003    -0.433523    -2.608356      63.85
 H      -0.737185    -0.089699    -3.688542      22.78
 C       0.116861     0.112666    -1.592807      12.19
 O       0.883114     1.199907    -1.900805     223.00
 C       0.675770     2.084207    -3.041218     122.12
 H       0.710436     1.574637    -3.860241      29.54
 H      -0.325354     2.473194    -2.982999      27.72
 H       1.479339     2.834645    -3.082867      26.00
 C       0.449591    -0.612501    -0.364420       7.49
 O       0.770666    -0.026465     0.915657     146.89
 C      -0.402226    -1.812155    -0.182961      31.91
 H      -0.429542    -2.079587     0.968498      20.50
 C      -1.424366    -1.511288    -2.447453      15.08
 C      -2.339086    -2.189940    -3.665431      82.97
 H      -2.230453    -1.450149    -4.449199      27.62
 O      -1.941136    -3.598779    -3.862559     229.99
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 H      -1.124897    -3.677953    -4.117769      32.93
 C      -3.833914    -2.274261    -3.260712      47.49
 H      -4.119213    -3.336496    -2.509413      23.15
 O      -4.153120    -0.957431    -2.656530     154.13
 H      -5.253168    -0.822114    -3.047002      22.72
 C      -4.628095    -2.568549    -4.754644      85.42
 O      -5.937422    -2.735394    -4.263824     262.95
 H      -6.560227    -3.166428    -4.988079      27.22
 H      -4.259313    -3.391241    -5.179902      26.57
 H      -4.418038    -1.515505    -5.216912      26.12
55
name = lig-ACN-frame_908
 C       4.019166    -0.763251     0.268497      53.25
 H       3.343189    -0.387350    -0.670643      19.40
 C       4.994899    -0.242481     2.345343      63.87
 H       5.294023     0.344694     3.075359      23.10
 C       6.135165    -0.969870     1.927657      12.64
 O       7.267121    -1.343569     2.829870     274.38
 C       7.385423    -0.904892     4.059649     104.96
 H       8.374569    -1.213532     4.407421      21.42
 H       6.440671    -1.408171     4.657430      28.00
 H       7.341435     0.129650     4.188133      31.17
 C       6.162992    -1.653324     0.673146      12.08
 O       7.314092    -2.376600     0.234742     196.50
 H       7.985203    -2.253159     0.938830      25.36
 C       5.067298    -1.473316    -0.156780      54.98
 H       5.163874    -1.921309    -1.247973      20.57
 C       3.914055     0.039695     1.477548      39.55
 C       2.677744     0.804569     2.124053      91.19
 H       3.018725     1.750698     2.497072      23.20
 O       2.033766     0.009791     3.352131     220.38
 H       1.752657    -0.655614     2.801524      26.69
 C       1.664766     1.179088     1.034193      96.07
 H       2.049766     1.727191     0.253550      22.24
 C       0.622318     2.102488     1.651993      95.42
 O       1.343340     3.459225     2.091051     279.58
 H       1.675440     3.878869     1.379451      33.34
 H       0.141902     1.775745     2.540175      24.60
 H      -0.007290     2.476794     0.779169      21.14
 C      -1.194026    -2.331416    -1.316316      49.14
 H      -2.002908    -3.007060    -0.938541      23.85
 C      -0.714781    -0.347325    -2.553850      44.03
 H      -0.619739     0.316563    -3.503015      20.06
 C       0.284242     0.080985    -1.600756       2.31
 O       1.039725     1.225556    -1.862505     201.18
 C       0.543662     2.104448    -3.004254     118.89
 H       0.651536     1.794705    -3.948779      27.58
 H      -0.413831     2.574292    -2.765666      27.01
 H       1.189589     2.879116    -2.823945      27.70
 C       0.309791    -0.669260    -0.373445      10.96
 O       0.776174    -0.043448     0.821766     174.75
 C      -0.450936    -1.831728    -0.192487      45.30
 H      -0.422692    -2.475959     0.846317      19.64
 C      -1.490968    -1.626168    -2.450122      28.31
 C      -2.345412    -2.233823    -3.510412     102.73
 H      -2.244235    -1.734098    -4.500628      25.33
 O      -1.879709    -3.551080    -3.839543     168.41
 H      -0.916161    -3.426564    -4.230151      26.40
 C      -3.875107    -2.287184    -3.388833      57.28
 H      -4.334674    -3.250088    -2.571203      21.78
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 O      -4.198062    -1.022589    -2.777211     232.92
 H      -5.188742    -0.868395    -2.564026      25.60
 C      -4.606450    -2.539194    -4.842809      98.13
 O      -5.952099    -2.720060    -4.250069     240.74
 H      -6.514737    -3.530780    -4.813235      25.61
 H      -4.284348    -3.272186    -5.456668      26.91
 H      -4.681672    -1.704092    -5.643072      25.63
55
name = lig-ACN-frame_909
 C       3.970356    -0.659576     0.241649      43.68
 H       2.996593    -0.503887    -0.469796      20.83
 C       5.091261    -0.153345     2.373909      63.32
 H       4.996148     0.402347     3.278528      16.90
 C       6.108206    -1.104988     2.032897      10.59
 O       7.251101    -1.405308     2.708019     249.58
 C       7.343528    -0.791589     4.217447      99.97
 H       8.236844    -1.140948     4.598156      24.91
 H       6.514514    -1.108547     5.012214      29.49
 H       7.351028     0.259696     4.061140      33.52
 C       6.199510    -1.592008     0.660049      19.82
 O       7.258756    -2.247232     0.230129     175.44
 H       7.928479    -2.427356     1.010630      21.20
 C       5.116694    -1.531166    -0.182690      56.89
 H       5.081559    -2.059223    -1.189380      21.38
 C       3.913326    -0.123216     1.530587      29.28
 C       2.745283     0.709082     2.010763      86.03
 H       3.104545     1.580834     2.399947      22.79
 O       2.013639     0.100788     3.309073     171.27
 H       1.479600    -0.855097     3.142016      20.88
 C       1.632051     1.123346     1.038639      78.28
 H       2.086066     1.347281     0.188779      22.32
 C       0.635182     2.334712     1.739997      96.01
 O       1.257017     3.486373     2.146821     279.68
 H       1.639195     3.798246     1.181150      26.20
 H       0.098093     1.923131     2.521077      24.89
 H      -0.235270     2.481131     0.955268      22.04
 C      -1.311325    -2.391719    -1.197514      48.05
 H      -1.761714    -3.459985    -1.026904      22.51
 C      -0.726756    -0.361740    -2.600365      59.16
 H      -1.243128     0.332380    -3.362537      20.66
 C       0.289909    -0.026814    -1.694839      -5.72
 O       1.147182     1.254935    -1.862089     197.71
 C       0.510188     2.190721    -2.839210     113.02
 H       0.557821     1.615841    -3.721937      26.43
 H      -0.581233     2.188741    -2.665528      26.92
 H       0.977559     3.037225    -2.904461      28.38
 C       0.177909    -0.548518    -0.330750       9.62
 O       0.860200    -0.112650     0.729404     154.40
 C      -0.435629    -1.853783    -0.293402      44.77
 H      -0.322462    -2.512106     0.725525      21.28
 C      -1.410627    -1.589716    -2.402647      23.10
 C      -2.324071    -2.187218    -3.528000      77.90
 H      -2.039393    -1.363842    -4.324281      24.92
 O      -1.810492    -3.572662    -3.857294      94.79
 H      -0.615570    -3.614833    -3.700741      21.81
 C      -3.878572    -2.243170    -3.555550      72.72
 H      -4.195208    -3.359734    -2.844833      22.92
 O      -4.264985    -1.059584    -2.906226     279.30
 H      -5.025595    -1.097388    -2.521335      32.79
 C      -4.642832    -2.493046    -4.759337     111.07
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 O      -6.047388    -2.749603    -4.325780     274.83
 H      -6.273707    -3.499111    -4.935199      27.50
 H      -4.265009    -3.393022    -5.053047      26.41
 H      -4.533809    -1.576470    -5.390683      25.64
55
name = lig-ACN-frame_910
 C       3.937727    -0.687584     0.181114      57.50
 H       2.941814    -0.894516    -0.352346      21.45
 C       5.117387    -0.196010     2.391213      61.85
 H       4.961699    -0.017179     3.536905      13.72
 C       6.106175    -1.112579     2.057444       7.45
 O       7.257518    -1.431463     2.796882     271.01
 C       7.333260    -0.715816     4.220014      87.80
 H       8.199243    -1.111311     4.601847      25.45
 H       6.369727    -0.989839     4.725032      32.34
 H       7.366029     0.410825     4.120960      32.03
 C       6.131611    -1.565442     0.732812      -2.67
 O       7.313456    -2.214093     0.223967     203.15
 H       8.025091    -2.457454     0.866564      24.02
 C       4.995510    -1.414218    -0.182487      52.73
 H       5.138474    -1.922669    -1.101252      21.44
 C       3.948693    -0.219538     1.562171      21.57
 C       2.717155     0.614032     2.069048     107.70
 H       3.153869     1.464570     2.365566      24.16
 O       2.044504     0.232778     3.192118     215.70
 H       1.966838    -0.946894     3.106323      20.48
 C       1.552739     1.140982     1.048477      89.10
 H       1.847279     1.621617     0.279836      24.47
 C       0.590663     2.292905     1.703418      89.93
 O       1.252064     3.563874     2.156287     225.12
 H       1.587777     4.281592     1.384438      27.20
 H       0.326151     1.898984     2.613552      24.85
 H      -0.289565     2.610353     0.993423      21.74
 C      -1.325148    -2.348925    -1.172454      56.46
 H      -1.612873    -3.466860    -1.392349      23.71
 C      -0.773255    -0.467041    -2.638227      42.89
 H      -1.012356     0.074148    -3.601764      22.51
 C       0.275474     0.153340    -1.723434       6.28
 O       1.110876     1.174274    -1.861434     248.32
 C       0.486363     2.145319    -2.714780     119.80
 H       0.538753     2.047201    -3.811476      25.32
 H      -0.525533     2.410268    -2.331219      26.69
 H       0.934967     2.993941    -2.511495      28.81
 C       0.168220    -0.497784    -0.453924      -7.94
 O       0.931424    -0.194013     0.767866     125.62
 C      -0.407951    -1.846336    -0.191066      29.03
 H      -0.024849    -2.163000     0.859182      18.82
 C      -1.515267    -1.636394    -2.367347      26.72
 C      -2.172051    -2.133348    -3.714472      72.86
 H      -1.923614    -1.530488    -4.738792      23.73
 O      -1.767436    -3.546489    -3.884164     126.62
 H      -0.774311    -3.599202    -3.323261      23.57
 C      -3.778483    -2.261311    -3.450051      52.23
 H      -3.907440    -3.254779    -2.511190      21.78
 O      -4.319604    -0.997307    -2.961549     174.98
 H      -5.396559    -1.139527    -2.956142      23.89
 C      -4.694304    -2.536026    -4.755133     104.01
 O      -6.123752    -2.776386    -4.470834     327.46
 H      -6.470385    -3.236676    -5.134587      33.16
 H      -4.322142    -3.264454    -5.435441      25.51
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 H      -4.642781    -1.724072    -5.474305      26.50
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name = lig-ACN-frame_911
 C       3.833591    -0.780269     0.310021      45.47
 H       3.035236    -0.513540    -0.348564      20.17
 C       4.959104    -0.417641     2.440896      25.31
 H       5.011155     0.250936     3.474906      17.84
 C       6.199226    -1.043063     2.043422       0.03
 O       7.259744    -1.394135     2.978259     292.77
 C       7.307912    -0.724313     4.102003     127.44
 H       8.097965    -1.048931     4.718173      23.01
 H       6.455929    -0.909106     4.775792      32.54
 H       7.411404     0.447566     3.979208      28.84
 C       6.172302    -1.643043     0.678039      23.40
 O       7.287309    -2.203501     0.194713     208.24
 H       7.883199    -2.076227     0.916161      24.83
 C       5.133721    -1.382794    -0.169760      61.11
 H       5.103648    -1.732372    -1.105481      23.35
 C       3.834919    -0.138022     1.540903      20.60
 C       2.719063     0.830285     1.999958     100.46
 H       3.159890     1.692714     2.252939      25.34
 O       2.065349     0.210730     3.242453     206.26
 H       1.975232    -0.867009     3.089178      22.09
 C       1.604545     1.186037     1.034465      93.14
 H       2.034044     1.498159     0.249823      23.52
 C       0.583149     2.172510     1.725645      88.47
 O       1.275988     3.599880     2.140991     271.14
 H       1.222714     4.058454     1.322518      29.68
 H       0.064692     1.891181     2.609426      24.05
 H      -0.274114     2.351532     0.962580      22.07
 C      -1.225490    -2.328521    -1.201621      26.80
 H      -1.781768    -3.176763    -0.622412      21.62
 C      -0.693615    -0.414076    -2.662806      42.93
 H      -0.407955    -0.162946    -3.665293      21.93
 C       0.016836     0.070139    -1.632062      10.48
 O       1.038206     1.095685    -1.942500     226.01
 C       0.483679     2.300897    -2.607587     104.26
 H       0.521536     2.070139    -3.748915      23.83
 H      -0.569964     2.384969    -2.327233      26.44
 H       1.163931     3.025434    -2.327745      25.96
 C       0.277399    -0.565763    -0.362904      21.99
 O       0.922687    -0.186787     0.725303     162.64
 C      -0.460797    -1.714902    -0.204481      44.67
 H      -0.357225    -2.385080     0.630629      22.71
 C      -1.530981    -1.582859    -2.473191      16.65
 C      -2.205643    -2.212864    -3.688607      84.09
 H      -1.956621    -1.421748    -4.657200      23.23
 O      -1.728648    -3.503876    -3.937488     218.03
 H      -0.832046    -3.629964    -3.726686      28.14
 C      -3.764678    -2.221748    -3.483878      50.87
 H      -3.815208    -3.034489    -2.394706      20.97
 O      -4.322306    -0.976164    -2.953126     136.52
 H      -5.406076    -0.663314    -3.343806      21.68
 C      -4.664700    -2.633628    -4.825661      88.27
 O      -6.157841    -2.781136    -4.570019     262.02
 H      -6.424015    -3.262738    -5.467765      26.92
 H      -4.306340    -3.509141    -5.381142      23.87
 H      -4.497940    -1.714729    -5.238169      27.76
55
name = lig-ACN-frame_912
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 C       3.891154    -0.796815     0.332184      57.95
 H       3.358332    -0.544580    -0.494959      22.84
 C       4.850320    -0.512651     2.463365      45.46
 H       4.850031     0.128232     3.523875      19.54
 C       6.120610    -1.080691     2.048462      24.94
 O       7.179693    -1.427717     2.844478     258.15
 C       7.289837    -0.606735     4.275934      94.21
 H       8.248229    -1.028623     4.650458      22.99
 H       6.418247    -0.645573     4.803321      33.72
 H       7.467863     0.471603     3.809572      26.29
 C       6.237088    -1.569277     0.754338       3.70
 O       7.339123    -2.255689     0.172985     210.02
 H       8.273667    -2.075674     0.544604      26.84
 C       5.053921    -1.379367    -0.125470      44.12
 H       5.175846    -1.753145    -1.072801      22.86
 C       3.803183    -0.098745     1.611983      30.40
 C       2.762018     0.937184     2.039761      89.65
 H       3.022108     1.830767     2.455743      24.87
 O       2.118096     0.212352     3.322714     216.47
 H       1.792987    -0.584105     3.003956      26.34
 C       1.642184     1.205877     0.997026     107.64
 H       1.852993     1.615501     0.161188      25.25
 C       0.627140     2.202657     1.710944     102.38
 O       1.207740     3.444215     2.045007     318.89
 H       1.146060     4.036751     1.290920      30.24
 H       0.345144     1.601303     2.633940      22.62
 H      -0.201442     2.410029     0.993929      22.71
 C      -1.304661    -2.215953    -1.292649      58.33
 H      -2.131595    -2.986363    -1.221900      22.94
 C      -0.680778    -0.478945    -2.710780      32.28
 H      -0.604106     0.063366    -3.601393      23.56
 C       0.042614     0.106921    -1.549184       1.29
 O       0.915168     1.038473    -2.008126     229.24
 C       0.500591     2.384709    -2.546303     106.35
 H       0.472015     2.355512    -3.751828      24.07
 H      -0.461151     2.755344    -2.213230      26.56
 H       1.165513     3.344639    -2.340109      23.76
 C       0.255662    -0.560265    -0.295321       3.70
 O       0.988251    -0.063089     0.786602     174.26
 C      -0.519739    -1.776024    -0.197981      59.36
 H      -0.566945    -2.113505     0.750152      24.26
 C      -1.402178    -1.612513    -2.508740      41.11
 C      -2.310137    -2.158571    -3.600594      69.15
 H      -2.150996    -1.331987    -4.540143      23.52
 O      -1.724309    -3.552512    -4.017364     174.71
 H      -0.868424    -3.408648    -4.131844      30.76
 C      -3.928031    -2.257037    -3.525790      73.12
 H      -4.363366    -3.317175    -2.791485      21.04
 O      -4.229338    -0.961362    -2.961407     204.39
 H      -5.151495    -0.759076    -3.450306      25.09
 C      -4.589241    -2.649229    -4.796306     106.86
 O      -6.069350    -2.756338    -4.663090     255.68
 H      -6.423783    -3.626239    -5.328535      23.78
 H      -4.127210    -3.686943    -4.963708      23.00
 H      -4.428301    -2.185344    -5.686178      25.89
55
name = lig-ACN-frame_913
 C       3.935070    -0.616469     0.268961      62.32
 H       3.050136    -0.609119    -0.219469      22.59
 C       4.884807    -0.436463     2.546464      44.41
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 H       4.729179    -0.437821     3.714722      16.95
 C       5.969394    -1.180720     2.117789      -1.31
 O       7.104230    -1.385728     2.876422     230.76
 C       7.298198    -0.552022     4.216185      71.95
 H       8.161376    -1.098741     4.771190      25.21
 H       6.549871    -0.713717     4.835493      35.02
 H       7.449427     0.685795     4.134934      26.46
 C       6.224963    -1.512153     0.682443       7.80
 O       7.351066    -2.286962     0.149754     192.14
 H       8.105673    -1.985537     0.770605      24.95
 C       5.110115    -1.469930    -0.021836      54.61
 H       5.066328    -1.888105    -1.041498      20.71
 C       3.866677    -0.155628     1.592399      13.24
 C       2.765832     0.817886     2.188617      92.10
 H       3.384272     1.676340     2.365834      22.96
 O       2.174423     0.308041     3.323457     332.06
 H       1.824281    -0.536160     3.137018      27.94
 C       1.637747     1.303516     0.969406      91.30
 H       2.173451     1.627354     0.214941      23.37
 C       0.595396     2.121376     1.609030     103.34
 O       1.175104     3.366718     1.988398     256.00
 H       1.325142     4.132481     1.163380      26.47
 H       0.435346     1.771719     2.723522      20.81
 H      -0.404340     2.108919     1.200828      24.10
 C      -1.479619    -2.230708    -1.239089      13.21
 H      -1.872432    -3.243966    -1.068250      22.38
 C      -0.651761    -0.434517    -2.670024      52.96
 H      -0.931640     0.194572    -3.440024      23.09
 C       0.125628     0.102824    -1.693717       4.64
 O       0.937781     1.213581    -2.028541     233.48
 C       0.444840     2.418370    -2.541075      88.17
 H       0.240888     2.386858    -3.765335      22.26
 H      -0.416222     2.735108    -1.967880      26.00
 H       1.568996     2.881988    -2.228896      19.43
 C       0.153937    -0.501107    -0.279991     -11.50
 O       0.978674    -0.071077     0.835439     120.95
 C      -0.563843    -1.771447    -0.116742      36.14
 H      -0.688962    -2.270169     0.726900      22.39
 C      -1.410531    -1.656701    -2.572401      20.95
 C      -2.365007    -2.232112    -3.659120      71.04
 H      -2.373877    -1.497987    -4.699279      21.88
 O      -1.820723    -3.509738    -4.087954     148.94
 H      -0.717459    -3.491101    -4.150572      23.76
 C      -3.938308    -2.275622    -3.458585      65.27
 H      -4.448007    -3.031381    -2.483695      21.33
 O      -4.182571    -0.953653    -3.004837     284.94
 H      -4.980046    -0.680038    -2.852335      31.86
 C      -4.537683    -2.764331    -4.885041      92.73
 O      -5.944399    -2.720787    -4.710817     278.02
 H      -6.251883    -3.604436    -5.315997      24.29
 H      -4.176335    -3.866539    -4.889755      22.84
 H      -4.165209    -2.230545    -5.676392      26.34
55
name = lig-ACN-frame_914
 C       4.011283    -0.556206     0.287477      56.65
 H       3.196208    -0.523696    -0.418840      24.72
 C       4.891300    -0.464183     2.563040      35.03
 H       4.704933    -0.052278     3.581406      17.32
 C       6.075934    -1.198646     2.140706       2.33
 O       7.094929    -1.311759     3.033742     273.04
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 C       7.265541    -0.627467     4.130189      71.85
 H       8.340211    -0.953485     4.513458      22.71
 H       6.522308    -0.696403     4.811884      32.20
 H       7.397576     0.601093     3.753143      27.08
 C       6.196965    -1.604544     0.738230       1.09
 O       7.285786    -2.207651     0.233057     209.07
 H       7.995594    -2.348718     0.838256      26.74
 C       4.998500    -1.451295    -0.170177      35.78
 H       5.062366    -2.105905    -1.131095      18.95
 C       3.887309    -0.129499     1.647192      39.27
 C       2.788859     0.762309     2.067981     105.70
 H       3.160423     1.722372     2.485388      21.63
 O       2.181715     0.398007     3.389876     227.96
 H       1.987490    -0.705628     3.421078      22.26
 C       1.742303     1.153556     1.093511      74.21
 H       2.049475     1.521586     0.160361      22.23
 C       0.510225     2.068166     1.621079      84.50
 O       1.159073     3.449433     1.943237     257.74
 H       1.321659     3.646828     0.917020      26.65
 H       0.148370     1.422808     2.567750      21.44
 H      -0.223463     2.161256     0.879766      24.50
 C      -1.412137    -2.278351    -1.130832      63.98
 H      -1.978269    -3.138547    -0.854324      22.78
 C      -0.794856    -0.458156    -2.722318      32.99
 H      -0.718307    -0.038653    -3.704805      21.42
 C       0.220626     0.070409    -1.651854      -3.63
 O       1.037303     1.259956    -1.948693     216.32
 C       0.422431     2.503530    -2.545152      82.26
 H      -0.219087     2.228960    -3.585764      22.65
 H      -0.319173     2.989525    -1.884299      26.23
 H       1.056521     3.572424    -2.885688      23.23
 C       0.114129    -0.444162    -0.353019       9.62
 O       0.880306    -0.151989     0.732915     125.87
 C      -0.724726    -1.636436    -0.193893      60.25
 H      -0.393542    -2.087367     0.648252      24.30
 C      -1.547104    -1.654306    -2.462404      11.42
 C      -2.338417    -2.248105    -3.720430      72.92
 H      -2.089823    -1.316079    -4.522487      23.17
 O      -1.941954    -3.535581    -4.167552     145.14
 H      -0.842801    -3.607091    -3.689111      21.47
 C      -3.827745    -2.303052    -3.429683      65.42
 H      -3.916877    -3.174210    -2.438367      22.51
 O      -4.166194    -0.872721    -3.057088     244.70
 H      -4.926263    -1.039239    -2.468163      27.84
 C      -4.440199    -2.890025    -4.775331      86.30
 O      -5.892930    -2.691531    -4.763826     312.95
 H      -6.324596    -3.134001    -5.492536      31.04
 H      -4.125587    -3.895016    -5.282285      22.74
 H      -4.091144    -2.100609    -5.432521      25.35
55
name = lig-ACN-frame_915
 C       3.985138    -0.631045     0.262353      51.61
 H       3.345878     0.000163    -0.441729      19.37
 C       4.943990    -0.492418     2.545990      58.87
 H       5.085838     0.101719     3.362826      16.93
 C       6.062739    -1.089148     2.128112       7.77
 O       7.147680    -1.484692     2.945891     245.80
 C       7.298708    -0.506079     4.226368      80.15
 H       8.333407    -0.786605     4.712280      22.77
 H       6.581059    -0.700604     4.981675      31.31
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 H       7.203028     0.709596     3.874277      26.77
 C       6.015786    -1.711207     0.842864       3.42
 O       7.263908    -2.173041     0.297380     190.15
 H       7.740804    -2.647747     1.030156      26.60
 C       5.092940    -1.386827    -0.109989      52.58
 H       5.068958    -1.683209    -1.254909      20.71
 C       3.931690    -0.122887     1.579152      14.88
 C       2.770428     0.811430     2.100265      83.52
 H       3.123901     1.895637     2.002869      22.58
 O       2.188311     0.430144     3.477643     180.34
 H       2.125521    -0.731933     3.326786      20.14
 C       1.545161     0.954118     1.063069      99.31
 H       2.095112     1.475870     0.237175      19.93
 C       0.645519     2.089255     1.621254      97.09
 O       1.059666     3.424521     1.849030     359.49
 H       1.540308     3.777696     1.211980      34.55
 H      -0.128361     2.006921     2.541813      22.36
 H      -0.006723     2.150854     0.786313      24.34
 C      -1.451695    -2.288297    -1.208169      28.97
 H      -2.008117    -3.186123    -0.976260      20.97
 C      -0.744468    -0.500186    -2.612917      48.30
 H      -0.716640    -0.257578    -3.699887      23.14
 C       0.101133     0.190917    -1.802131       6.26
 O       1.113254     1.255105    -1.876045     169.30
 C       0.271434     2.556069    -2.560743      51.94
 H      -0.574782     1.951871    -3.283316      20.55
 H      -0.137137     3.026187    -1.616034      22.28
 H       1.309621     3.033129    -3.094731      21.09
 C       0.116481    -0.404926    -0.491432       2.08
 O       0.852663    -0.227380     0.694481     159.15
 C      -0.698662    -1.483232    -0.130513      29.30
 H      -0.761195    -1.840298     0.892371      22.17
 C      -1.592246    -1.626266    -2.388074      45.81
 C      -2.234278    -2.125181    -3.607494      69.02
 H      -2.094109    -1.497023    -4.679939      23.11
 O      -1.964495    -3.611542    -4.201746     104.35
 H      -1.023642    -4.056514    -3.826330      23.77
 C      -3.695122    -2.332513    -3.453416      71.60
 H      -3.954837    -3.013157    -2.368306      21.39
 O      -4.186243    -0.937745    -3.132601     161.88
 H      -5.151046    -0.782220    -2.460807      22.47
 C      -4.421803    -2.785671    -4.663785      95.13
 O      -5.868059    -2.642302    -4.753001     301.51
 H      -5.993135    -3.164819    -5.466299      31.70
 H      -4.069207    -3.922653    -4.690308      22.70
 H      -3.954217    -2.272881    -5.572053      24.66
55
name = lig-ACN-frame_916
 C       3.931331    -0.571180     0.276834      54.91
 H       3.222300    -0.355001    -0.671178      19.67
 C       4.927774    -0.301851     2.548728      45.29
 H       4.727816    -0.056644     3.504669      15.50
 C       6.091750    -1.228624     2.155028       7.97
 O       7.189929    -1.532276     2.928583     215.24
 C       7.347438    -0.489584     4.236722      51.95
 H       8.406668    -0.658572     4.585628      24.77
 H       6.510693    -0.890482     4.920198      27.90
 H       7.148326     0.721083     3.899596      28.99
 C       6.091872    -1.770003     0.845421      -2.78
 O       7.225178    -2.246743     0.367921     124.95
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 H       7.883593    -2.572129     1.114157      25.33
 C       5.107340    -1.315722    -0.070185      32.08
 H       5.648333    -1.452841    -1.083562      19.78
 C       3.852407    -0.097545     1.623626      20.45
 C       2.674324     0.747768     2.119630     103.02
 H       3.143167     1.777161     2.478566      19.99
 O       2.289294     0.455015     3.451793     288.41
 H       1.965958    -0.548579     3.549038      23.87
 C       1.529306     1.004494     1.090649      95.51
 H       1.946155     1.257092     0.070108      19.88
 C       0.513879     2.110603     1.468327     102.71
 O       1.057211     3.441178     1.800660     320.94
 H       1.712058     3.658154     1.055429      28.95
 H       0.223592     1.615569     2.523789      21.60
 H      -0.378803     2.169168     0.897044      25.50
 C      -1.485508    -2.175262    -1.073097      62.69
 H      -1.915106    -3.181933    -0.851822      22.89
 C      -0.652214    -0.425160    -2.738336      31.16
 H      -0.814663     0.111768    -3.756789      19.97
 C       0.124341     0.269231    -1.661403      11.59
 O       0.953635     1.284991    -1.967012     248.14
 C       0.290132     2.397370    -2.474093     104.96
 H      -0.822819     2.271544    -3.125969      21.54
 H       0.143572     3.331774    -1.747180      23.23
 H       0.990420     2.950717    -3.348970      23.40
 C       0.068354    -0.438663    -0.446321      11.88
 O       0.883980    -0.260603     0.694915     141.44
 C      -0.790977    -1.576510    -0.214860      61.26
 H      -0.925657    -1.680371     0.921869      21.36
 C      -1.409975    -1.596588    -2.440556      20.31
 C      -2.182262    -2.260826    -3.630914      58.14
 H      -1.906796    -1.316686    -4.442361      23.63
 O      -1.917540    -3.627286    -4.139547     230.21
 H      -0.986969    -3.704621    -4.010768      27.86
 C      -3.795659    -2.177016    -3.360142      79.17
 H      -4.005368    -3.116141    -2.471340      22.23
 O      -4.196443    -0.944849    -3.177695     213.29
 H      -5.333658    -0.985080    -3.011181      22.16
 C      -4.397851    -2.794424    -4.640486      87.24
 O      -5.824384    -2.579976    -4.698749     279.01
 H      -6.288770    -3.389091    -5.148495      26.96
 H      -4.320230    -3.956960    -4.582537      22.99
 H      -3.794126    -2.470027    -5.639247      23.42
55
name = lig-ACN-frame_917
 C       4.006278    -0.541810     0.313599      46.54
 H       3.016224    -0.570164    -0.346739      22.28
 C       4.947123    -0.304653     2.499458      52.81
 H       4.864791     0.076062     3.489716      19.74
 C       5.963162    -1.251594     2.295485      -7.33
 O       7.204504    -1.417441     3.030511     252.95
 C       7.368121    -0.650941     4.089140      84.24
 H       8.399852    -0.749818     4.457212      22.24
 H       6.700659    -0.829616     5.129420      26.06
 H       7.112508     0.517425     3.700717      28.55
 C       6.137575    -1.626415     0.899226       6.68
 O       7.284743    -2.451069     0.382485     183.11
 H       8.002808    -2.200757     0.983880      24.07
 C       5.139109    -1.258002    -0.060735      62.60
 H       5.052639    -1.527262    -1.132213      22.62
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 C       3.790860    -0.108512     1.626776      21.40
 C       2.632259     0.778883     2.116807      91.28
 H       3.057012     1.918177     2.035274      20.97
 O       2.312301     0.406159     3.493084     307.04
 H       1.962631    -0.396147     3.476480      30.80
 C       1.609735     1.159206     0.971938      55.89
 H       2.347419     1.679508     0.180747      18.43
 C       0.358350     2.073937     1.472687      88.42
 O       1.077984     3.413247     1.722036     230.10
 H       1.622384     3.636157     0.745779      24.44
 H      -0.054478     1.727958     2.489044      22.49
 H      -0.466552     2.217924     0.751003      22.94
 C      -1.529592    -2.154357    -1.267783      -4.53
 H      -2.371279    -2.914258    -1.093162      20.67
 C      -0.610520    -0.371963    -2.715615      41.95
 H      -0.538495     0.222991    -3.718934      21.23
 C       0.047879     0.114480    -1.628389       6.04
 O       0.842540     1.264591    -2.021202     214.43
 C       0.262173     2.506012    -2.516531      69.84
 H      -0.989829     2.185885    -2.572588      22.59
 H       0.418406     3.258870    -1.586620      21.64
 H       0.811007     2.766880    -3.581004      22.40
 C       0.076401    -0.441522    -0.262759      11.44
 O       0.903366    -0.286496     0.764459      91.65
 C      -0.776109    -1.523160    -0.040041      24.42
 H      -0.643834    -2.211066     0.939072      21.93
 C      -1.267212    -1.679772    -2.573655      35.88
 C      -2.246967    -2.260659    -3.630196      75.78
 H      -2.221426    -1.735521    -4.772420      22.32
 O      -1.806444    -3.587621    -4.002220     224.83
 H      -0.943194    -3.644671    -3.990826      29.89
 C      -3.722286    -2.298867    -3.415243      70.77
 H      -4.133181    -2.629937    -2.285528      22.23
 O      -4.280182    -0.771177    -3.153868     195.66
 H      -5.121136    -0.809659    -3.540413      27.47
 C      -4.409022    -2.959972    -4.630961      78.76
 O      -5.826411    -2.484945    -4.625704     242.59
 H      -6.363529    -3.376790    -5.098126      24.83
 H      -4.108607    -4.063887    -4.727985      23.55
 H      -4.046267    -2.319385    -5.612333      22.42
55
name = lig-ACN-frame_918
 C       3.984987    -0.576715     0.364053      58.80
 H       3.271715    -0.265392    -0.484118      20.30
 C       4.867751    -0.363900     2.615263      38.66
 H       5.043609     0.407349     3.417086      16.54
 C       6.023666    -1.178246     2.211282       4.85
 O       7.068886    -1.457786     2.954345     245.88
 C       7.449279    -0.594730     4.175916      75.60
 H       8.489224    -0.822236     4.313155      23.46
 H       6.709872    -1.076126     5.075645      25.48
 H       7.274766     0.615493     4.060519      27.46
 C       6.226881    -1.608872     0.819539      -6.15
 O       7.205246    -2.514923     0.465180     201.22
 H       8.057710    -2.375778     0.884065      23.16
 C       5.200103    -1.278868    -0.053335      49.97
 H       5.256401    -1.910105    -0.895844      22.11
 C       3.866661    -0.065778     1.666350      21.54
 C       2.725503     0.921874     2.089703      84.80
 H       3.294256     1.874849     2.582483      20.71
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 O       2.254805     0.396781     3.476566     244.94
 H       2.092808    -0.535205     3.380014      25.63
 C       1.495404     1.118108     1.072554      89.09
 H       1.737942     1.487715    -0.092748      16.14
 C       0.464891     2.140831     1.455878      99.00
 O       1.034848     3.339494     1.626418     338.25
 H       1.256368     3.778415     0.722742      26.67
 H      -0.138083     1.964799     2.330557      23.96
 H      -0.255708     2.052481     0.582005      22.85
 C      -1.411404    -2.075534    -1.304719      46.57
 H      -2.106965    -2.975392    -1.227827      20.19
 C      -0.630232    -0.537548    -2.688354      22.64
 H      -0.434118    -0.056102    -3.704713      21.76
 C       0.068968     0.137289    -1.593582      -4.46
 O       0.858073     1.175463    -1.954946     142.37
 C       0.129943     2.589336    -2.495428      67.70
 H      -1.132191     2.769672    -2.617185      22.94
 H       0.687817     3.532309    -1.975548      22.30
 H       0.519837     2.658420    -3.591009      23.69
 C       0.025162    -0.507204    -0.242360     -25.28
 O       1.035148    -0.149398     0.828611     104.27
 C      -0.875299    -1.647494    -0.136584      62.83
 H      -0.818282    -2.334678     0.858657      22.59
 C      -1.395519    -1.625176    -2.641297      49.46
 C      -2.184973    -2.177200    -3.726374      66.02
 H      -2.059799    -1.268434    -4.585618      23.61
 O      -1.756684    -3.632423    -3.886694     203.76
 H      -0.929795    -3.604873    -3.459185      27.70
 C      -3.775963    -2.256880    -3.400298      61.07
 H      -3.944872    -3.081955    -2.426554      22.29
 O      -4.262746    -0.750878    -3.202582     228.24
 H      -4.999607    -0.638975    -3.729935      28.85
 C      -4.461646    -2.921433    -4.617813      88.32
 O      -5.842470    -2.511661    -4.538582     267.67
 H      -6.329881    -2.904310    -5.350951      27.91
 H      -4.510582    -4.037613    -4.616374      24.33
 H      -3.800265    -2.632028    -5.625594      23.91
55
name = lig-ACN-frame_919
 C       4.056263    -0.605522     0.324847      47.33
 H       3.421653    -0.228482    -0.462750      20.85
 C       4.919279    -0.378926     2.628395      33.67
 H       4.864775    -0.117531     3.801519      17.76
 C       6.060984    -0.986835     2.084845      22.92
 O       7.050667    -1.497137     2.977479     246.14
 C       7.504653    -0.601202     4.262411      75.17
 H       8.556527    -0.875491     4.372829      21.04
 H       6.844023    -0.991388     5.349586      24.15
 H       7.302403     0.499583     4.039339      27.91
 C       6.176232    -1.621371     0.853514      26.73
 O       7.122588    -2.550682     0.506521     171.80
 H       7.846868    -2.641400     1.272238      22.95
 C       5.157133    -1.386419    -0.083486      63.46
 H       5.266817    -1.568702    -1.081708      23.38
 C       3.922727     0.029724     1.680057      17.62
 C       2.789094     0.945434     2.189007      89.84
 H       3.038440     2.147196     2.257587      21.49
 O       2.181953     0.441183     3.366085     266.33
 H       2.135096    -0.680541     3.334795      20.88
 C       1.577996     1.115010     1.149481      69.47
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 H       2.309126     1.619804     0.254456      18.76
 C       0.425677     2.092159     1.420395     100.54
 O       1.028300     3.480338     1.567302     341.95
 H       1.256390     3.772177     0.773554      32.62
 H       0.022752     1.841771     2.343260      24.75
 H      -0.396965     2.175748     0.632055      22.71
 C      -1.523336    -2.289305    -1.304701      23.82
 H      -1.834896    -3.306712    -1.035255      20.37
 C      -0.536787    -0.474171    -2.727059      37.42
 H      -0.428797     0.007894    -3.702647      21.84
 C       0.060239     0.084904    -1.552280      -4.99
 O       0.836068     1.284892    -1.878331     163.58
 C       0.137495     2.543017    -2.511178      77.68
 H      -1.022581     2.415120    -2.038887      23.39
 H       0.737797     3.387765    -1.922483      22.00
 H       0.203353     2.449480    -3.603073      23.95
 C       0.086169    -0.474415    -0.248034      22.92
 O       0.932196    -0.257913     0.794707     130.30
 C      -0.723424    -1.638195    -0.209810      35.91
 H      -1.145827    -2.077869     0.800062      21.05
 C      -1.536202    -1.507946    -2.504686      18.68
 C      -2.218721    -2.196316    -3.755632      76.85
 H      -1.860371    -1.876926    -4.888288      25.08
 O      -1.874852    -3.588391    -3.840042     185.99
 H      -0.849849    -3.826581    -3.671737      25.00
 C      -3.743153    -2.109026    -3.489447      76.85
 H      -3.908719    -2.673412    -2.320875      22.35
 O      -4.156459    -0.892177    -3.267807     217.57
 H      -5.243766    -0.929490    -3.612809      22.66
 C      -4.513530    -2.883375    -4.549695      93.40
 O      -5.914842    -2.516827    -4.523886     310.89
 H      -6.182398    -2.593769    -5.344363      33.30
 H      -4.275537    -3.910897    -4.267106      25.72
 H      -4.213811    -2.673931    -5.713353      24.45
55
name = lig-ACN-frame_920
 C       4.087876    -0.444353     0.352719      61.76
 H       3.286579    -0.348057    -0.255821      24.93
 C       4.963924    -0.296846     2.532604      61.13
 H       4.658157    -0.446088     3.694523      18.65
 C       6.193054    -0.962498     2.215290      12.12
 O       7.117044    -1.444446     3.125312     285.55
 C       7.507992    -0.728210     4.190081     107.12
 H       8.597420    -0.848716     4.395029      21.57
 H       6.832226    -0.930194     5.331112      25.01
 H       7.322954     0.344409     4.012246      33.11
 C       6.094713    -1.653059     0.824109      -5.41
 O       7.096934    -2.594293     0.565592     120.99
 H       7.490822    -2.809892     1.474034      27.48
 C       5.054229    -1.398027    -0.119972      80.82
 H       5.065191    -1.730699    -1.107368      20.57
 C       3.981829     0.040531     1.609011      30.75
 C       2.653385     0.876179     2.125517      96.89
 H       3.210163     1.924174     2.454076      20.76
 O       2.133021     0.495418     3.371723     273.82
 H       1.935543    -0.668475     3.322012      19.99
 C       1.724413     1.149102     1.046478      41.45
 H       2.219435     1.405966    -0.127502      16.69
 C       0.471256     2.146454     1.473898      83.34
 O       0.967446     3.581874     1.542389     292.68
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 H       1.583685     3.721366     0.726983      26.72
 H       0.050107     2.000411     2.376887      24.43
 H      -0.344954     1.890961     0.680021      23.49
 C      -1.488022    -2.271255    -1.248652      47.12
 H      -2.191502    -3.064466    -1.257570      22.05
 C      -0.648011    -0.426141    -2.630846      47.98
 H      -0.588459     0.063733    -3.554735      23.81
 C       0.180325     0.217120    -1.660200      14.71
 O       0.840418     1.394111    -1.766887     247.72
 C       0.150210     2.341463    -2.413733     113.89
 H      -1.012295     2.509138    -1.909559      24.56
 H       0.694007     3.359481    -2.294990      24.67
 H      -0.052633     2.298024    -3.459728      25.84
 C       0.112475    -0.514502    -0.405400     -22.49
 O       0.850729    -0.354010     0.823431      17.83
 C      -0.699212    -1.719445    -0.207366      59.87
 H      -0.417082    -2.048842     0.853721      22.07
 C      -1.504114    -1.559055    -2.506587      32.31
 C      -2.196096    -2.197926    -3.705615      84.76
 H      -1.976715    -1.424982    -4.652102      26.03
 O      -2.045781    -3.639810    -3.803007     143.53
 H      -0.924359    -3.598225    -4.057492      23.77
 C      -3.664579    -2.191775    -3.553488      76.30
 H      -3.790862    -2.939415    -2.508026      23.63
 O      -4.147416    -0.776449    -3.372794     141.75
 H      -5.290472    -0.899227    -2.998606      22.33
 C      -4.546764    -2.923193    -4.536532      89.78
 O      -6.012570    -2.503264    -4.468129     220.32
 H      -6.381849    -2.683559    -5.479652      25.23
 H      -4.513438    -3.999154    -4.487767      25.57
 H      -4.068160    -2.610175    -5.599486      25.16
55
name = lig-ACN-frame_921
 C       4.015466    -0.359756     0.223116      38.92
 H       3.259695    -0.151398    -0.419620      23.44
 C       5.052303    -0.250397     2.559173      32.39
 H       4.950503     0.410366     3.569400      16.07
 C       6.138586    -1.089701     2.167289      12.10
 O       7.136450    -1.514735     3.066511     267.13
 C       7.547620    -0.653427     4.276984      67.61
 H       8.603311    -1.041927     4.465932      21.92
 H       6.783797    -1.212692     5.184092      23.63
 H       7.449254     0.371829     4.177360      30.86
 C       6.140196    -1.649511     0.931340      -0.46
 O       7.037103    -2.633751     0.616442     197.30
 H       7.669509    -2.844395     1.280262      24.99
 C       5.070196    -1.318147    -0.012312       9.14
 H       4.956962    -2.110697    -0.742899      20.03
 C       3.949597     0.068374     1.642530      12.74
 C       2.763928     0.818688     2.026867      84.18
 H       3.054741     1.971611     2.297812      22.53
 O       2.076750     0.488333     3.419671     228.10
 H       1.686609    -0.528572     3.492541      22.58
 C       1.527732     1.109177     0.978032      69.17
 H       1.890726     1.444514    -0.248870      14.68
 C       0.662560     2.216098     1.459172      99.99
 O       0.875279     3.581199     1.489487     308.18
 H       1.778318     3.880639     0.869263      25.80
 H       0.452350     1.885536     2.415304      23.95
 H      -0.288189     2.218695     0.775915      23.11
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 C      -1.466007    -2.160015    -1.234301      40.78
 H      -1.994499    -2.993709    -0.901224      25.27
 C      -0.776560    -0.340290    -2.665840      57.86
 H      -0.999526     0.072610    -3.580656      23.26
 C       0.168681     0.134995    -1.605853      -5.75
 O       0.940183     1.387264    -1.631528     190.25
 C       0.047090     2.400599    -2.439692      85.22
 H      -0.993283     2.629308    -1.795167      24.62
 H       0.699749     3.269329    -2.556623      25.82
 H      -0.118649     1.869268    -3.275354      26.29
 C       0.180086    -0.633358    -0.414878      10.29
 O       0.865024    -0.257872     0.789722      97.29
 C      -0.603723    -1.751505    -0.212249      61.56
 H      -0.494682    -2.537975     0.493310      23.78
 C      -1.338579    -1.623152    -2.492851      36.27
 C      -2.224831    -2.132517    -3.643583      62.08
 H      -1.784225    -1.683038    -4.678059      23.15
 O      -2.073687    -3.684324    -3.846006     147.88
 H      -1.091931    -4.132728    -3.790492      25.45
 C      -3.836092    -2.194346    -3.448935      63.00
 H      -4.103146    -2.631694    -2.262003      23.09
 O      -4.151743    -0.705389    -3.445636     203.52
 H      -4.948291    -0.526377    -2.741050      25.47
 C      -4.633172    -2.939911    -4.672317      88.30
 O      -6.017391    -2.497158    -4.409653     202.47
 H      -6.535242    -3.068984    -5.247978      25.23
 H      -4.577563    -4.003780    -4.584415      26.06
 H      -4.293033    -2.633838    -5.750796      24.38
55
name = lig-ACN-frame_922
 C       4.071744    -0.433413     0.312421      62.13
 H       3.490592    -0.130897    -0.530817      23.88
 C       5.052223    -0.123777     2.537242      64.02
 H       5.425417     0.563391     3.355959      18.30
 C       6.025115    -1.102875     2.320559      13.96
 O       7.165199    -1.535545     2.969208     210.25
 C       7.544324    -0.696988     4.330772      89.65
 H       8.636405    -0.962626     4.505694      23.37
 H       6.781946    -0.888439     5.404710      24.36
 H       7.454908     0.309889     4.177144      31.86
 C       6.086574    -1.682008     0.951520      16.31
 O       6.989590    -2.707551     0.589645     125.97
 H       7.777338    -2.521597     1.193015      22.94
 C       5.137074    -1.305529     0.080350      72.87
 H       5.226324    -1.750632    -0.992580      21.06
 C       3.975676     0.054525     1.578543      29.67
 C       2.657531     0.918295     2.068964      89.09
 H       3.061313     2.033412     2.144491      22.92
 O       2.111916     0.514373     3.352165     310.44
 H       2.087199    -0.418154     3.324601      28.54
 C       1.596768     1.025434     0.953556      84.32
 H       2.388438     1.492594     0.010076      19.30
 C       0.547365     2.147592     1.489706      81.01
 O       0.908192     3.657042     1.454046     287.21
 H       1.687680     3.870239     0.732503      25.78
 H       0.439617     2.051520     2.552301      23.34
 H      -0.510448     1.882091     1.092727      25.07
 C      -1.396426    -2.234370    -1.222843      35.14
 H      -1.872568    -3.190058    -1.290873      24.59
 C      -0.720300    -0.296885    -2.640467      59.42
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 H      -0.776468     0.430036    -3.465428      22.68
 C       0.086117     0.072867    -1.579382       3.18
 O       0.842952     1.343298    -1.635214     187.99
 C       0.097541     2.389551    -2.436803     115.18
 H      -0.770107     2.743096    -1.635999      25.35
 H       0.647053     3.240349    -2.666930      28.13
 H      -0.399879     2.136718    -3.308358      27.30
 C       0.297138    -0.622954    -0.301063      11.80
 O       0.894657    -0.108546     0.766557     156.80
 C      -0.490539    -1.839126    -0.192231      54.88
 H      -0.548950    -2.095921     0.804575      24.52
 C      -1.410751    -1.592951    -2.557028      16.24
 C      -2.325313    -2.331781    -3.598175      86.25
 H      -2.278257    -1.705697    -4.624044      25.50
 O      -2.056257    -3.698680    -3.874677     257.81
 H      -1.240812    -3.706897    -3.500860      31.71
 C      -3.908932    -2.023482    -3.466001      74.96
 H      -4.454055    -2.640380    -2.453411      24.47
 O      -4.158314    -0.696350    -3.478806     294.42
 H      -4.740453    -0.448754    -2.937632      34.53
 C      -4.673446    -2.849234    -4.625897      97.54
 O      -6.040571    -2.542924    -4.419238     320.48
 H      -6.665668    -3.181810    -4.667730      31.57
 H      -4.332103    -3.860416    -4.568760      25.59
 H      -4.346057    -2.409890    -5.623064      25.00
55
name = lig-ACN-frame_923
 C       4.130391    -0.521097     0.418329      38.32
 H       3.317212    -0.310718    -0.358366      25.97
 C       5.057879    -0.015137     2.541909      43.14
 H       4.776631     0.461839     3.459824      20.03
 C       6.039029    -1.152057     2.301702      11.22
 O       7.192806    -1.428899     3.090153     249.33
 C       7.512001    -0.771278     4.217602      92.33
 H       8.540625    -1.110244     4.506391      22.30
 H       6.666989    -1.202129     5.165003      24.29
 H       7.481742     0.279013     4.047521      30.78
 C       6.029909    -1.817787     1.041004      13.19
 O       6.949127    -2.708465     0.602333     175.25
 H       7.878914    -2.793903     1.056389      20.67
 C       5.201417    -1.359636    -0.059908      29.98
 H       5.578950    -1.337471    -1.197190      21.81
 C       3.920039     0.188273     1.690614      17.15
 C       2.733913     1.004457     2.081763     109.16
 H       3.025660     2.109614     2.384419      23.59
 O       2.199086     0.538198     3.276486     321.99
 H       2.200513    -0.338403     3.399124      31.99
 C       1.704850     1.283959     1.024818      66.60
 H       2.074189     1.507836    -0.174174      19.25
 C       0.468851     2.190142     1.549278      89.42
 O       0.915025     3.592850     1.407818     339.19
 H       1.219965     3.647441     0.560933      31.97
 H       0.333668     1.887176     2.641313      23.47
 H      -0.464075     2.027667     0.924982      25.18
 C      -1.190746    -2.346475    -1.329215      25.27
 H      -1.832451    -3.188550    -0.978789      22.35
 C      -0.704253    -0.446763    -2.587397      44.37
 H      -0.623678     0.070713    -3.637644      22.39
 C       0.101288     0.153957    -1.545642      27.96
 O       0.666992     1.288767    -1.758374     242.49
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 C       0.172830     2.421216    -2.329500     115.63
 H      -0.676815     3.072559    -1.615277      24.51
 H       1.040934     2.905196    -2.425598      27.50
 H      -0.256349     2.163780    -3.332354      24.71
 C       0.227035    -0.618102    -0.371383      11.85
 O       0.926801    -0.140856     0.828339      74.59
 C      -0.441466    -1.834673    -0.163190      57.85
 H      -0.518182    -2.256077     0.764071      24.01
 C      -1.558901    -1.587972    -2.466892      16.66
 C      -2.470995    -2.273892    -3.644533      88.35
 H      -2.076887    -1.702531    -4.590484      26.23
 O      -2.001355    -3.706610    -3.827855     199.00
 H      -1.078077    -3.818871    -3.741230      30.34
 C      -3.932642    -2.125295    -3.472967      81.23
 H      -4.268814    -2.469022    -2.266309      23.65
 O      -4.156659    -0.561346    -3.515509     172.12
 H      -5.077341    -0.511715    -3.080475      26.63
 C      -4.633646    -2.688156    -4.571614     108.16
 O      -6.148008    -2.589929    -4.392687     296.52
 H      -6.250031    -3.467994    -4.684512      29.77
 H      -4.481053    -3.768232    -4.589716      26.54
 H      -4.301552    -2.292004    -5.514862      27.03
55
name = lig-ACN-frame_924
 C       4.066362    -0.496897     0.400405      57.74
 H       3.192695    -0.197583    -0.345923      20.69
 C       5.087978    -0.102972     2.650241      69.71
 H       5.278582     0.275436     3.554390      22.38
 C       6.021072    -1.038631     2.282528       6.02
 O       7.125627    -1.440705     2.987716     218.69
 C       7.483099    -0.732036     4.284402      90.88
 H       8.459446    -1.153628     4.537979      23.77
 H       6.621791    -1.044956     5.252208      24.78
 H       7.470315     0.329876     4.316743      29.21
 C       6.024487    -1.831041     1.020744       8.60
 O       6.992651    -2.779165     0.621800     208.79
 H       7.539331    -2.897083     1.406454      22.84
 C       5.187139    -1.299386     0.073587      43.81
 H       5.248626    -1.821894    -1.038585      22.69
 C       4.073518     0.141315     1.627115      27.07
 C       2.914440     1.144202     2.059274      74.40
 H       3.395113     2.138887     2.283044      25.07
 O       2.244834     0.566502     3.347212     199.71
 H       1.950726    -0.389014     3.036502      25.14
 C       1.527764     1.368385     1.023688      50.88
 H       1.941642     1.984649     0.045219      19.25
 C       0.516013     2.230321     1.507657     106.94
 O       0.862001     3.534247     1.429791     328.74
 H       1.113703     3.843957     0.547916      30.42
 H       0.103450     2.123493     2.632504      22.95
 H      -0.398801     1.973250     0.895447      24.95
 C      -1.175907    -2.458461    -1.242049      47.65
 H      -1.611861    -3.500446    -1.016605      21.94
 C      -0.767925    -0.587791    -2.645438      46.21
 H      -0.840850    -0.095326    -3.704699      22.48
 C      -0.079503     0.027145    -1.601476       1.87
 O       0.703593     1.270565    -1.782712     186.22
 C       0.247211     2.577108    -2.347554     100.86
 H      -0.577305     3.210875    -1.492012      23.62
 H       0.993571     3.248780    -2.409679      27.91
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 H      -0.334802     2.586190    -3.365194      24.81
 C       0.212435    -0.516403    -0.219067       3.50
 O       0.973950    -0.193759     0.837859      80.15
 C      -0.429818    -1.820987    -0.286130      56.19
 H      -0.114912    -2.530810     0.437833      24.48
 C      -1.557297    -1.700838    -2.375779      39.72
 C      -2.262374    -2.148358    -3.603203      79.41
 H      -2.148566    -1.632177    -4.608606      26.97
 O      -2.022118    -3.669218    -3.766280     124.46
 H      -0.932872    -3.551192    -3.960930      25.40
 C      -3.898390    -1.993570    -3.384747      51.98
 H      -4.267624    -2.572201    -2.258579      23.88
 O      -4.163296    -0.554434    -3.474752     127.75
 H      -5.310551    -0.256374    -3.398869      23.52
 C      -4.757853    -2.671880    -4.603831      93.76
 O      -6.176200    -2.667819    -4.387010     231.44
 H      -6.751459    -3.398977    -5.019356      25.85
 H      -4.298488    -3.652788    -4.829242      25.21
 H      -4.545123    -2.040474    -5.418101      27.51
55
name = lig-ACN-frame_925
 C       4.061772    -0.387657     0.377856      43.34
 H       3.317908    -0.203591    -0.523464      21.94
 C       5.084189    -0.192529     2.660508      61.74
 H       5.214139     0.564726     3.310625      23.05
 C       6.133250    -1.098760     2.195097      17.33
 O       7.139567    -1.436919     2.978486     219.41
 C       7.439081    -0.726914     4.379235      60.47
 H       8.413781    -1.107488     4.567277      23.81
 H       6.554723    -1.072540     5.260815      23.40
 H       7.491468     0.343400     4.031039      25.63
 C       6.085363    -1.709803     0.970694       9.19
 O       6.979755    -2.798963     0.718177     194.86
 H       7.564523    -3.011586     1.453190      22.52
 C       5.030199    -1.388947     0.099695      46.96
 H       4.803633    -2.175014    -0.758564      21.94
 C       4.070955     0.209098     1.665602       3.35
 C       2.866663     1.121321     2.052736     108.37
 H       3.169898     2.109433     2.302444      25.59
 O       2.370064     0.686391     3.332130     202.44
 H       1.755449    -0.304775     3.170193      22.42
 C       1.681057     1.200305     1.056375      74.77
 H       1.911433     1.375184    -0.064042      19.99
 C       0.325292     2.186111     1.514723      70.80
 O       0.819628     3.689990     1.491284     212.50
 H       1.350862     3.780995     0.489647      24.15
 H       0.240516     1.969200     2.722813      21.92
 H      -0.582133     1.996303     0.931814      24.64
 C      -1.288494    -2.506555    -1.140912      44.80
 H      -1.355744    -3.655216    -1.250835      23.22
 C      -0.838043    -0.559072    -2.601284      34.44
 H      -0.929646     0.059394    -3.524759      22.90
 C      -0.059011     0.175612    -1.545035      -3.81
 O       0.759944     1.269410    -1.848838     189.23
 C       0.260720     2.682126    -2.331256      78.22
 H      -0.541564     3.040938    -1.344133      21.98
 H       1.176658     3.192578    -2.408754      25.82
 H      -0.305324     2.501009    -3.349329      23.73
 C       0.044758    -0.529269    -0.324964     -11.76
 O       1.054109    -0.111142     0.817602      53.10
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 C      -0.314941    -1.918226    -0.194473      23.31
 H       0.129094    -2.346430     0.742792      22.59
 C      -1.423380    -1.827387    -2.415959      22.71
 C      -2.322793    -2.233793    -3.538638      99.96
 H      -1.845621    -1.570128    -4.283246      26.40
 O      -2.047131    -3.540309    -3.761505     203.27
 H      -0.996732    -3.896828    -3.866587      24.35
 C      -3.911339    -1.917329    -3.471690      71.43
 H      -4.231763    -2.411342    -2.277908      23.76
 O      -4.151272    -0.546400    -3.383507     162.62
 H      -5.307209    -0.562309    -3.365494      23.83
 C      -4.750533    -2.615634    -4.631966      99.11
 O      -6.219280    -2.772878    -4.330161     235.24
 H      -6.489903    -2.987057    -5.373050      26.02
 H      -4.394987    -3.630889    -4.974483      25.00
 H      -4.636777    -1.977105    -5.421651      28.58
55
name = lig-ACN-frame_926
 C       4.121266    -0.354664     0.384119      42.42
 H       3.231468    -0.074880    -0.252120      24.15
 C       5.061859    -0.128396     2.486939      58.78
 H       5.036485     0.061973     3.529577      22.06
 C       6.136040    -1.012078     2.241811     -17.33
 O       7.301558    -1.463611     3.150119     241.64
 C       7.401524    -0.763800     4.253522     102.55
 H       8.277180    -1.070618     4.844933      24.51
 H       6.430515    -0.946146     5.088620      25.51
 H       7.346416     0.385865     4.336827      26.47
 C       6.117436    -1.714186     0.904229     -12.36
 O       6.883791    -2.785424     0.760307     134.73
 H       7.755186    -2.626440     1.322324      20.77
 C       4.912556    -1.546092     0.073614      44.61
 H       4.946806    -2.043260    -0.940779      19.25
 C       3.997229     0.268369     1.638628      37.64
 C       2.762409     1.076360     2.051616     106.82
 H       2.972557     2.081631     1.987517      27.69
 O       2.452185     0.802709     3.386032     237.58
 H       2.168755    -0.255451     3.542892      25.11
 C       1.615576     1.126387     0.966674      78.14
 H       2.252471     1.719267     0.241513      22.93
 C       0.472803     2.254756     1.522963      87.87
 O       0.707038     3.696978     1.536571     269.04
 H       1.546811     3.792086     0.836861      26.14
 H       0.076339     1.917969     2.655014      23.17
 H      -0.394544     2.127116     0.917692      25.46
 C      -1.135983    -2.499818    -1.082059      42.87
 H      -1.662797    -3.472523    -0.756514      23.33
 C      -0.855050    -0.393222    -2.424150      47.29
 H      -1.007184    -0.081685    -3.402402      25.41
 C      -0.050670     0.278370    -1.567910      10.11
 O       0.790096     1.319404    -1.924394     225.07
 C       0.275646     2.564945    -2.260336     110.74
 H      -0.429188     3.323977    -1.418488      23.34
 H       1.175280     3.270896    -2.380289      25.05
 H      -0.285207     2.582704    -3.307556      24.62
 C       0.148614    -0.520735    -0.282429     -29.12
 O       1.010108    -0.175680     0.734740     121.96
 C      -0.354133    -1.919605    -0.110018      40.99
 H      -0.212532    -2.542786     0.870908      24.45
 C      -1.359251    -1.719327    -2.287935      31.11
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 C      -2.361098    -2.186179    -3.565657      82.30
 H      -2.216765    -1.665884    -4.533974      26.29
 O      -2.127410    -3.661642    -3.842299     233.59
 H      -1.215966    -3.592552    -3.611803      29.79
 C      -3.901009    -2.043545    -3.495205      66.31
 H      -4.455029    -2.694615    -2.473622      23.62
 O      -4.166661    -0.491822    -3.315989     215.28
 H      -5.038601    -0.360524    -2.979136      28.77
 C      -4.685691    -2.541785    -4.661071     103.57
 O      -6.177289    -2.828948    -4.303873     288.12
 H      -6.600954    -2.979859    -5.075527      33.68
 H      -4.217090    -3.578500    -4.777814      25.28
 H      -4.620746    -1.998423    -5.492242      29.41
55
name = lig-ACN-frame_927
 C       4.046916    -0.478744     0.287121      51.37
 H       3.416675    -0.336342    -0.549026      24.67
 C       5.138919    -0.045880     2.516355      38.43
 H       4.877007     0.360761     3.613241      19.37
 C       6.182917    -0.990610     2.170767      18.12
 O       7.275770    -1.468196     3.020682     183.79
 C       7.354883    -0.681442     4.436153      71.00
 H       8.289298    -1.069158     4.893475      23.87
 H       6.341125    -1.088460     4.960493      24.52
 H       7.431808     0.408672     4.011373      23.79
 C       5.974950    -1.724401     1.033546      21.00
 O       6.866629    -2.812836     0.728985     115.33
 H       7.798515    -2.711127     1.126903      23.57
 C       5.000274    -1.468047     0.112720      63.90
 H       5.065575    -1.886978    -0.838431      24.01
 C       4.032321     0.204564     1.529157       4.53
 C       2.745474     1.100956     1.970333      95.80
 H       3.094807     2.018256     2.079199      28.34
 O       2.468591     0.844482     3.522170     227.27
 H       2.537810    -0.042659     3.593083      32.14
 C       1.523938     1.254417     1.003514      91.36
 H       1.727051     1.467344    -0.096065      21.23
 C       0.564536     2.218782     1.462598     104.23
 O       0.679414     3.645222     1.567141     340.95
 H       1.341602     4.069623     1.184033      35.17
 H       0.293765     1.956038     2.639450      23.54
 H      -0.276092     2.002097     0.843423      27.29
 C      -1.051660    -2.408987    -1.122033      43.73
 H      -1.773380    -3.223747    -0.923558      22.98
 C      -0.941089    -0.341740    -2.434357      28.39
 H      -1.064106     0.296063    -3.214375      22.70
 C       0.008493     0.201995    -1.397659       7.75
 O       0.841700     1.298288    -1.911775     209.34
 C       0.266716     2.606759    -2.281572      77.12
 H      -0.411982     2.871172    -1.149417      22.00
 H       1.200980     3.356555    -2.531554      23.22
 H      -0.489646     2.519099    -3.141138      24.13
 C       0.286163    -0.552085    -0.318038      38.93
 O       1.039700    -0.188195     0.750802     131.64
 C      -0.414631    -1.704313    -0.069975      39.34
 H      -0.158692    -2.157451     1.010825      21.91
 C      -1.530570    -1.630074    -2.255261      13.80
 C      -2.352320    -2.193890    -3.547163      75.57
 H      -1.901014    -1.529330    -4.267621      26.68
 O      -2.169880    -3.723749    -3.885632     237.58
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 H      -1.367964    -4.077088    -3.751774      32.49
 C      -3.972717    -1.954368    -3.382802      63.52
 H      -4.259835    -2.721432    -2.335953      23.88
 O      -4.164679    -0.556577    -3.255346     302.77
 H      -4.732376    -0.397651    -2.654533      33.90
 C      -4.691668    -2.617917    -4.716949      98.61
 O      -6.016077    -2.807962    -4.268154     275.33
 H      -6.443708    -3.389993    -4.975135      29.51
 H      -4.194817    -3.546215    -5.168065      25.61
 H      -4.603687    -1.888903    -5.420385      29.26
55
name = lig-ACN-frame_928
 C       3.958995    -0.568598     0.242108      43.90
 H       3.282760    -0.312195    -0.468006      22.69
 C       5.097843     0.012735     2.455957      57.01
 H       5.400759     0.978713     3.106236      21.30
 C       6.148026    -0.948467     2.249710      10.03
 O       7.202503    -1.352197     2.962278     229.68
 C       7.307290    -0.705016     4.399005      89.41
 H       8.299141    -1.097550     4.840941      24.45
 H       6.477801    -0.775477     5.162399      27.52
 H       7.332110     0.527082     4.390046      24.55
 C       6.022392    -1.855225     1.096339       1.67
 O       6.836087    -2.820917     0.669316     223.34
 H       7.532429    -2.958533     1.298990      23.62
 C       5.120408    -1.395454     0.026364      36.39
 H       5.165656    -2.074901    -0.720668      24.95
 C       4.012147     0.158128     1.545940      23.84
 C       2.937705     1.162748     1.995406      97.15
 H       3.237698     2.102599     2.057963      28.15
 O       2.481374     0.854564     3.470529     192.84
 H       2.258874    -0.060011     3.534460      28.78
 C       1.694178     1.229541     0.964548      88.36
 H       2.141741     1.661271     0.068525      23.15
 C       0.368793     2.154743     1.506992      85.29
 O       0.697004     3.648286     1.603002     286.44
 H       1.389589     3.626501     0.880510      28.66
 H       0.226957     1.746381     2.601682      23.30
 H      -0.568477     2.023074     0.994897      24.61
 C      -1.245165    -2.247932    -1.142930      51.39
 H      -1.175751    -3.305426    -1.027394      23.12
 C      -0.991728    -0.286424    -2.368395      44.31
 H      -1.284226     0.313296    -3.204323      23.97
 C       0.037316     0.192406    -1.586305      10.65
 O       0.893576     1.221943    -1.856485     208.32
 C       0.181249     2.565743    -2.230068      82.41
 H      -0.358112     3.322258    -1.248748      21.43
 H       1.158193     3.271964    -2.632009      22.79
 H      -0.488048     2.413642    -3.099668      23.98
 C       0.350824    -0.482479    -0.270191     -20.18
 O       1.147036    -0.104662     0.931359     115.96
 C      -0.443190    -1.660317    -0.084744      28.05
 H      -0.385580    -2.171748     0.984122      22.21
 C      -1.587130    -1.579910    -2.317197      41.50
 C      -2.330398    -2.263227    -3.444513     102.71
 H      -2.067192    -1.831656    -4.371453      25.67
 O      -2.243065    -3.656602    -3.870900     225.03
 H      -1.156802    -3.838173    -3.781550      25.94
 C      -3.838844    -2.033167    -3.420899      65.00
 H      -4.374857    -2.483066    -2.321740      22.12
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 O      -4.176464    -0.609374    -3.219694     230.17
 H      -4.978707    -0.538752    -2.505276      24.22
 C      -4.582176    -2.532086    -4.661713     109.54
 O      -5.957888    -2.845558    -4.258056     215.09
 H      -6.259825    -3.804920    -4.793112      26.51
 H      -4.143910    -3.487350    -5.048939      26.08
 H      -4.610511    -1.803003    -5.383398      29.06
55
name = lig-ACN-frame_929
 C       4.039043    -0.583218     0.379523      64.55
 H       3.247228    -0.599178    -0.278644      25.50
 C       5.143766     0.084231     2.310621      42.83
 H       5.353786     0.900971     3.151748      20.56
 C       5.985119    -1.024953     2.212073      24.88
 O       7.185625    -1.162834     3.105705     245.58
 C       7.307222    -0.708683     4.313237      98.44
 H       8.280441    -1.206677     4.719518      23.98
 H       6.454765    -1.193937     4.851069      26.63
 H       7.444465     0.552773     4.371954      24.20
 C       5.976365    -1.746792     0.982850      21.21
 O       6.854003    -2.887997     0.663921     137.58
 H       7.559124    -3.053829     1.341929      22.33
 C       5.112441    -1.451367    -0.013868      87.23
 H       5.184669    -1.834144    -0.952985      24.55
 C       3.979028     0.144100     1.522480      33.55
 C       2.974719     1.191613     2.068341     102.33
 H       3.549229     2.065585     2.167715      25.45
 O       2.517360     0.867829     3.310682     218.70
 H       1.867823    -0.010043     3.098383      23.78
 C       1.775576     1.290225     1.101221      74.03
 H       2.093513     1.662426     0.168959      24.17
 C       0.361884     2.161317     1.595926      92.54
 O       0.724275     3.526183     1.596820     220.02
 H       1.207009     3.857032     0.618078      25.32
 H       0.098044     1.979023     2.618869      25.06
 H      -0.410865     1.896775     0.861904      23.86
 C      -1.330505    -2.212806    -1.023550      55.82
 H      -1.673610    -3.215200    -1.036900      24.55
 C      -1.049857    -0.237964    -2.447130      64.54
 H      -1.204618     0.328724    -3.453597      21.36
 C       0.145777     0.148908    -1.510347      -7.01
 O       0.868251     1.317589    -1.845851     217.08
 C       0.213004     2.457027    -2.234438      75.68
 H      -0.324522     2.973720    -1.083986      21.29
 H       1.108743     3.209185    -2.783107      21.55
 H      -0.618474     2.265719    -2.905222      23.91
 C       0.276557    -0.421028    -0.180749      10.88
 O       1.177631    -0.072555     0.888066     136.00
 C      -0.435889    -1.642132    -0.106598      53.69
 H      -0.295181    -2.386110     0.722846      23.22
 C      -1.529534    -1.571812    -2.308636       6.29
 C      -2.355217    -2.164472    -3.548595      95.09
 H      -2.023034    -1.527631    -4.307261      26.15
 O      -2.196153    -3.623770    -3.741340     182.63
 H      -1.075339    -3.840410    -3.945432      24.41
 C      -3.832154    -2.067998    -3.344615      69.60
 H      -4.128768    -3.117280    -2.626619      22.36
 O      -4.171053    -0.629424    -3.198348     127.00
 H      -5.326152    -0.618545    -2.826172      21.80
 C      -4.500488    -2.489368    -4.614699      94.52
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 O      -5.951877    -2.913092    -4.271160     241.62
 H      -6.061493    -3.874021    -4.708396      27.52
 H      -3.942754    -3.323432    -5.022729      26.90
 H      -4.479126    -1.693142    -5.356724      28.04
55
name = lig-ACN-frame_930
 C       3.988959    -0.611318     0.332119      50.30
 H       3.096031    -0.521589    -0.322990      22.57
 C       5.219066     0.113706     2.325906      51.90
 H       5.099878     0.544971     3.373055      21.37
 C       6.047772    -1.040241     2.191711      14.51
 O       7.134818    -1.104508     2.889354     205.58
 C       7.274895    -0.676497     4.480622      79.78
 H       8.316017    -1.096298     4.779497      25.03
 H       6.516045    -0.897515     5.182222      28.85
 H       7.228664     0.586772     4.561423      24.08
 C       6.117241    -1.807749     0.907063       6.62
 O       6.828709    -2.884960     0.717320     138.19
 H       7.767852    -2.721631     1.171637      21.60
 C       5.017527    -1.480040    -0.022778      58.25
 H       4.997544    -1.840320    -1.049470      22.04
 C       4.034790     0.216528     1.536698      21.20
 C       2.933187     1.184415     1.934867      94.75
 H       3.294835     2.270962     2.061288      23.90
 O       2.497486     0.812625     3.313364     178.05
 H       1.817445    -0.122090     3.287197      22.07
 C       1.641155     1.428950     1.159131      83.48
 H       1.831015     1.832860     0.271943      23.79
 C       0.568705     2.135878     1.616914     122.84
 O       0.754913     3.529191     1.574076     279.84
 H       0.758420     3.843049     0.594652      27.74
 H       0.200217     1.938873     2.518804      26.68
 H      -0.270309     1.824512     0.947871      24.19
 C      -1.356518    -2.234270    -1.035726      34.13
 H      -2.061374    -2.799055    -0.521988      19.49
 C      -0.780930    -0.305201    -2.394681      22.83
 H      -0.762699     0.305149    -3.387392      19.94
 C       0.017719     0.233612    -1.445436      19.37
 O       0.925015     1.271467    -1.805998     229.16
 C       0.154507     2.456151    -2.258477      73.35
 H      -0.322925     3.194971    -1.171849      21.53
 H       0.917164     3.294918    -2.836427      21.87
 H      -0.645083     2.201902    -2.941313      23.56
 C       0.207982    -0.397070    -0.209556       4.65
 O       1.170562    -0.128430     0.761936      94.76
 C      -0.412733    -1.715752     0.007526      17.59
 H      -0.047134    -2.106783     0.933523      21.60
 C      -1.534321    -1.481496    -2.320412      41.25
 C      -2.261294    -2.040823    -3.539964      94.29
 H      -2.024941    -1.694246    -4.458883      27.65
 O      -2.046279    -3.565423    -3.601693     198.37
 H      -1.124683    -3.788794    -3.884378      28.40
 C      -3.891086    -2.024831    -3.343473      69.19
 H      -4.120682    -2.366627    -2.136847      19.69
 O      -4.190215    -0.700565    -3.093954     188.14
 H      -5.289295    -0.439272    -3.040959      24.44
 C      -4.577302    -2.577549    -4.642413     103.20
 O      -5.869080    -2.976982    -4.332242     324.54
 H      -6.070293    -3.651726    -4.851545      34.84
 H      -4.085402    -3.351495    -5.156005      28.35
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 H      -4.599112    -1.614969    -5.270497      28.14
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name = lig-ACN-frame_931
 C       3.915497    -0.539269     0.303875      46.95
 H       3.080792    -0.285865    -0.486271      20.92
 C       5.120294     0.020276     2.395576      59.66
 H       5.327261     0.607017     3.267913      22.80
 C       6.126627    -0.875539     2.012628      -8.24
 O       7.286658    -1.122254     2.930357     182.61
 C       7.207532    -0.633558     4.477157      79.43
 H       8.246054    -1.051182     4.686621      24.79
 H       6.492443    -1.160060     4.938273      29.73
 H       7.236445     0.633571     4.434537      23.64
 C       5.996240    -1.734123     0.897635      11.78
 O       6.901064    -2.920147     0.749747     160.28
 H       7.863204    -2.842156     1.141675      21.87
 C       4.982573    -1.522681     0.009188      53.96
 H       4.968248    -2.396693    -0.745736      23.77
 C       4.071621     0.271639     1.418072      20.03
 C       2.850527     1.154494     1.924263      95.06
 H       3.233845     2.290834     2.122318      23.29
 O       2.466761     0.761326     3.386307     178.86
 H       2.410178    -0.288492     3.283215      24.36
 C       1.727404     1.248534     0.861941      91.36
 H       2.106945     1.783310     0.146549      24.20
 C       0.457356     2.149657     1.719790      88.30
 O       0.785906     3.669133     1.549178     280.72
 H       0.619319     3.819562     0.703686      31.59
 H       0.604973     1.950311     2.659430      25.13
 H      -0.553808     1.980418     1.255212      22.68
 C      -1.355695    -2.128534    -0.972888      46.20
 H      -1.901596    -3.061324    -1.026096      20.28
 C      -0.563570    -0.395086    -2.480796      25.13
 H      -0.479346    -0.015975    -3.540399      17.72
 C       0.006968     0.333883    -1.358611      13.28
 O       0.922250     1.275385    -1.760308     208.66
 C       0.135351     2.521392    -2.291775      56.59
 H      -0.501072     3.218768    -1.251577      20.11
 H       1.021226     3.073053    -2.877615      21.43
 H      -0.644942     2.122288    -2.986889      23.41
 C       0.214903    -0.488154    -0.187923      17.05
 O       1.167120    -0.091153     0.687067     159.59
 C      -0.471298    -1.696024    -0.006875      76.71
 H      -0.564866    -2.244440     0.860528      23.19
 C      -1.453670    -1.479695    -2.213372      25.39
 C      -2.276759    -2.111536    -3.424557     106.26
 H      -1.987074    -1.518485    -4.196757      25.62
 O      -1.890773    -3.456230    -3.484423     319.77
 H      -1.020652    -3.496799    -3.446729      35.21
 C      -3.803280    -2.020222    -3.347639      64.18
 H      -4.159268    -3.086331    -2.662761      22.14
 O      -4.215815    -0.598830    -3.033263     248.49
 H      -5.089528    -0.637894    -2.698004      27.75
 C      -4.538684    -2.584392    -4.640041      95.21
 O      -5.925896    -3.095059    -4.363198     241.23
 H      -6.205076    -3.544482    -5.258598      29.70
 H      -3.882673    -3.325469    -4.999125      29.21
 H      -4.610922    -1.816561    -5.507206      26.96
55
name = lig-ACN-frame_932
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 C       4.027147    -0.505494     0.209451      33.64
 H       3.161647    -0.478407    -0.624850      22.60
 C       5.066051    -0.015094     2.340835      51.47
 H       4.989919     0.653068     3.123377      23.66
 C       6.319527    -0.761720     2.072579       7.41
 O       7.349047    -1.096055     2.979541     307.72
 C       7.204239    -0.679221     4.240974     106.71
 H       8.037251    -0.890932     4.931376      26.30
 H       6.393952    -1.098462     4.659976      32.13
 H       6.865008     0.510454     4.513141      24.59
 C       6.068702    -1.770011     0.965322      -9.45
 O       6.854189    -2.837173     0.748558     138.78
 H       7.497025    -2.770338     1.465247      23.16
 C       4.866077    -1.584641     0.055467      45.12
 H       4.526425    -2.368974    -0.787853      21.85
 C       3.996791     0.301292     1.452975      29.27
 C       2.852329     1.095078     1.982163      96.71
 H       3.144433     2.318405     2.076396      22.38
 O       2.472435     0.705694     3.322330     271.07
 H       2.486272    -0.157814     3.419521      32.08
 C       1.663852     1.214023     0.833006      90.09
 H       1.949920     1.424491    -0.044216      24.18
 C       0.521910     2.291945     1.664241      97.82
 O       0.768154     3.677617     1.554844     241.51
 H       0.685855     4.054189     0.564906      26.78
 H       0.763818     2.105916     2.621689      25.10
 H      -0.560176     1.992625     1.725077      24.27
 C      -1.430286    -2.125592    -1.023463      34.43
 H      -1.726706    -3.188865    -0.836109      19.90
 C      -0.535581    -0.438864    -2.520426      30.74
 H      -0.319233    -0.116038    -3.500517      18.59
 C       0.113513     0.167682    -1.469400       8.01
 O       0.845595     1.442915    -1.711952     211.06
 C       0.217505     2.468547    -2.337497      77.34
 H      -0.354029     3.253026    -1.273874      20.97
 H       0.904470     3.229980    -2.794582      22.54
 H      -0.596239     2.218557    -3.115343      22.50
 C       0.224157    -0.437445    -0.200443       5.62
 O       1.199477    -0.100184     0.723431     163.95
 C      -0.554730    -1.657311     0.086866      28.17
 H      -0.293869    -2.196969     0.994009      22.77
 C      -1.390286    -1.463848    -2.243063      48.75
 C      -2.197048    -2.031592    -3.280131     101.91
 H      -1.984283    -1.607725    -4.180284      25.88
 O      -1.759287    -3.454072    -3.429203     179.09
 H      -0.733426    -3.522182    -3.163656      25.98
 C      -3.847949    -2.041042    -3.374445      65.51
 H      -4.265952    -2.621516    -2.296203      21.24
 O      -4.189605    -0.620684    -2.990537     300.09
 H      -4.803314    -0.521670    -2.410517      32.12
 C      -4.446450    -2.596139    -4.656775      94.53
 O      -5.939920    -3.174795    -4.384414     136.56
 H      -6.053268    -3.813850    -5.359675      26.01
 H      -3.949160    -3.493077    -4.897250      26.86
 H      -4.446341    -1.842677    -5.605139      25.14
55
name = lig-ACN-frame_933
 C       4.063675    -0.470795     0.209902      52.94
 H       3.165639    -0.313671    -0.516908      20.96
 C       5.184900     0.087302     2.332835      55.04
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 H       5.064269     0.268565     3.317419      22.11
 C       6.217513    -0.826923     2.051355       3.26
 O       7.397193    -1.059344     2.809492     255.51
 C       7.087388    -0.663275     4.280119     111.39
 H       8.049988    -0.879729     4.698298      27.32
 H       6.309775    -1.176531     4.635689      32.26
 H       6.963465     0.527256     4.108316      26.47
 C       6.015124    -1.674536     1.010501      22.22
 O       6.823251    -2.772161     0.775496     219.90
 H       7.576327    -2.995650     1.341060      23.62
 C       4.948832    -1.607729     0.217912      49.78
 H       5.029506    -2.368146    -0.732698      20.07
 C       4.029517     0.149982     1.407972      17.77
 C       2.827162     1.130717     1.887180      87.91
 H       3.355818     2.261873     2.153524      21.94
 O       2.476210     0.676719     3.250741     293.04
 H       2.063088    -0.133267     3.060114      27.68
 C       1.622094     1.370162     1.086216      94.09
 H       1.974915     1.872298     0.337231      23.47
 C       0.676005     2.275354     1.646006     105.55
 O       0.758021     3.740619     1.510891     214.72
 H       0.782896     3.926879     0.407347      24.96
 H       0.666767     2.183004     2.691061      23.24
 H      -0.293833     2.019889     1.131335      22.02
 C      -1.355692    -2.158131    -0.883940      46.72
 H      -2.306926    -2.774392    -0.739442      17.62
 C      -0.525091    -0.376768    -2.569565      38.57
 H      -0.688281     0.081870    -3.474013      18.37
 C       0.335325     0.171977    -1.577294       5.34
 O       0.819042     1.404322    -1.639558     220.15
 C       0.196948     2.568097    -2.407032      66.59
 H      -0.611283     3.395647    -1.586461      21.16
 H       1.026082     3.019848    -2.811110      22.98
 H      -0.459424     2.149838    -3.272774      21.44
 C       0.215712    -0.440290    -0.207349      11.62
 O       1.123854    -0.198240     0.817941      94.68
 C      -0.576480    -1.535736     0.071794      53.90
 H      -0.312388    -2.068388     1.050174      20.50
 C      -1.428135    -1.493134    -2.205992       8.84
 C      -2.178015    -2.114994    -3.470592      81.14
 H      -1.917034    -1.528093    -4.279769      27.25
 O      -1.727957    -3.501042    -3.402613     169.84
 H      -0.553888    -3.571778    -3.485847      22.90
 C      -3.854918    -1.993619    -3.197963      56.96
 H      -4.267060    -2.855491    -2.301441      21.56
 O      -4.103799    -0.649986    -3.029925     232.12
 H      -5.059154    -0.572127    -2.607744      23.68
 C      -4.478593    -2.747780    -4.581795      86.30
 O      -5.801053    -3.161952    -4.469456     254.39
 H      -5.996425    -4.156473    -4.886890      27.70
 H      -3.722168    -3.474221    -4.925134      28.69
 H      -4.422725    -1.837648    -5.421438      26.59
55
name = lig-ACN-frame_934
 C       4.034597    -0.577682     0.254373      52.50
 H       3.356016    -0.416644    -0.585458      23.07
 C       5.173269     0.151785     2.356977      41.70
 H       5.157643     0.843724     3.180156      20.13
 C       6.149572    -0.847618     2.103504      23.52
 O       7.333873    -0.983318     2.729797     321.75
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 C       7.117251    -0.622088     4.208446     115.52
 H       7.944141    -0.934114     4.758645      28.37
 H       6.345935    -1.241251     4.552934      31.23
 H       6.809087     0.451091     4.607640      27.33
 C       6.033702    -1.734385     1.029003      11.59
 O       6.859822    -2.805621     0.780948      86.24
 H       7.703141    -2.457207     1.271872      20.67
 C       4.988086    -1.559938     0.082891      21.80
 H       5.000390    -2.404298    -0.759880      20.90
 C       4.087750     0.242139     1.494547      30.78
 C       3.017216     1.106982     1.962928     113.11
 H       3.520770     2.288585     2.048396      20.46
 O       2.468718     0.668681     3.200981     224.87
 H       1.892825    -0.278354     3.082411      20.38
 C       1.789478     1.386678     1.118691      70.51
 H       1.833497     1.593386     0.145410      20.49
 C       0.520189     2.287631     1.743648      78.00
 O       0.807952     3.806328     1.408971     258.38
 H       1.009392     3.893473     0.480009      28.60
 H       0.087283     2.171387     2.778375      22.53
 H      -0.311175     1.947813     1.120995      22.58
 C      -1.426404    -2.051277    -0.957281      54.35
 H      -2.107003    -2.850293    -0.482173      18.29
 C      -0.608132    -0.404208    -2.513669      40.40
 H      -0.809968     0.138419    -3.372137      18.83
 C       0.287427     0.148290    -1.542809       3.79
 O       0.888506     1.493610    -1.606555     218.54
 C       0.208410     2.542815    -2.517953      80.83
 H      -0.546864     3.365467    -1.627457      20.70
 H       0.907779     3.167550    -2.805389      25.13
 H      -0.416247     2.140800    -3.387852      22.57
 C       0.359855    -0.425692    -0.259811      10.69
 O       1.057382    -0.065635     0.921196     108.12
 C      -0.543062    -1.498429     0.064914      28.26
 H      -0.901751    -1.660652     1.189256      20.01
 C      -1.356554    -1.505442    -2.233411      28.12
 C      -2.223629    -2.210532    -3.431939      97.42
 H      -2.002453    -1.836638    -4.397142      24.30
 O      -1.807602    -3.570161    -3.460037     211.47
 H      -0.806331    -3.665722    -3.870027      24.44
 C      -3.705058    -2.205571    -3.254114      71.19
 H      -3.878326    -2.675836    -2.049728      19.65
 O      -4.054185    -0.640755    -3.062172      96.95
 H      -5.224111    -0.459152    -2.973039      22.90
 C      -4.354042    -2.735982    -4.440558      99.43
 O      -5.759069    -3.203049    -4.496680     300.97
 H      -5.724246    -4.024001    -4.804127      34.68
 H      -3.792134    -3.699345    -4.728437      26.05
 H      -4.245527    -1.875458    -5.327321      25.58
55
name = lig-ACN-frame_935
 C       3.994459    -0.606492     0.368278      58.27
 H       3.155868    -0.466820    -0.204992      22.98
 C       5.179278     0.161737     2.355068      58.51
 H       5.498134     1.087856     2.900203      23.49
 C       6.104441    -0.820719     2.086500     -11.20
 O       7.305512    -0.831536     2.848546     281.64
 C       7.195903    -0.691165     4.183712     111.25
 H       8.165770    -0.893729     4.593023      25.86
 H       6.335467    -1.237856     4.572368      30.50
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 H       6.968191     0.418769     4.293059      27.44
 C       5.981386    -1.847036     0.955234       7.33
 O       6.970686    -2.815360     0.832446     206.38
 H       7.912153    -2.801788     1.264497      22.08
 C       5.016035    -1.563149    -0.065328      56.01
 H       4.704156    -2.065734    -1.003305      22.54
 C       4.126554     0.267088     1.405488      25.50
 C       3.023590     1.204048     2.033813      82.47
 H       3.487065     2.275294     2.516132      21.05
 O       2.476005     0.686500     3.279402     175.74
 H       2.512422    -0.466573     3.111824      21.07
 C       1.730581     1.341889     1.038571      75.34
 H       2.154470     1.864132     0.181399      21.53
 C       0.454388     2.429509     1.626510      84.79
 O       0.831020     3.741342     1.377752     314.58
 H       1.190696     3.705212     0.537500      30.72
 H       0.563741     2.409320     2.803904      21.14
 H      -0.475561     2.147848     1.154119      23.69
 C      -1.420785    -1.960308    -0.955237      47.16
 H      -1.919988    -2.945123    -0.882473      21.24
 C      -0.619592    -0.330811    -2.465223      42.64
 H      -0.542022     0.088518    -3.477947      18.91
 C       0.196101     0.267064    -1.449690       6.34
 O       0.906299     1.563091    -1.701324     220.81
 C       0.276534     2.465132    -2.535588     107.02
 H      -0.780778     3.068241    -1.834634      22.24
 H       0.949310     3.087248    -3.002041      25.07
 H      -0.234922     1.950053    -3.365404      24.05
 C       0.456338    -0.442592    -0.155195       9.65
 O       1.036808     0.135100     0.993757     160.31
 C      -0.570737    -1.427009     0.003035      47.59
 H      -0.736339    -1.673687     1.179484      19.93
 C      -1.385388    -1.592122    -2.326712      22.46
 C      -2.119595    -2.241443    -3.366052      85.83
 H      -1.898788    -1.586296    -4.217282      22.31
 O      -1.940633    -3.720037    -3.543376     266.05
 H      -1.039086    -3.869206    -3.621922      29.55
 C      -3.655312    -2.136900    -3.151892      62.94
 H      -4.115753    -2.900734    -2.149362      20.98
 O      -3.962986    -0.754442    -3.127477     146.61
 H      -5.116027    -0.782606    -2.815424      21.94
 C      -4.256397    -2.822177    -4.467156      68.95
 O      -5.744167    -3.210098    -4.431718     251.88
 H      -5.824176    -3.825296    -5.178141      31.07
 H      -3.574771    -3.770702    -4.748177      24.68
 H      -4.003630    -1.989202    -5.318550      26.33
55
name = lig-ACN-frame_936
 C       3.933731    -0.604891     0.356023      40.13
 H       3.070260    -0.714143    -0.170631      21.56
 C       5.266035     0.208147     2.199655      29.79
 H       5.444906     0.743771     3.234781      21.73
 C       6.159931    -0.907029     2.009273      22.34
 O       7.315708    -0.800284     2.755245     269.01
 C       7.257267    -0.656302     4.338879     109.03
 H       8.228590    -1.064397     4.604270      27.44
 H       6.561225    -1.387247     4.863793      28.51
 H       7.096750     0.360910     4.787476      29.40
 C       6.058310    -1.801292     0.952478      -5.23
 O       7.017136    -2.844433     0.835463     177.98
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 H       7.526292    -2.600832     1.618423      22.73
 C       4.974343    -1.553925    -0.004892      41.49
 H       5.093619    -2.154671    -0.861234      20.76
 C       4.045764     0.342568     1.500135      12.56
 C       2.807269     1.259638     2.015780      89.29
 H       3.315085     2.395448     2.044210      22.25
 O       2.533265     0.675610     3.395604     215.15
 H       2.538692    -0.394203     3.384335      22.73
 C       1.617430     1.560522     1.090417      96.94
 H       1.974103     1.684607     0.015362      17.42
 C       0.616902     2.404876     1.527440     105.60
 O       0.878878     3.798137     1.308613     277.40
 H       1.223645     4.064792     0.299565      25.26
 H       0.460063     2.150871     2.707083      21.40
 H      -0.384394     2.152937     1.259115      23.88
 C      -1.322120    -2.034813    -0.934578      49.00
 H      -2.048813    -2.688209    -0.548317      18.87
 C      -0.552710    -0.292076    -2.452232      39.15
 H      -0.500683     0.114497    -3.524921      16.80
 C       0.187118     0.398610    -1.382918      18.64
 O       0.921717     1.446192    -1.735857     253.64
 C       0.235182     2.410193    -2.668372     102.21
 H      -0.681299     3.187994    -2.051282      22.66
 H       1.040835     3.146069    -2.812317      23.39
 H      -0.153375     1.963809    -3.534562      24.03
 C       0.308195    -0.238658    -0.158496      21.89
 O       1.015866     0.159429     0.983025     166.83
 C      -0.549353    -1.385291     0.084355      37.49
 H      -0.363880    -2.164782     0.956969      20.04
 C      -1.235909    -1.451646    -2.226125      31.80
 C      -2.107565    -2.323614    -3.415693      67.29
 H      -1.817232    -2.025137    -4.459635      21.52
 O      -1.998488    -3.811591    -3.598011     277.76
 H      -1.165729    -4.073994    -3.305951      32.25
 C      -3.657997    -2.199614    -3.201611      66.19
 H      -4.094139    -2.739161    -2.030629      20.51
 O      -3.950041    -0.820547    -3.144565     242.34
 H      -4.768275    -0.544450    -2.607759      25.07
 C      -4.270430    -2.921011    -4.516767      83.37
 O      -5.638510    -3.175216    -4.349239     187.80
 H      -6.057626    -3.570404    -5.313613      29.25
 H      -3.651002    -3.956252    -4.753638      23.58
 H      -4.251650    -2.165712    -5.415276      25.07
55
name = lig-ACN-frame_937
 C       3.897429    -0.568892     0.367055      45.75
 H       3.130798    -0.579345    -0.377056      21.63
 C       5.227597     0.224022     2.117870      38.69
 H       5.226639     0.847847     3.146053      24.27
 C       6.207807    -0.756589     2.025134       9.39
 O       7.383143    -0.839895     2.798719     252.44
 C       7.363631    -0.696583     4.395979      92.24
 H       8.458042    -0.928001     4.669926      26.51
 H       6.437315    -1.386115     4.630413      25.83
 H       7.124221     0.270868     4.591493      32.71
 C       6.142385    -1.763502     0.912553       4.46
 O       6.962193    -2.804404     0.836265     176.01
 H       7.754854    -2.855074     1.367797      23.02
 C       4.953218    -1.568285     0.177161      64.59
 H       4.660355    -2.227123    -0.580198      22.17
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 C       3.910843     0.307327     1.450492      26.19
 C       2.839130     1.226739     2.044794      93.84
 H       3.186055     2.305346     2.454879      22.27
 O       2.555776     0.750335     3.438577     273.97
 H       2.196948    -0.060675     3.282518      29.50
 C       1.699620     1.405011     1.031226      74.63
 H       2.053582     2.029747     0.041553      17.67
 C       0.545327     2.505895     1.563234      71.47
 O       0.942766     3.957411     1.261451     203.14
 H       0.977832     3.836782     0.152362      22.06
 H       0.408836     2.581402     2.783336      20.28
 H      -0.224730     2.218941     0.894641      21.80
 C      -1.195331    -2.024233    -0.848713      51.52
 H      -1.752570    -2.873085    -0.697448      20.99
 C      -0.488926    -0.322342    -2.460771      30.63
 H      -0.469909     0.213335    -3.507925      15.37
 C       0.117790     0.368823    -1.441612       7.31
 O       0.943238     1.475129    -1.811386     255.47
 C       0.285761     2.414703    -2.767710      95.34
 H      -0.738522     2.769803    -2.060242      21.60
 H       1.109611     3.193805    -3.162355      23.19
 H      -0.057956     2.005826    -3.661644      23.42
 C       0.027169    -0.112050    -0.043712      16.35
 O       0.978363     0.145232     0.929691     138.28
 C      -0.436771    -1.423582     0.153134      41.06
 H      -0.245553    -1.704283     1.253523      17.97
 C      -1.269820    -1.555027    -2.250152      21.55
 C      -2.081342    -2.359349    -3.418805      75.40
 H      -1.773295    -1.733515    -4.378927      20.66
 O      -1.964080    -3.865101    -3.532295     199.70
 H      -0.855339    -4.101995    -3.498318      23.43
 C      -3.607113    -2.323629    -3.379065      55.91
 H      -3.841685    -3.028617    -2.254072      20.01
 O      -3.978529    -0.765253    -3.161850     241.87
 H      -4.642844    -0.799050    -2.656725      30.51
 C      -4.271499    -2.938938    -4.521120      94.98
 O      -5.676211    -3.152470    -4.238707     217.39
 H      -6.018000    -3.783801    -5.067525      29.03
 H      -3.786837    -4.018477    -4.801677      25.19
 H      -3.994511    -2.216824    -5.290972      28.11
55
name = lig-ACN-frame_938
 C       3.889443    -0.605618     0.329098      47.29
 H       2.985420    -0.542506    -0.370740      19.74
 C       5.111289     0.255303     2.243480      58.30
 H       5.299557     1.229776     2.889585      22.02
 C       6.295899    -0.598585     2.033128      -1.99
 O       7.468042    -0.875296     2.908396     284.98
 C       7.386789    -0.726844     4.222330     111.60
 H       8.410904    -0.995726     4.720262      26.10
 H       6.712440    -1.425365     4.965540      27.70
 H       7.167657     0.224736     4.550681      30.70
 C       6.088707    -1.576121     1.054242      -6.65
 O       6.922243    -2.826537     0.788175     148.06
 H       7.807538    -2.505266     1.194804      23.30
 C       4.866267    -1.616781     0.239723      45.52
 H       4.743760    -2.493008    -0.388423      22.46
 C       4.009892     0.274142     1.440854      28.28
 C       2.943481     1.182811     2.082190     101.87
 H       3.507165     2.208114     2.034147      22.03
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 O       2.514922     0.816431     3.414487     276.13
 H       1.980913    -0.009373     3.429672      26.88
 C       1.661757     1.408009     1.137041      75.05
 H       2.298299     1.518967     0.048556      17.23
 C       0.545834     2.715723     1.504804      88.33
 O       0.969846     3.987680     1.222127     326.54
 H       1.021937     4.212173     0.311842      28.99
 H       0.231693     2.562281     2.719260      21.42
 H      -0.474332     2.555604     1.183964      23.76
 C      -1.134827    -2.133117    -0.879585      46.45
 H      -1.207332    -3.130500    -0.677118      22.26
 C      -0.613001    -0.495612    -2.522445      42.87
 H      -0.452490    -0.216413    -3.652063      17.33
 C       0.082978     0.369824    -1.473202      -0.95
 O       0.928087     1.502566    -1.879158     233.29
 C       0.325396     2.380627    -2.823344     104.24
 H      -0.660342     3.105474    -2.492633      24.42
 H       1.094989     3.317591    -3.005521      21.83
 H       0.037415     1.812328    -3.677853      23.97
 C       0.002999    -0.060209    -0.077294      12.08
 O       0.973305     0.199821     0.904378     155.16
 C      -0.483854    -1.400662     0.177121      34.60
 H      -0.478247    -1.888642     1.156938      19.34
 C      -1.281441    -1.679464    -2.210856      23.61
 C      -1.991783    -2.368800    -3.387071      85.55
 H      -1.512542    -1.948856    -4.410988      21.59
 O      -1.794957    -3.832173    -3.410353     199.33
 H      -0.809102    -4.063625    -3.983729      23.28
 C      -3.537721    -2.203994    -3.331214      62.25
 H      -4.131413    -2.887551    -2.356791      20.94
 O      -3.984051    -0.898513    -3.207910     245.36
 H      -4.953831    -0.840074    -2.874315      24.87
 C      -4.280112    -2.919808    -4.584226      97.57
 O      -5.773594    -3.150120    -4.160857     272.57
 H      -5.953175    -3.956511    -4.526690      33.98
 H      -3.694595    -3.931006    -4.814844      27.32
 H      -4.478298    -2.412809    -5.472132      27.98
55
name = lig-ACN-frame_939
 C       3.888622    -0.682566     0.369300      46.33
 H       2.856037    -0.841393    -0.209406      19.57
 C       5.299729     0.325591     2.414830      44.63
 H       5.185617     1.034560     3.319974      19.45
 C       6.313375    -0.591305     2.135241       9.07
 O       7.466119    -0.881987     2.763916     229.47
 C       7.415061    -0.685249     4.335934      80.60
 H       8.546587    -0.917729     4.506859      25.76
 H       6.564683    -1.526082     4.512990      25.94
 H       7.159720     0.215714     4.607609      30.21
 C       5.979008    -1.615385     1.086849       7.49
 O       6.851853    -2.666009     0.803630     139.87
 H       7.765209    -2.655709     1.268851      21.77
 C       4.884654    -1.652120     0.267754      61.23
 H       4.995870    -2.514116    -0.468040      21.24
 C       4.049170     0.247366     1.490198       8.70
 C       2.852163     1.210755     1.990453     100.61
 H       3.282313     2.244387     2.238385      22.84
 O       2.495360     0.889946     3.407740     194.46
 H       2.142297    -0.184612     3.214428      22.51
 C       1.630078     1.621174     1.155167      65.78
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 H       1.946954     2.152558     0.015884      16.19
 C       0.600030     2.684527     1.473000      90.82
 O       1.022839     4.096930     1.221804     264.67
 H       1.176660     4.105360     0.322654      30.51
 H       0.661540     2.805215     2.693940      20.87
 H      -0.265347     2.366491     0.895344      23.00
 C      -1.064394    -2.323215    -0.861947      42.42
 H      -1.459454    -3.283097    -0.565768      20.18
 C      -0.641506    -0.485873    -2.464812      38.55
 H      -0.655194    -0.235485    -3.564828      17.93
 C       0.023185     0.333386    -1.583867      10.13
 O       0.816132     1.420503    -1.856010     260.23
 C       0.331483     2.393840    -2.925776      89.38
 H      -0.583689     2.925780    -2.357170      23.73
 H       1.350447     2.973574    -3.167866      22.89
 H       0.021925     1.914226    -3.900026      22.66
 C       0.156827    -0.151345    -0.231184      -7.50
 O       0.907120     0.240571     0.962382     104.44
 C      -0.659169    -1.358812     0.069530      41.19
 H      -0.304198    -1.746158     0.984187      22.09
 C      -1.218743    -1.745012    -2.166017      24.27
 C      -1.895593    -2.434684    -3.335863      92.77
 H      -1.613950    -1.912138    -4.400020      21.94
 O      -1.657938    -3.789269    -3.297384     265.03
 H      -0.640400    -3.952436    -3.660281      24.75
 C      -3.608909    -2.279738    -3.396456      58.36
 H      -3.638430    -2.903262    -2.252657      21.48
 O      -3.988607    -0.889725    -3.239597     147.24
 H      -5.196580    -0.901017    -3.121211      21.91
 C      -4.391044    -2.900400    -4.561107     109.31
 O      -5.771134    -3.161492    -4.093791     295.33
 H      -5.993856    -4.093385    -4.270702      31.57
 H      -3.992227    -3.929490    -4.790878      27.12
 H      -4.249613    -2.233326    -5.346136      28.96
55
name = lig-ACN-frame_940
 C       3.900604    -0.677278     0.633414      38.07
 H       2.876765    -0.628783     0.010275      19.72
 C       5.249506     0.332620     2.390158      55.36
 H       5.383838     0.766217     3.374253      23.03
 C       6.157658    -0.740782     2.154599      12.21
 O       7.501749    -0.816563     2.731827     294.14
 C       7.461818    -0.691753     4.277950     112.38
 H       8.441126    -0.954640     4.827148      26.95
 H       6.685962    -1.462919     4.865382      26.25
 H       7.174265     0.183850     4.556080      33.98
 C       5.959064    -1.628469     1.134963      17.82
 O       6.913068    -2.572974     0.842960     214.31
 H       7.498876    -2.530259     1.598252      21.41
 C       4.905193    -1.628846     0.237802      56.05
 H       4.634138    -2.325631    -0.665586      21.39
 C       4.031681     0.309377     1.612974      20.46
 C       2.863888     1.373558     1.988243      86.48
 H       3.399705     2.345106     2.111671      24.79
 O       2.432066     0.889976     3.330193     191.17
 H       2.367965    -0.188958     3.556027      22.92
 C       1.644839     1.657987     0.974018      60.76
 H       2.219103     1.974229    -0.153394      17.77
 C       0.684464     2.718802     1.605873      93.44
 O       1.050315     4.141290     1.216188     250.11
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 H       1.485586     4.133070     0.232410      25.67
 H       0.104466     2.514220     2.631854      22.15
 H      -0.261426     2.602207     1.028199      22.75
 C      -1.099667    -2.334617    -0.889220      40.80
 H      -1.805688    -3.205281    -0.618883      20.15
 C      -0.687428    -0.462873    -2.487153      54.16
 H      -0.988577     0.070203    -3.367072      18.36
 C       0.068755     0.250805    -1.527894      10.64
 O       0.708739     1.421583    -1.911189     251.01
 C       0.358386     2.309218    -2.935206     113.02
 H      -0.296372     3.226104    -2.584936      26.13
 H       1.217732     3.004383    -3.240719      23.67
 H      -0.243286     1.772747    -3.788659      21.89
 C       0.207245    -0.320942    -0.256289      19.09
 O       0.786166     0.335937     0.905246     117.73
 C      -0.554357    -1.393415     0.091656      41.64
 H      -0.756205    -1.466542     1.113614      20.71
 C      -1.188925    -1.773729    -2.212969      24.78
 C      -1.967354    -2.403548    -3.366995      99.75
 H      -1.421928    -1.889737    -4.321494      22.46
 O      -1.578242    -3.870650    -3.217430     299.36
 H      -0.684339    -3.990405    -3.142360      31.45
 C      -3.519978    -2.437104    -3.325104      55.60
 H      -4.218306    -2.997146    -2.417754      21.33
 O      -3.985188    -0.858585    -3.275950      86.28
 H      -5.144146    -0.918147    -3.001364      22.25
 C      -4.402864    -2.960689    -4.475592     110.71
 O      -5.781258    -3.138005    -4.037561     213.70
 H      -5.985622    -4.172525    -4.484561      26.32
 H      -3.968139    -3.818007    -4.976781      27.47
 H      -4.571948    -2.261396    -5.266541      27.43
55
name = lig-ACN-frame_941
 C       3.814082    -0.594241     0.765703      51.92
 H       2.890995    -0.559899     0.092302      22.99
 C       5.151448     0.249822     2.451028      53.47
 H       5.403447     1.163692     2.881819      23.72
 C       6.089124    -0.770188     2.224097      -9.99
 O       7.446892    -0.768834     2.844550     262.53
 C       7.490505    -0.687021     4.191284     113.25
 H       8.596634    -0.895701     4.328056      25.48
 H       6.678329    -1.490230     4.647840      25.65
 H       7.316699     0.211772     4.543339      32.29
 C       6.007495    -1.719865     1.049804     -14.53
 O       7.082763    -2.596837     0.902945     156.60
 H       7.800739    -2.425107     1.543906      20.46
 C       4.762715    -1.480477     0.301697      49.76
 H       4.680962    -2.250682    -0.570419      19.90
 C       3.979678     0.422830     1.721496      32.92
 C       2.920556     1.376938     2.012184     104.64
 H       3.248825     2.385071     2.167792      24.89
 O       2.340001     0.945245     3.266013     246.14
 H       2.434896     0.057038     3.072447      29.80
 C       1.690054     1.524676     0.963806      58.78
 H       1.923814     1.778183    -0.292267      15.94
 C       0.640477     2.813873     1.497575      77.23
 O       1.084766     4.109125     1.327414     221.29
 H       1.453287     4.040404     0.240600      22.64
 H       0.947617     2.740171     2.597616      20.57
 H      -0.408734     2.536250     1.105783      22.83
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 C      -1.175904    -2.138392    -0.920674      33.56
 H      -1.810762    -3.095835    -0.586535      19.78
 C      -0.759618    -0.468426    -2.513223      57.12
 H      -1.011203    -0.010566    -3.421283      21.65
 C       0.120578     0.178876    -1.578063      -2.05
 O       0.707516     1.444911    -1.846557     253.19
 C       0.291778     2.293975    -2.981134     103.80
 H      -0.246030     3.142399    -2.584135      27.26
 H       1.255784     2.429106    -3.432057      25.33
 H      -0.294614     1.756507    -3.866461      22.70
 C       0.272536    -0.279307    -0.175798      -4.84
 O       0.717581     0.474558     0.825780     151.87
 C      -0.470390    -1.627162     0.168066      41.77
 H      -0.866549    -1.879563     1.094607      23.57
 C      -1.248165    -1.708547    -2.265307      35.80
 C      -1.996970    -2.552102    -3.323411      93.31
 H      -1.940157    -2.307222    -4.496498      19.59
 O      -1.639886    -3.927523    -3.179582     311.04
 H      -0.744560    -3.961557    -3.471797      29.77
 C      -3.588951    -2.338305    -3.249442      77.29
 H      -3.612481    -2.803051    -2.109353      21.90
 O      -3.922693    -0.983064    -3.284584     269.73
 H      -4.749277    -0.859328    -2.761007      26.40
 C      -4.330074    -2.991744    -4.505785      86.23
 O      -5.795529    -3.200297    -3.978695     236.96
 H      -6.292938    -3.852871    -4.613673      30.40
 H      -3.950406    -3.905804    -4.763785      29.20
 H      -4.151042    -2.184509    -5.268803      27.68
55
name = lig-ACN-frame_942
 C       3.674294    -0.532355     0.664613      34.45
 H       2.732610    -0.579228     0.173790      19.84
 C       5.204819     0.282932     2.565038      44.44
 H       5.594637     0.959412     3.236639      20.23
 C       6.112282    -0.770662     2.213337      15.79
 O       7.293161    -0.739651     2.762978     245.90
 C       7.561167    -0.657076     4.280566     103.69
 H       8.580736    -0.989691     4.470665      26.79
 H       6.930471    -1.530990     4.844887      25.97
 H       7.307777     0.184212     4.695859      32.79
 C       6.042087    -1.671886     1.151608       3.27
 O       7.140882    -2.603113     0.896663     150.16
 H       7.927846    -2.149826     1.394928      22.01
 C       4.804618    -1.508933     0.416000      31.99
 H       4.419463    -2.030471    -0.506649      22.38
 C       3.963126     0.388055     1.725830      -0.86
 C       2.787741     1.422747     1.989452     109.26
 H       3.189017     2.374361     2.140085      26.48
 O       2.232650     0.983453     3.257749     262.98
 H       1.945486     0.091216     3.356095      29.63
 C       1.633157     1.630244     0.923979      84.37
 H       2.319459     1.999715    -0.075372      19.83
 C       0.763795     2.688086     1.485996      93.28
 O       1.164251     4.129002     1.345021     268.82
 H       1.131293     4.567571     0.424781      28.27
 H       0.572282     2.500020     2.602334      23.24
 H      -0.369978     2.599819     1.217786      23.33
 C      -1.269881    -2.126526    -0.903900      32.56
 H      -1.819926    -3.188085    -0.760791      22.08
 C      -0.695364    -0.399276    -2.579072      64.87
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 H      -0.636049    -0.050333    -3.588105      22.18
 C       0.108194     0.180822    -1.560660      -0.08
 O       0.692897     1.427461    -1.754801     201.87
 C       0.295580     2.228163    -3.028885     104.94
 H      -0.134480     3.123043    -2.616910      27.96
 H       1.074081     2.636272    -3.533057      24.71
 H      -0.565384     1.711830    -3.570890      24.27
 C       0.187257    -0.372419    -0.209214       8.97
 O       0.669705     0.506833     0.898073     127.25
 C      -0.361126    -1.549095     0.096760      61.16
 H       0.032870    -2.030716     0.960331      23.30
 C      -1.369273    -1.690513    -2.285629       2.81
 C      -2.083253    -2.610535    -3.349013      90.01
 H      -1.466669    -2.123095    -4.243899      21.49
 O      -1.748224    -4.007356    -3.141033     226.27
 H      -1.007762    -4.393078    -3.859950      25.75
 C      -3.601022    -2.432291    -3.191879      86.44
 H      -4.270449    -2.914237    -2.306211      24.64
 O      -3.856438    -0.980951    -3.243641     293.95
 H      -4.506667    -0.801733    -2.742365      33.79
 C      -4.314990    -3.081465    -4.322918     111.96
 O      -5.719395    -3.238744    -4.017704     299.59
 H      -6.007297    -3.592256    -4.754664      36.30
 H      -3.897739    -3.965865    -4.524930      29.89
 H      -4.309326    -2.519516    -5.355259      26.13
55
name = lig-ACN-frame_943
 C       3.862541    -0.580716     0.672716      56.11
 H       3.045189    -0.623887     0.080408      24.99
 C       5.068559     0.312005     2.500791      56.11
 H       4.995716     0.683686     3.468608      25.74
 C       6.060799    -0.657947     2.246542       2.14
 O       7.403296    -0.717553     2.873993     259.16
 C       7.582918    -0.686074     4.313242     119.97
 H       8.631433    -0.751757     4.338557      27.17
 H       6.927568    -1.470745     4.902549      26.43
 H       7.402619     0.260260     4.646542      30.80
 C       5.945125    -1.619041     1.157047      -9.20
 O       7.039740    -2.506283     0.865239     160.94
 H       7.869396    -2.217386     1.361349      21.90
 C       4.761888    -1.593752     0.392344      57.64
 H       4.914005    -2.421696    -0.295261      19.66
 C       3.914008     0.401160     1.736200      32.85
 C       2.734614     1.344775     2.022491     106.17
 H       3.110064     2.277899     2.196554      27.38
 O       2.082476     1.060208     3.348690     192.82
 H       1.759723     0.050555     2.979410      24.42
 C       1.691952     1.706347     0.938110      56.88
 H       1.849468     1.895163    -0.246828      18.20
 C       0.718883     2.774687     1.522291     100.11
 O       1.231693     4.129447     1.409229     307.72
 H       0.872301     4.225297     0.624393      32.07
 H       0.558026     2.514076     2.552543      24.82
 H      -0.068921     2.652334     0.676128      23.23
 C      -1.257385    -2.193033    -0.892236      40.90
 H      -1.619171    -3.242388    -0.529202      21.11
 C      -0.608337    -0.555635    -2.590224      35.87
 H      -0.507815    -0.257560    -3.660558      19.05
 C       0.009928     0.274232    -1.561381      17.13
 O       0.674571     1.459746    -1.778703     266.28
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 C       0.286407     2.193637    -2.888173     125.46
 H      -0.076062     3.141071    -2.632176      28.47
 H       1.113507     2.171650    -3.459772      27.52
 H      -0.427643     1.705746    -3.555177      26.38
 C       0.195555    -0.170537    -0.260574       5.12
 O       0.632345     0.381255     0.905360     105.46
 C      -0.359289    -1.581123    -0.058190      34.14
 H       0.078199    -2.169429     0.781472      23.42
 C      -1.405401    -1.609221    -2.180669      45.49
 C      -2.059502    -2.553689    -3.239115      90.18
 H      -2.037976    -2.406399    -4.441958      21.35
 O      -1.874628    -4.104850    -3.108246     155.11
 H      -1.108214    -4.292416    -3.927395      24.35
 C      -3.608858    -2.485783    -3.167031      73.42
 H      -3.747593    -2.917092    -2.092654      24.22
 O      -3.797404    -0.919085    -3.181509     199.56
 H      -4.806165    -0.740355    -2.833368      24.82
 C      -4.312186    -3.274173    -4.312653      88.17
 O      -5.700644    -3.280493    -4.070261     247.29
 H      -6.047883    -3.846196    -4.898309      29.30
 H      -3.874200    -4.184742    -4.259189      28.62
 H      -3.916483    -2.615914    -5.275474      26.03
55
name = lig-ACN-frame_944
 C       3.892558    -0.643745     0.572338      45.30
 H       3.110773    -0.491224    -0.079726      24.21
 C       4.946340     0.296734     2.596458      34.77
 H       4.899893     1.070154     3.401525      20.25
 C       6.141932    -0.568663     2.322921       5.85
 O       7.420326    -0.708535     2.927840     290.30
 C       7.612741    -0.627399     4.337865     123.11
 H       8.575441    -0.944538     4.595430      28.04
 H       7.001889    -1.482437     4.838619      27.88
 H       7.250869     0.211835     4.763017      31.68
 C       5.973478    -1.515693     1.221538      15.43
 O       6.881163    -2.384031     0.831395     213.57
 H       7.569216    -2.401556     1.483270      24.25
 C       4.858576    -1.676292     0.382405      82.18
 H       4.480507    -2.313347    -0.352893      24.63
 C       3.832424     0.308876     1.644274      20.10
 C       2.771331     1.366997     2.073864      93.57
 H       3.259783     2.206382     2.273666      25.78
 O       1.956008     1.058969     3.337715     170.65
 H       1.460845     0.104830     3.499075      24.95
 C       1.622015     1.585288     1.038354      73.98
 H       2.132600     1.824317     0.018174      21.86
 C       0.618308     2.840215     1.462456      96.29
 O       1.262221     4.118755     1.483972     262.13
 H       1.418578     4.750105     0.675341      28.31
 H       0.269344     2.732965     2.443514      25.64
 H      -0.449432     2.853526     0.988306      24.23
 C      -1.169455    -2.231158    -0.911075      39.05
 H      -1.664437    -3.185636    -0.699023      22.69
 C      -0.551399    -0.626470    -2.534892      42.16
 H      -0.607180    -0.390749    -3.672645      20.56
 C      -0.045382     0.311483    -1.561128       8.05
 O       0.660430     1.495407    -1.771261     229.35
 C       0.307837     2.265097    -2.952222     123.16
 H       0.117392     3.194070    -2.600382      28.72
 H       1.096039     2.426736    -3.601309      27.08
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 H      -0.543017     1.849400    -3.348130      29.05
 C       0.067103    -0.241783    -0.245879      14.35
 O       0.702194     0.337857     0.906668     116.34
 C      -0.275778    -1.526415    -0.052667      64.46
 H      -0.313315    -1.870971     1.041283      23.22
 C      -1.379238    -1.779764    -2.206332      20.20
 C      -2.118946    -2.607070    -3.206321      84.86
 H      -1.474823    -2.146567    -4.163606      20.86
 O      -1.936098    -4.079309    -3.079890     259.12
 H      -1.068727    -4.288146    -3.408360      30.76
 C      -3.570502    -2.345893    -3.036580      85.63
 H      -4.006833    -2.778092    -2.108990      24.99
 O      -3.811433    -0.984858    -3.112052     184.34
 H      -5.025128    -0.874914    -3.221398      22.46
 C      -4.209920    -3.381255    -4.280635      69.98
 O      -5.765307    -3.343107    -4.168067     196.73
 H      -6.141691    -4.226313    -4.777912      29.08
 H      -3.921303    -4.398857    -4.206725      25.98
 H      -3.915851    -3.035580    -5.438821      24.24
55
name = lig-ACN-frame_945
 C       3.717294    -0.627340     0.458470      39.50
 H       2.942178    -0.785723    -0.311882      23.11
 C       4.971389     0.228588     2.640571      57.37
 H       5.155465     1.132061     3.364013      20.27
 C       6.074178    -0.523362     2.357398      20.44
 O       7.380571    -0.650640     2.902833     231.42
 C       7.559174    -0.635800     4.447852     112.02
 H       8.603932    -0.683883     4.522476      28.29
 H       6.903278    -1.408925     4.862342      27.92
 H       7.370403     0.342355     4.845047      29.60
 C       5.954445    -1.416704     1.282797      -1.11
 O       6.942893    -2.379733     0.841022     152.54
 H       7.645574    -2.582266     1.522888      22.95
 C       4.800469    -1.490675     0.410074      37.10
 H       5.145678    -2.287311    -0.216185      21.46
 C       3.851582     0.213640     1.712474       5.82
 C       2.604929     1.269052     2.113675     106.23
 H       3.003654     2.144729     2.243323      28.12
 O       1.925793     1.047928     3.364194     280.21
 H       1.853878     0.161749     3.218881      32.75
 C       1.455862     1.585926     1.046364      94.04
 H       2.022470     1.823280     0.099961      24.23
 C       0.560916     2.816761     1.413300      99.63
 O       1.300423     4.159742     1.585479     210.86
 H       1.687119     4.113582     0.515049      25.54
 H       0.278700     2.599250     2.368180      27.22
 H      -0.218926     2.907220     0.580028      24.26
 C      -1.062828    -2.330728    -0.854700      53.04
 H      -1.552216    -3.137250    -0.465741      25.16
 C      -0.628450    -0.597947    -2.543845      55.25
 H      -0.526313    -0.125621    -3.608079      22.24
 C      -0.011340     0.226893    -1.557709       0.05
 O       0.631258     1.504020    -1.781402     179.51
 C       0.288417     2.413353    -3.042464     116.32
 H       0.236021     3.344652    -2.634235      28.25
 H       1.083997     2.258254    -3.751229      26.78
 H      -0.534744     2.170331    -3.528618      30.14
 C       0.098226    -0.218918    -0.193904     -12.85
 O       0.799360     0.340878     0.921816     138.07
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 C      -0.392741    -1.579896     0.138744      18.66
 H      -0.150681    -1.851480     1.257066      24.04
 C      -1.125775    -1.881544    -2.201538      45.20
 C      -2.033815    -2.644319    -3.192232      91.24
 H      -1.988391    -2.401311    -4.439822      20.87
 O      -1.933027    -4.029885    -3.039644     292.46
 H      -1.072347    -4.198807    -2.881990      32.45
 C      -3.682321    -2.474454    -3.139318      78.84
 H      -4.027755    -2.908181    -2.201887      25.73
 O      -3.904933    -1.005531    -3.100608     175.50
 H      -5.062824    -0.808589    -3.328192      23.75
 C      -4.269175    -3.344890    -4.152875      85.76
 O      -5.741282    -3.401261    -4.264404     269.82
 H      -5.817381    -4.238726    -4.778322      30.59
 H      -3.823202    -4.320334    -3.786901      24.50
 H      -3.882618    -3.074640    -5.291968      23.89
55
name = lig-ACN-frame_946
 C       3.671114    -0.549954     0.629413      36.99
 H       2.646767    -0.562145     0.062498      21.16
 C       4.902999     0.265275     2.554628      34.98
 H       4.727046     0.867861     3.584798      24.38
 C       6.081145    -0.635468     2.356085       9.02
 O       7.324995    -0.544712     3.011401     260.33
 C       7.485804    -0.579863     4.412131     124.28
 H       8.512925    -0.931577     4.585584      27.23
 H       6.992820    -1.328300     4.970093      28.74
 H       7.133103     0.365011     4.846243      27.74
 C       5.972502    -1.481936     1.216568      17.44
 O       6.988467    -2.340226     0.909241     148.69
 H       7.723720    -2.180326     1.619650      18.85
 C       4.887923    -1.360523     0.359194      71.11
 H       4.746293    -1.963283    -0.595200      24.70
 C       3.638017     0.237206     1.773416      12.74
 C       2.538842     1.295734     2.069294     104.17
 H       3.039688     2.111332     2.236977      29.61
 O       1.941287     0.928558     3.411344     235.28
 H       1.857713     0.030856     3.651484      31.11
 C       1.509333     1.629042     0.964918      84.79
 H       1.775442     1.895839    -0.031534      23.69
 C       0.549344     2.807864     1.452203     111.34
 O       1.306846     4.052411     1.586782     272.12
 H       2.016135     4.136085     0.887204      31.10
 H      -0.187263     2.736362     2.137111      28.47
 H      -0.081318     2.986778     0.519197      25.32
 C      -0.934411    -2.399947    -0.760521      14.84
 H      -1.333641    -3.297705    -0.641241      25.81
 C      -0.636668    -0.544797    -2.505247      38.85
 H      -0.904036    -0.250320    -3.596261      21.71
 C       0.082321     0.240868    -1.527866      12.58
 O       0.531449     1.514981    -1.880964     221.66
 C       0.286700     2.425426    -3.017970     116.25
 H       0.421534     3.408057    -2.690095      27.82
 H       1.148331     2.263403    -3.715460      26.00
 H      -0.573168     2.270487    -3.430565      30.35
 C       0.160382    -0.286666    -0.120406       9.89
 O       0.777356     0.293367     0.913902     122.92
 C      -0.493244    -1.502278     0.253451      63.85
 H      -0.332415    -2.109510     1.224335      23.80
 C      -1.012137    -1.903639    -2.189664       4.85
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 C      -2.085881    -2.634972    -3.241582      69.69
 H      -1.548824    -2.290581    -4.366745      21.17
 O      -1.869810    -4.104045    -2.970347     174.09
 H      -0.786034    -4.226302    -2.701207      24.62
 C      -3.689556    -2.469219    -3.033979      87.79
 H      -3.857382    -2.858305    -2.106113      27.53
 O      -4.018862    -1.046885    -3.154397     272.68
 H      -5.017448    -0.859192    -3.004507      27.59
 C      -4.323721    -3.354517    -4.171112      91.58
 O      -5.710634    -3.456667    -4.322813     300.00
 H      -5.819359    -3.899854    -5.074050      34.91
 H      -3.996067    -4.465610    -3.983614      24.23
 H      -3.723897    -3.072383    -5.173415      24.51
55
name = lig-ACN-frame_947
 C       3.749938    -0.556477     0.807482      54.27
 H       2.957778    -0.645418    -0.101270      25.39
 C       4.810256     0.229178     2.559811      59.41
 H       4.984395     0.857806     3.579101      23.27
 C       5.870655    -0.599672     2.346163       0.41
 O       7.225407    -0.465360     3.016949     202.27
 C       7.379259    -0.549533     4.475253     113.89
 H       8.478852    -0.645178     4.680450      26.27
 H       6.727852    -1.270200     4.741047      28.56
 H       7.189769     0.425732     5.064702      26.70
 C       5.979685    -1.481990     1.140607      -8.10
 O       7.069016    -2.317342     0.980422     146.22
 H       7.835742    -1.955287     1.440465      21.22
 C       4.805632    -1.252249     0.235649      42.67
 H       4.634649    -1.745220    -0.775528      23.46
 C       3.646460     0.304355     1.842371      55.02
 C       2.592493     1.331313     2.141299     103.45
 H       2.970554     2.183555     2.407923      29.26
 O       1.927109     0.856738     3.446719     156.57
 H       2.117944    -0.225796     3.226851      25.83
 C       1.489994     1.571928     1.016992      96.57
 H       2.122016     1.789754     0.236834      27.66
 C       0.522475     2.824676     1.283694     113.44
 O       1.323258     3.936739     1.653919     304.37
 H       1.977407     3.961957     1.049074      35.08
 H       0.186249     2.600513     2.247172      27.75
 H      -0.246617     2.945912     0.476128      26.41
 C      -0.886348    -2.362931    -0.871682      48.59
 H      -1.103599    -3.303563    -0.548025      23.73
 C      -0.616646    -0.623500    -2.400420      65.17
 H      -0.942028    -0.013141    -3.278369      22.45
 C       0.054547     0.226082    -1.536555      18.47
 O       0.493925     1.542779    -1.834451     221.77
 C       0.285603     2.335056    -3.010154     126.04
 H       0.352761     3.295604    -2.541250      27.24
 H       0.943841     2.175139    -3.908990      26.53
 H      -0.623830     2.288040    -3.364191      30.65
 C       0.142323    -0.300464    -0.199329       0.82
 O       0.754674     0.330045     0.959193     128.81
 C      -0.476439    -1.515932     0.195130      48.32
 H      -0.520762    -1.495514     1.304441      25.05
 C      -1.158327    -1.880617    -2.114713      50.17
 C      -1.984675    -2.680660    -3.079474      89.59
 H      -1.779048    -2.360150    -4.331696      21.36
 O      -1.804199    -4.153035    -2.928570     192.82
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 H      -0.672367    -4.183946    -3.071768      25.02
 C      -3.593090    -2.422858    -2.970102      83.70
 H      -3.915094    -2.766797    -2.119989      28.41
 O      -4.117537    -1.106353    -3.199969     330.61
 H      -4.820581    -1.022471    -2.782424      35.74
 C      -4.191839    -3.443622    -4.218424      58.67
 O      -5.780981    -3.442204    -4.353159     218.10
 H      -5.810431    -3.758139    -5.338597      29.39
 H      -3.672055    -4.540762    -4.178126      22.99
 H      -3.935646    -2.910184    -5.209050      23.56
55
name = lig-ACN-frame_948
 C       3.664543    -0.548806     0.630660      39.62
 H       2.619749    -0.402384     0.069411      21.87
 C       4.848450     0.267199     2.825273      34.20
 H       5.094811     1.222817     3.454688      20.40
 C       5.889959    -0.615554     2.299393       5.42
 O       7.047589    -0.390790     2.943520     191.03
 C       7.204324    -0.517089     4.527741      91.67
 H       8.291259    -0.863422     4.595280      26.26
 H       6.770349    -1.242724     5.030065      29.79
 H       6.843249     0.521013     4.920894      25.12
 C       5.929641    -1.355859     1.144251      27.92
 O       7.086901    -2.258294     0.979901     187.56
 H       7.781373    -1.873996     1.532213      22.69
 C       4.900418    -1.298439     0.266327      49.22
 H       5.082039    -1.920291    -0.667219      24.09
 C       3.753756     0.359415     1.864882     -34.83
 C       2.521586     1.369688     2.317008      99.23
 H       2.903125     2.265108     2.483875      27.20
 O       1.924004     0.770394     3.434943     199.42
 H       1.865223    -0.336829     3.392550      24.78
 C       1.532621     1.531572     1.053448     106.01
 H       1.995972     1.585539     0.194408      27.44
 C       0.575766     2.690078     1.249094     104.79
 O       1.362159     3.901357     1.691247     220.42
 H       2.019299     4.144186     0.860863      28.04
 H      -0.113879     2.442644     2.064581      27.28
 H      -0.151708     2.951566     0.459641      25.93
 C      -0.944774    -2.390173    -0.775302      46.65
 H      -1.394165    -3.377374    -0.544644      22.01
 C      -0.693304    -0.569395    -2.476994      58.11
 H      -0.812614    -0.338637    -3.528708      22.51
 C       0.022675     0.224307    -1.498797      22.70
 O       0.511341     1.497375    -1.689484     196.52
 C       0.184738     2.258089    -3.011029     109.66
 H       0.478561     3.315130    -2.936300      26.67
 H       0.974278     1.866532    -3.706999      26.32
 H      -0.730991     2.035250    -3.349367      28.98
 C       0.176481    -0.164445    -0.161132      36.04
 O       0.684121     0.352801     0.955926     171.75
 C      -0.348951    -1.467281     0.058137      53.49
 H      -0.412993    -1.953655     1.012680      25.03
 C      -1.252747    -1.847007    -2.068678      10.19
 C      -2.012611    -2.728593    -3.005331      98.20
 H      -1.558567    -2.368970    -4.197043      22.05
 O      -1.697461    -4.130956    -2.889010     259.05
 H      -1.034251    -4.417944    -3.488052      29.82
 C      -3.611309    -2.629799    -3.062242      93.07
 H      -3.880390    -2.984947    -2.190027      29.20
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 O      -4.093159    -1.166239    -3.247907     265.50
 H      -4.979696    -0.975286    -2.881465      28.46
 C      -4.155240    -3.355784    -4.228766      81.52
 O      -5.689057    -3.401578    -4.322140     182.60
 H      -5.868697    -4.131576    -5.199058      26.38
 H      -3.790655    -4.566515    -4.183519      22.92
 H      -3.660473    -2.902264    -5.115524      25.71
55
name = lig-ACN-frame_949
 C       3.756004    -0.404320     0.612808      30.12
 H       2.860284    -0.597003    -0.086761      24.93
 C       4.802059     0.291278     2.734166      75.31
 H       4.895035     0.843986     3.684800      25.29
 C       5.867889    -0.459557     2.435651      15.94
 O       7.102683    -0.398125     3.071883     255.14
 C       7.034866    -0.489618     4.413825     121.76
 H       8.142423    -0.515118     4.728148      25.44
 H       6.391117    -1.171870     4.642439      29.20
 H       6.758643     0.561945     5.023676      25.11
 C       5.981663    -1.334001     1.218858       2.26
 O       7.002594    -2.109807     0.939654      93.76
 H       7.757396    -2.049879     1.649284      22.30
 C       4.823010    -1.329342     0.291472      15.38
 H       4.706928    -2.028038    -0.617173      21.05
 C       3.724110     0.370187     1.840498      40.61
 C       2.567038     1.207415     2.260667     111.96
 H       2.777850     2.066815     2.680885      28.10
 O       1.867182     0.690599     3.501861     236.82
 H       1.831778    -0.221884     3.354801      32.25
 C       1.592818     1.503110     1.076780      97.62
 H       2.136695     1.735847     0.326904      29.27
 C       0.664337     2.711834     1.298138     107.89
 O       1.369320     3.856241     1.691306     228.83
 H       1.716903     4.329175     0.742571      27.43
 H      -0.190712     2.721178     2.102698      25.67
 H       0.350759     2.788869     0.299471      25.81
 C      -1.086630    -2.278665    -0.772200      39.17
 H      -1.492346    -3.273762    -0.289388      26.05
 C      -0.765356    -0.546124    -2.480437      62.79
 H      -0.684282    -0.321629    -3.504545      25.17
 C      -0.053693     0.290566    -1.529934      -1.41
 O       0.509652     1.575409    -1.681441     208.81
 C       0.179348     2.048784    -2.951139     120.93
 H       0.307087     3.192956    -2.836595      25.98
 H       0.719078     1.580746    -3.796780      26.94
 H      -0.835745     1.952573    -3.121141      28.87
 C       0.103143    -0.278107    -0.170517      -4.87
 O       0.636432     0.386237     1.023487     124.69
 C      -0.204964    -1.582568     0.158358      42.21
 H       0.352328    -1.810368     1.000013      25.33
 C      -1.289563    -1.818372    -2.064159      30.14
 C      -2.083762    -2.731153    -3.124942      71.27
 H      -1.637444    -2.317839    -4.291283      21.89
 O      -1.604545    -4.142563    -2.838683     228.35
 H      -1.254503    -4.367179    -3.653534      30.36
 C      -3.675128    -2.670524    -3.062289      94.37
 H      -4.118043    -3.130237    -2.281338      28.69
 O      -3.944089    -1.296172    -3.262457     212.92
 H      -5.110054    -1.152492    -3.197637      23.33
 C      -4.185769    -3.379606    -4.348267      88.07
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 O      -5.520179    -3.355561    -4.285468     252.82
 H      -5.768061    -4.237037    -4.829709      26.14
 H      -3.722859    -4.584427    -4.227785      23.03
 H      -3.827764    -2.953171    -5.276204      26.40
55
name = lig-ACN-frame_950
 C       3.848524    -0.334778     0.605933      66.50
 H       3.054650    -0.157689    -0.096207      24.33
 C       4.739266     0.345353     2.677576      46.42
 H       4.365812     0.673403     3.591430      26.37
 C       5.955616    -0.423471     2.338379       6.49
 O       7.246009    -0.406004     3.078728     188.98
 C       6.922115    -0.433687     4.573877     110.86
 H       7.771316    -0.837278     5.187979      27.38
 H       6.311326    -1.167240     4.768191      30.09
 H       6.309102     0.610165     4.789081      24.37
 C       5.842259    -1.255477     1.275756      27.62
 O       6.995847    -2.016407     0.887839     158.03
 H       7.588278    -2.133412     1.672000      22.59
 C       4.795576    -1.278105     0.458734      73.83
 H       4.723301    -2.014887    -0.385976      22.26
 C       3.663457     0.330242     1.784448      28.05
 C       2.511427     1.129333     2.268026     114.48
 H       3.033005     1.952785     2.357026      28.55
 O       1.836577     0.578395     3.515750     262.65
 H       1.794268    -0.327040     3.514519      31.68
 C       1.572126     1.479605     1.167257     105.16
 H       2.099811     1.493861     0.376767      28.86
 C       0.709573     2.752228     1.266374     105.75
 O       1.436421     3.953103     1.682454     288.49
 H       1.627328     4.383348     0.887864      32.85
 H      -0.054942     2.351306     2.156836      25.33
 H       0.096593     2.977294     0.454470      26.85
 C      -1.134194    -2.215540    -0.660181       7.05
 H      -1.594757    -3.326940    -0.613477      23.50
 C      -0.748367    -0.523137    -2.421412      55.26
 H      -0.974515    -0.099637    -3.366470      23.21
 C      -0.131129     0.253050    -1.387655      26.22
 O       0.467367     1.525498    -1.673258     221.29
 C       0.112359     1.996297    -2.997133     114.05
 H       0.544281     3.093757    -3.127235      25.63
 H       0.658368     1.464486    -3.791552      27.06
 H      -0.926094     1.862425    -3.182820      27.89
 C       0.135315    -0.286819    -0.156495      24.99
 O       0.606487     0.372630     0.965076     138.20
 C      -0.152386    -1.700026     0.173066      51.28
 H       0.080032    -2.246910     1.018607      23.68
 C      -1.392032    -1.766526    -2.127159       6.22
 C      -2.055599    -2.745451    -3.072917      87.96
 H      -1.901304    -2.492011    -4.322525      21.72
 O      -1.558206    -4.093034    -2.844190     157.13
 H      -1.096814    -4.658423    -3.711096      24.21
 C      -3.573861    -2.721813    -3.165412      99.58
 H      -3.976227    -3.040843    -2.282878      27.84
 O      -3.832303    -1.323993    -3.226566     158.01
 H      -5.006773    -1.033592    -3.481730      21.93
 C      -4.008230    -3.478296    -4.431316      73.28
 O      -5.580221    -3.367796    -4.265341     298.78
 H      -5.987575    -3.846196    -4.881548      34.28
 H      -3.588287    -4.703045    -4.617782      23.30
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 H      -3.684880    -2.905635    -5.259020      28.47
55
name = lig-ACN-frame_951
 C       3.668665    -0.298019     0.482793      35.40
 H       3.071418    -0.214209    -0.351233      24.11
 C       4.819027     0.289938     2.756160      60.72
 H       4.955469     0.926105     3.559523      24.81
 C       6.052439    -0.275547     2.414719      13.14
 O       7.232629    -0.410709     3.095213     167.08
 C       6.784765    -0.446261     4.727993      83.47
 H       7.759239    -0.363258     5.208567      26.02
 H       6.077546    -1.113452     4.786262      29.54
 H       6.417538     0.730298     5.002988      23.89
 C       5.980603    -1.265190     1.310252      -0.54
 O       6.982811    -1.979191     0.854560     169.20
 H       7.690026    -2.008332     1.492846      24.52
 C       4.781529    -1.298448     0.419113      24.73
 H       5.000978    -1.971961    -0.440454      22.03
 C       3.686939     0.309715     1.829665      18.70
 C       2.418005     1.154858     2.354917      99.60
 H       2.498024     2.002736     2.844108      26.24
 O       1.854310     0.522571     3.478993     232.78
 H       2.062701    -0.498530     3.318392      26.30
 C       1.489629     1.457612     1.028263     102.66
 H       2.065335     1.720038     0.247076      27.00
 C       0.686874     2.777907     1.341284      86.19
 O       1.486827     4.049916     1.686646     256.92
 H       1.821229     4.280133     0.817081      31.27
 H       0.049222     2.845039     2.387722      24.06
 H       0.071444     2.913699     0.454426      25.26
 C      -1.162814    -2.316257    -0.822528      65.51
 H      -1.525740    -3.337240    -0.361967      24.06
 C      -0.829058    -0.524526    -2.348890      62.53
 H      -1.021387    -0.098500    -3.349139      21.74
 C      -0.133031     0.199100    -1.357798       2.32
 O       0.373096     1.434880    -1.663999     157.66
 C       0.076576     1.987396    -3.098492      95.26
 H       0.622170     3.099003    -3.080769      24.30
 H       0.521312     1.255051    -3.728971      26.06
 H      -0.950377     2.214403    -3.380772      26.35
 C       0.224608    -0.422653    -0.059198      18.58
 O       0.611838     0.376136     0.986461     200.02
 C      -0.285382    -1.680628     0.090903      52.29
 H      -0.131423    -2.050120     1.072746      26.72
 C      -1.387333    -1.738425    -1.950804      31.83
 C      -1.914192    -2.746059    -3.111349      92.63
 H      -1.158740    -2.260003    -3.918960      21.68
 O      -1.521909    -4.094586    -2.821911     214.21
 H      -0.843490    -4.193705    -3.689082      25.17
 C      -3.449949    -2.808666    -3.209090      84.14
 H      -3.861546    -3.383630    -2.410155      27.04
 O      -3.755625    -1.263908    -3.237290     179.08
 H      -4.888552    -1.249541    -3.305219      22.78
 C      -4.046844    -3.468573    -4.457519      84.26
 O      -5.556203    -3.420745    -4.286535     269.98
 H      -5.705453    -3.622545    -5.230581      30.13
 H      -3.773442    -4.762004    -4.490551      22.52
 H      -3.785103    -3.004810    -5.370862      26.06
55
name = lig-ACN-frame_952
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 C       3.732301    -0.426241     0.636290      48.93
 H       2.888981    -0.456832     0.066748      24.96
 C       4.867676     0.331823     2.737218      58.42
 H       4.747620     1.064461     3.512911      22.39
 C       6.039291    -0.383882     2.365615      16.44
 O       7.144974    -0.367252     3.359268     230.71
 C       6.807465    -0.360762     4.665750     122.63
 H       7.637074    -0.697879     5.238970      28.74
 H       6.264225    -1.203400     4.911448      30.56
 H       6.142613     0.624128     5.048248      24.03
 C       5.924442    -1.137241     1.217167      16.99
 O       7.073796    -2.042278     0.831233     147.99
 H       7.955236    -1.779535     1.275856      21.22
 C       4.825312    -1.171719     0.353212      69.92
 H       4.804533    -1.800841    -0.515706      25.51
 C       3.686629     0.429742     1.867273       2.58
 C       2.467194     1.247070     2.303525     102.63
 H       2.822478     2.152826     2.563499      26.12
 O       1.831577     0.424528     3.449571     160.43
 H       1.875211    -0.738052     3.361879      20.31
 C       1.496849     1.569210     1.126072      83.19
 H       1.874186     1.631109     0.111163      23.95
 C       0.633582     2.920750     1.454291      94.42
 O       1.500898     4.036353     1.640587     223.71
 H       2.110282     4.079419     0.706185      26.27
 H      -0.065181     2.555779     2.403003      24.11
 H      -0.082862     3.153885     0.635286      24.74
 C      -1.091484    -2.503086    -0.720635      30.10
 H      -1.622898    -3.476077    -0.627427      20.11
 C      -0.954862    -0.540745    -2.237582      52.91
 H      -1.075872    -0.113579    -3.291901      23.35
 C      -0.068739     0.146172    -1.421243      33.19
 O       0.250069     1.469554    -1.737337     227.84
 C       0.133478     1.929367    -3.057541     109.35
 H       0.951705     2.890810    -3.001560      23.85
 H       0.408935     1.402370    -3.948265      26.91
 H      -0.961199     2.256336    -3.212813      25.79
 C       0.188399    -0.404684    -0.213273       0.49
 O       0.598265     0.319565     1.060425      75.16
 C      -0.446562    -1.690817     0.230647      43.63
 H      -0.227599    -2.049273     1.261449      24.07
 C      -1.410827    -1.848916    -2.040755      23.18
 C      -1.769084    -2.687682    -3.137842     104.72
 H      -1.540970    -2.486251    -4.235737      24.05
 O      -1.408780    -4.143491    -2.859075     258.18
 H      -0.552895    -4.354788    -3.052323      31.95
 C      -3.343458    -2.663109    -3.304615      97.73
 H      -3.582513    -3.038164    -2.318014      25.88
 O      -3.723812    -1.346756    -3.248531     319.13
 H      -4.590654    -1.145894    -3.054447      30.67
 C      -4.109618    -3.445883    -4.444272      90.78
 O      -5.482825    -3.450169    -4.364326     212.25
 H      -6.031973    -3.912363    -5.246592      26.20
 H      -3.554898    -4.642515    -4.367285      23.18
 H      -3.780983    -3.063734    -5.404099      26.04
55
name = lig-ACN-frame_953
 C       3.704201    -0.445070     0.903138      50.72
 H       2.785342    -0.712531     0.436817      23.30
 C       4.849011     0.498459     2.637420      58.86
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 H       4.837926     0.795517     3.717867      25.06
 C       5.907571    -0.441323     2.471486     -11.84
 O       7.068025    -0.334987     3.333495     216.77
 C       6.771712    -0.399903     4.812730     115.16
 H       7.731660    -0.294193     5.258541      27.82
 H       6.073445    -1.096100     4.993692      28.98
 H       6.327988     0.693343     5.214748      24.97
 C       6.150762    -1.183424     1.086283      -9.55
 O       7.078276    -2.037791     0.810959     156.03
 H       7.912227    -1.693623     1.317701      22.71
 C       4.927802    -1.074870     0.298964      45.26
 H       4.853112    -1.715073    -0.544508      24.79
 C       3.767873     0.454144     1.822367      52.93
 C       2.563215     1.217070     2.275672      98.39
 H       2.865651     2.020358     2.802795      26.35
 O       1.809670     0.507221     3.387525     175.91
 H       1.976042    -0.562457     3.045851      22.49
 C       1.390478     1.626124     1.242404      60.61
 H       2.082590     1.843087     0.351564      22.13
 C       0.579140     2.891905     1.525085      92.12
 O       1.517092     3.995179     1.647948     197.39
 H       1.949187     4.065805     0.595776      25.05
 H       0.169521     2.991626     2.643513      23.29
 H      -0.270436     3.031239     0.712228      23.30
 C      -1.094869    -2.502966    -0.693663      73.47
 H      -1.254041    -3.475594    -0.434645      27.14
 C      -1.016914    -0.606977    -2.292608      43.47
 H      -1.507118    -0.196672    -3.255075      20.87
 C      -0.119929     0.153444    -1.485102       3.99
 O       0.215588     1.473973    -1.727272     202.83
 C       0.184027     1.977470    -3.074245     105.12
 H       0.957051     2.972115    -3.271920      23.69
 H       0.388806     1.084023    -3.644581      26.25
 H      -0.776470     2.438568    -3.377337      26.36
 C       0.070969    -0.355655    -0.013478       2.39
 O       0.577688     0.255022     1.025373     116.96
 C      -0.498299    -1.672575     0.290787      45.34
 H      -0.397352    -2.009403     1.392534      22.75
 C      -1.223411    -1.991775    -1.975817      16.43
 C      -1.782758    -2.865875    -3.344704      84.40
 H      -1.120384    -2.410214    -4.088099      22.62
 O      -1.330119    -4.175224    -2.936710     297.70
 H      -0.447435    -3.929563    -2.759819      30.58
 C      -3.382500    -2.703430    -3.265514      82.91
 H      -3.751217    -3.264008    -2.409829      24.43
 O      -3.692261    -1.245563    -3.297396     308.26
 H      -4.516088    -1.178894    -3.089996      32.02
 C      -3.907886    -3.452036    -4.472140      71.21
 O      -5.521258    -3.447118    -4.395361     214.06
 H      -5.569760    -4.342201    -5.049372      25.42
 H      -3.597075    -4.714442    -4.427716      21.62
 H      -3.609527    -2.990822    -5.443260      24.28
55
name = lig-ACN-frame_954
 C       3.751854    -0.605530     0.760534      29.08
 H       2.808387    -0.906745     0.203452      21.79
 C       4.976802     0.543092     2.692331      39.16
 H       5.036083     1.382230     3.500104      22.60
 C       5.963292    -0.414061     2.411667      32.60
 O       6.994700    -0.369222     3.268641     189.01
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 C       6.765625    -0.350276     4.911237      89.35
 H       7.700803    -0.598970     5.320358      27.19
 H       6.325936    -1.316121     5.143177      27.50
 H       6.180843     0.647160     5.149930      24.71
 C       6.058618    -1.055102     1.229712      20.59
 O       7.178963    -2.032659     0.781849     218.93
 H       7.946459    -2.177159     1.350783      26.59
 C       4.971673    -1.066932     0.356243      54.01
 H       4.990567    -1.624683    -0.550898      24.83
 C       3.734735     0.527093     1.891041      -5.43
 C       2.431345     1.272261     2.369565     105.83
 H       2.736310     2.252493     2.587587      25.62
 O       1.819453     0.614261     3.352144     285.27
 H       1.735483    -0.386049     3.380627      25.58
 C       1.415563     1.539604     1.236017      82.98
 H       1.633777     1.940109     0.185058      22.10
 C       0.551145     2.825932     1.681474      87.92
 O       1.518028     3.950554     1.633902     234.66
 H       1.599606     4.236030     0.666416      28.12
 H      -0.057423     2.750943     2.691785      24.79
 H      -0.278396     2.903679     0.810351      23.66
 C      -1.031088    -2.456170    -0.697618      47.36
 H      -1.303040    -3.367596    -0.394633      30.36
 C      -0.921121    -0.702369    -2.318545      55.47
 H      -1.385452    -0.225890    -3.226901      21.15
 C      -0.314945     0.144369    -1.343125       7.32
 O       0.222556     1.507620    -1.643567     145.85
 C       0.205020     1.967680    -3.138658      95.42
 H       1.212709     2.700549    -3.069434      24.09
 H       0.463647     1.225713    -3.934261      26.33
 H      -0.778276     2.395527    -3.450395      26.11
 C      -0.135720    -0.300718    -0.045992       0.26
 O       0.633592     0.348661     1.101619     114.82
 C      -0.507489    -1.599287     0.301736      43.42
 H      -0.412083    -1.988050     1.400749      21.42
 C      -1.167922    -2.076258    -2.103266      33.28
 C      -1.765484    -2.886288    -3.153413     101.58
 H      -1.580893    -2.605500    -4.213138      22.69
 O      -1.288798    -4.260678    -3.081467     202.47
 H      -0.247066    -4.257521    -2.614053      24.72
 C      -3.323481    -2.797695    -3.299667      69.48
 H      -3.781167    -3.088294    -2.312200      23.55
 O      -3.638410    -1.206011    -3.355206     193.78
 H      -4.645243    -0.924903    -3.412194      24.06
 C      -3.936898    -3.443192    -4.514676      85.02
 O      -5.385411    -3.485841    -4.437384     286.89
 H      -5.765185    -4.103521    -5.081416      30.11
 H      -3.397120    -4.626860    -4.530333      22.97
 H      -3.516853    -2.909606    -5.459468      24.90
55
name = lig-ACN-frame_955
 C       3.763535    -0.457106     0.751991      49.07
 H       2.863976    -0.508473     0.003993      21.63
 C       4.862019     0.600763     2.604344      61.06
 H       5.148856     1.572511     3.119892      22.12
 C       6.060470    -0.212940     2.464270      -6.69
 O       7.102151    -0.443095     3.438276     253.24
 C       6.807389    -0.394982     4.736362     121.21
 H       7.774479    -0.198182     5.187097      27.82
 H       6.067563    -1.198201     5.056967      27.94
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 H       6.277929     0.507687     5.193009      27.35
 C       6.130287    -1.177218     1.245077      -6.71
 O       7.145028    -1.936480     0.812287     152.35
 H       7.709835    -1.968392     1.615663      23.77
 C       4.977893    -1.170290     0.394218      46.36
 H       5.191534    -1.797263    -0.483590      23.42
 C       3.716709     0.362630     1.872708      40.64
 C       2.480821     1.337044     2.219922      76.06
 H       2.799680     2.284467     2.651319      23.90
 O       1.740274     0.679700     3.549894     195.33
 H       1.848283    -0.126442     3.279327      31.05
 C       1.338563     1.568330     1.153097      90.45
 H       2.090809     1.619794     0.225689      21.05
 C       0.564190     2.727712     1.727320      99.48
 O       1.423694     3.900878     1.664470     280.15
 H       1.452911     4.068128     0.805805      33.02
 H       0.367375     2.535146     2.805307      25.11
 H      -0.496916     3.068438     1.123382      22.89
 C      -0.979295    -2.466177    -0.729164      58.46
 H      -1.422405    -3.392269    -0.538747      22.23
 C      -0.785565    -0.674302    -2.345738      58.64
 H      -0.653813    -0.396161    -3.386264      21.68
 C      -0.450735     0.302836    -1.326149       8.42
 O       0.158248     1.459727    -1.675054     211.69
 C       0.268028     1.896797    -3.042359     108.43
 H       0.984993     2.875220    -3.072407      24.33
 H       0.498736     1.044627    -3.776231      24.21
 H      -0.664841     2.425266    -3.290407      26.18
 C      -0.134406    -0.142376     0.100171      -1.84
 O       0.555509     0.329691     1.109434     148.69
 C      -0.570120    -1.571966     0.270769      37.23
 H      -0.285388    -1.968764     1.318751      23.35
 C      -1.146367    -2.006707    -2.034159      29.20
 C      -1.767458    -2.928229    -3.127366      71.72
 H      -1.313826    -2.352512    -3.999782      24.43
 O      -1.317184    -4.377137    -3.184289     192.33
 H      -0.229141    -4.466509    -2.857070      26.09
 C      -3.370301    -2.691809    -3.237532      77.42
 H      -4.000794    -3.134248    -2.340066      24.92
 O      -3.504719    -1.307280    -3.423726     176.62
 H      -4.707183    -1.247253    -3.504514      21.06
 C      -3.887079    -3.474762    -4.570160      71.93
 O      -5.284599    -3.516220    -4.460792     291.33
 H      -5.466340    -3.771160    -5.284930      32.67
 H      -3.444303    -4.673787    -4.775971      23.04
 H      -3.627974    -2.779605    -5.494878      25.07
55
name = lig-ACN-frame_956
 C       3.835568    -0.383799     0.642583      31.18
 H       2.958722    -0.414331    -0.139594      21.05
 C       4.955487     0.615850     2.580083      52.01
 H       4.626336     1.159320     3.483702      23.06
 C       6.099590    -0.215172     2.437525       6.63
 O       7.225203    -0.451349     3.323918     235.09
 C       6.814075    -0.357719     4.809159     100.95
 H       7.667463    -0.509070     5.483195      25.98
 H       6.335199    -1.405581     5.033651      26.77
 H       6.198457     0.542978     4.806729      27.10
 C       6.029529    -1.125078     1.333530       6.50
 O       7.171537    -1.870421     0.939074     183.55
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 H       8.078674    -1.951837     1.441594      22.50
 C       4.930361    -1.228659     0.470146      58.16
 H       4.738051    -1.900209    -0.395312      22.25
 C       3.621485     0.385824     1.840207      28.13
 C       2.505370     1.197275     2.209326      71.91
 H       3.006452     2.224749     2.490001      21.99
 O       1.756408     0.798195     3.616636     140.47
 H       1.596552    -0.157138     3.791704      25.87
 C       1.380603     1.518163     1.135751      79.43
 H       1.536849     1.962354    -0.021531      19.72
 C       0.556589     2.703130     1.714870     100.66
 O       1.302787     3.895323     1.712152     245.16
 H       1.691581     4.111962     0.807971      28.86
 H       0.555529     2.404764     2.760810      25.36
 H      -0.647083     2.594522     1.476140      24.25
 C      -1.031173    -2.416654    -0.680453      52.24
 H      -1.122564    -3.471665    -0.318992      22.92
 C      -0.667584    -0.621370    -2.311723      67.86
 H      -0.468898    -0.414360    -3.320289      21.20
 C      -0.418227     0.296395    -1.311906      17.74
 O       0.138537     1.531239    -1.656160     234.13
 C       0.255960     1.904158    -2.971094     122.07
 H       1.152099     2.645825    -2.967479      24.76
 H       0.689667     1.039714    -3.640090      24.12
 H      -0.600059     2.103331    -3.522738      27.25
 C      -0.272605    -0.231614     0.006925       7.04
 O       0.473923     0.349672     1.170324     104.50
 C      -0.555531    -1.519015     0.305489      55.76
 H      -0.338183    -1.908702     1.305409      22.22
 C      -1.147230    -1.978131    -1.990356      34.09
 C      -1.706667    -2.912790    -3.179664      77.77
 H      -1.313576    -2.609739    -4.199162      23.36
 O      -1.431254    -4.357383    -3.189562     266.94
 H      -0.525792    -4.282888    -3.453342      30.31
 C      -3.268386    -2.798869    -3.316746      82.67
 H      -3.845938    -3.150341    -2.326099      23.30
 O      -3.429922    -1.379089    -3.486685     152.50
 H      -4.568688    -0.874205    -3.420548      20.82
 C      -3.712527    -3.436069    -4.543477      67.73
 O      -5.296938    -3.514525    -4.507304     235.31
 H      -5.768236    -4.059144    -5.312426      28.17
 H      -3.191778    -4.587099    -4.617655      23.87
 H      -3.271295    -2.792340    -5.461227      25.50
55
name = lig-ACN-frame_957
 C       3.787996    -0.365258     0.581964      54.70
 H       2.931519    -0.546702    -0.141143      21.23
 C       4.889970     0.508288     2.693014      60.26
 H       4.877754     0.846778     3.674827      23.44
 C       6.060652    -0.272123     2.465664       3.45
 O       7.272075    -0.374919     3.180179     208.92
 C       6.836166    -0.366901     4.813345      83.54
 H       7.812806    -0.195507     5.322418      26.78
 H       6.064302    -1.300338     4.857237      24.62
 H       6.274275     0.420020     5.165286      29.30
 C       6.061600    -1.143964     1.323687      -0.20
 O       7.180177    -1.863020     1.040111     152.89
 H       7.744754    -1.507913     1.810445      18.31
 C       4.883058    -1.232980     0.511843      50.65
 H       5.153650    -2.063481    -0.196960      21.01
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 C       3.865728     0.441295     1.774906      27.89
 C       2.406267     1.123549     2.273214      86.31
 H       2.692521     2.290828     2.461393      21.96
 O       1.868012     0.928375     3.558556     204.33
 H       1.595302    -0.193701     3.519917      22.78
 C       1.308310     1.445347     1.197058      73.75
 H       1.913725     1.522918     0.055610      20.06
 C       0.534915     2.598103     1.837868      99.44
 O       1.181734     3.979990     1.732468     142.98
 H       1.538224     3.962816     0.650592      24.60
 H       0.241728     2.482835     2.836103      26.12
 H      -0.321835     2.840547     1.030454      22.44
 C      -1.110760    -2.396510    -0.622300      35.76
 H      -1.356204    -3.557037    -0.455862      25.37
 C      -0.683800    -0.732435    -2.328644      46.81
 H      -0.917021    -0.314413    -3.277027      21.08
 C      -0.244007     0.242447    -1.324707       8.23
 O       0.099180     1.632984    -1.492306     166.88
 C       0.334112     1.921111    -3.069871      99.68
 H       0.751895     2.920095    -3.052731      26.86
 H       1.011178     1.066766    -3.520850      25.24
 H      -0.596817     2.115626    -3.487933      27.48
 C      -0.241532    -0.181410     0.063660       8.18
 O       0.344865     0.372310     1.147832     161.59
 C      -0.591489    -1.586007     0.377681      39.61
 H      -0.371435    -1.841337     1.370229      20.30
 C      -1.124209    -2.010611    -2.081295      32.60
 C      -1.650799    -2.840605    -3.237676     104.19
 H      -1.270405    -2.304385    -4.137773      25.33
 O      -1.453935    -4.269818    -3.106096     280.07
 H      -1.064044    -4.614603    -3.801336      33.62
 C      -3.132336    -2.789697    -3.344093      67.80
 H      -3.580400    -3.343461    -2.335101      23.65
 O      -3.387815    -1.329362    -3.524760     213.72
 H      -4.502460    -1.175546    -3.192127      22.04
 C      -3.760020    -3.528735    -4.599271      71.71
 O      -5.184172    -3.477155    -4.574935     242.40
 H      -5.274759    -4.464342    -5.126919      23.85
 H      -3.402437    -4.722437    -4.635300      22.47
 H      -3.401950    -2.937501    -5.609001      23.64
55
name = lig-ACN-frame_958
 C       3.837812    -0.391228     0.693807      37.75
 H       2.914282    -0.403401     0.142568      23.34
 C       4.864127     0.342461     2.838463      48.50
 H       4.739096     1.128307     3.476412      21.58
 C       6.022886    -0.333851     2.450660       6.07
 O       7.176384    -0.216815     3.270444     289.85
 C       6.948745    -0.346027     4.609586     111.45
 H       7.926241    -0.643334     5.087747      25.99
 H       6.437260    -1.447889     4.965535      25.74
 H       6.480714     0.465478     4.898268      30.59
 C       6.056473    -1.136233     1.303711      16.08
 O       7.191653    -1.882256     1.142233     226.01
 H       7.889574    -1.924046     1.787814      22.10
 C       4.969190    -1.295605     0.418319      61.51
 H       4.828694    -1.952725    -0.460047      22.69
 C       3.752629     0.495246     1.763883      23.07
 C       2.522848     1.260886     2.214532      90.45
 H       2.918799     2.416553     2.227805      22.22
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 O       2.000733     0.889558     3.522777     185.02
 H       1.603942    -0.150566     3.545734      22.99
 C       1.283323     1.356777     1.362488      80.73
 H       1.809121     1.776641     0.209394      21.07
 C       0.441912     2.700401     1.752815      93.84
 O       1.089891     3.987789     1.755630     209.16
 H       1.248771     4.190543     0.724409      26.12
 H       0.076711     2.492423     2.715966      26.44
 H      -0.560983     2.589010     1.075248      23.76
 C      -1.164732    -2.459161    -0.719758      43.53
 H      -1.787057    -3.427770    -0.319129      20.81
 C      -0.694838    -0.632211    -2.319591      51.44
 H      -0.931208    -0.332767    -3.351345      20.78
 C      -0.131346     0.197159    -1.303247       1.54
 O       0.067640     1.635921    -1.543968     198.28
 C       0.349688     2.001134    -2.948452     124.41
 H       0.759863     2.915874    -3.049089      27.94
 H       1.091686     1.241750    -3.422347      26.96
 H      -0.458222     1.656854    -3.564655      26.04
 C      -0.119949    -0.339015     0.055101      12.00
 O       0.215729     0.425563     1.220011     170.41
 C      -0.680848    -1.576413     0.334382      56.18
 H      -0.638011    -1.990966     1.278065      25.33
 C      -1.068672    -2.052921    -1.976223      32.17
 C      -1.562332    -2.796749    -3.268711      91.75
 H      -0.920084    -2.618062    -4.091732      23.92
 O      -1.389973    -4.226846    -2.991662     160.75
 H      -1.210776    -4.561079    -4.045087      27.50
 C      -3.142047    -2.648547    -3.456348      65.36
 H      -3.636207    -3.027109    -2.377260      23.11
 O      -3.430278    -1.312157    -3.510796     284.02
 H      -4.389651    -1.096886    -3.436954      26.33
 C      -3.699498    -3.595701    -4.651712      77.65
 O      -5.120113    -3.475325    -4.629199     281.34
 H      -5.759745    -4.096361    -5.200338      28.52
 H      -3.348321    -4.782948    -4.609739      24.20
 H      -3.201378    -3.155956    -5.682858      24.84
55
name = lig-ACN-frame_959
 C       3.872447    -0.472000     0.746861      60.17
 H       3.162412    -0.504129    -0.006005      24.13
 C       4.724182     0.377882     2.770267      47.54
 H       4.870414     0.822126     3.705382      22.34
 C       5.911305    -0.316445     2.507721      15.38
 O       7.093118    -0.092585     3.175944     295.42
 C       7.105939    -0.386653     4.640866      93.38
 H       8.181363    -0.399033     4.946446      26.44
 H       6.221979    -1.267469     4.724943      24.94
 H       6.756103     0.306382     5.270467      31.10
 C       6.118764    -1.206813     1.328054      -9.96
 O       7.235822    -1.995198     1.129606     184.11
 H       7.805795    -1.843255     1.915769      24.92
 C       4.965132    -1.194226     0.382732      56.74
 H       4.990734    -1.844088    -0.483669      24.55
 C       3.711175     0.353753     1.938450      52.64
 C       2.575086     1.353084     2.181533      82.50
 H       2.957319     2.483148     2.501601      22.02
 O       2.168379     0.826496     3.575024     189.98
 H       1.947976    -0.044505     3.354930      28.55
 C       1.240243     1.590560     1.286060      66.30
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 H       1.343299     1.550292    -0.002956      18.44
 C       0.312327     2.722212     1.700154     108.18
 O       1.006354     3.982673     1.739312     270.59
 H       1.120389     4.355575     0.965510      33.57
 H      -0.001822     2.637965     2.731210      26.23
 H      -0.610980     2.809175     0.953014      23.65
 C      -1.223228    -2.476147    -0.706923      31.49
 H      -1.798690    -3.521970    -0.505142      20.92
 C      -0.652399    -0.647284    -2.241553      53.85
 H      -0.537339    -0.178300    -3.269592      21.63
 C      -0.138717     0.224724    -1.272771      24.32
 O       0.061714     1.531707    -1.564261     228.21
 C       0.357769     1.971341    -2.859162     134.38
 H       0.403063     2.948024    -2.682181      29.13
 H       1.326248     1.570417    -3.176944      27.46
 H      -0.431812     2.043634    -3.590334      26.86
 C       0.008930    -0.394759    -0.003757      -8.76
 O       0.150216     0.409997     1.344595      41.97
 C      -0.739082    -1.669474     0.279222      35.80
 H      -0.942011    -1.794120     1.323515      24.01
 C      -1.051463    -1.912938    -2.114653      38.75
 C      -1.528466    -2.832573    -3.198953     106.27
 H      -1.110644    -2.478692    -4.061325      27.04
 O      -1.296147    -4.226031    -2.894412     150.58
 H      -0.982422    -4.867526    -3.798037      26.20
 C      -3.130724    -2.650152    -3.566539      62.64
 H      -3.668851    -3.271660    -2.610517      23.10
 O      -3.505346    -1.178137    -3.563073     280.24
 H      -4.332990    -1.118456    -3.693283      31.72
 C      -3.572181    -3.562856    -4.678990      79.09
 O      -5.148164    -3.452247    -4.659306     282.65
 H      -5.282225    -3.838824    -5.451081      32.11
 H      -3.236382    -4.614148    -4.227706      24.83
 H      -3.148441    -3.333120    -5.803792      24.47
55
name = lig-ACN-frame_960
 C       3.751475    -0.463621     0.697058      53.90
 H       2.995400    -0.412083    -0.035732      23.56
 C       4.797033     0.402040     2.835204      21.04
 H       4.487779     0.965262     3.726503      19.37
 C       5.911420    -0.381013     2.449383      22.68
 O       7.089926     0.033019     3.112228     203.61
 C       7.208616    -0.384034     4.715646      80.27
 H       8.218955    -0.799162     4.693170      25.79
 H       6.767210    -1.557751     4.945234      24.34
 H       6.930152     0.358578     5.277039      29.15
 C       6.088373    -1.263987     1.377770       9.32
 O       7.213179    -2.061523     1.118560     193.00
 H       8.011265    -1.806699     1.742637      20.22
 C       5.116408    -1.135938     0.454474      59.35
 H       5.273190    -1.615892    -0.478786      24.11
 C       3.575378     0.253745     1.833457      -2.74
 C       2.444703     1.314403     2.290636      67.27
 H       3.086204     2.412981     2.318461      21.93
 O       2.271791     0.821075     3.588426     220.49
 H       2.084797    -0.079137     3.612288      28.46
 C       1.119947     1.638471     1.175201      45.18
 H       1.859958     1.985959     0.166628      20.97
 C       0.220935     2.779954     1.690422     106.64
 O       0.943126     4.066797     1.740628     218.65
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 H       1.102621     4.115298     0.744736      28.21
 H      -0.205124     2.376864     2.620925      25.93
 H      -0.700354     2.860968     0.938656      24.19
 C      -1.237374    -2.382976    -0.829882      58.85
 H      -1.648259    -3.443810    -0.684091      21.93
 C      -0.530621    -0.652262    -2.336066      58.90
 H      -0.562286    -0.287006    -3.430048      19.84
 C      -0.180507     0.098383    -1.185507       5.46
 O       0.060131     1.467441    -1.445664     167.66
 C       0.372468     2.098916    -2.840535     116.89
 H       0.546586     3.050056    -2.600271      28.03
 H       1.222954     1.775459    -3.372589      27.79
 H      -0.433685     1.687769    -3.501971      23.78
 C      -0.066491    -0.364305     0.220443      27.11
 O       0.230703     0.338140     1.296316     137.31
 C      -0.670892    -1.604044     0.292590      57.30
 H      -0.876464    -2.041463     1.314811      23.68
 C      -1.147823    -1.979906    -2.077477      40.55
 C      -1.599407    -2.800374    -3.298093      95.72
 H      -1.021798    -2.670123    -4.086973      28.43
 O      -1.207502    -4.244487    -2.786440     204.54
 H      -0.498762    -4.404036    -3.436111      28.07
 C      -3.078455    -2.605110    -3.512524      76.29
 H      -3.774444    -2.930076    -2.519023      22.57
 O      -3.462938    -1.182889    -3.678934     275.59
 H      -4.400937    -1.093275    -3.593560      27.39
 C      -3.630518    -3.477228    -4.673808      98.66
 O      -5.015454    -3.436914    -4.740746     299.26
 H      -5.489892    -3.993021    -5.362659      32.06
 H      -3.332515    -4.609164    -4.487014      25.64
 H      -3.178397    -3.233903    -5.772050      25.19
55
name = lig-ACN-frame_961
 C       3.806823    -0.473384     0.571954      46.26
 H       3.091214    -0.622557    -0.251229      23.00
 C       4.652214     0.273219     2.644770      46.57
 H       4.942657     1.079063     3.401153      21.44
 C       5.995654    -0.298336     2.580246       6.79
 O       7.150793     0.062146     3.268281     312.08
 C       7.387753    -0.423059     4.559180     102.14
 H       8.420895    -0.466499     4.805817      25.40
 H       6.468954    -1.217713     4.876547      26.31
 H       7.126725     0.341003     5.183034      29.27
 C       6.088274    -1.247152     1.451170     -14.96
 O       7.151897    -2.075281     1.123316     164.76
 H       7.996160    -1.870889     1.644394      22.90
 C       4.980045    -1.133515     0.367274      39.94
 H       5.165263    -1.586789    -0.578349      23.40
 C       3.602465     0.349496     1.820261      43.60
 C       2.377098     1.146621     2.223670      87.42
 H       2.777153     2.361689     2.386733      22.30
 O       2.210344     0.888926     3.698998     128.10
 H       1.909357    -0.194147     3.708953      23.20
 C       1.162818     1.522486     1.359754      79.33
 H       1.461432     1.725950     0.119437      19.13
 C       0.156547     2.801089     1.651928      86.84
 O       0.840499     4.099355     1.714838     147.74
 H       1.475429     4.398308     0.821924      25.66
 H      -0.166942     2.885147     2.760316      24.97
 H      -0.735172     2.830478     0.944622      24.77
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 C      -1.203265    -2.313200    -0.739764      33.46
 H      -1.602236    -3.246999    -0.422670      22.10
 C      -0.467965    -0.748363    -2.337822      54.32
 H      -0.407497    -0.177744    -3.302569      20.61
 C      -0.158607     0.070050    -1.223594       3.61
 O       0.142595     1.523511    -1.351791     185.32
 C       0.331780     2.096052    -2.713333     124.19
 H       0.387400     3.139128    -2.697876      28.12
 H       1.132805     1.641156    -3.063675      29.06
 H      -0.624731     2.105122    -3.406756      25.62
 C      -0.274657    -0.330901     0.115579      -1.87
 O       0.433438     0.386750     1.229496     124.04
 C      -0.694165    -1.694112     0.361417      50.52
 H      -0.454914    -2.294588     1.321743      22.29
 C      -1.141029    -1.891238    -2.202582      38.27
 C      -1.567927    -2.842741    -3.259118     103.99
 H      -1.210058    -2.605858    -4.134634      28.89
 O      -1.173355    -4.202115    -2.805354     287.00
 H      -0.317959    -4.178006    -2.740749      35.71
 C      -3.184849    -2.606941    -3.468619      67.45
 H      -3.505783    -2.915088    -2.312262      22.05
 O      -3.331805    -1.239133    -3.829545     250.84
 H      -4.282645    -0.882207    -3.420345      22.80
 C      -3.577075    -3.478442    -4.712427      79.45
 O      -5.033742    -3.370905    -4.812549     282.59
 H      -5.285213    -4.394252    -5.213633      26.14
 H      -3.096107    -4.512918    -4.643503      25.80
 H      -3.047357    -2.768334    -5.476332      25.98
55
name = lig-ACN-frame_962
 C       3.800302    -0.394101     0.513870      50.05
 H       2.971814    -0.367354    -0.290205      23.58
 C       4.784294     0.358826     2.646967      21.77
 H       4.348172     1.035909     3.469641      21.14
 C       5.965366    -0.352899     2.493817      50.82
 O       7.175899     0.106540     3.262500     246.45
 C       7.485239    -0.383423     4.626481      83.41
 H       8.434490    -0.845066     4.534945      22.00
 H       6.977143    -1.540005     4.780643      21.58
 H       7.267518     0.247299     5.376569      28.05
 C       6.023902    -1.162772     1.347504      24.40
 O       7.073716    -2.047996     1.134851     173.26
 H       7.686592    -1.945321     1.843669      22.74
 C       5.046049    -1.213539     0.434665      66.50
 H       5.143509    -1.956991    -0.355321      23.39
 C       3.610528     0.292129     1.624693       5.12
 C       2.418475     1.201908     2.298170      61.99
 H       2.990717     2.353380     2.381243      21.96
 O       2.050141     0.921387     3.748557     148.88
 H       1.610385    -0.140890     3.838781      23.04
 C       1.185239     1.494201     1.404013      47.67
 H       1.955560     1.965357     0.428182      23.04
 C       0.245512     2.792660     1.731378     110.49
 O       0.757385     4.139398     1.651342     194.29
 H       1.368563     4.064290     0.783232      27.61
 H      -0.414109     2.592231     2.677754      25.98
 H      -0.494534     2.576505     0.901144      25.56
 C      -1.245487    -2.418613    -0.755972      70.79
 H      -1.662146    -3.329192    -0.755798      27.86
 C      -0.413618    -0.592568    -2.372226      63.60
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 H      -0.134676    -0.444848    -3.415989      22.30
 C      -0.129800     0.279365    -1.289043       8.21
 O       0.209051     1.539990    -1.298293     201.69
 C       0.266518     2.075807    -2.577276     128.23
 H       0.653614     3.027422    -2.244308      26.20
 H       0.920043     1.724171    -3.219611      29.45
 H      -0.752812     1.799419    -3.161443      24.65
 C      -0.264972    -0.294647     0.093831      -2.29
 O       0.409763     0.189830     1.178817     111.09
 C      -0.676432    -1.596526     0.358639      44.80
 H      -0.488175    -1.938100     1.469105      22.00
 C      -1.072552    -1.921525    -2.017773      10.40
 C      -1.578752    -2.841937    -3.202550      96.10
 H      -1.132793    -2.568387    -4.023496      27.37
 O      -1.215671    -4.170312    -2.885454     223.56
 H      -0.343286    -4.052055    -2.267181      26.42
 C      -3.111245    -2.745330    -3.426774      76.24
 H      -4.108740    -2.963754    -2.746501      22.00
 O      -3.211966    -1.255490    -3.923309     119.16
 H      -4.355294    -0.858167    -3.645719      21.06
 C      -3.513986    -3.397336    -4.693522      96.97
 O      -5.067485    -3.369922    -4.883748     216.56
 H      -5.432367    -4.269479    -5.479766      25.80
 H      -3.252043    -4.457709    -4.753915      25.66
 H      -3.129024    -2.941421    -5.619539      26.44
55
name = lig-ACN-frame_963
 C       3.841480    -0.412423     0.425782      35.85
 H       3.073928    -0.503383    -0.478389      22.76
 C       4.741736     0.490717     2.631525      46.74
 H       4.804581     0.784404     3.729092      21.97
 C       5.961354    -0.219684     2.465416      15.24
 O       7.109116     0.109880     3.139223     177.43
 C       7.567051    -0.506874     4.688399      67.01
 H       8.607814    -0.421280     4.676862      24.88
 H       6.887970    -1.465144     5.000292      23.98
 H       7.357413     0.288272     5.389301      26.84
 C       6.070235    -1.121037     1.318659      -1.69
 O       7.062178    -2.041741     1.164460     168.78
 H       7.706417    -2.026518     1.934089      23.08
 C       4.930928    -1.250787     0.339910      36.15
 H       5.065358    -2.103092    -0.367416      21.41
 C       3.685825     0.362442     1.821818      27.21
 C       2.438393     1.241666     2.404523      79.62
 H       3.008706     2.395403     2.626896      21.82
 O       1.928043     0.924176     3.677851     268.43
 H       1.529285     0.032791     3.609396      28.44
 C       1.293026     1.538588     1.405564      52.75
 H       1.612258     1.716558     0.151113      19.53
 C       0.249810     2.606436     1.723166      95.95
 O       0.730713     4.101384     1.586782     213.92
 H       1.042197     4.206133     0.758894      33.05
 H      -0.116757     2.569432     2.891615      24.64
 H      -0.556856     2.621644     1.010593      25.27
 C      -1.200300    -2.409428    -0.668245      65.50
 H      -1.653204    -3.223283    -0.357195      23.28
 C      -0.468398    -0.609585    -2.315859      67.65
 H      -0.319119    -0.339829    -3.324922      22.26
 C      -0.192626     0.224885    -1.210627      17.71
 O       0.323499     1.584126    -1.231214     200.42
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 C       0.263825     2.190073    -2.575744     118.73
 H       0.391043     3.306062    -2.757155      26.28
 H       0.834884     1.664880    -3.132886      29.13
 H      -0.905716     2.230731    -2.907312      25.65
 C      -0.139247    -0.309935     0.012542      12.66
 O       0.440135     0.145900     1.260878      68.42
 C      -0.780212    -1.563378     0.248674      42.10
 H      -0.951368    -1.820522     1.345316      25.09
 C      -0.980441    -1.854650    -1.997391      25.26
 C      -1.565967    -2.746064    -3.088723     100.40
 H      -1.143107    -2.456459    -3.918622      29.69
 O      -1.285727    -4.228346    -2.932858     147.30
 H      -0.328686    -4.297464    -2.237263      25.88
 C      -3.081140    -2.630524    -3.575236      65.57
 H      -3.594710    -2.922888    -2.442789      23.36
 O      -3.136317    -1.282893    -3.902287     154.09
 H      -4.362604    -1.119153    -4.102175      20.46
 C      -3.630112    -3.529922    -4.844318      99.18
 O      -5.005767    -3.355047    -4.909951     315.80
 H      -5.309942    -3.902280    -5.669827      29.56
 H      -3.302430    -4.513979    -4.687982      27.62
 H      -3.028894    -3.031508    -5.597649      28.47
55
name = lig-ACN-frame_964
 C       3.826412    -0.341642     0.643167      39.40
 H       2.861349    -0.362137    -0.025391      23.03
 C       4.795474     0.503190     2.735091      15.91
 H       4.688563     1.323370     3.459213      17.45
 C       6.008390    -0.119917     2.320595       7.89
 O       7.141278     0.044129     3.173644     248.19
 C       7.531325    -0.470062     4.590619      79.75
 H       8.566045    -0.760445     4.619050      26.33
 H       7.097195    -1.540627     4.773863      27.00
 H       6.959319     0.283986     5.225852      26.33
 C       5.986612    -1.127576     1.300581       0.14
 O       7.109407    -2.060216     1.193850     145.25
 H       7.864666    -1.773684     1.857209      20.03
 C       4.966043    -1.209871     0.340653      59.40
 H       4.934960    -1.728536    -0.650145      22.44
 C       3.626451     0.454738     1.839810       8.14
 C       2.449705     1.310020     2.330141      74.29
 H       2.807727     2.528831     2.617438      21.43
 O       1.834268     0.860508     3.604474     277.12
 H       1.525472     0.045568     3.514357      31.43
 C       1.319548     1.466638     1.317321      71.93
 H       1.903336     1.629934     0.192000      21.79
 C       0.245890     2.571434     1.679971      98.44
 O       0.710284     3.948650     1.556628     222.23
 H       0.773518     4.178886     0.600557      29.06
 H       0.301997     2.531856     2.934137      23.43
 H      -0.679616     2.162810     1.465078      26.93
 C      -1.172038    -2.330624    -0.720494      51.05
 H      -1.701856    -3.226459    -0.622634      23.04
 C      -0.565743    -0.621676    -2.233746      50.93
 H      -0.813022    -0.162515    -3.152738      23.55
 C      -0.110176     0.304836    -1.188473     -16.56
 O       0.408502     1.654668    -1.278495     151.17
 C       0.204838     2.292258    -2.616569     109.50
 H       0.817313     3.229500    -2.260888      24.09
 H       0.693989     1.887095    -3.359081      28.98
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 H      -0.934972     2.146392    -3.065282      24.57
 C      -0.008064    -0.371477     0.237423      -3.81
 O       0.526553     0.237610     1.355147     128.13
 C      -0.833342    -1.485866     0.433991      64.37
 H      -1.049795    -1.824003     1.442428      25.24
 C      -1.072739    -1.994667    -2.054796      29.54
 C      -1.452474    -2.810856    -3.272564     105.56
 H      -0.837941    -2.552778    -3.996684      28.08
 O      -1.396378    -4.226172    -2.912285     254.70
 H      -0.357363    -4.426223    -2.836619      28.80
 C      -3.003661    -2.625000    -3.628923      56.50
 H      -3.868365    -2.898293    -2.689841      21.97
 O      -3.168041    -1.206507    -3.900362     211.54
 H      -4.208920    -1.004786    -4.262818      23.85
 C      -3.517408    -3.625070    -4.845093     106.54
 O      -4.997386    -3.302550    -4.941887     324.93
 H      -5.377478    -3.878891    -5.484167      34.97
 H      -3.419665    -4.644057    -4.694709      27.61
 H      -3.200821    -3.404771    -5.810245      28.21
55
name = lig-ACN-frame_965
 C       3.719142    -0.320814     0.830095      55.10
 H       2.896674    -0.352369     0.079199      24.58
 C       4.852858     0.595749     2.704183      63.09
 H       4.968443     1.248735     3.517310      21.91
 C       6.002263    -0.142485     2.426751      -8.38
 O       7.266221    -0.002485     3.129686     251.20
 C       7.336489    -0.472651     4.410318     108.28
 H       8.411343    -0.277960     4.607448      24.20
 H       6.905599    -1.504723     4.521383      27.56
 H       7.057714     0.125656     5.384814      27.09
 C       6.071002    -1.200220     1.279555      -8.04
 O       7.100026    -2.006051     1.208179     175.48
 H       7.789706    -1.583341     1.768416      18.88
 C       4.925991    -0.996225     0.436018      53.04
 H       5.006665    -1.607966    -0.501134      23.14
 C       3.701149     0.553691     1.941796      38.28
 C       2.399782     1.315088     2.264231      78.87
 H       2.869566     2.503874     2.475812      22.97
 O       1.820098     0.821590     3.523645     208.13
 H       1.773808    -0.223473     3.372172      25.55
 C       1.306143     1.472619     1.219334      85.48
 H       1.732368     1.717510     0.121892      23.60
 C       0.341041     2.500081     1.778391     112.65
 O       0.654976     3.821953     1.479191     161.16
 H       0.761399     3.842923     0.349948      25.53
 H       0.212974     2.240492     2.987754      24.24
 H      -0.563694     2.494374     1.298438      26.36
 C      -1.244210    -2.318845    -0.672296      -0.24
 H      -1.584516    -3.337061    -0.359243      24.03
 C      -0.668100    -0.480567    -2.142318      55.69
 H      -0.767846    -0.043369    -3.131513      26.03
 C       0.022542     0.209210    -1.115883      -4.17
 O       0.391387     1.581946    -1.416857     181.04
 C       0.228938     2.331756    -2.615999     117.72
 H       0.483354     3.503127    -2.511381      25.08
 H       0.711417     1.965820    -3.404238      29.11
 H      -0.961657     2.660974    -2.751479      25.49
 C      -0.007507    -0.306173     0.330225       9.28
 O       0.611441     0.267383     1.422377     146.95
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 C      -0.795523    -1.490385     0.515174      55.35
 H      -0.909850    -1.864516     1.484679      26.49
 C      -1.049459    -1.853494    -2.035838       0.86
 C      -1.492365    -2.912119    -3.413460      86.77
 H      -0.959809    -2.817529    -4.271819      26.64
 O      -1.435519    -4.252559    -2.913431     272.88
 H      -0.776820    -4.604230    -3.335791      33.21
 C      -2.935404    -2.668374    -3.786091      58.23
 H      -3.563423    -3.090179    -2.702680      22.66
 O      -3.212192    -1.139092    -3.947301     244.28
 H      -4.125102    -1.125173    -3.952737      28.57
 C      -3.481988    -3.595955    -4.809813     114.50
 O      -4.948165    -3.253933    -4.942600     298.43
 H      -5.366965    -4.113805    -5.242786      27.86
 H      -3.314820    -4.472764    -4.370515      28.31
 H      -2.862290    -3.522848    -5.632044      29.24
55
name = lig-ACN-frame_966
 C       3.720663    -0.292611     0.868127      52.76
 H       2.887079    -0.416808     0.233885      24.01
 C       5.003113     0.737641     2.746442      43.67
 H       5.044803     1.227109     3.650844      24.48
 C       6.040622    -0.251503     2.514053      24.56
 O       7.288038     0.015395     2.947115     249.29
 C       7.263503    -0.498524     4.443591      80.16
 H       8.278605    -0.698691     4.876006      23.58
 H       6.932156    -1.534835     4.426393      26.80
 H       6.322270     0.117709     4.709094      24.65
 C       5.996080    -0.974674     1.414569       5.34
 O       7.126448    -1.960504     1.159694     192.95
 H       7.833169    -1.930576     1.798554      24.89
 C       4.908368    -0.948122     0.508865      56.49
 H       4.787929    -1.578002    -0.379404      22.84
 C       3.733700     0.585078     1.995040       8.45
 C       2.501063     1.365123     2.314681      91.27
 H       2.658553     2.565718     2.740863      23.27
 O       1.880058     0.815204     3.443363     176.20
 H       1.822130    -0.354099     3.444922      21.20
 C       1.349870     1.518132     1.280806      73.99
 H       1.417936     1.743785     0.193460      23.94
 C       0.252205     2.433904     1.779507      97.82
 O       0.664257     3.839914     1.416398     172.91
 H       1.117311     3.840689     0.434753      26.71
 H       0.165716     2.538710     2.988909      24.98
 H      -0.583762     1.924015     1.441934      27.52
 C      -1.216400    -2.232758    -0.600488      41.73
 H      -1.624528    -3.340291    -0.438588      24.23
 C      -0.680001    -0.439996    -2.124827      52.69
 H      -0.547995     0.140106    -3.073441      25.45
 C      -0.002559     0.186514    -1.097252      17.16
 O       0.431328     1.491777    -1.430354     170.21
 C       0.161330     2.372628    -2.636685     108.25
 H       0.899493     3.188767    -2.285249      24.55
 H       0.501271     1.973461    -3.518572      27.97
 H      -1.030666     2.337688    -2.954471      24.82
 C      -0.096959    -0.264950     0.232008      11.89
 O       0.603958     0.135481     1.368655      97.00
 C      -0.707550    -1.540573     0.405748      73.82
 H      -0.740377    -1.878090     1.383116      24.67
 C      -1.109110    -1.792186    -1.991989      -0.94
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 C      -1.489564    -2.812988    -3.332225      75.48
 H      -0.706910    -2.584847    -4.011259      24.84
 O      -1.442198    -4.313894    -2.918082     193.30
 H      -0.785726    -4.755344    -3.584754      27.53
 C      -2.956060    -2.517393    -3.751214      74.86
 H      -3.556920    -2.745173    -2.602515      22.53
 O      -3.252946    -1.224080    -4.004954     324.40
 H      -4.004997    -1.033985    -3.722880      33.67
 C      -3.523609    -3.556184    -4.798303     115.72
 O      -4.836809    -3.256971    -4.950848     244.41
 H      -5.376315    -4.126591    -5.470701      25.60
 H      -3.438883    -4.477144    -4.462500      27.24
 H      -3.170986    -3.409847    -5.778287      26.46
55
name = lig-ACN-frame_967
 C       3.792483    -0.197361     0.891185      65.36
 H       2.852411    -0.261821     0.476275      25.58
 C       4.980680     0.762113     2.817643      79.18
 H       4.996557     1.591437     3.460702      20.68
 C       6.046285    -0.035886     2.502972      -5.11
 O       7.410031    -0.020964     3.026004     235.41
 C       7.175747    -0.551986     4.374684     101.73
 H       8.008363    -0.178845     5.032361      25.26
 H       6.892961    -1.540347     4.300043      28.54
 H       6.419081     0.060368     5.126159      26.34
 C       6.032745    -1.075108     1.335646      -3.86
 O       7.027470    -1.840415     1.061434     108.39
 H       7.606468    -1.782304     1.905767      16.78
 C       4.887829    -1.066342     0.549364      57.29
 H       5.032150    -1.682247    -0.330037      21.22
 C       3.874251     0.665996     2.003741      25.88
 C       2.553483     1.432497     2.403417      51.97
 H       3.003905     2.613709     2.621873      23.12
 O       1.947586     0.809936     3.545442     195.29
 H       1.737653    -0.291424     3.151801      21.18
 C       1.310817     1.429787     1.383004      71.46
 H       1.892882     1.722907     0.543935      27.40
 C       0.204842     2.521563     1.748816     109.73
 O       0.602391     3.828928     1.388483     278.20
 H       1.138805     3.840141     0.654530      32.43
 H       0.187874     2.465547     2.942255      25.86
 H      -0.810907     2.506001     1.393146      26.05
 C      -1.208053    -2.300342    -0.750095      21.72
 H      -1.729891    -3.395622    -0.504624      19.89
 C      -0.644030    -0.570938    -2.234197      40.29
 H      -0.739095    -0.317555    -3.347789      21.19
 C      -0.191698     0.326328    -1.184475       5.46
 O       0.532583     1.498529    -1.393477     178.25
 C       0.134937     2.219275    -2.623005     117.09
 H       0.522182     3.267754    -2.497859      27.01
 H       0.552084     1.836716    -3.535995      26.13
 H      -0.979362     2.684244    -2.520829      25.90
 C      -0.090995    -0.285119     0.154681       6.60
 O       0.658701     0.084072     1.262677     138.51
 C      -0.626755    -1.537846     0.395817      58.77
 H      -0.529013    -1.969990     1.371837      25.98
 C      -1.228554    -1.829626    -1.990055      55.74
 C      -1.451965    -2.674336    -3.062549      98.53
 H      -0.780723    -2.465111    -3.940885      25.91
 O      -1.442013    -4.234540    -2.933240     139.96
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 H      -0.451947    -4.357376    -3.578919      23.50
 C      -2.991947    -2.569728    -3.572650      55.72
 H      -3.856535    -2.987210    -2.733775      24.15
 O      -3.275234    -1.166712    -4.114998     230.56
 H      -4.256206    -0.955559    -3.849320      25.10
 C      -3.425842    -3.533320    -4.805142      95.32
 O      -4.939460    -3.245074    -4.956441     235.85
 H      -5.252724    -3.966025    -5.773791      25.01
 H      -3.189564    -4.477327    -4.617758      28.49
 H      -2.754965    -3.258272    -5.569792      28.71
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name = lig-ACN-frame_968
 C       3.873338    -0.175271     0.863597      49.41
 H       3.088530    -0.222230     0.124883      26.94
 C       5.022902     0.787694     2.820984     -10.05
 H       5.180488     1.100487     3.919786      17.83
 C       6.216745     0.053583     2.276213      -3.18
 O       7.390155    -0.028173     3.167655     236.20
 C       7.189402    -0.552865     4.465677      94.85
 H       8.196814    -0.504878     4.916567      24.33
 H       7.121960    -1.574967     4.523228      29.11
 H       6.104913    -0.091034     4.827276      24.18
 C       5.947510    -0.965336     1.412918      -5.76
 O       7.047689    -1.796057     0.992689     147.92
 H       7.946335    -1.699299     1.506641      20.57
 C       4.809847    -1.137407     0.553695      63.96
 H       4.597384    -1.827089    -0.245065      22.84
 C       3.819077     0.780413     1.974058      21.85
 C       2.482340     1.352010     2.457179      84.20
 H       2.486301     2.595646     2.785631      22.69
 O       2.068764     0.862801     3.752009     195.58
 H       1.741790    -0.229871     3.663630      23.59
 C       1.327021     1.478138     1.361075      83.68
 H       1.560946     1.774981     0.427329      28.16
 C       0.202303     2.533983     1.750980     107.41
 O       0.569313     3.901402     1.421316     256.43
 H       0.902772     3.921954     0.543602      30.99
 H      -0.082611     2.521880     2.859120      26.78
 H      -0.622171     2.061030     1.144786      26.58
 C      -1.207884    -2.406810    -0.587288      49.84
 H      -1.545304    -3.569803    -0.414777      20.58
 C      -0.645913    -0.555793    -2.334129      55.96
 H      -0.544106    -0.176451    -3.408301      20.43
 C      -0.290601     0.305820    -1.245396     -14.05
 O       0.549380     1.527782    -1.407255     190.21
 C       0.127425     2.197789    -2.556928     132.86
 H       0.719834     3.050019    -2.686741      28.53
 H       0.179707     1.497522    -3.383821      25.25
 H      -1.063785     2.019858    -2.621817      25.05
 C      -0.059320    -0.310037     0.016384     -27.67
 O       0.785577     0.145825     1.201784      69.81
 C      -0.645148    -1.639409     0.296578      67.24
 H      -0.421178    -2.024911     1.319082      26.21
 C      -1.192764    -1.795740    -1.919355      -6.97
 C      -1.709777    -2.761611    -3.151975      98.07
 H      -1.133532    -2.228247    -4.024799      25.91
 O      -1.336810    -4.058276    -2.930341     225.01
 H      -0.275084    -4.353121    -2.994044      25.67
 C      -3.105440    -2.613781    -3.566023      81.79
 H      -3.705316    -2.629849    -2.493745      24.48
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 O      -3.278156    -1.154871    -4.115032     101.88
 H      -4.453840    -1.082375    -4.240043      20.96
 C      -3.384646    -3.437145    -4.739225     105.00
 O      -4.900855    -3.261340    -4.973259     271.60
 H      -5.197826    -4.029727    -5.534557      28.57
 H      -3.272727    -4.431922    -4.673739      27.36
 H      -3.015842    -2.852158    -5.587790      25.96
55
name = lig-ACN-frame_969
 C       3.759800    -0.055114     0.821305      50.58
 H       2.867209     0.052941     0.138199      23.40
 C       5.075538     0.744121     2.671540      69.96
 H       4.860953     1.094280     3.749803      20.49
 C       6.228560     0.121801     2.365467      11.69
 O       7.331849     0.021584     3.147148     203.44
 C       7.219112    -0.651997     4.597984      91.00
 H       7.980232    -0.259308     5.259583      24.52
 H       7.033503    -1.586127     4.415032      29.39
 H       6.329584    -0.119430     5.305809      24.86
 C       6.105536    -0.973309     1.251269      -5.51
 O       7.079190    -1.799611     0.932968     154.25
 H       7.831512    -1.480241     1.454200      22.31
 C       4.806029    -1.071942     0.688004      56.77
 H       4.741272    -1.955441     0.045642      22.55
 C       3.856764     0.749021     1.966095      19.72
 C       2.389837     1.385769     2.497273      61.20
 H       2.774389     2.589220     2.711532      22.25
 O       2.174795     0.894979     3.935397     203.76
 H       1.949635    -0.025507     3.882800      29.04
 C       1.361988     1.566941     1.343113      68.73
 H       1.985169     2.030742     0.723060      29.32
 C       0.174830     2.462545     1.706901     100.01
 O       0.515906     3.945812     1.497794     158.61
 H       0.815722     4.183539     0.467132      25.55
 H      -0.069479     2.464117     2.745034      27.93
 H      -0.844175     2.227457     1.141429      25.43
 C      -1.202223    -2.408011    -0.693902      16.71
 H      -1.568195    -3.482814    -0.438034      26.37
 C      -0.735898    -0.525593    -2.226412      51.67
 H      -0.719657    -0.289731    -3.316421      24.77
 C      -0.075312     0.236012    -1.230676       9.97
 O       0.451445     1.459218    -1.378230     191.19
 C       0.044887     2.131002    -2.665094     120.98
 H       0.594308     2.996291    -2.657996      29.31
 H       0.465252     1.692639    -3.613045      26.20
 H      -0.944925     2.721534    -2.576407      26.65
 C      -0.009389    -0.346004     0.093442      23.45
 O       0.785732     0.139401     1.037996     119.01
 C      -0.508892    -1.581483     0.415684      22.93
 H      -0.371521    -1.877672     1.513309      24.16
 C      -1.236652    -1.917722    -2.024681      20.20
 C      -1.693006    -2.628329    -3.240884      80.05
 H      -1.216493    -2.408215    -4.325491      22.38
 O      -1.237207    -4.038904    -2.899667     243.69
 H      -0.429192    -3.742554    -2.730174      32.62
 C      -3.262028    -2.461737    -3.537244      72.04
 H      -4.211340    -2.807917    -2.858204      23.50
 O      -3.287443    -1.209077    -4.019789     147.09
 H      -4.490276    -1.027223    -4.318178      20.36
 C      -3.549158    -3.388245    -4.773606     106.08
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 O      -4.855160    -3.321144    -4.976569     352.02
 H      -5.160902    -4.088110    -5.256252      32.16
 H      -3.058009    -4.282948    -4.612789      26.46
 H      -2.810749    -3.067968    -5.577154      27.23
55
name = lig-ACN-frame_970
 C       3.749052    -0.082566     0.797017      53.47
 H       2.741342    -0.427538     0.310856      21.56
 C       4.963311     0.789348     2.691115      28.18
 H       5.200037     1.560439     3.451509      22.06
 C       6.161116    -0.071975     2.375279      -8.19
 O       7.354504     0.063076     3.254217     186.11
 C       7.205824    -0.638999     4.606222      94.03
 H       8.207883    -0.504397     4.894431      24.67
 H       7.198319    -1.611444     4.585960      28.87
 H       6.163051    -0.249710     5.103398      24.79
 C       6.141433    -0.784495     1.221487      13.09
 O       7.173024    -1.813856     0.874144     177.54
 H       7.865721    -1.934793     1.555613      23.70
 C       4.828311    -0.954470     0.670368      30.06
 H       4.692748    -1.745364    -0.094238      23.08
 C       3.725426     0.744531     1.950922      20.68
 C       2.584194     1.445368     2.612239      86.08
 H       2.700031     2.691912     2.795479      23.50
 O       2.243044     0.915766     3.915168     228.76
 H       2.008674     0.068656     3.814915      31.92
 C       1.364270     1.542721     1.400939      76.01
 H       1.779709     1.815784     0.539563      27.81
 C       0.137055     2.551510     1.657257     103.15
 O       0.425842     3.914580     1.618271     192.02
 H       0.960475     3.978962     0.623469      24.88
 H      -0.052180     2.255251     2.630020      28.52
 H      -0.848137     2.354885     0.957003      24.93
 C      -1.076713    -2.298219    -0.696525      76.10
 H      -1.585300    -3.216803    -0.493117      24.66
 C      -0.804519    -0.568403    -2.145661      64.93
 H      -1.031909     0.068075    -2.971891      26.22
 C       0.017387     0.034519    -1.228702       1.90
 O       0.328598     1.462962    -1.459111     179.44
 C       0.094040     2.213312    -2.700021     124.40
 H       0.736170     3.006646    -2.588997      28.18
 H       0.081089     1.525655    -3.648237      24.61
 H      -1.043427     2.303436    -2.795199      27.31
 C       0.069364    -0.356514     0.101485      -8.70
 O       0.919578     0.257075     1.040613     152.80
 C      -0.545877    -1.666885     0.332376      52.81
 H      -0.586233    -2.138817     1.363187      25.80
 C      -1.219682    -1.792651    -2.011632      36.33
 C      -1.708178    -2.666005    -3.192393      84.90
 H      -1.077040    -2.071281    -4.095856      22.71
 O      -1.206668    -4.007332    -2.930491     279.01
 H      -0.344391    -4.180197    -2.629588      29.64
 C      -3.251460    -2.542946    -3.607626      82.92
 H      -3.732449    -2.725921    -2.562727      23.47
 O      -3.364708    -1.053902    -3.932229     151.24
 H      -4.547119    -0.668061    -3.897328      19.91
 C      -3.444272    -3.446270    -4.744476      98.38
 O      -5.039364    -3.398034    -5.023264     246.53
 H      -5.123066    -4.188403    -5.639252      27.60
 H      -3.365544    -4.422211    -4.405531      24.73
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 H      -3.037145    -3.008554    -5.697845      25.08
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name = lig-ACN-frame_971
 C       3.714909    -0.227688     0.914402      27.74
 H       2.811799    -0.612638     0.281404      25.17
 C       5.007459     0.784386     2.696998      60.39
 H       5.063403     1.414688     3.549942      24.86
 C       6.080395    -0.060288     2.524434      13.78
 O       7.256366     0.055187     3.304107     272.84
 C       7.259072    -0.626492     4.503192     118.26
 H       7.972654    -0.357020     5.200635      25.03
 H       7.021920    -1.548169     4.331284      29.48
 H       6.401801    -0.126983     5.264799      25.56
 C       6.186017    -0.885845     1.262425      -9.60
 O       7.167366    -1.712737     0.825629     176.53
 H       7.690679    -2.053685     1.652234      22.87
 C       4.970848    -0.854629     0.411107      13.79
 H       4.908735    -1.598830    -0.439578      22.11
 C       3.788308     0.752947     2.010643      20.19
 C       2.564363     1.542047     2.546278      80.68
 H       2.947101     2.613025     2.933619      24.53
 O       2.270773     0.911239     3.798774     192.21
 H       1.941235    -0.094809     3.579688      24.77
 C       1.383252     1.658923     1.392864      70.24
 H       1.825538     2.177464     0.676024      29.39
 C       0.084480     2.479629     1.732750     107.28
 O       0.403465     3.930682     1.709978     224.95
 H       1.013591     4.236389     1.006137      30.77
 H      -0.507880     2.441544     2.543345      29.07
 H      -0.485517     2.045229     0.771660      26.06
 C      -1.092619    -2.417819    -0.725653      45.23
 H      -1.370223    -3.355210    -0.549613      21.70
 C      -0.805777    -0.404164    -2.260189      53.14
 H      -1.198380     0.057360    -3.105292      22.05
 C      -0.010007     0.205569    -1.261508      13.95
 O       0.293028     1.456421    -1.492170     189.21
 C       0.059922     2.152995    -2.719620     118.52
 H       0.645898     3.054331    -2.749687      28.86
 H       0.621394     1.602685    -3.624464      25.30
 H      -0.951193     2.635221    -2.786908      27.41
 C       0.238864    -0.403725     0.148845      -1.77
 O       1.002764     0.192707     1.183616     113.89
 C      -0.462028    -1.578344     0.380481      57.72
 H      -0.504040    -2.050840     1.377411      25.87
 C      -1.289511    -1.807275    -1.965834       3.09
 C      -1.609152    -2.646137    -3.128943     102.41
 H      -0.975449    -2.296753    -4.180409      23.32
 O      -1.312776    -4.046363    -2.998780     187.53
 H      -0.163436    -3.843280    -3.056328      24.41
 C      -3.059928    -2.514816    -3.559866      71.31
 H      -3.849869    -2.854267    -2.805696      25.46
 O      -3.437020    -0.967961    -3.830839     248.07
 H      -4.396733    -1.011990    -3.373475      24.54
 C      -3.662131    -3.532403    -4.749478      90.59
 O      -5.090803    -3.447120    -5.045835     255.19
 H      -5.316629    -4.273025    -5.780358      25.09
 H      -3.169771    -4.510589    -4.629045      25.14
 H      -2.988327    -3.315424    -5.642836      26.00
55
name = lig-ACN-frame_972
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 C       3.859892    -0.320089     0.944417      72.63
 H       2.892768    -0.143631     0.445402      24.14
 C       5.023528     0.793403     2.780137      41.51
 H       4.975356     1.286076     3.697901      22.57
 C       6.105595    -0.097285     2.459335       9.47
 O       7.202346     0.099031     3.247339     238.39
 C       7.214093    -0.642127     4.584110      94.87
 H       8.228348    -0.554046     4.766222      25.68
 H       7.189732    -1.629565     4.495135      29.60
 H       6.243274    -0.315659     5.198785      26.30
 C       6.029551    -0.943640     1.320541      12.09
 O       7.177911    -1.614322     0.835209     187.07
 H       7.975696    -1.709247     1.477327      21.26
 C       5.088847    -0.776186     0.361606      48.53
 H       5.243513    -1.254219    -0.650789      23.51
 C       3.867595     0.652712     1.917224       1.91
 C       2.555240     1.519954     2.415576      91.09
 H       2.858394     2.604460     2.576177      26.06
 O       2.196677     0.893054     3.688459     161.69
 H       1.902209    -0.218289     3.396502      21.93
 C       1.429933     1.746725     1.527759      76.34
 H       1.748617     1.964611     0.592038      28.17
 C       0.081024     2.448413     1.717374     110.42
 O       0.370535     3.938967     1.812718     261.00
 H       0.791690     3.997042     1.046490      35.02
 H      -0.264312     2.053667     2.600497      29.00
 H      -0.663669     2.540191     0.825538      24.76
 C      -1.040855    -2.367150    -0.625372      64.86
 H      -1.206807    -3.322119    -0.550830      27.84
 C      -0.853338    -0.464321    -2.219217      71.19
 H      -0.855421    -0.100203    -3.196995      25.01
 C      -0.151136     0.295895    -1.213179      -9.49
 O       0.388143     1.631194    -1.434665     169.43
 C       0.108512     2.163401    -2.774274     108.75
 H       0.640883     3.140465    -2.595167      25.94
 H       0.364730     1.451310    -3.733566      23.96
 H      -0.966428     2.200686    -3.008412      26.48
 C       0.309437    -0.318451     0.030207     -43.80
 O       1.019985     0.113696     1.270849      15.54
 C      -0.363465    -1.597134     0.379728      14.54
 H      -0.164497    -1.794988     1.408003      26.40
 C      -1.214255    -1.752943    -1.954077      18.18
 C      -1.617098    -2.615581    -3.254799      77.08
 H      -0.799346    -2.158045    -4.128037      22.93
 O      -1.366984    -4.079547    -3.041080     120.30
 H      -0.380620    -4.504073    -3.585977      23.64
 C      -3.206587    -2.471906    -3.589160      85.43
 H      -3.534887    -2.785620    -2.526061      25.18
 O      -3.401386    -1.104812    -3.704957     277.53
 H      -4.383166    -0.853475    -3.771654      25.53
 C      -3.678315    -3.500059    -4.783341      87.63
 O      -5.087133    -3.456761    -5.003324     205.57
 H      -5.283286    -4.552516    -5.350902      24.55
 H      -3.628624    -4.492403    -4.280116      21.37
 H      -3.254182    -3.181521    -5.775164      23.80
55
name = lig-ACN-frame_973
 C       3.863000    -0.157763     0.739894      36.59
 H       3.189669    -0.437514    -0.029437      25.21
 C       4.963051     0.701136     2.787363      49.74
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 H       5.178053     1.488649     3.496249      21.20
 C       6.049931    -0.060057     2.452271      22.16
 O       7.243662     0.055352     3.255217     242.69
 C       7.232611    -0.676003     4.536534     114.37
 H       8.061573    -0.369750     5.119354      26.43
 H       6.999194    -1.672314     4.402063      30.17
 H       6.566568    -0.175160     5.361112      27.30
 C       6.160703    -0.910729     1.329691      20.75
 O       7.228848    -1.555014     0.868882     163.18
 H       7.950150    -1.334296     1.443564      18.82
 C       5.082828    -0.844497     0.401582       6.15
 H       5.155390    -1.138705    -0.685364      22.60
 C       3.840694     0.658369     1.973840      27.78
 C       2.689427     1.410267     2.408370      92.32
 H       3.072155     2.356918     2.779604      26.57
 O       2.078977     0.901669     3.589956     184.19
 H       1.823417    -0.222837     3.512885      23.06
 C       1.385273     1.521060     1.322683      76.97
 H       1.810664     2.006366     0.445911      26.47
 C       0.134271     2.516667     1.789579     108.67
 O       0.351389     3.883102     1.915290     243.93
 H       0.641823     4.426707     1.092133      28.37
 H      -0.273686     2.288090     2.747057      27.75
 H      -0.607963     1.958630     1.076725      25.02
 C      -0.952653    -2.263084    -0.633240      67.84
 H      -1.346112    -3.133708    -0.225317      33.17
 C      -0.774123    -0.440759    -2.087707      35.95
 H      -0.819729    -0.069721    -3.113050      25.25
 C      -0.146109     0.414883    -1.122185       3.48
 O       0.428174     1.713901    -1.413416     175.06
 C       0.145512     2.203530    -2.789127     103.79
 H       0.395046     3.251245    -3.234717      25.71
 H       0.862567     1.506839    -3.473621      24.79
 H      -0.884975     2.208502    -2.905406      27.38
 C       0.195100    -0.270403     0.100452       4.34
 O       0.945381     0.166902     1.185509     154.83
 C      -0.196092    -1.548755     0.288960      84.71
 H      -0.101911    -2.107858     1.168250      28.02
 C      -1.127102    -1.859550    -1.952618       9.10
 C      -1.665916    -2.683607    -3.298836      69.53
 H      -1.142883    -2.183216    -4.380593      21.42
 O      -1.412656    -4.040801    -3.071450     219.13
 H      -0.695372    -4.303234    -3.730258      27.44
 C      -3.233441    -2.590042    -3.556844      92.62
 H      -3.891922    -3.089001    -2.719216      24.45
 O      -3.414876    -1.162214    -3.675261     293.42
 H      -4.182699    -1.044958    -3.976296      33.31
 C      -3.620311    -3.397499    -4.686898      94.55
 O      -5.156946    -3.443824    -4.929218     249.99
 H      -5.301968    -4.411989    -5.405775      25.18
 H      -3.055337    -4.397987    -4.482622      24.16
 H      -2.954254    -3.266620    -5.571582      26.63
55
name = lig-ACN-frame_974
 C       3.893435     0.008549     0.602594      67.44
 H       2.999434     0.125599     0.114411      23.50
 C       4.947490     0.637206     2.743779      36.27
 H       4.779687     1.359656     3.606964      22.87
 C       6.159996    -0.093667     2.547717       6.20
 O       7.313284    -0.011357     3.257491     259.79
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 C       7.238127    -0.632995     4.538078     106.61
 H       8.248019    -0.707739     4.897126      25.02
 H       7.043005    -1.688320     4.398367      28.09
 H       6.295669    -0.232491     4.985620      27.21
 C       6.212222    -0.781682     1.231642      -3.68
 O       7.368972    -1.513117     0.898950     176.07
 H       8.071044    -1.606371     1.603242      24.81
 C       5.048016    -0.886811     0.428293      40.81
 H       5.203197    -1.691786    -0.356450      20.30
 C       3.767118     0.547082     1.858422      14.38
 C       2.513831     1.391719     2.360589     100.92
 H       2.791390     2.394464     2.524110      27.00
 O       1.953607     0.868816     3.601068     267.97
 H       1.777099    -0.109057     3.448971      27.25
 C       1.491481     1.535517     1.232979      91.10
 H       1.756726     1.852584     0.140948      22.18
 C       0.229802     2.369135     1.879415      87.60
 O       0.356185     3.885965     1.980359     152.21
 H       0.622135     4.168945     0.904316      25.35
 H       0.129464     2.046223     2.947600      25.09
 H      -0.703214     2.493617     1.252378      23.02
 C      -0.909703    -2.371324    -0.715186      27.19
 H      -1.342100    -3.382166    -0.455460      26.08
 C      -0.645679    -0.409978    -2.100913      56.85
 H      -1.030600     0.132343    -3.017805      23.73
 C      -0.065392     0.464884    -1.102938      11.26
 O       0.393303     1.773527    -1.409269     188.18
 C       0.170534     2.163587    -2.807091     103.86
 H       0.575813     3.252055    -2.418694      22.99
 H       0.799264     1.541449    -3.626336      25.14
 H      -0.732832     2.026589    -3.158805      29.08
 C       0.088676    -0.143883     0.136683       6.56
 O       0.896407     0.276945     1.140958     153.96
 C      -0.150197    -1.597220     0.248775      25.26
 H       0.207422    -1.898392     1.221490      24.36
 C      -1.084660    -1.774341    -2.048495      18.96
 C      -1.764554    -2.663102    -3.111173      92.36
 H      -1.270309    -2.240955    -4.241435      21.85
 O      -1.384017    -4.069252    -3.111090     255.64
 H      -0.554771    -4.104207    -3.288416      33.85
 C      -3.221745    -2.621109    -3.394269      80.39
 H      -3.839159    -2.889024    -2.483464      25.19
 O      -3.468237    -1.179125    -3.701948     262.55
 H      -4.419436    -1.087908    -3.561423      26.76
 C      -3.617875    -3.431847    -4.752647      86.17
 O      -5.055245    -3.443772    -4.844439     289.35
 H      -5.160195    -4.016695    -5.522688      33.58
 H      -3.421291    -4.597086    -4.720918      21.94
 H      -3.405634    -2.725815    -5.534538      25.31
55
name = lig-ACN-frame_975
 C       3.951673    -0.014754     0.559924      32.43
 H       3.329948    -0.119804    -0.284019      24.05
 C       4.889182     0.549154     2.751597      47.50
 H       4.730685     0.737197     3.880199      22.73
 C       6.147850    -0.055083     2.408078       7.52
 O       7.407470    -0.035537     3.226726     227.66
 C       7.223224    -0.698850     4.558799     111.66
 H       8.126592    -0.431415     5.115978      25.54
 H       6.904842    -1.775870     4.474411      26.82
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 H       6.654160    -0.162741     5.337936      27.55
 C       6.255009    -0.756378     1.257242      11.58
 O       7.428855    -1.436151     0.883260     179.80
 H       7.758892    -1.957890     1.721219      21.54
 C       5.067907    -0.883759     0.381961      -7.58
 H       4.920781    -1.697766    -0.391837      18.57
 C       3.810382     0.617090     1.871708      24.78
 C       2.476755     1.394071     2.297456      93.03
 H       2.778565     2.344559     2.667231      26.97
 O       1.864192     0.844573     3.580535     277.88
 H       1.716440     0.004404     3.516152      33.39
 C       1.385906     1.724320     1.282308      77.01
 H       2.061893     2.284942     0.399585      23.13
 C       0.298186     2.392008     1.910385     118.55
 O       0.438293     3.836509     2.008622     244.97
 H       0.774881     4.092992     1.058222      27.88
 H       0.215308     1.817059     2.897517      24.29
 H      -0.541603     1.816492     1.416748      26.21
 C      -0.767576    -2.374547    -0.783887      69.22
 H      -0.800738    -3.551600    -0.880342      23.23
 C      -0.628104    -0.358293    -2.258456      59.40
 H      -0.753710     0.096627    -3.315780      20.75
 C      -0.057488     0.388143    -1.255033       4.15
 O       0.285995     1.707158    -1.398564     205.92
 C       0.239639     2.219374    -2.765521     112.31
 H       0.540024     3.405549    -3.026638      24.92
 H       1.010902     1.703830    -3.470823      25.65
 H      -0.674778     2.284849    -3.067945      29.33
 C       0.069106    -0.254307     0.086160     -20.70
 O       0.848056     0.266155     1.173675      59.11
 C      -0.257078    -1.595425     0.206884      79.95
 H       0.006771    -2.111044     1.159665      24.94
 C      -1.069840    -1.698366    -1.918617      17.75
 C      -1.695083    -2.579712    -3.062361      63.30
 H      -1.236187    -1.975208    -4.117554      24.11
 O      -1.300404    -4.093466    -3.085808     204.72
 H      -0.413521    -4.103083    -2.644868      28.44
 C      -3.304138    -2.568871    -3.324208      78.63
 H      -3.823594    -2.967852    -2.442587      27.02
 O      -3.575911    -1.235873    -3.697817     232.48
 H      -4.593654    -0.771441    -3.437041      22.45
 C      -3.604599    -3.403848    -4.717237      83.40
 O      -5.028909    -3.443126    -4.770907     309.21
 H      -5.361341    -4.032381    -5.433222      30.86
 H      -2.941510    -4.335422    -4.990022      24.35
 H      -3.023977    -2.819099    -5.430186      27.49
55
name = lig-ACN-frame_976
 C       4.009507    -0.107193     0.643753      57.26
 H       3.085339    -0.124336     0.039727      24.13
 C       4.886600     0.431078     2.835463      27.74
 H       4.733825     0.868641     3.909885      21.79
 C       6.163819     0.030032     2.404655      -4.88
 O       7.330446    -0.082787     3.215156     247.10
 C       7.265805    -0.657404     4.590935      97.42
 H       8.301410    -0.805575     4.975543      24.83
 H       6.878632    -1.768897     4.546194      27.28
 H       6.462109    -0.129242     5.004818      28.29
 C       6.245739    -0.885269     1.164297       5.45
 O       7.404128    -1.386895     0.830966     165.29
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 H       7.995613    -1.824145     1.519149      21.15
 C       5.175049    -0.847518     0.330497      79.72
 H       5.384310    -1.278289    -0.691581      23.09
 C       3.802266     0.699310     1.808161      18.41
 C       2.612446     1.423263     2.425634      97.94
 H       3.005985     2.303283     2.787976      26.25
 O       1.855569     0.827006     3.511033     261.47
 H       1.688726    -0.134681     3.364568      27.16
 C       1.414321     1.635529     1.336666      62.52
 H       1.494832     2.178292     0.181412      19.42
 C       0.167407     2.442447     1.983100      99.33
 O       0.516825     3.793815     2.021904     283.56
 H       0.862006     4.158975     1.285477      33.71
 H       0.075078     2.463236     3.099290      23.99
 H      -0.826254     2.496709     1.405688      24.17
 C      -0.651926    -2.326414    -0.858697      12.32
 H      -0.836015    -3.522147    -0.504764      17.77
 C      -0.706710    -0.435354    -2.396804      57.08
 H      -0.666282    -0.214778    -3.509639      21.70
 C      -0.084029     0.318995    -1.322879       7.70
 O       0.227747     1.697422    -1.397534     194.36
 C       0.276708     2.294979    -2.759743     100.76
 H       0.857587     3.351370    -2.420417      23.19
 H       0.855407     1.573749    -3.387566      26.18
 H      -0.608758     2.298343    -3.188222      28.20
 C       0.195269    -0.292243     0.017103       3.68
 O       0.779617     0.266286     1.091396     118.40
 C      -0.290618    -1.610502     0.335524      48.18
 H      -0.104675    -2.081812     1.349877      24.36
 C      -1.111036    -1.734863    -2.086713      42.09
 C      -1.633786    -2.582193    -3.138866      79.66
 H      -1.166389    -2.280263    -4.318934      23.21
 O      -1.250557    -3.960547    -2.996640     148.65
 H      -0.158209    -4.070525    -2.533765      23.14
 C      -3.226643    -2.598898    -3.375537      87.41
 H      -3.896207    -3.015470    -2.661275      26.94
 O      -3.690588    -1.181755    -3.642567     150.55
 H      -4.926288    -1.381166    -3.661506      20.30
 C      -3.472332    -3.314732    -4.585997      95.73
 O      -5.052013    -3.450254    -4.734847     198.56
 H      -5.014352    -4.450551    -5.281937      24.15
 H      -3.209605    -4.391942    -4.335573      23.45
 H      -3.287210    -2.737778    -5.433410      26.74
55
name = lig-ACN-frame_977
 C       3.945380    -0.148373     0.704070      41.85
 H       3.085397    -0.113598    -0.047322      25.13
 C       4.927704     0.490326     2.825211      58.02
 H       4.857243     1.137838     3.744311      22.72
 C       6.132280    -0.158740     2.477483      30.85
 O       7.271398    -0.122171     3.213027     285.60
 C       7.219242    -0.629950     4.520947     111.42
 H       8.271076    -0.469825     4.873015      24.92
 H       6.776234    -1.752573     4.485023      25.88
 H       6.808598    -0.048228     5.332907      27.83
 C       6.233457    -0.783758     1.257605       2.28
 O       7.461456    -1.434666     0.697526     171.60
 H       8.081402    -1.314397     1.401845      22.24
 C       5.189094    -0.761877     0.223111      17.41
 H       5.354613    -1.171370    -0.818532      24.75
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 C       3.936642     0.538026     1.948283      22.94
 C       2.552442     1.432576     2.360172      92.14
 H       2.714741     2.391448     2.630526      27.91
 O       1.942957     0.783639     3.512593     206.12
 H       1.826290    -0.335984     3.228969      23.23
 C       1.280064     1.549269     1.412691      78.08
 H       1.805824     2.081878     0.328379      22.17
 C       0.094316     2.512327     2.038298      99.27
 O       0.636889     3.957297     2.064495     234.04
 H       0.941517     3.930307     1.096516      26.76
 H      -0.304653     1.783682     2.825931      25.24
 H      -0.723676     2.289565     1.304984      25.74
 C      -0.752530    -2.322938    -0.801888      33.94
 H      -1.362891    -3.391710    -0.737240      16.04
 C      -0.703107    -0.472624    -2.388956      52.88
 H      -0.990220     0.150311    -3.230705      20.40
 C      -0.116135     0.286558    -1.335554      12.99
 O       0.173604     1.648962    -1.423019     229.03
 C       0.326834     2.294401    -2.690860     127.04
 H       0.876320     3.372460    -2.417111      25.29
 H       0.978689     1.929964    -3.445162      28.34
 H      -0.472526     2.719810    -3.071064      29.42
 C       0.224824    -0.279673    -0.093321      16.03
 O       0.798175     0.288043     1.080991     152.00
 C      -0.216701    -1.558718     0.208088      72.53
 H      -0.114848    -1.849742     1.273888      24.97
 C      -0.989260    -1.811303    -2.163107      18.91
 C      -1.639449    -2.643848    -3.323157     100.13
 H      -1.101971    -2.142424    -4.386955      23.68
 O      -1.228858    -3.930372    -2.887177     155.30
 H      -0.048485    -3.746218    -3.000619      23.53
 C      -3.132200    -2.461889    -3.361541      94.15
 H      -3.282921    -2.897504    -2.418155      27.53
 O      -3.752135    -1.183134    -3.529304     200.31
 H      -4.884193    -1.350454    -3.938852      20.55
 C      -3.590066    -3.403425    -4.596089     105.45
 O      -4.965552    -3.493970    -4.702825     265.03
 H      -5.240600    -4.513720    -5.199343      24.07
 H      -3.027548    -4.376591    -4.503072      26.10
 H      -2.992270    -3.116099    -5.411400      28.82
55
name = lig-ACN-frame_978
 C       3.955118    -0.157661     0.682275      52.75
 H       3.094787    -0.142757    -0.077801      23.29
 C       5.039975     0.596879     2.870633       9.96
 H       5.131043     1.135464     3.815208      21.30
 C       6.063931    -0.354385     2.509228      -8.53
 O       7.286216    -0.125251     3.208142     251.53
 C       7.260472    -0.607042     4.574885      99.42
 H       8.313762    -0.849265     4.894871      24.37
 H       6.712038    -1.711532     4.760074      26.09
 H       6.624417     0.087191     5.117347      27.60
 C       6.297650    -0.791568     1.051865      12.85
 O       7.408247    -1.393455     0.654816     167.76
 H       8.216839    -1.279415     1.246122      25.08
 C       5.141071    -0.654139     0.318011      83.57
 H       5.162631    -1.190908    -0.659767      22.45
 C       3.715795     0.485809     1.971188      -3.25
 C       2.445082     1.289416     2.302707     104.79
 H       2.852442     2.203801     2.526666      25.90
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 O       2.073995     0.740786     3.598870     173.29
 H       1.927649    -0.427231     3.556927      21.21
 C       1.270195     1.643647     1.363141      70.02
 H       1.678127     2.385677     0.373306      19.69
 C       0.210491     2.528667     1.923344      93.49
 O       0.664091     3.936587     2.141636     189.15
 H       1.088936     4.529657     1.306450      26.82
 H       0.072308     2.623012     3.126884      20.74
 H      -0.644594     2.665941     1.258691      24.17
 C      -0.982656    -2.354155    -0.892896      34.89
 H      -1.194541    -3.407173    -0.430300      24.65
 C      -0.663100    -0.407782    -2.330507      64.38
 H      -1.110391    -0.029704    -3.192239      24.77
 C      -0.070341     0.351246    -1.333689      29.97
 O       0.134761     1.640765    -1.453066     245.33
 C       0.384748     2.414769    -2.651982     113.07
 H       1.118606     3.271369    -2.288556      24.33
 H       0.735721     1.707604    -3.314591      28.65
 H      -0.506065     2.632365    -3.016020      28.81
 C       0.229346    -0.228341    -0.083415      25.16
 O       0.791936     0.230602     1.083989     139.93
 C      -0.179039    -1.584192     0.020631      19.75
 H      -0.101443    -1.997914     1.016884      23.24
 C      -0.892807    -1.794393    -2.174784      31.98
 C      -1.503516    -2.473360    -3.331764      72.19
 H      -1.030822    -2.511054    -4.499646      22.17
 O      -1.207436    -4.029975    -2.917144     125.74
 H      -0.272713    -4.280534    -3.322318      24.93
 C      -3.162805    -2.535245    -3.380319      73.63
 H      -3.554464    -2.922982    -2.503372      25.96
 O      -3.709842    -1.173396    -3.419368     255.93
 H      -4.722622    -1.208742    -3.696219      24.53
 C      -3.525303    -3.539230    -4.580171     101.31
 O      -4.984426    -3.550517    -4.679234     284.14
 H      -5.259248    -4.205276    -5.413932      28.50
 H      -3.179921    -4.535685    -4.319219      25.23
 H      -3.279064    -3.041785    -5.453399      27.10
55
name = lig-ACN-frame_979
 C       3.849928    -0.074935     0.745631      39.70
 H       2.958948    -0.227914     0.095746      26.88
 C       4.894001     0.468995     2.702231      56.28
 H       4.928112     1.054525     3.570798      26.36
 C       6.098767    -0.238000     2.424876      15.36
 O       7.329726    -0.221564     3.198279     256.88
 C       7.287245    -0.610050     4.652921      95.07
 H       8.314225    -0.625149     5.095151      24.35
 H       6.545810    -1.606131     4.616336      23.71
 H       6.864213     0.184721     5.358372      27.04
 C       6.204047    -0.773902     1.154168      16.22
 O       7.409876    -1.371050     0.569020     124.94
 H       8.009293    -1.428808     1.398217      23.98
 C       5.145587    -0.710522     0.243143      47.55
 H       5.215239    -1.034552    -0.818147      23.42
 C       3.719452     0.517913     1.963994      33.86
 C       2.508702     1.233737     2.430581     111.07
 H       2.837776     2.185229     2.708615      25.37
 O       2.132072     0.724404     3.730772     251.98
 H       1.926682    -0.303914     3.674480      24.62
 C       1.378302     1.600071     1.286235      62.26
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 H       1.784262     1.774235     0.097218      19.28
 C       0.285985     2.685346     1.918270      91.05
 O       0.727601     3.961280     2.232469     252.41
 H       0.984970     4.281540     1.154418      22.92
 H      -0.085460     1.792320     2.817936      21.91
 H      -0.634488     2.527932     1.368497      24.66
 C      -0.944131    -2.307521    -0.951837      64.93
 H      -1.251145    -3.335445    -0.979169      26.95
 C      -0.617978    -0.391376    -2.376687      55.07
 H      -0.513535     0.090832    -3.308919      23.84
 C      -0.014746     0.407712    -1.311624      -8.31
 O       0.139879     1.858420    -1.376362     212.30
 C       0.392673     2.416306    -2.680689     135.94
 H       1.153237     3.283207    -2.472933      26.78
 H       0.855657     1.924002    -3.431678      31.11
 H      -0.319973     3.031978    -3.046811      30.17
 C       0.186792    -0.308390    -0.076275       3.17
 O       0.758934     0.246828     1.069138     134.71
 C      -0.248980    -1.667524     0.035379      57.72
 H       0.112814    -2.181468     0.874651      23.81
 C      -1.002014    -1.721284    -2.207423      34.12
 C      -1.502214    -2.679856    -3.275900      84.83
 H      -1.020505    -2.016747    -4.266619      21.57
 O      -1.227075    -4.084335    -3.060253     260.36
 H      -0.468135    -4.229658    -3.380006      34.46
 C      -3.110718    -2.667038    -3.397996      90.08
 H      -3.407713    -3.211693    -2.565922      27.62
 O      -3.631539    -1.208753    -3.379031     299.10
 H      -4.478923    -1.239590    -3.329661      32.56
 C      -3.504621    -3.532201    -4.556369     107.52
 O      -5.056172    -3.607394    -4.651163     315.47
 H      -5.183887    -4.153490    -5.329361      32.05
 H      -3.060547    -4.470968    -4.319777      27.07
 H      -3.026416    -3.323428    -5.432956      28.94
55
name = lig-ACN-frame_980
 C       3.825374    -0.163179     0.554118      62.38
 H       3.005210    -0.132814    -0.124718      23.94
 C       4.906805     0.374262     2.814060      36.57
 H       4.737896     0.802549     3.752275      23.44
 C       6.191093    -0.056686     2.382085      -1.98
 O       7.322603    -0.313579     3.206135     218.59
 C       7.252793    -0.559064     4.636624      97.46
 H       8.320760    -0.853132     4.743562      24.83
 H       6.737521    -1.632643     5.088742      25.72
 H       6.820979     0.297319     5.191941      26.80
 C       6.168903    -0.826543     1.097227      -3.39
 O       7.366547    -1.328882     0.579438     181.91
 H       7.914063    -1.777876     1.216063      24.48
 C       4.987565    -0.700768     0.231750      64.80
 H       5.194067    -1.137047    -0.758937      24.10
 C       3.775017     0.514029     1.859979       4.46
 C       2.581278     1.359322     2.547706      81.78
 H       2.803018     2.396268     2.785410      24.97
 O       2.106988     0.709641     3.841106     289.11
 H       1.924950    -0.126133     3.712932      31.44
 C       1.484480     1.454699     1.320273      73.08
 H       2.272367     2.032257     0.568636      21.53
 C       0.323217     2.522463     1.867337      62.88
 O       0.805719     3.972864     2.292730     196.75
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 H       1.140597     4.396179     1.382414      27.08
 H      -0.024060     2.101632     3.135051      20.47
 H      -0.331874     2.786169     1.110732      23.39
 C      -0.831701    -2.324180    -0.991625      31.03
 H      -1.149040    -3.260538    -0.839414      19.68
 C      -0.465390    -0.292964    -2.460340      59.81
 H      -0.457224     0.063620    -3.498844      21.45
 C      -0.087744     0.432520    -1.311497      -0.73
 O       0.150353     1.934787    -1.307855     173.21
 C       0.460338     2.544994    -2.730200     104.36
 H       1.329452     3.193730    -2.538316      25.70
 H       0.610569     1.711262    -3.311002      27.47
 H      -0.470289     2.878966    -3.048919      26.74
 C       0.139978    -0.294733    -0.055886      -1.34
 O       0.686792     0.246885     1.107733     128.90
 C      -0.244460    -1.671258     0.175548      65.36
 H      -0.038646    -2.203029     1.070357      24.84
 C      -1.135882    -1.634372    -2.229392      15.62
 C      -1.631377    -2.744122    -3.339274      79.48
 H      -1.173902    -2.594751    -4.542992      23.28
 O      -1.193131    -4.127149    -3.235144     237.09
 H      -0.252087    -4.045721    -3.240515      30.13
 C      -3.085960    -2.684085    -3.335293      96.52
 H      -3.415615    -3.076232    -2.423552      27.52
 O      -3.495912    -1.370702    -3.367638     304.04
 H      -4.449352    -1.450986    -3.325105      28.93
 C      -3.624797    -3.573780    -4.593890     104.64
 O      -4.996277    -3.624616    -4.615229     320.25
 H      -5.263363    -4.427220    -5.088106      29.41
 H      -3.280525    -4.573086    -4.439929      25.67
 H      -3.260106    -3.138956    -5.428889      28.94
55
name = lig-ACN-frame_981
 C       3.746618    -0.081702     0.563716      40.62
 H       3.020249     0.016736    -0.193065      23.19
 C       4.975981     0.377708     2.876109      54.28
 H       4.837209     0.493055     3.925299      22.67
 C       6.148861    -0.144582     2.382820       0.70
 O       7.280536    -0.390487     3.143242     238.01
 C       7.275084    -0.521813     4.585811      99.89
 H       8.257835    -0.588709     5.077685      25.26
 H       6.383251    -1.382470     4.773419      26.46
 H       6.941265     0.423646     5.119010      27.37
 C       6.152273    -0.718762     1.036968      23.82
 O       7.303985    -1.332724     0.569189     173.81
 H       7.691312    -1.826068     1.333103      24.16
 C       5.089569    -0.829538     0.197890      51.73
 H       5.078794    -1.487988    -0.654893      29.85
 C       3.783070     0.503864     1.885247       1.67
 C       2.578099     1.246690     2.524334     111.10
 H       3.025665     2.247856     2.782550      24.17
 O       2.102789     0.775193     3.844058     312.28
 H       1.998866    -0.146100     3.733818      29.01
 C       1.477423     1.542424     1.581132      89.22
 H       1.734886     1.726723     0.455261      20.81
 C       0.475361     2.518425     1.831684      90.93
 O       0.890949     3.839036     2.322312     302.46
 H       1.196706     4.255558     1.600059      33.55
 H      -0.419546     2.212230     2.834196      22.09
 H      -0.226134     2.398267     1.066091      25.40
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 C      -0.791481    -2.284289    -0.948869      59.44
 H      -0.989847    -3.221456    -0.833130      24.26
 C      -0.492209    -0.372465    -2.460241      62.30
 H      -0.693937     0.193175    -3.432877      19.52
 C      -0.111389     0.517669    -1.277790      -1.73
 O       0.184480     1.857340    -1.320817     219.97
 C       0.457488     2.516518    -2.646032     116.33
 H       1.242372     3.236522    -2.636860      28.05
 H       0.825665     1.850224    -3.427741      26.53
 H      -0.339502     3.211805    -3.032726      25.60
 C       0.108523    -0.191188    -0.013918      -0.46
 O       0.679263     0.257775     1.194356      94.13
 C      -0.253532    -1.569332     0.084481      75.44
 H      -0.206900    -1.940091     1.109837      23.37
 C      -0.967981    -1.683865    -2.282471      28.28
 C      -1.575873    -2.652280    -3.432648      52.30
 H      -1.414005    -1.970561    -4.535916      23.82
 O      -1.113198    -4.150697    -3.338094     152.76
 H       0.024021    -4.182350    -3.165346      23.93
 C      -3.176681    -2.905891    -3.327085      85.54
 H      -3.521820    -3.401517    -2.467214      26.91
 O      -3.464332    -1.425446    -3.385739     173.60
 H      -4.558699    -1.165604    -3.700533      23.20
 C      -3.598746    -3.607184    -4.564115     106.60
 O      -5.086512    -3.622260    -4.541885     270.43
 H      -5.454049    -4.459439    -5.242303      24.25
 H      -3.098085    -4.516135    -4.725088      27.14
 H      -3.333280    -2.996226    -5.334510      28.50
55
name = lig-ACN-frame_982
 C       3.958993    -0.052701     0.694460      77.66
 H       2.985329    -0.054655     0.263298      25.55
 C       4.869572     0.360083     2.788795      60.50
 H       4.778642     0.812792     3.811056      24.07
 C       6.078223    -0.332295     2.381783       7.75
 O       7.324238    -0.460065     3.044220     221.52
 C       7.194527    -0.413839     4.523086     105.83
 H       8.171639    -0.837525     4.766021      25.33
 H       6.480076    -1.364756     4.947637      26.27
 H       6.825715     0.544851     4.894100      28.28
 C       6.171373    -0.668953     1.020776       2.46
 O       7.306921    -1.394208     0.564992     149.70
 H       7.911385    -1.581115     1.396319      22.65
 C       4.941227    -0.800382     0.224160      43.23
 H       5.134349    -1.375216    -0.648169      20.72
 C       3.830602     0.424828     2.007960      41.60
 C       2.608594     1.168453     2.535939      99.59
 H       2.986405     2.251630     2.688070      23.23
 O       2.131467     0.819873     3.796493     292.26
 H       1.925485    -0.250238     3.989890      23.94
 C       1.453066     1.485701     1.530551      81.28
 H       2.149465     1.975693     0.737940      22.41
 C       0.323350     2.592861     1.920206      87.76
 O       1.006903     3.726643     2.331088     276.70
 H       1.293594     4.140461     1.488839      28.93
 H      -0.288429     1.863845     2.814415      21.54
 H      -0.104139     2.967245     1.024769      22.27
 C      -0.790144    -2.277036    -1.010729      36.15
 H      -1.076097    -3.235236    -0.794968      27.01
 C      -0.609517    -0.365721    -2.311347      67.09
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 H      -0.690287     0.150725    -3.319119      25.22
 C      -0.087541     0.414488    -1.308871      14.74
 O       0.229054     1.793434    -1.396881     216.35
 C       0.482492     2.492509    -2.566742     111.30
 H       1.201595     3.132225    -2.154733      26.20
 H       0.801156     1.847428    -3.449537      26.16
 H      -0.554285     2.966971    -2.824244      25.36
 C       0.122852    -0.056893     0.021083       8.78
 O       0.663402     0.255637     1.333002     116.77
 C      -0.281684    -1.388508     0.039914      41.39
 H      -0.102432    -1.967649     0.995493      22.85
 C      -0.744814    -1.850843    -2.315008      26.25
 C      -1.500790    -2.691169    -3.349869      65.36
 H      -1.248830    -2.163278    -4.518870      19.80
 O      -1.025442    -4.030823    -3.432118     147.72
 H       0.189792    -3.898350    -3.721937      18.85
 C      -3.049703    -2.914764    -3.337987      82.09
 H      -3.392537    -3.380602    -2.407420      25.15
 O      -3.562572    -1.473227    -3.380365     113.99
 H      -4.672093    -1.407395    -3.968206      19.76
 C      -3.639238    -3.590492    -4.643898      94.37
 O      -5.168436    -3.681591    -4.458442     226.26
 H      -5.541596    -4.121519    -5.488892      23.18
 H      -3.301565    -4.611950    -4.712335      25.64
 H      -3.322639    -3.035959    -5.420373      27.55
55
name = lig-ACN-frame_983
 C       3.828865    -0.091349     0.721296      33.16
 H       3.022344    -0.190678    -0.052074      25.25
 C       4.995378     0.276196     2.931579      39.73
 H       5.045907     0.939062     3.880004      19.03
 C       6.076337    -0.377622     2.344314      11.39
 O       7.276721    -0.507157     3.009141     239.85
 C       7.194300    -0.391527     4.410166     106.04
 H       8.148434    -0.474348     4.925218      25.65
 H       6.312611    -1.098665     4.828689      27.40
 H       6.970464     0.632769     4.719731      27.75
 C       6.172275    -0.914043     0.995131      45.19
 O       7.319223    -1.443574     0.561465     144.72
 H       8.023219    -1.287274     1.217105      24.93
 C       5.086983    -0.725029     0.238491      58.40
 H       4.847973    -0.912028    -0.770608      23.99
 C       3.746969     0.422934     2.086677       0.86
 C       2.553495     1.279002     2.521129      98.54
 H       2.958406     2.362889     2.741529      21.47
 O       2.136917     0.809758     3.865547     199.96
 H       2.016428    -0.369896     3.655839      20.35
 C       1.413519     1.452555     1.434714      88.02
 H       1.694831     1.703822     0.383166      21.69
 C       0.295624     2.516461     1.913868      77.50
 O       1.146640     3.752601     2.424300     174.22
 H       1.411571     4.282691     1.458578      25.06
 H      -0.378159     2.584677     2.986286      21.49
 H      -0.566346     2.577947     1.259588      24.91
 C      -0.680062    -2.282581    -0.926445      58.77
 H      -0.929466    -3.296675    -0.559877      22.10
 C      -0.631150    -0.417791    -2.359234      51.61
 H      -0.838009     0.107008    -3.292351      26.53
 C      -0.016743     0.411807    -1.246025       9.13
 O       0.258025     1.698912    -1.378224     218.60
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 C       0.488796     2.522201    -2.571797     107.92
 H       1.148519     3.319139    -2.469594      27.45
 H       0.955572     1.871781    -3.407545      26.14
 H      -0.468375     3.097439    -3.049005      25.17
 C       0.118864    -0.162445     0.077260      17.03
 O       0.656463     0.274073     1.288066     166.69
 C      -0.349403    -1.483197     0.115438      52.07
 H      -0.200620    -1.926088     1.172220      24.38
 C      -0.781334    -1.795680    -2.269742      31.81
 C      -1.413597    -2.687966    -3.417433      65.82
 H      -1.216266    -2.005875    -4.546987      20.81
 O      -0.881646    -3.988977    -3.520517     158.51
 H       0.348664    -3.887511    -3.856251      17.72
 C      -2.983945    -2.718637    -3.393208      84.88
 H      -3.233821    -3.368979    -2.515167      25.78
 O      -3.687083    -1.540416    -3.363717     223.97
 H      -4.767839    -2.049699    -3.600986      18.91
 C      -3.723854    -3.638398    -4.645820      95.79
 O      -5.120252    -3.682234    -4.397498     272.08
 H      -5.566699    -4.189599    -5.261853      24.20
 H      -3.290299    -4.667826    -4.682706      25.80
 H      -3.660476    -3.167887    -5.533434      28.30
55
name = lig-ACN-frame_984
 C       3.788780    -0.197316     0.766539      51.91
 H       2.929545     0.220672     0.122735      22.42
 C       4.922687     0.240937     2.881117      51.51
 H       5.111932     0.551307     3.972043      22.52
 C       6.104568    -0.409873     2.324483       5.78
 O       7.294294    -0.568295     2.985965     235.20
 C       7.238163    -0.282162     4.405303     108.35
 H       8.181696    -0.675521     4.786980      26.09
 H       6.465507    -1.072286     4.822754      28.36
 H       6.930085     0.684359     4.629362      30.52
 C       6.100448    -1.075433     1.088914      -9.08
 O       7.405930    -1.523858     0.506045     174.17
 H       8.027625    -1.414833     1.223876      22.19
 C       5.001240    -0.627606     0.144001      15.60
 H       5.392830    -0.931598    -0.810954      23.31
 C       3.774453     0.445080     2.118950       5.86
 C       2.540202     1.337487     2.532044      77.96
 H       2.871660     2.494172     2.766427      21.04
 O       2.103587     0.808004     3.867919     220.62
 H       2.065458    -0.351874     3.822322      21.47
 C       1.270062     1.539933     1.436817      87.93
 H       1.742237     1.952966     0.582122      23.91
 C       0.428715     2.601306     2.039147     108.43
 O       1.178212     3.754872     2.408396     233.24
 H       1.485973     4.292327     1.504827      26.31
 H       0.199240     1.795037     2.941910      21.29
 H      -0.270631     2.889520     1.232323      24.22
 C      -0.632441    -2.396502    -0.884650      21.85
 H      -0.768963    -3.575626    -1.035733      18.40
 C      -0.509421    -0.376286    -2.357112      56.52
 H      -0.769502     0.150248    -3.216061      21.52
 C      -0.042499     0.295545    -1.273965       7.02
 O       0.325617     1.809098    -1.328583     166.71
 C       0.501348     2.482001    -2.650076      89.69
 H       1.045571     3.228696    -2.259956      26.92
 H       1.063466     1.887736    -3.497552      24.61
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 H      -0.633056     2.806391    -3.016681      23.56
 C       0.099173    -0.326469     0.035839       7.79
 O       0.610599     0.191606     1.206580     117.93
 C      -0.331890    -1.653581     0.323768      59.63
 H      -0.486214    -2.125273     1.354510      23.20
 C      -0.958081    -1.754009    -2.158204       8.44
 C      -1.364507    -2.483239    -3.551430      51.39
 H      -0.870292    -1.759123    -4.530229      23.23
 O      -0.815783    -4.003122    -3.612678     133.41
 H       0.332467    -3.846397    -3.288833      21.38
 C      -3.012232    -2.845524    -3.506620      64.82
 H      -3.028005    -3.353532    -2.488737      25.35
 O      -3.838477    -1.541797    -3.344912     252.97
 H      -4.811527    -1.627746    -3.197382      27.21
 C      -3.626716    -3.642781    -4.615669     111.52
 O      -5.099549    -3.675005    -4.284320     321.23
 H      -5.497878    -4.295082    -4.793619      31.44
 H      -3.126583    -4.679736    -4.616732      25.63
 H      -3.341008    -3.225672    -5.495160      28.94
55
name = lig-ACN-frame_985
 C       3.840392    -0.113182     0.741945      53.03
 H       2.938785     0.022484    -0.004959      22.82
 C       4.906314     0.191549     2.829176      50.93
 H       4.611999     0.604442     3.830383      18.75
 C       6.054743    -0.519641     2.349371      -8.62
 O       7.331166    -0.583702     3.003518     205.67
 C       7.328454    -0.259899     4.440903     125.60
 H       8.361282    -0.455365     4.740588      25.09
 H       6.610894    -0.847202     5.041115      28.91
 H       7.219887     0.745197     4.642679      31.65
 C       6.089595    -1.020230     0.965447      22.30
 O       7.327870    -1.562736     0.497148     121.76
 H       7.859282    -1.952345     1.301324      23.04
 C       4.999760    -0.747031     0.213740      85.40
 H       4.779219    -0.822621    -0.856418      24.30
 C       3.777137     0.419920     1.987975      17.06
 C       2.534385     1.198435     2.556519      95.85
 H       2.996429     2.358887     2.741350      21.52
 O       2.039218     0.853523     3.820017     314.87
 H       2.066250    -0.139197     3.859346      26.28
 C       1.450630     1.522274     1.443145      67.85
 H       1.820020     1.870651     0.560662      23.06
 C       0.434768     2.612327     2.157741      96.55
 O       1.224081     3.791075     2.408043     295.91
 H       1.328180     4.144921     1.544669      31.07
 H      -0.149063     2.556721     3.247783      22.27
 H      -0.545900     2.840383     1.727949      24.71
 C      -0.749048    -2.490624    -0.959230      32.35
 H      -0.947575    -3.711959    -0.779887      18.27
 C      -0.506065    -0.406729    -2.317811      51.33
 H      -0.445374    -0.022520    -3.290267      23.67
 C       0.019805     0.413629    -1.200056       0.79
 O       0.370551     1.728863    -1.286642     194.13
 C       0.486589     2.408456    -2.617279      93.39
 H       0.896180     3.322731    -2.608074      27.30
 H       1.133948     1.723869    -3.288551      25.33
 H      -0.615285     2.609649    -3.220268      23.46
 C       0.076409    -0.428535     0.061881     -14.34
 O       0.597926     0.234313     1.207235      95.54
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 C      -0.317206    -1.841260     0.214557      65.07
 H      -0.078103    -2.223619     1.234389      24.90
 C      -0.958222    -1.743710    -2.170633      34.69
 C      -1.422201    -2.499907    -3.462597      79.97
 H      -1.049077    -1.893095    -4.561448      23.91
 O      -0.911983    -3.835474    -3.659260     169.22
 H       0.235013    -3.860673    -3.765576      23.05
 C      -2.982001    -2.773726    -3.474364      72.22
 H      -3.146881    -3.529668    -2.555294      26.92
 O      -3.852623    -1.547555    -3.322214     290.66
 H      -4.583529    -1.956402    -3.298838      34.09
 C      -3.564038    -3.672963    -4.619941      95.38
 O      -5.009442    -3.707988    -4.198412     300.81
 H      -5.421013    -4.329466    -4.788744      28.91
 H      -3.247261    -4.808126    -4.503458      24.24
 H      -3.546549    -3.228471    -5.549198      28.21
55
name = lig-ACN-frame_986
 C       3.855297    -0.022643     0.562440      54.42
 H       2.943231    -0.171410    -0.134070      25.97
 C       4.892778     0.132861     2.825561      49.29
 H       5.165896     0.517413     3.794158      21.54
 C       6.059041    -0.560015     2.374351      10.23
 O       7.264436    -0.609152     3.045882     250.96
 C       7.480043    -0.208055     4.443381     116.35
 H       8.465767    -0.508934     4.828413      25.58
 H       6.780958    -0.785136     5.024248      30.17
 H       7.233343     0.745859     4.523085      32.48
 C       6.159421    -0.885617     0.982482      17.48
 O       7.197339    -1.631381     0.485703     182.74
 H       7.555235    -2.185425     1.261934      23.94
 C       4.930828    -0.877452     0.166605      16.65
 H       5.113136    -1.443575    -0.817884      19.38
 C       3.752790     0.346239     1.968233      24.73
 C       2.600627     1.150797     2.455788      93.46
 H       3.102890     2.297946     2.663883      20.90
 O       1.978471     0.836813     3.796079     325.85
 H       1.843879    -0.010630     3.883927      32.69
 C       1.437610     1.442939     1.550598      80.81
 H       1.790831     1.835912     0.719627      25.16
 C       0.389190     2.624844     2.252067      96.89
 O       1.279940     3.868989     2.393605     273.18
 H       1.347187     4.284165     1.586498      30.78
 H       0.379379     2.042573     3.259249      21.76
 H      -0.261387     2.496876     1.442116      25.18
 C      -0.908791    -2.485285    -1.022403      32.06
 H      -1.429783    -3.612026    -1.009414      23.39
 C      -0.486492    -0.428310    -2.245058      64.15
 H      -0.463011     0.046520    -3.221419      24.93
 C      -0.017494     0.267419    -1.151712      12.51
 O       0.424122     1.666405    -1.243520     192.65
 C       0.467463     2.246992    -2.573596     100.24
 H       0.762391     3.141434    -2.363885      28.77
 H       1.227955     1.720574    -3.263292      26.35
 H      -0.688223     2.128865    -3.086464      24.01
 C       0.151296    -0.311153     0.093714      13.62
 O       0.589287     0.245994     1.280935     136.88
 C      -0.194753    -1.788190    -0.001054      20.58
 H       0.101026    -2.498973     0.736510      24.40
 C      -0.864213    -1.820074    -2.232545      24.77
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 C      -1.535632    -2.470193    -3.383956      81.19
 H      -1.481729    -1.525227    -4.297165      22.98
 O      -0.969240    -3.724028    -3.707269     229.48
 H      -0.129648    -3.530525    -4.034570      30.07
 C      -2.984201    -2.693840    -3.346412      86.25
 H      -3.227010    -3.328510    -2.351105      25.32
 O      -3.774147    -1.614417    -3.300774     267.14
 H      -4.612691    -1.905526    -3.720430      26.21
 C      -3.594198    -3.668640    -4.596930      86.30
 O      -4.916295    -3.801262    -4.148336     236.61
 H      -5.653767    -4.008922    -4.989070      22.78
 H      -2.875744    -4.629107    -4.699078      23.78
 H      -3.480836    -3.287641    -5.590873      26.73
55
name = lig-ACN-frame_987
 C       3.849040    -0.127881     0.513173      63.17
 H       2.977177     0.284682    -0.017439      18.71
 C       4.899354     0.074244     2.813612      57.52
 H       4.587547     0.505503     3.724172      20.48
 C       6.091047    -0.431250     2.359883     -14.93
 O       7.255855    -0.679092     3.078563     233.44
 C       7.492614    -0.185193     4.424362     133.06
 H       8.536632    -0.541345     4.397727      25.15
 H       6.985113    -0.704406     5.127963      31.89
 H       7.436330     0.769968     4.623635      33.66
 C       6.038080    -0.913763     1.010057      11.33
 O       7.135260    -1.744840     0.467414     131.03
 H       7.776455    -1.927286     1.144788      26.84
 C       5.013726    -0.863475     0.141735      78.90
 H       5.245127    -1.548981    -0.721287      23.98
 C       3.821553     0.245379     1.888998       0.94
 C       2.574544     1.181290     2.483888      89.27
 H       3.028971     2.349122     2.664664      21.67
 O       1.988931     0.805741     3.774020     311.14
 H       2.041442    -0.207275     3.699958      25.30
 C       1.352846     1.485682     1.547312      98.49
 H       1.609701     1.810421     0.620980      24.51
 C       0.625829     2.542411     2.204118     127.35
 O       1.211528     3.838751     2.410927     283.10
 H       1.277935     4.187506     1.429670      27.43
 H       0.073259     2.378048     3.188762      24.89
 H      -0.275866     2.977234     1.892894      24.32
 C      -0.878434    -2.331174    -1.021632      42.22
 H      -1.202910    -3.434149    -0.806352      26.18
 C      -0.433042    -0.476935    -2.299017      62.72
 H      -0.728695     0.147435    -3.188523      24.36
 C       0.015414     0.276973    -1.139970      15.27
 O       0.441481     1.516702    -1.207375     210.90
 C       0.452179     2.108521    -2.505930     113.97
 H       0.560849     3.054410    -2.432672      30.41
 H       1.245983     1.742346    -3.193523      27.56
 H      -0.653197     2.122585    -3.103632      24.50
 C       0.216390    -0.405899     0.104474      10.71
 O       0.561395     0.175943     1.387485     111.11
 C      -0.079411    -1.736533     0.014514      55.86
 H       0.014049    -2.148917     0.963120      24.70
 C      -0.917074    -1.768900    -2.279750      44.60
 C      -1.614245    -2.292027    -3.480947      68.39
 H      -1.433737    -1.673387    -4.574727      24.12
 O      -0.942136    -3.681754    -3.814586     178.48
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 H      -0.064230    -3.645973    -3.821224      31.35
 C      -3.113131    -2.891113    -3.278730      74.75
 H      -3.202203    -3.549947    -2.292105      24.47
 O      -3.779162    -1.504680    -3.277931     114.00
 H      -4.820864    -1.573748    -3.827535      21.48
 C      -3.465017    -3.599966    -4.480924      86.85
 O      -4.932257    -3.912623    -4.142398     221.74
 H      -5.449802    -3.921615    -5.143146      22.75
 H      -3.064610    -4.718133    -4.536656      21.88
 H      -3.423648    -2.856172    -5.267038      24.31
55
name = lig-ACN-frame_988
 C       3.842739    -0.223387     0.579112      60.28
 H       3.258710    -0.060775    -0.258582      25.74
 C       4.779151     0.099364     2.813225      46.90
 H       4.749679     0.243776     3.862335      25.21
 C       6.118394    -0.359281     2.350611      -5.83
 O       7.234292    -0.726153     3.056722     259.07
 C       7.556675    -0.221108     4.399800     125.75
 H       8.596559    -0.363424     4.728703      26.20
 H       7.000067    -0.664938     5.087055      32.98
 H       7.325647     0.719274     4.338634      34.43
 C       6.117894    -1.107037     1.017585      13.81
 O       7.103634    -1.812167     0.513481     183.87
 H       7.898715    -1.677478     1.090143      22.91
 C       5.029103    -0.776427     0.093600      54.07
 H       4.980020    -0.839561    -1.019029      23.40
 C       3.714369     0.326103     1.873191      28.65
 C       2.589918     1.157052     2.438193      88.48
 H       3.179371     2.222307     2.713026      21.81
 O       2.088754     0.736595     3.731948     268.79
 H       2.089576    -0.401537     3.949287      22.27
 C       1.415767     1.411027     1.464926      67.41
 H       1.703952     1.694006     0.445942      23.29
 C       0.449926     2.616733     2.230995     103.56
 O       1.239498     3.806546     2.422511     248.26
 H       1.469547     4.460804     1.528860      24.84
 H       0.487752     2.076669     3.222433      23.66
 H      -0.339689     2.373958     1.557675      26.03
 C      -0.691692    -2.318728    -0.957757      -0.39
 H      -1.003329    -3.354469    -0.834012      20.45
 C      -0.413618    -0.366252    -2.369123      52.91
 H      -0.425994     0.214525    -3.363481      21.16
 C       0.096995     0.158173    -1.170047      12.32
 O       0.470738     1.527814    -1.205193     206.78
 C       0.444798     2.136171    -2.505165     110.27
 H       0.695079     3.038861    -2.374960      29.59
 H       1.185437     1.571969    -3.077771      28.03
 H      -0.606678     1.854017    -2.997636      24.18
 C       0.286074    -0.422330     0.138952      -0.32
 O       0.527175     0.109734     1.411071     108.91
 C      -0.110909    -1.780361     0.229673      72.68
 H      -0.119355    -2.416462     1.062542      25.73
 C      -1.031259    -1.629481    -2.263497     -31.75
 C      -1.613740    -2.480219    -3.551303      99.70
 H      -1.804475    -1.546239    -4.387282      27.35
 O      -0.893930    -3.605354    -3.935629     192.78
 H       0.051363    -3.469588    -3.417738      23.16
 C      -3.048828    -2.730172    -3.226576      70.62
 H      -3.294602    -3.255495    -2.157552      25.73
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 O      -3.818625    -1.451251    -3.220947     136.49
 H      -4.997833    -1.744591    -3.338454      21.37
 C      -3.576728    -3.643304    -4.387433      97.67
 O      -4.947798    -3.993650    -4.231174     315.00
 H      -5.342051    -4.358894    -5.006316      28.07
 H      -2.736618    -4.431421    -4.667503      22.65
 H      -3.401953    -3.050157    -5.357577      24.61
55
name = lig-ACN-frame_989
 C       3.812571    -0.179071     0.606926      74.62
 H       2.908946    -0.185122     0.159031      22.12
 C       4.855986     0.115893     2.768823      39.40
 H       4.784270     0.561243     3.758705      21.76
 C       5.985904    -0.534688     2.265420      -0.16
 O       7.264828    -0.779326     3.033734     236.88
 C       7.489387    -0.213736     4.356070     135.80
 H       8.505213    -0.603011     4.546060      25.60
 H       6.915324    -0.646115     4.999625      34.71
 H       7.400978     0.755806     4.472821      34.46
 C       6.065167    -1.044109     1.007508      -2.34
 O       7.208861    -1.907370     0.561497     156.83
 H       7.957180    -1.952793     1.303463      20.47
 C       5.075821    -0.724228     0.120531      38.97
 H       5.483262    -0.920436    -0.869341      23.03
 C       3.722484     0.297005     1.928981      10.03
 C       2.548773     1.129845     2.387932     102.03
 H       2.874236     2.316508     2.495208      20.97
 O       2.191543     0.691390     3.734189     215.08
 H       2.193526    -0.511278     3.577351      19.46
 C       1.402425     1.371943     1.499618      83.91
 H       1.836670     1.745201     0.476630      20.73
 C       0.418839     2.498381     2.157393      93.33
 O       1.220341     3.772254     2.445411     228.64
 H       1.215131     4.062568     1.390247      24.33
 H       0.092775     2.147517     3.139555      24.68
 H      -0.499465     3.015301     1.654952      22.78
 C      -0.646096    -2.397083    -1.023246      55.12
 H      -0.940389    -3.360040    -1.058987      25.73
 C      -0.437993    -0.368747    -2.334536      41.11
 H      -0.280013     0.142823    -3.338036      22.75
 C       0.229050     0.211889    -1.170485     -13.10
 O       0.512200     1.582913    -1.185009     174.15
 C       0.491619     2.188236    -2.524887     121.63
 H       0.786506     3.110064    -2.383349      29.86
 H       1.096392     1.816024    -3.336128      28.02
 H      -0.536560     2.432929    -2.969651      26.82
 C       0.263029    -0.503270     0.198579     -14.19
 O       0.582280     0.179723     1.363270     129.11
 C      -0.210377    -1.848542     0.253599      59.67
 H       0.016541    -2.419206     1.167684      24.58
 C      -0.947056    -1.702457    -2.166687      23.24
 C      -1.588144    -2.369064    -3.380551      82.96
 H      -1.406334    -1.682929    -4.406449      23.44
 O      -0.794917    -3.544239    -4.014795      64.77
 H       0.290595    -3.599439    -3.488952      22.78
 C      -3.149747    -2.647439    -3.232812      78.45
 H      -3.116508    -3.183448    -2.130748      25.68
 O      -3.852186    -1.432401    -3.145660     254.52
 H      -4.805788    -1.839845    -2.942011      26.20
 C      -3.647134    -3.633526    -4.414996      86.65
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 O      -4.997165    -4.103118    -4.288459     324.93
 H      -5.147243    -4.705460    -4.932630      31.37
 H      -3.071444    -4.647117    -4.213831      21.31
 H      -3.567498    -3.114314    -5.416907      23.76
55
name = lig-ACN-frame_990
 C       3.846226    -0.137918     0.566959      61.21
 H       3.121027    -0.022142    -0.191706      25.56
 C       4.969153     0.187155     2.762603      57.38
 H       5.008119     0.825296     3.704002      21.76
 C       6.042307    -0.737575     2.425083      12.43
 O       7.184062    -0.783187     2.954865     250.47
 C       7.390028    -0.284087     4.320842     129.37
 H       8.388569    -0.596170     4.576397      26.85
 H       6.766824    -0.602583     4.950097      35.70
 H       7.394083     0.728186     4.285096      32.93
 C       6.186905    -1.079664     0.937055      11.80
 O       7.217626    -1.900512     0.638935     145.69
 H       7.567492    -2.167130     1.533162      20.27
 C       5.078933    -0.714074     0.085849      74.34
 H       4.990115    -0.997168    -0.930231      22.00
 C       3.817185     0.244795     1.899814      13.49
 C       2.563491     1.144179     2.484296      81.18
 H       3.098279     2.203657     2.695097      21.03
 O       2.253615     0.687288     3.746628     239.63
 H       2.209116    -0.497981     3.870123      20.77
 C       1.269383     1.420186     1.501723      80.48
 H       1.642534     1.927747     0.457136      20.93
 C       0.435937     2.485582     2.124128     100.52
 O       1.167060     3.665972     2.424384     297.09
 H       1.421675     4.252980     1.754484      31.00
 H      -0.000270     2.227597     3.042550      26.43
 H      -0.381321     2.561338     1.144934      23.24
 C      -0.710388    -2.584472    -0.946312      32.86
 H      -0.869551    -3.542292    -0.872166      27.72
 C      -0.351886    -0.440213    -2.138491      72.09
 H      -0.793443     0.128743    -2.969766      26.76
 C       0.211694     0.258221    -1.104519      22.03
 O       0.583514     1.604715    -1.228649     203.06
 C       0.554578     2.387472    -2.525205     111.79
 H       1.159075     3.229203    -2.339968      27.62
 H       1.039082     1.708264    -3.132661      28.38
 H      -0.515106     2.466521    -2.833099      27.02
 C       0.196432    -0.438497     0.077694      15.42
 O       0.602875     0.153209     1.300533     125.70
 C      -0.201620    -1.837213     0.112738      47.38
 H      -0.198658    -2.424415     1.108867      21.72
 C      -0.754773    -1.762112    -2.178939      25.96
 C      -1.504773    -2.207218    -3.386812      53.33
 H      -1.594565    -1.171672    -4.066427      23.75
 O      -0.751728    -3.473910    -3.985838      72.65
 H       0.354282    -3.492848    -3.773947      24.64
 C      -3.171151    -2.767280    -3.262534      64.64
 H      -3.496452    -3.498257    -2.352083      23.10
 O      -3.908475    -1.396777    -3.064981     246.79
 H      -4.724481    -1.370128    -2.952226      33.57
 C      -3.622606    -3.651820    -4.378678      90.85
 O      -5.087401    -4.168229    -4.257146     215.52
 H      -5.355258    -4.689400    -5.211225      21.31
 H      -2.795830    -4.478309    -4.402608      22.89
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 H      -3.322326    -3.193415    -5.418552      22.10
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name = lig-ACN-frame_991
 C       4.003788    -0.109460     0.535896      46.22
 H       3.229627     0.269285    -0.175139      25.38
 C       4.994547     0.154085     2.720836      47.25
 H       5.137745     0.641421     3.758034      17.42
 C       5.943079    -0.676350     2.269195      12.32
 O       7.286625    -0.860676     3.024335     251.17
 C       7.321138    -0.334804     4.305033     137.30
 H       8.201762    -0.637503     4.815579      26.26
 H       6.573732    -0.619849     4.799953      36.38
 H       7.219500     0.685384     4.252464      31.50
 C       6.077271    -1.148378     1.010462       7.82
 O       7.226078    -1.888751     0.666196     138.74
 H       7.808170    -2.155897     1.381593      24.62
 C       5.131106    -0.800013     0.037158      61.75
 H       5.413951    -0.901487    -1.011609      21.38
 C       3.801072     0.375032     1.889796      27.35
 C       2.699631     1.119159     2.463430      99.59
 H       3.040606     2.217865     2.672364      21.83
 O       2.241696     0.688563     3.868833     215.17
 H       2.204231    -0.397460     3.848451      23.00
 C       1.431107     1.403790     1.537919      55.76
 H       1.844035     1.723127     0.417569      20.83
 C       0.327807     2.491051     2.045849      90.91
 O       1.145177     3.641505     2.436757     292.10
 H       1.321868     3.968527     1.625937      32.26
 H       0.081573     2.074440     3.010292      25.05
 H      -0.734933     2.693919     1.358147      23.30
 C      -0.664215    -2.596793    -0.950877      62.95
 H      -1.080558    -3.563175    -0.829726      25.39
 C      -0.361799    -0.461720    -2.143999      38.51
 H      -0.674599     0.107298    -3.027482      26.40
 C       0.163932     0.347122    -1.123302      23.99
 O       0.655707     1.668860    -1.235162     206.95
 C       0.644901     2.406277    -2.487128     130.79
 H       1.193039     3.362780    -2.205790      26.64
 H       0.977106     2.037454    -3.416335      28.56
 H      -0.218334     2.867488    -2.854963      29.24
 C       0.204132    -0.371066     0.097792      11.81
 O       0.563518     0.040281     1.297900     100.88
 C      -0.159900    -1.782647     0.100546      38.94
 H      -0.062732    -2.124036     1.237864      23.53
 C      -0.721012    -1.903344    -2.142192      23.61
 C      -1.521936    -2.312714    -3.433866      78.85
 H      -1.687884    -1.523168    -4.346865      23.81
 O      -0.784778    -3.303837    -3.951332     213.16
 H       0.038343    -2.974350    -3.948991      34.13
 C      -3.182197    -2.728578    -3.199301      80.50
 H      -3.105833    -3.211145    -2.098792      25.21
 O      -3.859735    -1.427487    -3.019853     235.65
 H      -4.764185    -1.786415    -3.268018      26.94
 C      -3.644071    -3.718827    -4.456910      71.84
 O      -4.997139    -4.166124    -4.201031     235.12
 H      -5.573441    -4.216667    -5.217771      21.95
 H      -2.982553    -4.631545    -4.472510      22.14
 H      -3.816419    -3.068691    -5.435087      21.20
55
name = lig-ACN-frame_992
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 C       4.061803     0.009038     0.491304      60.74
 H       3.221716     0.228347    -0.285307      23.10
 C       4.915346     0.117540     2.753062      60.24
 H       4.689541     0.503481     3.818660      22.12
 C       6.143429    -0.580523     2.290498      -3.74
 O       7.270821    -0.967147     2.985487     231.53
 C       7.214474    -0.326562     4.412637     120.45
 H       8.119344    -0.696628     4.808988      26.65
 H       6.491352    -0.676578     4.853072      38.04
 H       7.278200     0.726786     4.486480      32.08
 C       6.079579    -1.317040     0.995054      12.82
 O       7.224672    -1.896600     0.609513     162.78
 H       7.848608    -1.688189     1.371016      16.43
 C       5.187668    -0.840920     0.048132      38.43
 H       5.504579    -1.000319    -1.013460      21.06
 C       3.937231     0.404946     1.815051      24.16
 C       2.609617     1.187603     2.540295      94.10
 H       2.995742     2.225106     2.712441      23.26
 O       2.262290     0.700031     3.882555     343.35
 H       2.151070    -0.189929     3.877561      30.84
 C       1.465951     1.294303     1.533028      80.02
 H       1.972125     1.575859     0.472346      20.47
 C       0.408901     2.354981     2.104264      88.43
 O       1.066084     3.659556     2.393503     250.12
 H       1.360281     4.275773     1.568326      25.96
 H      -0.173616     2.053811     3.006521      24.88
 H      -0.379652     2.807022     1.245096      21.64
 C      -0.573164    -2.450506    -0.932144      44.72
 H      -0.916899    -3.524995    -0.684784      23.07
 C      -0.421283    -0.438669    -2.331568      47.83
 H      -0.245341    -0.090640    -3.357980      25.69
 C       0.133008     0.336368    -1.201487      -5.63
 O       0.674553     1.672480    -1.244416     173.73
 C       0.728757     2.497209    -2.490864     104.89
 H       1.558542     3.328117    -2.215659      24.27
 H       1.218154     1.833009    -3.151443      26.92
 H      -0.261894     2.783853    -2.595173      27.22
 C       0.236052    -0.412279     0.089708      -9.73
 O       0.641756     0.083230     1.447221      92.31
 C      -0.125800    -1.746418     0.193685      36.28
 H       0.096584    -2.373977     1.173249      23.49
 C      -0.894384    -1.757149    -2.182750      19.47
 C      -1.652730    -2.297558    -3.371185     103.61
 H      -1.658743    -1.279600    -3.935964      25.55
 O      -0.767242    -3.353293    -4.048035     167.80
 H       0.117944    -2.990964    -4.072734      29.18
 C      -3.006153    -2.716573    -3.192599      92.83
 H      -3.225948    -3.490540    -2.300006      27.12
 O      -3.836123    -1.562966    -3.033644     168.13
 H      -4.906720    -1.642586    -3.528554      22.99
 C      -3.666304    -3.658714    -4.410416      87.59
 O      -4.947311    -4.145732    -4.092343     292.40
 H      -5.543523    -4.257061    -4.945469      24.56
 H      -2.965667    -4.464682    -4.652976      24.47
 H      -3.422926    -3.042150    -5.440514      23.39
55
name = lig-ACN-frame_993
 C       4.112779     0.067907     0.389217      40.07
 H       3.369987     0.304800    -0.493599      23.91
 C       5.021242     0.035390     2.774399      32.76
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 H       4.912309     0.290692     3.856078      19.41
 C       6.121915    -0.619372     2.301095      15.61
 O       7.216581    -0.930012     3.127071     280.43
 C       7.213191    -0.435849     4.446604     118.57
 H       8.063570    -0.766397     5.011807      24.97
 H       6.446646    -0.669434     4.899417      38.10
 H       7.096803     0.624979     4.220321      31.42
 C       6.163307    -1.189392     1.039233      15.28
 O       7.280811    -1.966783     0.528038     202.55
 H       8.102733    -2.071864     1.168164      23.60
 C       5.141965    -0.789368     0.098258      41.93
 H       5.162400    -1.094245    -0.964648      20.88
 C       3.888070     0.451959     1.831892      23.07
 C       2.660411     1.164634     2.520773     106.30
 H       2.865634     2.202541     2.726266      23.84
 O       2.304439     0.714299     3.840431     344.27
 H       2.111639    -0.157890     3.801295      30.69
 C       1.412290     1.303367     1.636506      96.09
 H       1.737121     1.678906     0.588460      21.54
 C       0.538284     2.393360     2.026877     107.22
 O       0.997553     3.668219     2.409289     281.48
 H       1.040087     4.135514     1.367770      23.70
 H       0.070957     1.974391     3.005229      24.41
 H      -0.228932     2.082243     1.270967      25.16
 C      -0.640879    -2.291351    -0.951703      37.36
 H      -0.699339    -3.494238    -1.101099      22.71
 C      -0.356495    -0.303472    -2.382252      58.25
 H      -0.563686     0.329240    -3.298482      23.23
 C       0.156295     0.280006    -1.240240      -1.99
 O       0.666834     1.589311    -1.215583     187.26
 C       0.804345     2.457593    -2.452243     114.82
 H       1.478563     3.471554    -2.181457      24.17
 H       1.043092     1.996274    -3.445918      26.20
 H      -0.019743     2.907300    -2.858085      28.51
 C       0.301946    -0.332495     0.178884      -5.74
 O       0.714696     0.070878     1.425273     134.68
 C      -0.041004    -1.729652     0.193233      50.24
 H       0.111881    -2.359573     1.125473      23.23
 C      -1.006877    -1.584793    -2.092759      21.77
 C      -1.535611    -2.221682    -3.399022      67.44
 H      -1.775043    -1.549780    -4.193805      28.02
 O      -0.815337    -3.406111    -4.147703      99.82
 H       0.352834    -3.320994    -3.958918      23.29
 C      -3.104510    -2.917842    -3.230605      81.68
 H      -3.090561    -3.547239    -2.235264      25.43
 O      -3.838267    -1.647005    -3.029817     115.46
 H      -4.845921    -1.873487    -3.616785      22.94
 C      -3.470134    -3.595691    -4.388459      89.03
 O      -4.952886    -4.092326    -3.965388     278.72
 H      -5.189321    -4.528672    -4.684028      31.63
 H      -2.858841    -4.424054    -4.466128      25.60
 H      -3.851672    -2.941259    -5.341968      22.67
55
name = lig-ACN-frame_994
 C       4.072471     0.142792     0.561008      51.07
 H       3.351483     0.586614    -0.205805      24.54
 C       4.938193     0.051966     2.696272      51.30
 H       4.903758     0.360957     3.711939      22.01
 C       6.111598    -0.743895     2.351026       7.81
 O       7.212184    -0.978560     3.205001     250.06
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 C       7.173009    -0.432395     4.540999     123.85
 H       8.134440    -0.824240     4.920211      26.90
 H       6.505110    -0.837824     4.987145      38.25
 H       7.258108     0.639548     4.816416      30.03
 C       6.339650    -1.049961     0.925898      10.83
 O       7.265032    -1.999162     0.457865     185.28
 H       7.677139    -2.368234     1.267358      23.12
 C       5.220578    -0.745046     0.126744      39.44
 H       5.495345    -1.044104    -0.906096      18.70
 C       3.934038     0.413888     1.870567      35.05
 C       2.794304     1.161127     2.468806     104.45
 H       3.206799     2.128724     2.573965      24.01
 O       2.364260     0.691090     3.813691     262.92
 H       2.175597    -0.400284     3.782460      23.39
 C       1.624505     1.398702     1.548429      66.23
 H       2.081229     1.644371     0.599965      22.94
 C       0.363615     2.358665     2.103815      90.62
 O       0.928566     3.704515     2.331276     287.15
 H       1.180162     4.357197     1.589830      27.38
 H       0.014192     2.044599     3.193927      22.86
 H      -0.429759     2.746871     1.529267      22.85
 C      -0.740090    -2.209106    -1.002317      24.71
 H      -1.020441    -3.425305    -0.939430      24.06
 C      -0.409195    -0.205257    -2.210631      58.17
 H      -0.735940     0.488985    -3.079090      22.90
 C       0.287996     0.354787    -1.071600      19.94
 O       0.697650     1.618565    -1.239086     217.48
 C       0.788715     2.388709    -2.439027      99.78
 H       1.659097     3.137859    -1.906410      22.52
 H       1.427502     1.785614    -3.174070      25.25
 H      -0.123377     2.827904    -2.530956      26.80
 C       0.318873    -0.371646     0.099758      31.11
 O       0.757091     0.049937     1.373732     109.83
 C      -0.003696    -1.699873     0.090228      57.57
 H       0.239994    -2.204683     0.992013      23.70
 C      -0.928176    -1.489314    -2.237468      12.63
 C      -1.563867    -2.344751    -3.496472     106.36
 H      -1.486687    -1.556317    -4.141977      28.05
 O      -0.840099    -3.356256    -4.135091     176.58
 H       0.212071    -3.713053    -3.697950      23.49
 C      -2.948145    -2.801151    -3.141526      80.11
 H      -3.029963    -3.555290    -2.251705      25.10
 O      -3.891579    -1.748876    -3.014429     266.45
 H      -4.798517    -2.049405    -3.253814      28.41
 C      -3.551615    -3.743873    -4.408923      87.73
 O      -4.857694    -4.056004    -3.912502     310.08
 H      -5.294327    -4.753897    -4.443976      27.50
 H      -3.038189    -4.504430    -4.790669      26.85
 H      -3.418200    -2.976885    -5.360654      23.94
55
name = lig-ACN-frame_995
 C       4.178654     0.051307     0.520907      56.75
 H       3.430104     0.305915    -0.237060      21.28
 C       5.055605    -0.033178     2.822267      28.53
 H       4.923425     0.293598     3.812431      19.45
 C       6.167212    -0.727343     2.342931      18.90
 O       7.177777    -1.019582     3.203980     201.91
 C       7.202740    -0.491382     4.729295      81.56
 H       8.189205    -0.871729     5.094071      25.34
 H       6.505599    -0.909699     5.148469      36.45
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 H       6.953673     0.606135     4.610281      29.00
 C       6.317179    -1.040742     0.941225      19.26
 O       7.221481    -1.976111     0.432325     164.12
 H       7.832946    -2.306293     1.095967      26.73
 C       5.300527    -0.551530     0.065295      54.65
 H       5.124715    -0.793231    -0.975544      25.04
 C       3.969619     0.340799     1.919575      20.38
 C       2.836723     1.244780     2.537545      96.93
 H       3.153188     2.158912     2.861565      25.19
 O       2.444812     0.670972     3.760904     205.37
 H       2.305054    -0.514046     3.673605      21.39
 C       1.520003     1.449478     1.434631      83.59
 H       1.724196     1.952779     0.584607      22.53
 C       0.369713     2.453317     2.113035     101.11
 O       0.890717     3.773526     2.345581     350.60
 H       1.058342     3.929617     1.506577      34.08
 H       0.082610     1.851767     3.096944      24.40
 H      -0.399285     2.044833     1.498038      26.28
 C      -0.782050    -2.260667    -1.099921      39.83
 H      -1.441430    -3.256812    -0.834486      24.12
 C      -0.514347    -0.150973    -2.103960      66.07
 H      -0.414767     0.508865    -3.021687      22.24
 C       0.253678     0.404727    -1.110386      10.07
 O       0.805403     1.728948    -1.091649     226.71
 C       0.833051     2.359964    -2.386492     118.36
 H       1.466582     3.428420    -2.534844      24.23
 H       0.908913     1.700763    -3.362036      25.17
 H      -0.047664     2.704290    -2.839367      27.72
 C       0.462664    -0.360119     0.123856       7.96
 O       0.903047     0.112775     1.311484     142.97
 C      -0.068071    -1.736063    -0.010512      58.80
 H       0.024990    -2.432152     0.720480      25.11
 C      -0.814682    -1.598238    -2.318904      37.47
 C      -1.544631    -2.150019    -3.525691     101.20
 H      -1.875639    -1.607431    -4.270694      28.80
 O      -0.791202    -3.384913    -4.087140     181.63
 H      -0.107113    -3.470920    -3.354045      28.68
 C      -2.902739    -2.876229    -3.229505      89.50
 H      -2.726892    -3.386823    -2.226901      25.29
 O      -3.924625    -1.789629    -2.968206     285.78
 H      -4.563487    -2.313863    -2.977689      34.99
 C      -3.504412    -3.801653    -4.354677      95.48
 O      -4.831106    -4.071818    -3.872240     193.36
 H      -5.412463    -4.573037    -4.763874      22.73
 H      -3.041209    -4.667789    -4.387237      26.47
 H      -3.734936    -3.179147    -5.373457      22.60
55
name = lig-ACN-frame_996
 C       4.171118     0.066399     0.541252      49.35
 H       3.329594     0.209575    -0.093133      21.10
 C       5.054236    -0.068748     2.882659      48.51
 H       5.054865     0.027516     3.973940      20.55
 C       6.229583    -0.638079     2.364991      -1.22
 O       7.266003    -1.088926     3.316033     254.53
 C       7.172764    -0.623187     4.657414     122.43
 H       8.182040    -0.653732     5.145900      24.61
 H       6.584894    -1.108027     5.198638      35.24
 H       7.006997     0.530311     4.757870      29.53
 C       6.237841    -1.083267     0.975325      14.27
 O       7.206181    -1.932804     0.426450     193.65
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 H       8.066792    -1.847536     0.964593      24.42
 C       5.420629    -0.476737    -0.018554      48.57
 H       5.737307    -0.813438    -0.994301      24.12
 C       4.042579     0.356854     1.950903      12.98
 C       2.781352     1.269412     2.453103      98.33
 H       3.141360     2.191964     2.593024      25.47
 O       2.466437     0.632569     3.768160     269.79
 H       2.271741    -0.400796     3.510748      23.37
 C       1.521737     1.543900     1.585499      93.76
 H       1.927355     1.914852     0.743889      21.74
 C       0.458432     2.345013     2.132579     106.40
 O       0.790718     3.776177     2.309133     333.42
 H       1.144312     4.453533     1.711225      29.83
 H       0.272617     2.207605     3.267861      22.18
 H      -0.448950     2.586350     1.637167      22.59
 C      -0.742825    -2.322733    -1.158128      40.15
 H      -1.143136    -3.432319    -1.173678      21.37
 C      -0.464221    -0.169018    -2.268539      58.18
 H      -0.807615     0.349719    -3.141897      21.80
 C       0.223477     0.439329    -1.045144     -21.38
 O       0.861238     1.796180    -1.042546     144.09
 C       0.766334     2.395274    -2.493860      81.40
 H       1.702653     3.179537    -2.353454      23.06
 H       1.288852     1.508380    -3.043617      22.91
 H      -0.208859     2.785546    -2.505353      24.60
 C       0.492017    -0.417312     0.049377       2.25
 O       1.079968     0.137549     1.239554     134.53
 C      -0.103278    -1.734280     0.036183      46.87
 H      -0.092290    -2.161689     0.965605      23.97
 C      -0.861165    -1.501754    -2.316786      22.66
 C      -1.563806    -2.109258    -3.613715      96.66
 H      -1.335010    -1.457697    -4.291550      28.44
 O      -0.731083    -3.322266    -4.002089     273.38
 H       0.051414    -3.435826    -3.697748      34.51
 C      -2.943856    -2.834956    -3.253717      95.55
 H      -2.790947    -3.632828    -2.456673      25.12
 O      -3.895582    -1.874144    -2.916080     280.24
 H      -4.843133    -2.191188    -2.971807      26.81
 C      -3.387711    -3.823301    -4.276283      91.07
 O      -4.912590    -4.157535    -3.839110     240.20
 H      -5.341740    -4.169674    -4.863896      23.80
 H      -2.738673    -4.605839    -4.338812      27.32
 H      -3.315263    -3.474977    -5.414347      25.25
55
name = lig-ACN-frame_997
 C       4.214061     0.140473     0.548842      61.61
 H       3.508282     0.536718    -0.169825      21.67
 C       5.045763    -0.026908     2.853951      51.75
 H       4.598976     0.253916     3.868607      19.38
 C       6.277899    -0.703707     2.459283       3.83
 O       7.311675    -1.149243     3.260602     256.28
 C       7.192609    -0.701606     4.640531     109.12
 H       8.209060    -0.919402     4.989638      24.35
 H       6.649719    -1.319621     5.029318      35.82
 H       6.648088     0.322124     4.744309      28.93
 C       6.335685    -1.028365     1.025074      25.04
 O       7.251585    -1.873728     0.459477     144.56
 H       8.100091    -1.977741     1.049479      23.24
 C       5.397118    -0.505311     0.109034      64.51
 H       5.555726    -0.496656    -0.959454      25.96
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 C       4.022082     0.430068     1.872683      29.30
 C       2.861592     1.169903     2.513189     121.51
 H       3.198549     2.070023     2.801186      26.18
 O       2.440642     0.641292     3.762733     353.80
 H       2.119280    -0.156383     3.697359      31.42
 C       1.725566     1.458850     1.544061      63.97
 H       2.041614     2.118854     0.816057      23.17
 C       0.404221     2.435600     2.241011      86.58
 O       0.739876     3.851186     2.356741     267.08
 H       1.048059     3.900187     1.278360      23.01
 H       0.197609     1.885149     3.179465      23.65
 H      -0.388780     1.956891     1.561030      23.12
 C      -0.584331    -2.260550    -1.100489      37.84
 H      -0.668533    -3.355365    -1.120618      21.80
 C      -0.338091    -0.103136    -2.304269      78.97
 H      -0.582441     0.677115    -2.968833      22.89
 C       0.240383     0.458758    -1.182451      15.02
 O       0.781200     1.725299    -1.153723     248.72
 C       0.815308     2.387057    -2.392947     112.33
 H       1.473539     3.375835    -2.384335      24.46
 H       0.920554     1.767371    -3.408504      23.60
 H      -0.163322     2.787691    -2.825074      25.29
 C       0.409956    -0.333822     0.008026       0.32
 O       1.180707     0.020702     1.158642      93.66
 C      -0.121677    -1.702459     0.077772      49.19
 H      -0.000518    -2.354087     0.934689      23.04
 C      -0.984295    -1.456090    -2.262540      27.50
 C      -1.438285    -2.189204    -3.543345     109.43
 H      -1.734771    -1.604630    -4.278849      29.74
 O      -0.706514    -3.280565    -3.964858     276.84
 H       0.192855    -2.951587    -4.089437      30.28
 C      -2.877524    -2.788088    -3.245008      84.60
 H      -2.592314    -3.201495    -2.250366      25.99
 O      -3.915872    -1.844487    -2.832032     185.66
 H      -4.785605    -2.404896    -3.462676      22.09
 C      -3.443605    -3.890699    -4.284680      99.27
 O      -4.836842    -4.230977    -3.922305     321.11
 H      -5.363080    -4.304077    -4.616720      34.00
 H      -2.945140    -4.829789    -4.089571      25.41
 H      -3.464208    -3.438705    -5.333796      25.85
55
name = lig-ACN-frame_998
 C       4.265524     0.285690     0.494031      44.51
 H       3.737467     0.680603    -0.420707      23.65
 C       5.082384     0.006459     2.790721      55.14
 H       5.078356     0.210434     3.939799      20.33
 C       6.149665    -0.764372     2.431149      25.78
 O       7.311886    -1.158216     3.151503     258.23
 C       7.215030    -0.882086     4.667627     123.45
 H       8.141138    -0.672291     5.189597      28.28
 H       6.669948    -1.440643     5.127043      37.98
 H       6.810349     0.198272     4.715860      29.64
 C       6.413127    -0.940340     1.097362      18.74
 O       7.383234    -1.822345     0.512221     196.10
 H       7.915082    -2.266202     1.188537      23.77
 C       5.347500    -0.528268     0.241126      40.99
 H       5.521654    -0.884388    -0.794537      19.58
 C       4.087128     0.425288     1.930172      33.12
 C       2.947803     1.158498     2.579380     101.92
 H       3.280864     2.078740     2.805942      25.22
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 O       2.378599     0.627014     3.832648     330.18
 H       2.100353    -0.257462     3.693996      28.23
 C       1.726729     1.417405     1.529283      57.24
 H       2.028504     1.680888     0.534663      20.59
 C       0.489009     2.313538     2.284839      82.87
 O       0.669677     3.788751     2.347462     235.52
 H       0.915714     4.401627     1.437151      24.35
 H       0.322963     2.167527     3.310549      22.95
 H      -0.490999     2.296086     1.580119      21.23
 C      -0.539415    -2.165859    -1.116666      54.83
 H      -0.718202    -3.163493    -1.106275      24.10
 C      -0.438352    -0.133299    -2.326952      69.34
 H      -0.322531     0.240860    -3.362627      21.41
 C       0.310580     0.376397    -1.202903       9.25
 O       0.727978     1.673116    -1.271262     194.75
 C       0.785798     2.489545    -2.450467      96.45
 H       1.548148     3.323421    -2.095819      24.13
 H       1.437287     1.854657    -3.237886      24.28
 H      -0.277788     2.914581    -2.552776      24.24
 C       0.362375    -0.253260     0.091792      19.73
 O       1.265135     0.003286     1.067252     140.01
 C      -0.031827    -1.564889     0.066702      46.72
 H       0.412280    -2.230685     0.899910      21.39
 C      -0.833171    -1.416772    -2.227215      34.33
 C      -1.547721    -2.111302    -3.463640      82.29
 H      -1.530798    -1.410785    -4.185811      28.05
 O      -0.657997    -3.292226    -3.963197     106.12
 H       0.467570    -3.100418    -4.279746      23.95
 C      -2.841761    -2.913737    -3.090278      82.23
 H      -2.800818    -3.637214    -2.298102      27.23
 O      -3.936586    -1.787123    -2.841409     114.33
 H      -4.948026    -2.154263    -3.422288      22.55
 C      -3.442306    -3.890677    -4.245812      99.38
 O      -4.793681    -4.268575    -3.979224     295.33
 H      -4.950184    -4.709898    -4.816208      28.11
 H      -2.632333    -4.706127    -4.412779      25.06
 H      -3.356061    -3.545858    -5.316152      25.96
55
name = lig-ACN-frame_999
 C       4.368744     0.353610     0.595929      39.19
 H       3.392433     0.659888     0.045827      23.15
 C       5.133801    -0.017437     2.896970      39.72
 H       4.943563     0.317889     4.012960      20.22
 C       6.257835    -0.780825     2.418425      15.47
 O       7.284635    -1.165578     3.232989     269.70
 C       7.217852    -0.979365     4.605846     132.83
 H       8.240511    -1.205164     4.761001      25.72
 H       6.764597    -1.695346     5.021345      36.41
 H       6.731523    -0.041804     4.941304      30.96
 C       6.390382    -1.035677     0.994850      20.87
 O       7.436304    -1.719784     0.572661     173.30
 H       8.064735    -1.942017     1.276324      24.47
 C       5.436541    -0.579516     0.112502      60.02
 H       5.478843    -1.061786    -0.896713      20.04
 C       4.088311     0.492667     1.943039      25.15
 C       2.820807     1.260976     2.559191      93.77
 H       3.121865     2.195856     2.856099      24.52
 O       2.356866     0.604801     3.881123     246.29
 H       2.272329    -0.510249     3.669236      20.93
 C       1.671195     1.398611     1.583817     109.62
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 H       2.080597     2.248825     0.951692      21.48
 C       0.600646     2.242573     2.169521     100.35
 O       0.638558     3.710265     2.349746     305.51
 H       1.007571     4.191668     1.618917      30.40
 H       0.666328     1.821580     3.123677      23.09
 H      -0.491707     1.827276     1.825603      23.76
 C      -0.585600    -2.193240    -1.027390      55.32
 H      -0.831607    -3.147928    -0.936992      26.49
 C      -0.426758    -0.138075    -2.341004      61.58
 H      -0.377641     0.514039    -3.296825      21.89
 C       0.238762     0.436399    -1.251527      11.96
 O       0.768627     1.704193    -1.283534     191.60
 C       0.824408     2.604007    -2.478796     102.46
 H       1.317437     3.520035    -2.066151      25.21
 H       1.319582     2.166435    -3.482254      24.70
 H      -0.177981     2.930303    -3.106109      23.59
 C       0.424462    -0.188350     0.032294      10.01
 O       1.362022     0.094925     1.126100     145.95
 C       0.088995    -1.567655     0.040544      32.08
 H       0.298139    -2.176948     1.072024      18.92
 C      -0.785183    -1.561817    -2.309187      29.41
 C      -1.508407    -2.195641    -3.368725      80.15
 H      -1.903921    -1.530314    -4.111019      26.83
 O      -0.745653    -3.260974    -3.996828     112.29
 H       0.346341    -3.178276    -3.445292      21.15
 C      -3.031438    -2.936908    -3.047307      91.70
 H      -2.857403    -3.353732    -2.111068      26.58
 O      -3.856147    -1.816485    -2.870894     250.36
 H      -4.816735    -2.066401    -3.191328      26.51
 C      -3.246936    -3.788939    -4.253368      82.79
 O      -4.764385    -4.332294    -4.057247     205.10
 H      -5.070243    -5.122650    -4.818381      25.57
 H      -2.639256    -4.797290    -4.248324      22.95
 H      -3.241366    -3.056028    -5.025946      25.75
55
name = lig-ACN-frame_1000
 C       4.415191     0.232783     0.650361      38.02
 H       3.737522     0.571866    -0.249713      23.01
 C       5.102571    -0.026929     2.936173      67.31
 H       4.979065     0.048103     4.063108      24.20
 C       6.219803    -0.645126     2.428858       6.98
 O       7.278344    -1.195650     3.193319     282.14
 C       7.250618    -1.154204     4.668091     127.61
 H       8.209309    -1.169947     5.140919      26.04
 H       6.630496    -1.825751     4.988665      34.63
 H       6.964297    -0.186759     5.062268      30.75
 C       6.318835    -1.074449     1.031271      15.47
 O       7.521489    -1.688071     0.540077     184.86
 H       8.347058    -1.678420     1.163224      21.60
 C       5.380378    -0.502056     0.015850      44.18
 H       5.315648    -0.468174    -1.098999      22.11
 C       4.196389     0.570275     2.089121      23.14
 C       2.824864     1.244224     2.658508     101.01
 H       2.952625     2.245589     3.004652      23.06
 O       2.389319     0.612718     3.825376     269.51
 H       2.294857    -0.588994     3.799037      18.63
 C       1.782038     1.581600     1.521634      76.43
 H       2.239105     1.895423     0.542510      19.89
 C       0.477703     2.134287     2.274264      94.98
 O       0.652776     3.579847     2.322215     300.84
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 H       1.071456     3.845887     1.522943      30.04
 H       0.272378     1.832955     3.260301      23.38
 H      -0.380609     1.828818     1.480779      22.48
 C      -0.588163    -2.263787    -0.981002      39.69
 H      -0.911780    -3.229193    -0.769800      21.40
 C      -0.342176    -0.198350    -2.350426      66.74
 H      -0.915439     0.361619    -3.185205      20.85
 C       0.194576     0.583958    -1.250076       3.46
 O       0.840303     1.858203    -1.334024     193.67
 C       0.833873     2.673975    -2.519621      95.98
 H       1.131481     3.649859    -2.238084      26.06
 H       1.662317     2.190857    -3.228132      24.13
 H      -0.351697     2.672467    -2.803920      23.45
 C       0.604735    -0.243562    -0.052799       5.34
 O       1.345370     0.198600     1.093149     123.31
 C       0.131836    -1.575584     0.058111      29.75
 H       0.227813    -2.219419     1.117972      20.24
 C      -0.799503    -1.563284    -2.185314      21.09
 C      -1.641408    -2.363449    -3.368310      87.76
 H      -1.750837    -1.551957    -4.136841      26.50
 O      -0.786513    -3.245322    -4.039327     174.57
 H      -0.124724    -3.789533    -3.381274      26.45
 C      -2.937302    -2.899273    -2.946089     103.19
 H      -3.077265    -3.546139    -2.151766      28.18
 O      -3.862556    -1.775694    -2.916816     306.51
 H      -4.601631    -2.100565    -3.064550      36.26
 C      -3.348976    -3.772168    -4.225908      89.39
 O      -4.626156    -4.356533    -4.136221     213.44
 H      -4.740959    -4.771517    -5.233481      22.72
 H      -2.414949    -4.541696    -4.363597      23.77
 H      -3.210952    -3.341809    -5.167288      26.01
55
name = lig-ACN-frame_1001
 C       4.243213     0.272650     0.713656      74.13
 H       3.553015     0.969230     0.107912      19.41
 C       5.103191     0.005225     3.019951      58.92
 H       5.009976     0.039713     4.093659      24.76
 C       6.223059    -0.699531     2.385460      -3.06
 O       7.321291    -1.221151     3.167554     216.49
 C       7.195920    -1.268045     4.716062     115.26
 H       8.203849    -1.672540     4.958117      25.44
 H       6.544473    -1.903726     5.103292      34.18
 H       6.949725    -0.291533     4.953600      32.42
 C       6.393124    -0.977635     0.988920      23.00
 O       7.478927    -1.636373     0.469916     166.44
 H       8.107291    -1.890402     1.238895      24.01
 C       5.439982    -0.468838     0.199904      54.14
 H       5.780507    -0.591885    -0.837588      23.86
 C       4.175654     0.575765     2.057748      19.64
 C       3.016497     1.288017     2.647368     103.42
 H       3.461841     2.198905     3.064159      22.32
 O       2.392986     0.595870     3.810080     264.44
 H       2.134877    -0.449955     3.479781      17.68
 C       1.795156     1.512184     1.550012      68.65
 H       1.997196     2.459546     0.869906      20.22
 C       0.422054     2.117260     2.183483      94.04
 O       0.652097     3.490305     2.332168     218.78
 H       0.941568     3.996782     1.374369      24.42
 H       0.465977     1.638987     3.195984      20.92
 H      -0.592892     1.993553     1.570075      21.58
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 C      -0.520739    -2.251249    -0.922398      52.19
 H      -0.878264    -3.317583    -0.850831      20.17
 C      -0.401483    -0.239187    -2.286328      38.82
 H      -0.591366     0.227107    -3.308222      20.95
 C       0.360092     0.547358    -1.241032       5.45
 O       0.878423     1.954432    -1.292555     202.93
 C       0.789550     2.693778    -2.554217     108.31
 H       1.004072     3.668625    -2.301296      26.50
 H       1.534721     2.317314    -3.413060      24.48
 H      -0.211610     2.680840    -3.293486      22.87
 C       0.726571    -0.198504    -0.134843      15.30
 O       1.296117     0.211793     1.003480     146.82
 C       0.151825    -1.570687     0.075938      36.97
 H       0.596879    -2.015472     1.124807      21.59
 C      -0.887817    -1.555651    -2.106906      44.51
 C      -1.535976    -2.231865    -3.241937      67.55
 H      -1.893510    -1.497663    -4.103612      25.40
 O      -0.754260    -3.327883    -4.124525     177.97
 H      -0.375985    -3.863030    -3.605862      34.21
 C      -2.994157    -2.956184    -3.027286      90.86
 H      -2.814175    -3.397177    -2.107227      27.02
 O      -3.895893    -1.691287    -2.913264     211.79
 H      -4.827541    -2.034345    -3.123214      26.38
 C      -3.286603    -3.781504    -4.223094      98.38
 O      -4.590791    -4.408867    -4.237945     294.37
 H      -4.975138    -4.476898    -5.163887      28.12
 H      -2.559554    -4.740836    -4.214779      22.74
 H      -3.214724    -3.094235    -4.965604      26.52
55
name = lig-ACN-frame_1002
 C       4.260403     0.352525     0.694040      32.54
 H       3.497477     0.610009    -0.087630      22.39
 C       5.224195    -0.027075     2.923801      48.13
 H       5.042852     0.287794     3.886302      20.88
 C       6.287019    -0.800908     2.539721      35.18
 O       7.319744    -1.273541     3.224529     280.53
 C       7.143163    -1.355352     4.599515     143.70
 H       8.104192    -1.814191     4.981981      27.76
 H       6.328461    -1.893047     4.730909      36.08
 H       7.152233    -0.529222     5.229438      32.85
 C       6.445385    -0.818238     1.125414      10.98
 O       7.414208    -1.599812     0.406963     195.57
 H       7.983787    -2.130020     0.947977      26.12
 C       5.352381    -0.349434     0.256988      45.70
 H       5.263809    -0.602154    -0.794905      21.26
 C       4.134277     0.437491     2.114591      35.86
 C       2.970482     1.310314     2.599104      91.45
 H       3.177234     2.400564     2.921427      22.89
 O       2.431482     0.628795     3.780479     353.58
 H       2.194828    -0.234498     3.572587      30.13
 C       1.699587     1.503887     1.582373      90.52
 H       2.264903     2.033225     0.640324      19.80
 C       0.513377     2.083736     2.107595      95.66
 O       0.629447     3.541376     2.398403     231.18
 H       0.718255     4.025615     1.424072      25.51
 H       0.211429     1.687167     3.183429      21.94
 H      -0.316599     1.584182     1.453378      23.62
 C      -0.488757    -2.208876    -0.864193      40.07
 H      -0.579460    -3.363686    -0.578176      23.25
 C      -0.396293    -0.114563    -2.198692      67.43
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 H      -0.398193     0.317223    -3.204153      22.80
 C       0.516288     0.490855    -1.398733      12.08
 O       0.822196     1.894293    -1.307516     191.57
 C       0.766441     2.695528    -2.631065     100.99
 H       0.822040     3.689079    -2.338378      27.24
 H       1.660745     2.330199    -3.282766      25.06
 H      -0.377671     2.508739    -2.986772      22.79
 C       0.693796    -0.205997    -0.112663      16.18
 O       1.403532     0.217461     1.018307     149.34
 C       0.297533    -1.509235     0.060997      36.03
 H       0.555651    -2.114315     1.019143      19.19
 C      -0.852698    -1.529101    -2.047201      24.56
 C      -1.494150    -2.237107    -3.336753      62.57
 H      -1.528983    -1.242422    -4.066845      23.34
 O      -0.739371    -3.280324    -4.124477     193.77
 H      -0.015230    -3.653684    -3.547107      27.41
 C      -3.003336    -2.800850    -3.004130      88.24
 H      -3.189399    -3.343915    -2.147442      27.25
 O      -3.898487    -1.718523    -2.907889     173.07
 H      -5.029522    -1.930861    -3.268596      22.50
 C      -3.208959    -3.821674    -4.298299      83.28
 O      -4.685209    -4.432027    -4.284750     314.12
 H      -4.792359    -4.667789    -5.122420      31.09
 H      -2.355940    -4.612608    -4.440084      24.35
 H      -3.032908    -3.321798    -5.155311      27.67
55
name = lig-ACN-frame_1003
 C       4.269159     0.366357     0.735529      48.76
 H       3.455222     0.464179     0.051056      23.33
 C       5.155419     0.014637     2.992133      57.77
 H       5.266889     0.211024     4.001842      20.39
 C       6.330325    -0.748717     2.472016       4.12
 O       7.403334    -1.328570     3.245964     290.48
 C       7.101563    -1.512247     4.688719     123.92
 H       7.765705    -2.330057     5.097936      25.74
 H       6.188898    -1.841010     4.842331      36.06
 H       7.188444    -0.513062     4.969479      31.63
 C       6.382193    -0.797430     1.050037      25.54
 O       7.336973    -1.551457     0.369721     154.53
 H       8.082089    -1.803392     0.977226      26.48
 C       5.435221    -0.337970     0.215378      63.98
 H       5.589182    -0.673316    -0.797912      21.30
 C       4.099450     0.483935     2.073889      17.51
 C       2.805096     1.229347     2.594480     126.03
 H       3.229283     2.295925     2.858185      21.53
 O       2.446603     0.712742     3.834115     363.66
 H       2.390699    -0.142059     3.799499      32.95
 C       1.898872     1.482415     1.448348      80.77
 H       2.124604     2.327401     0.575071      19.31
 C       0.478070     2.155775     2.159873      81.84
 O       0.567134     3.572073     2.417371     285.50
 H       0.769520     4.049180     1.683642      32.02
 H       0.220267     1.504054     3.187039      19.42
 H      -0.302439     2.265318     1.362746      21.01
 C      -0.434888    -2.163074    -0.886871      65.16
 H      -0.856935    -3.311715    -0.808322      22.41
 C      -0.371839    -0.165251    -2.312051      41.88
 H      -0.958530     0.363319    -3.019572      20.05
 C       0.555556     0.513090    -1.281614      21.32
 O       0.798641     1.832523    -1.421937     238.76
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 C       0.706301     2.593923    -2.576652     113.13
 H       0.862607     3.659753    -2.263227      25.05
 H       1.493933     2.322529    -3.358012      25.38
 H      -0.276202     2.463372    -3.266952      23.28
 C       0.763770    -0.147443    -0.031805      25.68
 O       1.540019     0.130243     1.069859     153.70
 C       0.409120    -1.524759     0.082231      33.98
 H       0.665416    -1.947626     1.052036      17.04
 C      -0.732812    -1.475810    -2.110839      20.97
 C      -1.523327    -2.200263    -3.346485      62.37
 H      -1.788446    -1.395293    -4.280327      22.12
 O      -0.691203    -3.168039    -4.015774     156.17
 H       0.431084    -3.102780    -3.678937      22.18
 C      -2.924876    -2.784476    -3.141091      92.09
 H      -2.770744    -3.359427    -2.295469      26.25
 O      -3.922727    -1.684868    -2.933476     184.31
 H      -4.786313    -2.288243    -3.509179      21.94
 C      -3.341358    -3.823255    -4.360347     105.69
 O      -4.628300    -4.367278    -4.297990     314.33
 H      -4.814573    -5.013261    -5.007933      29.72
 H      -2.682634    -4.670525    -4.021723      24.89
 H      -3.224171    -3.459302    -5.275951      27.69
55
name = lig-ACN-frame_1004
 C       4.303691     0.276051     0.672788      48.27
 H       3.638609     0.804745     0.048219      21.73
 C       5.145069     0.022526     3.030126      64.20
 H       4.809360     0.154955     4.049651      25.25
 C       6.280739    -0.596182     2.449856       0.12
 O       7.392252    -1.375806     3.172787     167.67
 C       7.023200    -1.603263     4.779354     107.89
 H       7.795858    -2.360301     4.979696      26.79
 H       6.091476    -1.784570     4.870124      36.17
 H       7.344876    -0.868580     5.510765      27.96
 C       6.371963    -0.880702     1.024627      29.54
 O       7.400963    -1.562245     0.350791     181.84
 H       8.253345    -1.585913     0.940512      25.23
 C       5.425430    -0.307083     0.122675      51.35
 H       5.598835    -0.297520    -0.959451      23.84
 C       4.170465     0.558850     2.142895      15.14
 C       2.993256     1.281386     2.598779      88.56
 H       3.287291     2.393444     2.947649      20.92
 O       2.364400     0.774022     3.957504     299.99
 H       2.274253    -0.230081     3.904433      22.60
 C       1.781509     1.509331     1.523754      90.87
 H       2.478214     2.114180     0.675713      19.24
 C       0.484376     2.233937     1.999537      99.88
 O       0.561460     3.613888     2.503142     281.88
 H       0.959680     4.150561     1.758204      28.62
 H       0.389103     1.621964     3.101483      18.72
 H      -0.360148     1.790904     1.448050      23.76
 C      -0.343367    -2.137702    -1.002691      47.52
 H      -0.760150    -3.238146    -0.721202      18.69
 C      -0.253977    -0.130572    -2.280127      66.51
 H      -0.570705     0.549092    -3.025232      21.00
 C       0.356045     0.451420    -1.253374      18.13
 O       0.837362     1.813648    -1.399256     208.55
 C       0.659960     2.534195    -2.682953      94.36
 H       0.722617     3.602238    -2.241471      24.19
 H       1.526384     2.295622    -3.365883      24.61
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 H      -0.429901     2.539972    -3.104242      23.58
 C       0.877829    -0.239042    -0.047710       9.88
 O       1.643308     0.125815     1.063819     168.96
 C       0.374527    -1.571729     0.061958      36.19
 H       0.673624    -2.147037     0.858812      23.02
 C      -0.742371    -1.536424    -2.226472      31.00
 C      -1.501109    -2.045103    -3.388052      69.08
 H      -1.666022    -0.975573    -4.030561      23.79
 O      -0.611040    -3.097260    -3.905591      49.07
 H       0.496330    -2.701877    -3.646970      25.01
 C      -2.904600    -2.863762    -3.244670      92.72
 H      -2.996706    -3.377299    -2.363340      28.28
 O      -3.920650    -1.740151    -3.008604     246.50
 H      -4.839177    -1.909836    -3.360016      27.59
 C      -3.275590    -3.811039    -4.355403     111.58
 O      -4.690072    -4.275587    -4.215666     254.04
 H      -4.815078    -4.777730    -5.267237      23.62
 H      -2.530824    -4.630694    -4.398680      26.65
 H      -3.097122    -3.332547    -5.208859      29.00
55
name = lig-ACN-frame_1005
 C       4.325119     0.360340     0.716081      68.40
 H       3.733403     0.892971     0.010033      21.88
 C       5.171344     0.026271     2.977740     103.17
 H       5.118672     0.064318     4.108961      30.35
 C       6.330753    -0.669516     2.475607       9.86
 O       7.205539    -1.318236     3.231405     283.98
 C       7.042142    -1.656785     4.659636     107.35
 H       7.473748    -2.616104     4.745166      25.88
 H       6.118007    -1.910223     4.758125      33.58
 H       7.362208    -0.799697     5.272122      27.49
 C       6.363244    -0.852182     1.022013      36.14
 O       7.541471    -1.601881     0.384410     175.16
 H       8.295587    -1.854392     0.965525      27.35
 C       5.421773    -0.328446     0.107123      57.99
 H       5.507255    -0.336758    -1.006131      23.57
 C       4.249023     0.514657     2.056504      10.91
 C       2.952869     1.420863     2.785119      89.24
 H       3.396111     2.536187     3.063282      21.47
 O       2.344918     0.858608     3.976955     320.53
 H       2.053969    -0.203168     3.676472      19.33
 C       1.882076     1.566427     1.611302      75.00
 H       2.103296     2.246104     0.607015      17.12
 C       0.518768     2.158633     2.022264      81.44
 O       0.596976     3.600233     2.476002     204.63
 H       1.037023     4.437533     1.848698      25.24
 H       0.073428     1.671993     3.069370      19.62
 H      -0.195978     2.267694     1.204801      21.14
 C      -0.344405    -2.255871    -1.117229      94.72
 H      -0.541429    -3.384961    -1.071452      17.57
 C      -0.284776    -0.164436    -2.302077      63.50
 H      -0.141343     0.142370    -3.321352      20.50
 C       0.423265     0.534076    -1.140909       9.38
 O       0.868127     1.777229    -1.320409     175.72
 C       0.613467     2.524371    -2.723907      77.75
 H       0.837109     3.736461    -2.586859      22.16
 H       1.190612     2.100882    -3.499118      25.61
 H      -0.397605     2.254453    -3.015350      24.01
 C       0.848471    -0.333606    -0.075399      23.51
 O       1.640065     0.156770     1.003583     166.81
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 C       0.366683    -1.632710    -0.026122      39.38
 H       0.543242    -2.274725     0.761922      24.36
 C      -0.754907    -1.400897    -2.176564      26.84
 C      -1.474957    -2.052937    -3.410549      62.19
 H      -1.637043    -1.330015    -4.433448      22.56
 O      -0.538482    -3.025618    -3.892941     190.63
 H       0.391909    -2.852144    -3.576107      30.47
 C      -2.941294    -2.793291    -3.167844      96.39
 H      -2.805249    -3.393870    -2.318609      26.97
 O      -3.878739    -1.785348    -3.107380     314.54
 H      -4.580781    -2.156741    -3.383637      33.06
 C      -3.163985    -3.760791    -4.444201      90.83
 O      -4.706464    -4.176658    -4.157532     234.54
 H      -5.122514    -4.434521    -5.231233      24.97
 H      -2.601715    -4.627204    -4.494957      26.85
 H      -3.279041    -3.282336    -5.312038      27.26
55
name = lig-ACN-frame_1006
 C       4.380666     0.508911     0.683627      13.67
 H       3.516529     0.763487     0.062634      20.74
 C       5.234688     0.007002     2.915756      20.54
 H       5.223044     0.315885     4.030729      19.57
 C       6.226331    -0.774954     2.365662      37.13
 O       7.169474    -1.297777     3.245306     269.10
 C       6.966584    -1.715191     4.526436     149.08
 H       7.709972    -2.460438     4.636136      28.13
 H       6.063127    -1.745008     4.884550      36.11
 H       7.478931    -1.029901     5.276290      29.23
 C       6.562870    -0.897961     0.971936      17.02
 O       7.556517    -1.583794     0.470993     220.95
 H       7.998616    -1.928580     1.249244      23.67
 C       5.491618    -0.378867     0.210851      50.08
 H       5.629126    -0.753715    -0.851652      21.58
 C       4.127625     0.627308     2.190178      11.73
 C       2.927166     1.407998     2.742837      79.06
 H       3.357690     2.524567     3.122078      19.27
 O       2.366380     0.937749     3.934861     268.66
 H       2.038141    -0.234700     3.802085      17.91
 C       1.906766     1.620528     1.614039      57.11
 H       2.549955     2.459372     0.993345      18.99
 C       0.522095     2.231368     2.051528     100.86
 O       0.662812     3.571389     2.482528     266.00
 H       1.041944     3.773254     1.493042      24.07
 H      -0.126467     1.480658     2.723613      21.14
 H      -0.000933     2.076004     1.111932      22.70
 C      -0.395232    -2.310948    -1.153740      39.43
 H      -0.589701    -3.353476    -1.281492      22.03
 C      -0.235094    -0.051546    -2.249949      53.35
 H      -0.438914     0.591684    -3.153747      19.20
 C       0.503097     0.469182    -1.270619      12.59
 O       0.936665     1.903705    -1.330391     225.49
 C       0.558991     2.383491    -2.632438     106.14
 H       0.950437     3.563355    -2.471764      23.02
 H       1.135263     1.898492    -3.380415      26.76
 H      -0.415563     2.511414    -2.857603      27.15
 C       0.741658    -0.226624    -0.030410       2.08
 O       1.612502     0.140091     1.004391      91.35
 C       0.396894    -1.770460    -0.108671      28.95
 H       0.749036    -2.249897     0.802419      15.67
 C      -0.859450    -1.440484    -2.189241      34.42
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 C      -1.429155    -2.117933    -3.394003      82.10
 H      -1.737467    -1.165691    -4.163654      23.04
 O      -0.459789    -3.061242    -3.965776     247.44
 H       0.125659    -3.163699    -3.379310      33.94
 C      -2.729776    -2.780094    -3.208775     100.04
 H      -2.852064    -3.318471    -2.296583      27.87
 O      -3.897468    -1.790162    -3.193879     256.92
 H      -4.564664    -2.332205    -3.399345      28.89
 C      -3.286900    -3.687370    -4.414920     116.53
 O      -4.604962    -4.047538    -4.136241     317.97
 H      -5.052779    -4.479197    -4.947806      28.38
 H      -2.701350    -4.492440    -4.409078      29.46
 H      -3.047725    -3.189954    -5.292111      29.31
55
name = lig-ACN-frame_1007
 C       4.500870     0.454780     0.778714      43.98
 H       3.843226     0.679182    -0.077526      23.03
 C       5.113923     0.090894     2.910655      45.63
 H       5.224621     0.123652     4.039488      21.88
 C       6.165542    -0.798284     2.408532      30.40
 O       7.262843    -1.309026     3.080950     230.42
 C       6.957356    -1.761009     4.640844     114.43
 H       7.275383    -2.734368     4.684038      27.81
 H       5.963896    -1.999534     4.637623      33.53
 H       7.362421    -0.919085     5.267835      30.97
 C       6.487511    -0.865522     1.018840       4.88
 O       7.610063    -1.612165     0.540096     181.71
 H       8.288443    -2.066352     1.164666      23.03
 C       5.463556    -0.288153     0.229722      65.46
 H       5.283179    -0.426180    -0.873184      22.15
 C       4.223486     0.678301     2.070051      41.01
 C       2.947163     1.372588     2.649794      91.79
 H       3.246154     2.582467     2.796436      19.97
 O       2.364162     0.942136     3.942374     277.34
 H       2.366087    -0.256994     3.913781      18.10
 C       1.858124     1.615533     1.604258      75.14
 H       2.163096     1.933028     0.564913      17.49
 C       0.529813     2.173986     1.932166     100.91
 O       0.746302     3.555059     2.439711     306.34
 H       0.924121     4.292108     1.959004      31.84
 H       0.309711     1.672001     3.006948      18.09
 H      -0.261858     2.228807     1.228025      22.93
 C      -0.391145    -2.229810    -1.094869      45.50
 H      -0.675990    -3.177602    -0.935931      20.16
 C      -0.367990    -0.119586    -2.283406      63.08
 H      -1.092720     0.542836    -2.893082      18.32
 C       0.588319     0.521271    -1.241925      14.02
 O       0.956365     1.851686    -1.323392     229.82
 C       0.604307     2.432565    -2.573297     100.96
 H       1.065982     3.576439    -2.761867      22.74
 H       0.855739     1.826194    -3.394715      27.33
 H      -0.398291     2.474184    -2.596373      28.34
 C       0.728146    -0.309182    -0.041804      23.47
 O       1.548317     0.166398     1.031065     132.80
 C       0.445119    -1.649723    -0.114702      50.45
 H       0.872625    -2.490198     0.535334      16.49
 C      -0.781740    -1.418074    -2.204338      24.39
 C      -1.367505    -2.068695    -3.451865      64.68
 H      -1.303990    -1.255797    -4.369291      24.10
 O      -0.400293    -3.092525    -4.062451     157.78
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 H       0.029866    -3.726106    -3.335402      26.07
 C      -2.825002    -2.809041    -3.265444      94.50
 H      -2.677624    -3.393693    -2.324812      25.09
 O      -3.837109    -1.753291    -3.230793     218.82
 H      -4.819136    -2.246025    -3.406990      21.26
 C      -3.132069    -3.690919    -4.338389     120.02
 O      -4.600371    -3.948773    -4.127823     334.22
 H      -4.753424    -4.497330    -4.766542      34.72
 H      -2.684933    -4.548503    -4.440061      29.58
 H      -3.153157    -3.231775    -5.332811      27.13
55
name = lig-ACN-frame_1008
 C       4.393800     0.473279     0.650406      60.24
 H       3.688285     1.139126     0.124633      19.23
 C       5.143015     0.027610     3.061834      86.57
 H       4.720949     0.214864     4.050908      25.07
 C       6.247024    -0.709049     2.505166      -0.81
 O       7.322093    -1.390824     3.175026     273.05
 C       6.918739    -1.782762     4.507713     122.50
 H       7.593301    -2.540146     4.781553      26.74
 H       5.841634    -1.696994     4.638065      34.32
 H       7.241991    -1.013348     5.314095      28.39
 C       6.408146    -0.929288     1.033785      27.91
 O       7.538135    -1.585280     0.534040     192.24
 H       8.123246    -1.598487     1.354667      23.83
 C       5.608306    -0.288840     0.086938      48.05
 H       5.898813    -0.335056    -1.007475      21.22
 C       4.253080     0.700437     2.107186       3.48
 C       2.919480     1.450533     2.566400      65.92
 H       3.283745     2.571281     2.976732      18.66
 O       2.434262     0.918844     3.871610     293.21
 H       2.345552    -0.179123     3.780794      16.53
 C       1.795788     1.436797     1.304293     116.37
 H       2.253199     2.214908     0.693900      21.35
 C       0.543989     2.241416     1.977052      93.55
 O       0.808914     3.601327     2.454869     318.71
 H       0.899532     3.975536     1.602790      29.68
 H       0.137984     1.641311     2.903963      19.75
 H      -0.255204     2.044045     1.252969      21.91
 C      -0.363428    -2.152314    -1.052582      80.00
 H      -0.594670    -3.138843    -0.952225      26.60
 C      -0.444048    -0.037660    -2.180032      62.37
 H      -0.674406     0.550180    -3.162513      18.99
 C       0.388346     0.449751    -1.240897      22.80
 O       1.009688     1.735128    -1.282684     197.78
 C       0.585535     2.533906    -2.612480      94.83
 H       1.380226     3.487618    -2.589705      22.86
 H       0.719497     1.872814    -3.444864      25.79
 H      -0.314865     2.931988    -2.583462      28.15
 C       0.933016    -0.212354    -0.119267       9.33
 O       1.449976     0.098202     1.090195     206.43
 C       0.461885    -1.600880    -0.054122      39.77
 H       0.842119    -2.127824     0.945895      15.87
 C      -0.678601    -1.471105    -2.241885      28.00
 C      -1.311038    -2.134245    -3.529255      68.68
 H      -1.566996    -1.381440    -4.400505      23.17
 O      -0.390603    -3.079531    -4.125044      96.15
 H      -0.101279    -3.902827    -3.273802      22.72
 C      -2.759715    -2.677313    -3.222516      77.96
 H      -2.898219    -3.201953    -2.200336      23.47
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 O      -3.734235    -1.656804    -3.208041     193.31
 H      -4.734491    -2.267751    -3.622414      18.05
 C      -3.090892    -3.816109    -4.411775      91.42
 O      -4.606184    -3.955842    -4.158642     325.01
 H      -5.052944    -4.502214    -4.799895      30.59
 H      -2.525717    -4.574938    -4.178773      29.35
 H      -2.812384    -3.334935    -5.424119      26.66
55
name = lig-ACN-frame_1009
 C       4.479268     0.501376     0.585491      54.44
 H       3.945621     1.044770    -0.170403      20.28
 C       5.146213     0.011299     3.055123     109.02
 H       5.171499     0.055157     4.104849      29.94
 C       6.350913    -0.666609     2.487626       2.85
 O       7.284567    -1.408425     3.215675     275.79
 C       6.926738    -1.754396     4.553598     101.33
 H       7.447429    -2.676051     4.772875      26.09
 H       5.913211    -2.302166     4.538332      27.46
 H       7.186256    -0.810985     5.150145      26.56
 C       6.357441    -0.879068     1.095926      31.54
 O       7.417080    -1.545229     0.558739     199.34
 H       8.201422    -1.766971     1.042661      28.98
 C       5.558796    -0.199253     0.097394      45.78
 H       6.018913    -0.275556    -0.913579      21.44
 C       4.229009     0.611885     2.056005       7.82
 C       2.965052     1.410402     2.478722     105.79
 H       3.033914     2.644529     2.534644      17.02
 O       2.505495     0.899051     3.724429     356.50
 H       2.219970     0.012736     3.557947      23.10
 C       1.819702     1.512091     1.415091      81.16
 H       2.067279     1.703574     0.448029      18.55
 C       0.539116     2.216105     2.003254      98.26
 O       0.853226     3.597807     2.385747     251.90
 H       1.223495     4.270298     1.576338      23.43
 H       0.274356     1.579364     2.887787      19.54
 H      -0.250308     2.488988     1.321737      20.40
 C      -0.281481    -2.187606    -1.059044      60.55
 H      -0.526599    -3.258407    -1.005845      21.62
 C      -0.472044    -0.059264    -2.233419      55.05
 H      -0.415602     0.558531    -3.185657      17.82
 C       0.348976     0.553399    -1.160544      22.37
 O       0.957268     1.740519    -1.428232     220.61
 C       0.666923     2.603009    -2.502462      99.42
 H       1.576251     3.338442    -2.427610      23.05
 H       0.780145     2.111462    -3.544572      23.71
 H      -0.221836     3.068035    -2.440782      27.25
 C       0.911055    -0.351451    -0.168202      22.73
 O       1.426784     0.116117     1.109475     165.30
 C       0.448102    -1.589796    -0.013724      30.83
 H       0.434054    -2.062466     1.044143      17.77
 C      -0.655562    -1.457898    -2.263556      20.50
 C      -1.282531    -2.135813    -3.473931      88.68
 H      -1.329319    -1.276549    -4.174922      24.34
 O      -0.449016    -3.087660    -4.150320     138.94
 H       0.169648    -3.653729    -3.295958      23.86
 C      -2.670985    -2.721968    -3.264029      73.38
 H      -2.638921    -3.294860    -2.204634      22.57
 O      -3.647463    -1.524820    -3.213302     168.05
 H      -4.604930    -2.087766    -3.761204      18.83
 C      -3.186506    -3.818262    -4.278037     107.02
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 O      -4.543876    -3.997844    -4.219184     288.70
 H      -4.710918    -4.442271    -5.207098      24.25
 H      -2.785686    -4.725309    -4.175989      26.40
 H      -2.977341    -3.555828    -5.426680      23.74
55
name = lig-ACN-frame_1010
 C       4.509471     0.620235     0.697913      33.55
 H       3.790068     1.065333     0.043270      23.44
 C       5.153548     0.054537     2.862037      50.09
 H       4.889169     0.285684     3.833471      18.66
 C       6.257446    -0.674384     2.473032      27.38
 O       7.252683    -1.372543     3.147141     260.19
 C       6.929639    -1.804906     4.678868      94.62
 H       7.852413    -2.354335     4.960289      26.66
 H       5.752141    -2.048764     4.609223      25.38
 H       6.828182    -1.012589     5.496155      30.07
 C       6.466141    -0.748834     1.093753      35.09
 O       7.371741    -1.596765     0.473292     196.32
 H       7.963784    -1.954225     1.202478      22.28
 C       5.637201    -0.212309     0.212226      66.53
 H       5.554333    -0.299564    -0.868474      23.78
 C       4.231852     0.547557     1.950933      36.04
 C       3.047174     1.385338     2.376560      94.06
 H       3.667725     2.348383     2.715059      21.04
 O       2.521127     0.907055     3.618040     392.60
 H       2.428535     0.053842     3.615056      31.53
 C       1.798530     1.518672     1.447274     102.50
 H       2.125199     2.247894     0.800566      20.87
 C       0.589652     2.274311     1.954769     103.37
 O       0.915824     3.609095     2.374969     264.91
 H       1.337566     4.209200     1.514145      24.21
 H       0.249553     1.960697     2.918146      21.39
 H      -0.181378     1.837053     1.285577      21.52
 C      -0.239337    -2.305801    -1.174597      43.55
 H      -0.654879    -3.400174    -1.062174      15.51
 C      -0.333304    -0.105192    -2.272424      62.23
 H      -0.992268     0.400720    -2.987065      19.31
 C       0.372858     0.505378    -1.263148      19.05
 O       0.952582     1.766900    -1.442779     244.92
 C       0.761701     2.737472    -2.492848     106.53
 H       1.537218     3.566336    -2.379826      23.68
 H       0.668429     2.216281    -3.517105      23.87
 H      -0.160110     3.225758    -2.341030      26.42
 C       0.755722    -0.215568    -0.017364       3.68
 O       1.418449     0.105302     1.101520     174.92
 C       0.327547    -1.715997    -0.017120      46.12
 H       0.583662    -2.391715     0.843186      20.23
 C      -0.645900    -1.444972    -2.172105      47.10
 C      -1.247493    -2.047779    -3.476446      71.17
 H      -1.435966    -1.332549    -4.223485      27.47
 O      -0.454302    -3.129301    -4.128394     219.32
 H       0.465312    -3.284867    -3.722263      29.33
 C      -2.731834    -2.726114    -3.222940      73.80
 H      -2.771183    -3.161318    -2.073114      22.62
 O      -3.516084    -1.511241    -3.248584     225.51
 H      -4.565703    -1.678409    -3.522335      22.93
 C      -3.120829    -3.810354    -4.225107      87.70
 O      -4.607734    -4.001719    -4.240236     263.85
 H      -5.013741    -4.762110    -5.097630      24.06
 H      -2.491921    -4.563565    -3.955825      27.85
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 H      -2.724743    -3.257534    -5.234138      24.88
55
name = lig-ACN-frame_1011
 C       4.543246     0.651184     0.503399      33.55
 H       3.875051     1.056093    -0.251260      21.92
 C       5.106629     0.074497     2.922159      12.66
 H       4.898748     0.122907     3.964359      20.84
 C       6.259083    -0.718543     2.420101      19.14
 O       7.209876    -1.343362     3.290741     263.48
 C       6.932799    -1.724074     4.603879     131.12
 H       7.765912    -2.456071     4.914006      25.98
 H       6.091960    -2.622893     4.683449      27.91
 H       6.978368    -0.716379     5.109955      30.78
 C       6.612740    -0.738249     0.991368      -2.97
 O       7.418587    -1.710466     0.409026     209.24
 H       8.014105    -2.205286     1.094039      22.62
 C       5.586815    -0.067878     0.116781      60.00
 H       5.868945    -0.518052    -0.806102      21.11
 C       4.183557     0.609710     1.946368      24.16
 C       3.044481     1.389055     2.465242      98.65
 H       3.256723     2.535907     2.528949      20.32
 O       2.516300     0.925010     3.668572     378.74
 H       2.435973    -0.000808     3.519256      25.95
 C       1.894869     1.565771     1.369353      76.02
 H       2.118335     1.870853     0.444333      18.50
 C       0.615529     2.257008     2.050255      99.85
 O       0.949882     3.643750     2.316997     307.25
 H       1.157874     4.152527     1.487602      26.77
 H       0.363176     1.693221     2.859899      20.99
 H      -0.124940     2.574336     1.270135      17.47
 C      -0.260244    -2.356022    -1.167118      31.93
 H      -0.340992    -3.559473    -1.352957      17.93
 C      -0.283695    -0.123750    -2.290542      46.52
 H      -0.605507     0.593789    -3.058677      18.78
 C       0.510699     0.481618    -1.267269       2.96
 O       1.029683     1.790546    -1.316988     160.76
 C       0.734891     2.867055    -2.529883      86.20
 H       1.575901     3.431049    -2.317515      24.51
 H       0.962490     2.342395    -3.594166      23.00
 H      -0.255212     3.373687    -2.475092      24.01
 C       0.481940    -0.305974    -0.005807      13.12
 O       1.446162     0.183252     1.083167     129.59
 C       0.324804    -1.672242    -0.054049      46.25
 H       0.821480    -2.178037     0.731522      17.43
 C      -0.661716    -1.576932    -2.300114      21.12
 C      -1.316488    -2.135006    -3.479500      92.48
 H      -1.439806    -1.374537    -4.129486      25.96
 O      -0.424869    -3.121481    -4.085644     273.16
 H       0.318500    -2.881827    -3.846881      33.79
 C      -2.717481    -2.627756    -3.112388      72.68
 H      -2.970966    -3.171125    -2.022080      21.01
 O      -3.470195    -1.452720    -3.288442     301.51
 H      -4.261796    -1.783983    -3.218939      30.53
 C      -3.101883    -3.752066    -4.246672      81.02
 O      -4.584794    -3.967270    -4.174501     240.06
 H      -4.793730    -4.817006    -5.007665      24.84
 H      -2.689463    -4.710130    -4.034413      23.90
 H      -2.781585    -3.537127    -5.394062      23.39
55
name = lig-ACN-frame_1012
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 C       4.519802     0.611088     0.466447      66.06
 H       3.867677     1.117210    -0.284834      19.39
 C       5.149826    -0.032900     2.847415      95.27
 H       4.988519    -0.024931     3.947137      28.04
 C       6.281879    -0.667122     2.412760       3.31
 O       7.206574    -1.294099     3.202418     269.23
 C       6.968252    -1.659614     4.593474      90.74
 H       7.987989    -2.105211     4.901841      24.60
 H       5.814425    -2.212261     4.563656      23.97
 H       6.694821    -0.988595     5.429568      27.80
 C       6.517782    -0.778528     0.972665      31.06
 O       7.452370    -1.791796     0.362497     228.50
 H       8.289924    -1.924166     0.895848      25.64
 C       5.808724    -0.101834    -0.029199      40.21
 H       5.931580     0.005633    -1.020004      21.56
 C       4.301690     0.745692     1.873915      10.29
 C       2.906211     1.539259     2.443022      84.94
 H       3.206945     2.541405     2.785052      20.19
 O       2.498970     0.944878     3.794931     307.62
 H       2.114448    -0.039681     3.735964      18.32
 C       1.833357     1.530867     1.309435     107.79
 H       2.267544     2.139035     0.617551      19.96
 C       0.692469     2.320421     1.945601     103.06
 O       0.979649     3.675935     2.400911     335.08
 H       1.191446     4.216332     1.729722      31.61
 H       0.499464     1.924065     2.843660      21.19
 H      -0.302978     1.954553     1.409609      20.70
 C      -0.264067    -2.299101    -1.181398      52.49
 H      -0.110180    -3.452174    -1.143869      20.35
 C      -0.233117    -0.161110    -2.331302      70.37
 H      -0.095203     0.173714    -3.359449      20.61
 C       0.467881     0.467476    -1.249053       6.60
 O       1.048748     1.840094    -1.280307     212.70
 C       0.817247     2.802446    -2.438723      91.15
 H       1.291558     3.682870    -2.296478      25.42
 H       0.934166     2.253820    -3.509030      22.71
 H      -0.357539     3.065025    -2.369465      23.18
 C       0.593792    -0.194748    -0.010651      13.82
 O       1.372576     0.128065     1.017852     193.73
 C       0.344654    -1.672267    -0.080206      30.22
 H       0.589370    -2.240085     0.746195      17.18
 C      -0.561554    -1.496341    -2.291922      31.54
 C      -1.324037    -2.191365    -3.498817      94.54
 H      -1.556741    -1.508876    -4.197838      26.94
 O      -0.427177    -3.127536    -4.060818     233.77
 H       0.546830    -2.866525    -3.760085      26.24
 C      -2.704174    -2.718714    -3.244373      62.98
 H      -2.670663    -3.103991    -2.045406      21.97
 O      -3.544937    -1.361352    -3.293569     233.08
 H      -4.433985    -1.555169    -3.141018      27.68
 C      -3.180458    -3.733609    -4.187430      92.92
 O      -4.501839    -3.892135    -4.061508     269.09
 H      -4.963934    -4.448692    -4.934351      25.41
 H      -2.492735    -4.584622    -4.015837      25.45
 H      -2.890655    -3.220978    -5.260794      24.20
55
name = lig-ACN-frame_1013
 C       4.688711     0.574584     0.516490      74.71
 H       4.043198     1.134875    -0.212883      21.54
 C       5.099607     0.032850     2.688343      66.38
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 H       4.745670     0.146282     3.781866      22.47
 C       6.300140    -0.659022     2.251241       1.13
 O       7.301265    -1.228312     3.061697     221.34
 C       6.925114    -1.599349     4.604056      81.12
 H       7.841348    -2.263381     4.938702      25.60
 H       6.083051    -2.557567     4.617597      24.72
 H       6.903818    -0.571256     4.965842      26.42
 C       6.520767    -0.942139     0.863002      26.75
 O       7.412573    -1.760078     0.378910     218.65
 H       8.258737    -1.724271     0.831897      27.07
 C       5.808876    -0.056263     0.006309      58.58
 H       6.319340    -0.209358    -0.871472      22.48
 C       4.317678     0.788072     1.877629      23.13
 C       2.993748     1.431463     2.454861      98.53
 H       3.120496     2.462548     2.564089      21.43
 O       2.483444     1.017180     3.821069     273.64
 H       2.288459    -0.124904     3.577978      15.68
 C       1.809107     1.565278     1.377388      86.67
 H       2.179036     1.881212     0.441899      17.31
 C       0.613414     2.341307     1.957471      99.76
 O       0.963925     3.667652     2.474414     315.94
 H       1.316463     4.214083     1.826276      29.89
 H       0.500341     1.793616     2.783393      20.97
 H      -0.359054     2.435174     1.221692      19.60
 C      -0.199613    -2.203049    -1.160210      54.82
 H      -0.711490    -3.178680    -1.172869      17.05
 C      -0.052972    -0.087970    -2.426747      50.80
 H      -0.298032     0.492577    -3.361926      19.19
 C       0.397295     0.615045    -1.296289      14.23
 O       1.049998     1.808495    -1.293039     235.97
 C       0.774525     2.643301    -2.296680     104.47
 H       1.298570     3.507668    -2.086788      24.44
 H       1.282145     2.283281    -3.392640      22.48
 H      -0.405813     2.825802    -2.493433      23.08
 C       0.770242    -0.270991    -0.170513      -1.82
 O       1.378702     0.177630     1.084538     172.14
 C       0.361047    -1.586261    -0.040859      49.53
 H       0.548198    -2.132006     0.840594      21.23
 C      -0.591795    -1.504632    -2.302785      25.63
 C      -1.204654    -2.041535    -3.543205      78.94
 H      -1.235943    -1.325749    -4.260153      25.74
 O      -0.408607    -3.219060    -4.087678      86.08
 H       0.691598    -3.292018    -3.530112      22.20
 C      -2.738325    -2.608303    -3.208375      60.93
 H      -3.031067    -3.159824    -2.093015      19.61
 O      -3.561373    -1.386131    -3.274106     168.82
 H      -4.677643    -1.760891    -3.201007      20.74
 C      -3.107761    -3.668586    -4.252083      82.84
 O      -4.610749    -3.860444    -3.930741     314.81
 H      -4.958877    -4.390771    -4.654302      30.53
 H      -2.546927    -4.673019    -4.089683      24.56
 H      -2.946835    -3.314162    -5.392870      24.71
55
name = lig-ACN-frame_1014
 C       4.707159     0.786228     0.442137      31.99
 H       4.247797     1.329049    -0.421116      20.78
 C       5.210560     0.069871     2.719608      42.35
 H       5.176478    -0.036979     3.879698      13.55
 C       6.256026    -0.721541     2.236049      29.17
 O       7.357155    -1.241527     3.057008     302.35
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 C       6.998196    -1.494698     4.374125     114.64
 H       7.913866    -1.958612     4.935134      26.57
 H       5.783207    -1.966569     4.420670      24.97
 H       6.691058    -0.649502     5.077569      31.09
 C       6.472785    -0.912046     0.879538      19.12
 O       7.464723    -1.786431     0.324900     220.33
 H       8.017081    -2.212676     1.068547      24.16
 C       5.788840    -0.114372     0.022379      62.80
 H       5.724844     0.031580    -1.016654      23.11
 C       4.239246     0.670302     1.809752      51.65
 C       3.049067     1.435153     2.412034     113.01
 H       3.461740     2.342071     2.639182      26.01
 O       2.537418     1.035655     3.684662     239.87
 H       2.314662    -0.120561     3.840471      17.26
 C       1.884093     1.529439     1.424670      68.64
 H       2.236727     2.249130     0.597228      17.54
 C       0.527897     2.376052     2.033110      87.60
 O       0.935362     3.640064     2.573880     286.62
 H       1.291934     4.148130     1.716987      25.26
 H      -0.160246     1.867103     2.604102      23.17
 H      -0.128796     2.613145     1.074154      18.13
 C      -0.316102    -2.165365    -1.144680      82.49
 H      -0.675267    -3.090401    -0.876200      17.42
 C      -0.028009    -0.029772    -2.492055      68.43
 H      -0.440404     0.643984    -3.299432      18.37
 C       0.515390     0.484255    -1.286497      22.22
 O       1.049582     1.749281    -1.205436     196.57
 C       0.755144     2.681969    -2.360884      83.64
 H       0.978541     3.673408    -1.965729      23.55
 H       1.370258     2.227099    -3.318761      22.11
 H      -0.449971     2.763915    -2.651244      23.39
 C       0.894491    -0.243555    -0.161422       6.26
 O       1.374309     0.219626     1.117577     191.71
 C       0.420628    -1.545712    -0.068613      38.26
 H       0.581229    -1.949451     0.961295      17.77
 C      -0.447275    -1.324929    -2.361001      37.33
 C      -1.156677    -2.072263    -3.532994      83.57
 H      -1.161744    -1.400257    -4.370641      27.53
 O      -0.416895    -3.264922    -4.107508     112.22
 H       0.297428    -3.692999    -3.232698      22.46
 C      -2.633651    -2.439387    -3.258164      74.28
 H      -2.531745    -3.028308    -2.128862      20.36
 O      -3.598368    -1.420161    -3.257959     183.92
 H      -4.589282    -2.149651    -3.538825      16.65
 C      -3.219800    -3.586210    -4.279816      86.95
 O      -4.645915    -3.847209    -3.857468     340.76
 H      -4.962506    -4.469862    -4.366004      36.42
 H      -2.688629    -4.666197    -4.036143      23.77
 H      -3.210323    -3.360454    -5.417987      25.37
55
name = lig-ACN-frame_1015
 C       4.674380     0.861010     0.470676      38.87
 H       4.070102     1.630153    -0.029540      19.32
 C       5.253853     0.027212     2.751884      45.50
 H       4.949532     0.451170     3.779333      17.26
 C       6.345512    -0.776517     2.284704      11.20
 O       7.356802    -1.227513     2.958483     269.80
 C       6.997019    -1.374649     4.354036     112.50
 H       7.789717    -2.108324     4.745147      25.45
 H       6.079422    -2.292611     4.337119      25.32
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 H       6.991413    -0.305297     4.804694      28.50
 C       6.513361    -0.893265     0.802554     -12.97
 O       7.446457    -1.794265     0.298574     225.12
 H       7.870532    -2.317544     1.073184      24.11
 C       5.644192    -0.047132    -0.089424      76.06
 H       6.090064    -0.370227    -1.042175      24.16
 C       4.299955     0.590734     1.775479      18.45
 C       3.086194     1.480861     2.365412     103.61
 H       3.367023     2.445643     2.472380      24.15
 O       2.626076     0.984846     3.619336     297.60
 H       2.286773    -0.031725     3.338643      19.92
 C       1.805372     1.663274     1.506596      67.38
 H       2.160203     2.146589     0.473080      14.54
 C       0.613403     2.393766     1.927432      83.79
 O       0.906704     3.618310     2.672829     228.30
 H       1.362887     4.496519     2.104208      24.33
 H       0.146118     1.833222     2.880215      19.38
 H       0.026473     2.446476     0.937776      19.23
 C      -0.342022    -2.009005    -1.145271      76.01
 H      -0.553607    -2.958645    -1.255621      22.68
 C      -0.047604     0.009571    -2.398340      54.99
 H      -0.032779     0.567950    -3.377224      19.31
 C       0.798560     0.464324    -1.325049      -0.61
 O       1.016783     1.870099    -1.221449     214.26
 C       0.775876     2.699201    -2.349246      89.03
 H       1.060678     3.831758    -2.082483      21.65
 H       1.406843     2.560139    -3.390826      22.39
 H      -0.428486     2.539595    -2.617485      21.30
 C       0.921406    -0.246757    -0.053029       6.35
 O       1.401809     0.237168     1.098719     170.11
 C       0.447552    -1.584120    -0.085973      52.12
 H       0.474483    -2.379139     0.761008      17.76
 C      -0.412770    -1.459850    -2.404783      16.33
 C      -1.097257    -2.073653    -3.662914      85.55
 H      -1.076102    -1.384864    -4.564847      22.94
 O      -0.439237    -3.270153    -4.058764     250.84
 H      -0.099711    -3.779815    -3.278294      27.77
 C      -2.576970    -2.550635    -3.358562      64.92
 H      -2.608877    -2.936388    -2.171896      20.54
 O      -3.654586    -1.400136    -3.249802     130.03
 H      -4.672111    -1.911857    -3.648449      18.80
 C      -3.309251    -3.550373    -4.192576      93.23
 O      -4.633391    -3.789367    -3.783527     289.69
 H      -5.019051    -4.458969    -4.492105      27.43
 H      -2.514861    -4.515746    -4.335872      23.10
 H      -3.285061    -3.057533    -5.205978      24.96
55
name = lig-ACN-frame_1016
 C       4.673125     0.718856     0.440625      70.21
 H       4.218630     1.441303    -0.218686      21.19
 C       5.173997    -0.015010     2.682024     112.51
 H       5.159418     0.032145     3.792016      26.63
 C       6.294193    -0.629482     2.095140      -1.76
 O       7.427003    -1.272333     2.915931     249.26
 C       7.095477    -1.402949     4.418202      82.51
 H       7.990938    -1.766816     4.958051      24.30
 H       5.851592    -1.705993     4.718067      23.25
 H       6.921675    -0.313233     4.883129      27.70
 C       6.405860    -0.807476     0.741791      41.21
 O       7.330800    -1.746325     0.276126     212.81
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 H       8.098439    -1.808117     0.885376      27.05
 C       5.678106    -0.059853    -0.118956      46.00
 H       5.774497     0.237569    -1.184677      20.21
 C       4.355782     0.742705     1.855562      42.24
 C       3.129798     1.533074     2.349611     132.40
 H       3.490148     2.442952     2.648956      22.51
 O       2.715408     0.885397     3.603562     304.10
 H       2.320949     0.044643     3.449573      23.92
 C       1.947760     1.680087     1.317084      65.45
 H       2.252770     2.211184     0.228009      12.85
 C       0.658275     2.451959     1.968152      81.03
 O       0.883534     3.640754     2.735398     252.36
 H       1.384296     4.210023     1.963184      25.71
 H       0.199219     1.508483     2.579107      19.76
 H      -0.215766     2.724661     1.349795      20.46
 C      -0.276178    -2.121394    -1.246239      76.98
 H      -0.657550    -2.980157    -0.984311      21.80
 C       0.122470    -0.101431    -2.351239      52.32
 H       0.027822     0.522022    -3.254343      20.73
 C       0.883771     0.560704    -1.322142      14.74
 O       1.062323     1.957997    -1.243137     208.89
 C       0.795237     2.765523    -2.376337      94.19
 H       0.985343     3.896433    -1.895207      21.47
 H       1.582720     2.380208    -3.229218      22.64
 H      -0.216099     2.841387    -2.838425      24.71
 C       0.908489    -0.242455    -0.091760      -8.76
 O       1.461375     0.270483     1.178990     116.57
 C       0.410619    -1.600231    -0.071720      29.72
 H       0.690516    -2.234869     0.911157      16.91
 C      -0.484591    -1.330509    -2.494353      33.11
 C      -1.120278    -2.069164    -3.704947      71.72
 H      -1.019453    -1.311617    -4.627008      23.00
 O      -0.407781    -3.307066    -4.056353     257.98
 H      -0.110754    -3.583428    -3.344223      34.72
 C      -2.753400    -2.499153    -3.255995      69.09
 H      -2.605356    -3.130975    -2.196458      21.12
 O      -3.593817    -1.369117    -3.252642     231.05
 H      -4.545103    -1.870538    -3.471152      20.06
 C      -3.248864    -3.529802    -4.316838      90.13
 O      -4.646063    -3.780126    -3.700112     238.04
 H      -5.197799    -4.399318    -4.555992      27.04
 H      -2.838779    -4.708505    -4.370418      21.86
 H      -3.393247    -3.097092    -5.296372      24.62
55
name = lig-ACN-frame_1017
 C       4.578680     0.697962     0.437476      72.71
 H       3.957276     1.192170    -0.274181      21.15
 C       5.170051    -0.001084     2.676494      71.03
 H       4.868415    -0.281042     3.650460      23.43
 C       6.360574    -0.604267     2.150619      -0.31
 O       7.310508    -1.292263     2.929069     222.76
 C       7.194730    -1.264950     4.390078      96.36
 H       7.986525    -1.928627     4.718699      25.00
 H       6.251623    -2.185805     4.635375      24.41
 H       7.228496    -0.189690     4.869830      27.43
 C       6.426411    -0.788808     0.674952      33.27
 O       7.300278    -1.703937     0.217735     202.44
 H       8.096481    -1.715742     0.768802      28.70
 C       5.670588     0.009026    -0.196832      56.73
 H       5.936929    -0.081364    -1.264709      22.83
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 C       4.371010     0.877970     1.768686      23.04
 C       3.173438     1.569236     2.386560     101.57
 H       3.340514     2.531768     2.763341      22.75
 O       2.755109     0.835745     3.594164     312.94
 H       2.510820     0.057536     3.354735      30.86
 C       2.051403     1.667484     1.246867      69.21
 H       2.679108     2.151529     0.263820      15.16
 C       0.672711     2.430670     2.005508      76.00
 O       0.933044     3.660739     2.748153     283.47
 H       1.300623     4.315927     2.236182      32.06
 H       0.319421     1.768821     3.009659      19.30
 H       0.096379     2.497259     1.101268      21.07
 C      -0.201223    -2.233901    -1.238152      48.84
 H      -0.710126    -3.090210    -1.223287      20.11
 C       0.338961    -0.038791    -2.518312      49.78
 H       0.005908     0.640186    -3.267090      21.58
 C       0.727699     0.540063    -1.234423      -5.68
 O       1.097372     1.942621    -1.245173     171.54
 C       0.919193     2.868864    -2.454233      83.29
 H       1.235074     4.081147    -2.069992      21.12
 H       1.690169     2.702273    -3.350925      23.72
 H      -0.084853     2.794295    -2.819571      25.46
 C       0.986180    -0.160336    -0.055500      18.37
 O       1.480955     0.256766     1.108090     195.80
 C       0.405845    -1.484852    -0.184661      28.88
 H       0.392680    -2.070837     0.863153      19.85
 C      -0.457223    -1.357878    -2.362452     -19.49
 C      -1.262306    -2.073567    -3.582593      72.75
 H      -1.462748    -1.507210    -4.656132      22.32
 O      -0.404027    -3.265659    -4.059026     142.77
 H       0.370085    -3.484109    -3.405510      25.57
 C      -2.639330    -2.466674    -3.301615      75.24
 H      -2.787469    -2.954941    -2.196675      21.42
 O      -3.556475    -1.326397    -3.245215     272.74
 H      -4.337562    -1.719633    -3.126330      28.90
 C      -3.367432    -3.549865    -4.366415      79.19
 O      -4.641046    -3.773861    -3.704667     253.30
 H      -5.304157    -4.481868    -4.326853      25.54
 H      -2.466422    -4.402794    -4.288648      23.00
 H      -3.347885    -3.180567    -5.353743      26.47
55
name = lig-ACN-frame_1018
 C       4.529706     0.807067     0.270405      23.40
 H       3.709031     1.234659    -0.277857      24.80
 C       5.221136     0.097700     2.630088      41.65
 H       4.862382     0.219972     3.586508      22.84
 C       6.298217    -0.623200     2.158809      34.31
 O       7.182391    -1.295310     2.907967     276.90
 C       7.320044    -1.265481     4.306990      98.25
 H       8.311306    -1.588263     4.518871      25.31
 H       6.186026    -1.742496     4.946918      24.81
 H       7.213990    -0.161885     4.740695      28.39
 C       6.507868    -0.670842     0.785443      29.15
 O       7.398407    -1.699099     0.131897     221.30
 H       7.913679    -2.194724     0.872552      22.36
 C       5.618225     0.004023    -0.158536      70.24
 H       5.661209    -0.343314    -1.162765      23.75
 C       4.441601     0.807304     1.767784      55.36
 C       3.170158     1.546479     2.397488     126.28
 H       3.398163     2.577781     2.600557      23.46
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 O       2.753187     0.830392     3.566414     288.86
 H       2.385358    -0.066581     3.264691      22.76
 C       1.987273     1.673543     1.529104      89.02
 H       2.095940     2.251006     0.442865      15.17
 C       0.853643     2.405708     1.953120      92.08
 O       0.996948     3.675823     2.715087     291.25
 H       1.294171     4.254441     2.005355      30.37
 H       0.389860     1.516341     2.732001      20.02
 H      -0.033745     2.530301     1.362337      22.13
 C      -0.169138    -2.055822    -1.226328      43.74
 H      -0.330419    -3.084486    -1.008926      21.40
 C       0.257863    -0.080676    -2.512996      59.42
 H       0.306951     0.387972    -3.462608      24.07
 C       0.672585     0.672188    -1.406076       6.76
 O       1.138157     1.952726    -1.309020     211.97
 C       1.051488     2.869677    -2.458000      87.32
 H       1.271081     4.013617    -1.840538      20.50
 H       1.753939     2.575994    -3.356493      24.46
 H       0.097175     2.915776    -2.839623      27.37
 C       0.913805    -0.190027    -0.180512       0.15
 O       1.557004     0.291580     1.032549     136.70
 C       0.454211    -1.495031    -0.088669      44.19
 H       0.458896    -2.063223     0.913190      18.38
 C      -0.330915    -1.416681    -2.459743      35.28
 C      -1.159674    -2.047814    -3.508633      79.25
 H      -1.066139    -1.032649    -4.242801      22.90
 O      -0.463617    -3.181672    -4.043714      72.10
 H       0.677764    -3.043880    -3.676619      21.62
 C      -2.710670    -2.574338    -3.346948      73.08
 H      -2.695142    -3.203463    -2.334878      22.13
 O      -3.502381    -1.242515    -3.231898     249.22
 H      -4.306677    -1.558791    -2.991287      29.07
 C      -3.332617    -3.496777    -4.258175     116.88
 O      -4.641906    -3.791059    -3.750437     287.58
 H      -4.887780    -4.560307    -4.253201      30.08
 H      -2.886512    -4.619151    -4.409812      22.25
 H      -3.538202    -3.094522    -5.203889      25.26
55
name = lig-ACN-frame_1019
 C       4.599987     0.829664     0.333291      33.70
 H       4.081867     1.274748    -0.516673      24.69
 C       5.237521     0.281160     2.642469      54.64
 H       5.416017     0.421012     3.652998      21.98
 C       6.260137    -0.621950     2.114457      10.55
 O       7.168336    -1.410890     2.866259     249.21
 C       7.367428    -1.153176     4.309411      94.15
 H       8.345177    -1.588530     4.513356      26.88
 H       6.646207    -1.968390     5.137466      25.17
 H       7.394082    -0.020391     4.501626      29.42
 C       6.564399    -0.672737     0.667105      24.63
 O       7.435093    -1.585793     0.180310     218.20
 H       7.721772    -2.170443     0.951494      20.93
 C       5.596881    -0.086400    -0.110163      77.46
 H       5.674651    -0.174757    -1.167876      27.00
 C       4.287337     0.871020     1.634734      36.76
 C       3.218894     1.477768     2.387499      92.52
 H       3.644802     2.342066     2.911778      22.63
 O       2.742719     0.830237     3.597571     194.56
 H       2.166338    -0.162332     3.385897      18.62
 C       1.996653     1.675157     1.389034      73.77
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 H       2.614538     2.380698     0.659617      17.29
 C       0.697719     2.391555     2.141000      89.67
 O       1.094570     3.653894     2.625924     260.54
 H       1.548866     4.346629     1.881378      25.99
 H       0.105572     1.858180     3.075404      20.59
 H       0.228314     2.510397     1.154125      20.07
 C      -0.120718    -2.033575    -1.108890      57.38
 H      -0.566117    -3.078382    -1.223941      20.81
 C       0.085988    -0.039528    -2.587746      55.42
 H       0.114789     0.330815    -3.594762      20.96
 C       0.740048     0.600027    -1.461877       9.50
 O       1.181827     1.961312    -1.387879     226.01
 C       1.119196     2.852316    -2.445597     102.93
 H       1.726073     3.999959    -2.088529      21.07
 H       1.874801     2.514068    -3.248334      24.47
 H       0.167752     3.020216    -2.808585      26.85
 C       0.857664    -0.016025    -0.201256       3.15
 O       1.598587     0.303295     0.952779     148.65
 C       0.496112    -1.432324    -0.018169      39.41
 H       0.865551    -1.965010     0.846922      19.10
 C      -0.234135    -1.414272    -2.394666      25.27
 C      -1.060182    -1.967504    -3.602459      60.14
 H      -1.364404    -1.286224    -4.610052      21.50
 O      -0.485663    -3.152066    -4.081136      83.11
 H       0.754974    -3.158527    -3.976619      21.86
 C      -2.642967    -2.449137    -3.187459      67.65
 H      -2.690594    -2.909553    -2.171955      22.81
 O      -3.399873    -1.272112    -3.185313     194.84
 H      -4.522492    -1.405569    -3.003840      22.60
 C      -3.321658    -3.483779    -4.340893      82.20
 O      -4.690803    -3.853785    -3.776722     344.99
 H      -5.038653    -4.555285    -4.156839      33.71
 H      -2.518015    -4.355569    -4.394917      24.00
 H      -3.239752    -3.004957    -5.282649      26.60
55
name = lig-ACN-frame_1020
 C       4.656758     0.748688     0.318169      40.35
 H       3.984817     1.411031    -0.275246      22.95
 C       5.368118     0.335164     2.533174      62.13
 H       4.978201     0.561029     3.503653      18.55
 C       6.325657    -0.559580     2.076023      35.11
 O       7.120467    -1.493129     2.849548     309.32
 C       7.470799    -1.083404     4.267747      85.67
 H       8.537710    -1.445691     4.448689      25.84
 H       6.383856    -1.542347     4.887950      25.33
 H       7.333171     0.002879     4.515524      31.13
 C       6.445560    -0.783647     0.735688      11.50
 O       7.518583    -1.505498     0.240034     210.85
 H       8.041118    -1.809206     0.989026      28.57
 C       5.632347    -0.060610    -0.266017      65.58
 H       5.987262    -0.137193    -1.293455      27.47
 C       4.375175     0.841826     1.784990      58.39
 C       3.054769     1.506889     2.418116     101.82
 H       3.171279     2.621787     2.579343      20.63
 O       2.733250     0.773270     3.653548     189.86
 H       2.303404    -0.282183     3.260135      16.95
 C       2.002202     1.711389     1.365742      80.25
 H       2.004043     2.321381     0.450803      15.45
 C       0.615029     2.427164     2.100076      81.92
 O       1.187235     3.686848     2.599155     207.98
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 H       1.640380     4.116660     1.624318      23.24
 H       0.282202     1.795820     3.065221      20.63
 H      -0.435785     2.492830     1.613402      20.78
 C      -0.106919    -2.090524    -1.132326      51.56
 H      -0.443351    -3.195911    -0.724137      18.60
 C       0.099763     0.043326    -2.550259      64.24
 H      -0.357858     0.706018    -3.306142      22.17
 C       0.763764     0.637694    -1.477792       3.33
 O       1.228729     1.903944    -1.395872     183.29
 C       1.206685     2.866719    -2.566138      89.17
 H       1.735282     3.936362    -1.995273      20.81
 H       1.531553     2.519692    -3.600333      24.49
 H       0.174170     3.169223    -2.749980      26.08
 C       0.882713    -0.008624    -0.136291      15.77
 O       1.670655     0.424337     0.872624     175.80
 C       0.510477    -1.310024    -0.087932      49.87
 H       0.722227    -1.724612     0.822360      21.14
 C      -0.346605    -1.328555    -2.364865       1.01
 C      -1.137388    -2.011122    -3.589016      65.40
 H      -1.031964    -1.068843    -4.436614      23.42
 O      -0.459120    -3.236324    -4.193635     117.22
 H       0.612636    -3.322873    -3.767854      22.78
 C      -2.520002    -2.401400    -3.189715      90.50
 H      -2.392895    -2.899033    -2.250205      24.77
 O      -3.343639    -1.185156    -3.102418     160.46
 H      -4.365068    -1.889882    -3.119960      19.34
 C      -3.251664    -3.433557    -4.235800      96.80
 O      -4.616093    -3.862607    -3.844820     266.64
 H      -4.830712    -4.604662    -4.601552      25.66
 H      -2.657025    -4.385431    -4.342137      22.87
 H      -3.479920    -2.984827    -5.189938      23.49
55
name = lig-ACN-frame_1021
 C       4.571883     0.715634     0.305757      60.38
 H       3.897798     1.261038    -0.388880      19.29
 C       5.422420     0.308624     2.689986      45.72
 H       5.500971     0.122129     3.782232      20.48
 C       6.400427    -0.583595     2.119458      25.29
 O       7.091694    -1.458250     2.880788     237.27
 C       7.451707    -1.015967     4.148678     110.44
 H       8.481690    -1.510821     4.449378      25.39
 H       6.793500    -1.476972     5.211279      25.13
 H       7.593155     0.053528     4.110487      31.78
 C       6.424420    -0.844175     0.649621      27.75
 O       7.624010    -1.483823     0.267404     201.90
 H       8.251497    -1.528835     1.025360      28.34
 C       5.697967    -0.018568    -0.243001      53.33
 H       5.810624    -0.000022    -1.354522      21.71
 C       4.462771     0.896465     1.672215      18.87
 C       3.044411     1.590834     2.400436      74.99
 H       3.364623     2.484764     3.106821      23.95
 O       2.696774     0.749086     3.612307     210.35
 H       2.391179    -0.268610     3.361696      22.05
 C       1.690637     1.806551     1.350089     126.38
 H       2.351775     2.484035     0.824843      20.20
 C       0.693263     2.445869     2.097937     107.46
 O       1.199402     3.696459     2.565906     267.40
 H       1.499358     4.425334     1.793719      25.66
 H       0.734554     1.766991     3.074645      20.10
 H      -0.296144     2.545863     1.547243      23.30
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 C      -0.101913    -1.954229    -1.212732      49.96
 H      -0.285385    -3.209089    -1.169406      20.21
 C       0.037770    -0.006347    -2.407025      38.94
 H      -0.249281     0.649428    -3.299363      22.18
 C       0.748714     0.720465    -1.375091      18.12
 O       1.340915     1.982575    -1.496178     225.62
 C       1.159981     2.835271    -2.607774      92.07
 H       2.067119     3.776564    -2.403648      20.90
 H       1.544631     2.298683    -3.501006      24.53
 H       0.115775     3.306893    -2.632500      23.86
 C       0.978107     0.000720    -0.265935      12.42
 O       1.735991     0.443634     0.826817     175.10
 C       0.465451    -1.360263    -0.093394      50.59
 H       0.448981    -1.848114     0.790457      22.26
 C      -0.478289    -1.337596    -2.385031      36.84
 C      -1.035633    -2.050989    -3.573220      75.69
 H      -1.174872    -1.229997    -4.558260      22.84
 O      -0.424346    -3.257423    -4.237819     201.99
 H       0.202372    -3.585232    -3.573006      28.10
 C      -2.521916    -2.484553    -3.258872      83.87
 H      -2.506065    -2.968136    -2.328728      24.98
 O      -3.333254    -1.165351    -2.996065     162.10
 H      -4.451126    -1.349391    -3.101885      22.89
 C      -3.163134    -3.387081    -4.163956     112.15
 O      -4.489139    -3.816749    -3.864055     224.47
 H      -4.783559    -4.622843    -4.733206      23.08
 H      -2.468782    -4.205309    -4.285848      24.21
 H      -3.010612    -2.869879    -5.124714      24.54
55
name = lig-ACN-frame_1022
 C       4.574162     0.708793     0.339553      46.28
 H       3.841885     0.993127    -0.417680      23.17
 C       5.388809     0.242188     2.653725      78.52
 H       5.173421     0.640028     3.690911      21.50
 C       6.259533    -0.620043     2.046375      17.28
 O       7.109904    -1.473103     2.867608     284.59
 C       7.558032    -0.936973     4.173398      78.84
 H       8.575817    -1.581394     4.356544      24.79
 H       6.515319    -0.989199     4.895755      25.08
 H       7.744128     0.120233     4.202767      30.15
 C       6.621407    -0.732306     0.662506      -0.38
 O       7.684367    -1.485368     0.215195     201.13
 H       8.106185    -1.782773     1.122427      21.13
 C       5.674830    -0.027578    -0.142884      70.44
 H       5.894543    -0.185927    -1.245713      26.14
 C       4.388096     0.980163     1.785742      61.72
 C       3.165741     1.522315     2.412240     102.77
 H       3.468142     2.676821     2.696214      19.75
 O       2.653525     0.737099     3.506852     267.01
 H       2.343533    -0.009628     3.138565      28.06
 C       2.001834     1.848767     1.337619      73.29
 H       1.941365     2.479578     0.442253      17.07
 C       0.640449     2.476918     2.203840      90.17
 O       1.162643     3.766174     2.584508     288.26
 H       1.388679     4.233327     1.767666      29.75
 H       0.111970     1.992991     3.113441      22.20
 H      -0.243369     2.557429     1.498873      21.77
 C      -0.153750    -2.012595    -1.216294      41.49
 H      -0.450881    -3.249280    -1.232889      19.82
 C      -0.095131     0.121801    -2.436900      59.99
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 H       0.027080     0.443222    -3.521148      21.35
 C       0.687464     0.739347    -1.438519     -11.49
 O       1.447062     2.023083    -1.527015     201.50
 C       1.123005     2.797232    -2.711109      98.72
 H       1.813790     3.856608    -2.738511      22.89
 H       1.104381     2.271573    -3.670675      25.84
 H      -0.042193     3.139137    -2.722589      24.68
 C       1.036756    -0.073013    -0.197798       8.18
 O       1.724769     0.430694     0.811922     155.49
 C       0.453216    -1.349946    -0.121380      55.97
 H       0.762525    -1.876872     0.752498      21.35
 C      -0.392720    -1.268340    -2.419962      14.31
 C      -1.091044    -2.083239    -3.642855      59.78
 H      -1.155970    -1.351998    -4.690839      23.05
 O      -0.342100    -3.206968    -4.193244     228.22
 H       0.091888    -3.691654    -3.647725      32.34
 C      -2.606997    -2.422852    -3.069581      84.30
 H      -2.547444    -2.958144    -2.228245      26.23
 O      -3.271363    -1.196666    -2.922726     315.74
 H      -4.113763    -1.433132    -3.075075      30.52
 C      -3.043497    -3.423058    -4.332540      82.83
 O      -4.371334    -3.743976    -3.882571     229.13
 H      -4.898760    -4.716883    -4.378130      24.39
 H      -2.417982    -4.229685    -4.222170      24.88
 H      -3.091664    -3.054489    -5.390231      23.23
55
name = lig-ACN-frame_1023
 C       4.619501     0.695598     0.431949      29.14
 H       3.861201     1.132831    -0.174232      24.89
 C       5.264292     0.260656     2.550263      54.93
 H       5.281121     0.228797     3.654993      23.11
 C       6.282052    -0.687250     2.118628      20.69
 O       7.142425    -1.447703     2.842335     261.49
 C       7.612112    -0.862561     4.157948      92.64
 H       8.336200    -1.599770     4.755312      26.60
 H       6.709497    -0.920671     5.074938      25.86
 H       8.048327     0.092381     3.976839      31.37
 C       6.679083    -0.573024     0.759717      20.19
 O       7.699137    -1.468895     0.193857     220.48
 H       7.976507    -2.202841     0.781349      24.22
 C       5.695497    -0.055680    -0.126503      60.58
 H       5.695840    -0.146375    -1.243529      24.25
 C       4.395957     0.873439     1.721338      48.87
 C       3.226448     1.610084     2.333803      98.55
 H       3.376187     2.615392     3.018078      22.84
 O       2.625763     0.763743     3.398803     261.23
 H       2.226680     0.018759     3.040552      25.99
 C       2.108864     1.741806     1.387319      98.44
 H       2.459278     2.458937     0.655732      22.15
 C       0.672247     2.519093     2.171041      90.53
 O       1.075840     3.834042     2.626793     308.91
 H       1.484348     4.309286     1.998914      33.73
 H       0.433444     1.884262     3.039721      22.99
 H      -0.025822     2.587305     1.303563      22.65
 C      -0.181993    -2.007814    -1.220370      42.86
 H      -0.535947    -3.137044    -0.848467      20.69
 C      -0.066529     0.204056    -2.570993      38.09
 H      -0.331901     0.910898    -3.398229      20.63
 C       0.738854     0.738178    -1.452369       0.60
 O       1.441580     1.932200    -1.589452     178.52
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 C       0.991765     2.763261    -2.844442      82.47
 H       1.703776     3.700852    -2.754534      23.69
 H       1.234523     2.227102    -3.772307      24.36
 H      -0.135221     3.128203    -2.535016      23.48
 C       0.904811     0.026042    -0.281319      -0.09
 O       1.757761     0.409001     0.911556     131.79
 C       0.520976    -1.401846    -0.160393      30.51
 H       0.779756    -1.971134     0.788185      20.00
 C      -0.356788    -1.265019    -2.485254      13.28
 C      -1.115275    -2.001436    -3.521425      90.78
 H      -1.374427    -1.167409    -4.424173      23.64
 O      -0.319690    -3.133703    -4.146930     170.11
 H       0.467533    -3.181247    -3.469916      25.81
 C      -2.426867    -2.480051    -3.190223      93.55
 H      -2.522502    -3.040589    -2.383085      26.38
 O      -3.272088    -1.230356    -2.864804     274.52
 H      -4.084335    -1.484009    -2.941937      30.59
 C      -3.021317    -3.443365    -4.309264      97.01
 O      -4.346865    -3.699243    -3.892365     269.90
 H      -4.612796    -4.585349    -4.532883      24.14
 H      -2.466546    -4.268047    -4.400515      25.37
 H      -2.945851    -2.873330    -5.296404      23.48
55
name = lig-ACN-frame_1024
 C       4.616717     0.722288     0.256685     113.18
 H       4.162379     1.199713    -0.592101      22.21
 C       5.341007     0.061463     2.738462      42.00
 H       4.926102     0.023747     3.716570      22.15
 C       6.430349    -0.584037     2.133003      32.54
 O       7.202081    -1.436392     2.967399     273.03
 C       7.616099    -0.853519     4.143001     104.67
 H       8.422348    -1.682670     4.485971      22.87
 H       6.712912    -0.314708     4.744425      25.17
 H       8.214099     0.032977     3.919055      27.10
 C       6.643502    -0.670909     0.711049       2.57
 O       7.645772    -1.385114     0.184603     227.02
 H       7.897695    -1.924388     0.946704      29.21
 C       5.759575    -0.032911    -0.135057      55.53
 H       5.989654    -0.240500    -1.189088      24.13
 C       4.403032     0.836853     1.736507      52.88
 C       3.150472     1.564272     2.392099     113.44
 H       3.686299     2.594955     2.731584      21.50
 O       2.637652     0.786102     3.419653     235.00
 H       2.283897    -0.134545     2.867649      19.13
 C       1.969164     1.843080     1.328584     119.57
 H       2.322553     2.269525     0.440948      22.80
 C       0.925136     2.526628     1.982032     113.52
 O       0.966881     3.849052     2.678950     282.97
 H       1.472496     4.470628     2.006103      28.01
 H       0.647185     1.918897     2.795342      24.48
 H      -0.065190     2.501050     1.445761      24.42
 C      -0.126246    -1.869183    -1.263223      62.32
 H      -0.549403    -2.933508    -1.428572      22.23
 C       0.051501     0.060791    -2.537116      72.72
 H      -0.536838     0.575312    -3.270912      23.58
 C       0.754784     0.703794    -1.538280       5.33
 O       1.369754     1.923258    -1.757929     216.97
 C       0.959321     2.701337    -2.797666     111.93
 H       1.532487     3.650742    -2.756747      24.97
 H       1.049044     2.173824    -3.752281      25.64
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 H      -0.281966     2.971365    -2.975553      24.25
 C       0.918899     0.036168    -0.174681       6.94
 O       1.701779     0.366367     0.906194     145.52
 C       0.584964    -1.297670    -0.207296      54.57
 H       0.636467    -1.862839     0.826831      20.20
 C      -0.385008    -1.183219    -2.369811      42.74
 C      -1.016609    -1.862414    -3.588339      71.71
 H      -1.139113    -1.062001    -4.516208      23.80
 O      -0.320454    -3.000779    -4.031310     157.85
 H       0.793493    -3.187323    -4.031754      23.24
 C      -2.389104    -2.597863    -3.200779      84.54
 H      -2.207991    -3.153209    -2.359743      25.93
 O      -3.266724    -1.322242    -2.862346     185.23
 H      -4.308814    -1.738010    -2.833104      22.40
 C      -3.003952    -3.374783    -4.301605     110.50
 O      -4.380164    -3.696395    -3.914770     329.24
 H      -4.779483    -4.251921    -4.532110      30.69
 H      -2.424044    -4.168405    -4.379310      27.69
 H      -3.005453    -2.805644    -5.290319      24.61
55
name = lig-ACN-frame_1025
 C       4.717513     0.739596     0.309558      30.62
 H       3.896021     1.320069    -0.183123      20.80
 C       5.220036     0.039114     2.610178      61.44
 H       5.035867    -0.050922     3.622470      24.73
 C       6.490997    -0.536553     2.186377      39.40
 O       7.221645    -1.458526     2.967255     260.28
 C       7.756875    -0.769681     4.203090     105.23
 H       8.082789    -1.531979     4.988920      25.80
 H       6.821494    -0.448389     4.936852      25.11
 H       8.521181     0.003826     3.976302      26.77
 C       6.546267    -0.733223     0.782535      32.39
 O       7.664762    -1.393424     0.197085     197.94
 H       8.418048    -1.628348     0.821228      33.62
 C       5.783991     0.008239    -0.233699      49.62
 H       6.123305    -0.042622    -1.247872      23.07
 C       4.460510     0.723341     1.749722      21.72
 C       3.204843     1.478638     2.267564      71.48
 H       3.316926     2.519570     2.838344      21.38
 O       2.637151     0.782201     3.523408     137.39
 H       2.237185    -0.337314     3.270040      18.03
 C       2.145206     1.886806     1.139075      93.35
 H       2.244438     2.417451     0.251232      21.90
 C       0.794649     2.537726     1.979734      87.51
 O       0.957456     3.813784     2.640182     225.47
 H       1.213837     4.656920     1.908744      25.49
 H       0.635519     1.869527     2.705760      23.60
 H       0.059976     2.600607     1.116147      21.69
 C      -0.056982    -1.940683    -1.196368      54.36
 H      -0.121689    -2.987434    -0.944495      20.94
 C       0.097723     0.111951    -2.537178      36.46
 H       0.312718     0.609124    -3.471870      20.02
 C       0.837107     0.694258    -1.444924      20.73
 O       1.342423     1.927900    -1.764743     219.45
 C       0.875005     2.714369    -2.949991      85.07
 H       1.317940     3.640819    -2.839340      26.06
 H       1.256273     2.357545    -3.942479      23.74
 H      -0.341661     2.837333    -2.645297      22.21
 C       1.030404     0.060685    -0.265720      23.58
 O       1.595961     0.469181     0.929864     158.66
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 C       0.519164    -1.262790    -0.154249      39.84
 H       0.838017    -1.885632     0.803099      19.10
 C      -0.487866    -1.185667    -2.440692       7.49
 C      -1.017043    -1.832994    -3.612134      87.23
 H      -1.078289    -1.000874    -4.511481      25.20
 O      -0.280166    -2.986205    -4.028398      25.73
 H       0.847094    -2.611835    -3.644802      22.02
 C      -2.367695    -2.417899    -3.150944      94.06
 H      -2.210538    -3.093671    -2.382244      26.31
 O      -3.264838    -1.488204    -2.858846     225.38
 H      -4.340579    -2.110245    -2.862935      18.84
 C      -3.043406    -3.380371    -4.356827     100.85
 O      -4.406725    -3.663359    -3.925241     335.68
 H      -4.775298    -4.321528    -4.437778      31.42
 H      -2.587183    -4.252810    -4.513810      27.04
 H      -3.084270    -2.781091    -5.334394      25.54
55
name = lig-ACN-frame_1026
 C       4.773735     0.768121     0.408425      47.79
 H       4.306622     1.404994    -0.460857      22.56
 C       5.239856     0.010728     2.593388      48.63
 H       4.969732     0.102885     3.603822      22.55
 C       6.374739    -0.669698     2.138636      20.10
 O       7.281004    -1.386367     3.022973     287.99
 C       7.808650    -0.763800     4.319747      92.17
 H       8.285529    -1.665389     4.803582      26.03
 H       7.081920     0.064360     4.584379      29.02
 H       8.713459    -0.134578     3.988287      28.74
 C       6.667579    -0.688615     0.702626      29.45
 O       7.683400    -1.444237     0.204838     166.20
 H       8.342183    -1.438859     0.956993      25.72
 C       5.821144     0.001576    -0.147158      55.32
 H       5.977364     0.120227    -1.184255      31.79
 C       4.378399     0.694363     1.683798      46.03
 C       3.250183     1.474728     2.209412      98.41
 H       3.814082     2.383370     2.672449      23.25
 O       2.633747     0.792420     3.542388     156.59
 H       2.216044    -0.248585     3.270966      18.21
 C       2.148854     1.827552     1.201923      90.71
 H       2.791527     2.276647     0.563436      22.20
 C       0.727941     2.554483     1.908910      88.74
 O       0.969864     3.772442     2.571852     268.07
 H       1.183979     4.442011     1.758048      26.16
 H       0.326060     1.898334     2.532847      25.49
 H      -0.065165     2.634052     1.113341      22.78
 C      -0.103978    -1.998558    -1.176663      57.20
 H      -0.406406    -2.968055    -1.157342      21.17
 C       0.161932     0.101869    -2.535296      56.59
 H       0.244302     0.424051    -3.591995      20.64
 C       0.848371     0.750741    -1.529613       6.71
 O       1.421659     2.047039    -1.730684     174.51
 C       0.809020     2.755886    -2.993881      89.40
 H       1.147613     3.652525    -2.838391      27.10
 H       1.109694     2.219461    -3.948657      24.37
 H      -0.444151     2.747564    -3.236683      23.56
 C       1.084244     0.046629    -0.257060      11.77
 O       1.516967     0.633426     0.895044     199.93
 C       0.529086    -1.268227    -0.094351      45.09
 H       0.801182    -1.769665     0.892690      20.31
 C      -0.339794    -1.199694    -2.369736       3.84
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 C      -1.101535    -1.863888    -3.619327      69.02
 H      -1.301381    -1.126337    -4.524444      25.06
 O      -0.205273    -2.958398    -4.094287      54.44
 H       0.722307    -3.256155    -3.258111      18.81
 C      -2.397976    -2.547494    -3.317550      99.04
 H      -2.082660    -3.089951    -2.488201      25.15
 O      -3.417520    -1.508821    -2.791767     186.56
 H      -4.399526    -2.214085    -3.005490      17.43
 C      -3.045233    -3.349963    -4.352539     110.06
 O      -4.423169    -3.578604    -3.902091     311.20
 H      -4.659619    -4.540701    -4.390782      25.00
 H      -2.452596    -4.210094    -4.461712      25.59
 H      -3.059150    -2.787005    -5.331177      25.33
55
name = lig-ACN-frame_1027
 C       4.784391     0.793325     0.277416      30.27
 H       4.266171     1.557071    -0.443469      20.91
 C       5.243851    -0.029030     2.637234      39.66
 H       4.998443    -0.071355     3.711117      22.72
 C       6.357978    -0.813253     2.125345      10.74
 O       7.309935    -1.276899     3.045808     291.78
 C       7.850961    -0.716891     4.240740     113.97
 H       7.796748    -1.559186     4.960964      28.08
 H       7.293714    -0.114462     4.984342      30.08
 H       8.957543    -0.370153     4.114559      28.31
 C       6.777791    -0.709066     0.754244      16.65
 O       7.772355    -1.511051     0.209076     210.68
 H       8.222871    -1.962612     0.939741      22.81
 C       5.883686     0.045117    -0.099796      57.96
 H       6.255613    -0.062836    -1.110954      26.34
 C       4.341825     0.640823     1.718458      24.40
 C       3.164341     1.491291     2.422560      97.92
 H       3.502052     2.549132     2.645565      24.42
 O       2.676746     0.850007     3.470697     324.94
 H       2.289024     0.049744     3.062261      27.20
 C       2.032651     1.898737     1.393582      88.40
 H       2.183884     2.458435     0.562004      22.71
 C       0.808988     2.543215     1.773833     110.65
 O       0.975346     3.788884     2.498467     320.68
 H       1.450543     4.402753     2.007249      32.84
 H       0.430670     1.935169     2.472481      26.22
 H       0.191316     2.685662     0.868656      23.51
 C      -0.167572    -1.907408    -1.126045      47.12
 H      -0.690443    -2.759896    -0.992278      24.03
 C       0.245380     0.004640    -2.596951      46.77
 H      -0.386628     0.595947    -3.314540      20.21
 C       0.919524     0.800790    -1.560165      -4.94
 O       1.389175     2.179627    -1.782526     222.25
 C       0.853223     2.753022    -2.949538      94.33
 H       1.087484     3.689140    -3.103637      26.41
 H       1.383851     2.316138    -3.870138      24.28
 H      -0.380631     2.599065    -2.768035      23.09
 C       1.012896     0.092781    -0.321683       4.65
 O       1.457260     0.617332     0.835410     164.13
 C       0.589704    -1.302157    -0.123080      46.75
 H       0.451310    -1.641865     0.876519      19.81
 C      -0.257660    -1.275597    -2.400176      31.63
 C      -0.984353    -1.941540    -3.558291      76.03
 H      -0.979852    -1.138089    -4.370519      24.34
 O      -0.166019    -2.923807    -4.212998     137.54
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 H       0.247525    -3.648626    -3.436144      23.97
 C      -2.504083    -2.578134    -3.191952      82.14
 H      -2.543836    -3.426892    -2.568201      24.04
 O      -3.513372    -1.551754    -2.777027     262.67
 H      -4.477632    -1.971299    -2.914925      21.96
 C      -3.079608    -3.363829    -4.445403      96.26
 O      -4.408815    -3.545371    -3.892916     247.00
 H      -5.023832    -4.357419    -4.556280      23.33
 H      -2.588051    -4.346856    -4.521451      25.25
 H      -3.093176    -2.863523    -5.431126      25.22
55
name = lig-ACN-frame_1028
 C       4.769993     0.745114     0.385655      57.17
 H       4.091019     1.365300    -0.270287      21.09
 C       5.175832    -0.113856     2.548215      61.86
 H       5.020709    -0.162963     3.681582      24.00
 C       6.415415    -0.696583     2.241608      27.55
 O       7.346099    -1.273420     3.015392     266.64
 C       7.830340    -0.720292     4.288878     102.89
 H       7.895129    -1.579207     4.999872      26.46
 H       7.318009     0.164073     4.306845      30.69
 H       8.945532    -0.349153     4.109803      26.13
 C       6.712821    -0.802296     0.824339      12.57
 O       7.876707    -1.567075     0.246978     245.87
 H       8.007435    -2.395749     0.776899      29.36
 C       6.025465     0.051932    -0.134776      35.65
 H       6.313433     0.167792    -1.199649      19.09
 C       4.407140     0.720280     1.702735      26.78
 C       3.163993     1.616115     2.340551      81.32
 H       3.535065     2.443862     2.935090      23.07
 O       2.632240     0.812317     3.552345     283.45
 H       2.271614     0.069922     3.340288      29.45
 C       2.045959     1.896583     1.275461      98.37
 H       2.694085     2.417149     0.666098      22.49
 C       0.717057     2.619329     1.821915     107.70
 O       0.984958     3.850453     2.469580     341.33
 H       1.474549     4.338604     1.855572      32.36
 H      -0.008190     2.067017     2.320004      25.52
 H       0.164167     2.765136     0.891445      23.32
 C      -0.208414    -1.886339    -1.117912      57.48
 H      -0.668990    -2.748090    -0.670692      24.12
 C       0.268553     0.056522    -2.624463      52.08
 H       0.091538     0.596188    -3.642310      19.45
 C       0.980603     0.775373    -1.643435      14.28
 O       1.338712     2.137826    -1.712405     229.95
 C       0.883009     2.774368    -2.973497      84.84
 H       1.233624     3.753020    -2.763065      24.70
 H       1.108486     2.121363    -3.890210      21.96
 H      -0.365456     2.817253    -3.133404      23.84
 C       1.016180     0.156336    -0.374358       6.98
 O       1.465498     0.536878     0.908688     157.17
 C       0.560713    -1.161117    -0.156194      35.97
 H       0.678053    -1.483567     0.803651      19.46
 C      -0.225741    -1.322558    -2.409482      36.47
 C      -1.037560    -2.036749    -3.494782      84.92
 H      -1.400589    -1.264448    -4.221455      24.44
 O      -0.196164    -2.961945    -4.317495     212.53
 H       0.275677    -3.510218    -3.734890      29.83
 C      -2.517320    -2.551376    -3.140497      86.97
 H      -2.389880    -3.148751    -2.255657      24.18
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 O      -3.480870    -1.568689    -2.775382     290.84
 H      -4.183196    -2.138141    -3.093945      24.12
 C      -3.141146    -3.352600    -4.455697      86.22
 O      -4.470508    -3.579683    -3.944817     242.09
 H      -5.120083    -4.215288    -4.788875      22.21
 H      -2.613304    -4.340098    -4.730277      23.05
 H      -3.149377    -2.731025    -5.343721      24.35
55
name = lig-ACN-frame_1029
 C       4.899729     0.697034     0.369994      73.61
 H       4.497067     1.204668    -0.484610      22.87
 C       5.148908    -0.118793     2.648786      33.16
 H       4.614203    -0.054748     3.688319      21.69
 C       6.470193    -0.597016     2.146847       8.38
 O       7.410404    -1.382378     3.028770     231.64
 C       7.795225    -0.666520     4.263710     112.68
 H       7.561816    -1.155691     5.229249      27.81
 H       7.251173     0.168347     4.539304      31.57
 H       8.931314    -0.439493     4.137067      26.33
 C       6.767762    -0.864616     0.704793      12.27
 O       7.834245    -1.557620     0.347405     219.79
 H       7.963057    -2.248370     1.098792      25.66
 C       5.999268     0.037698    -0.016888      54.43
 H       6.346126     0.144273    -1.081437      21.64
 C       4.411894     0.800248     1.767202      14.44
 C       3.184129     1.498095     2.314755      84.38
 H       3.526005     2.477284     2.433590      23.10
 O       2.586719     0.819921     3.626312     250.31
 H       2.320028    -0.047692     3.178256      23.18
 C       2.063053     1.824458     1.246039      82.16
 H       2.235553     2.207248     0.288669      19.84
 C       0.629194     2.726216     1.746962      84.86
 O       0.996946     3.931541     2.488126     250.51
 H       1.204943     4.727375     1.783924      25.93
 H       0.390121     2.026890     2.531670      22.00
 H      -0.013789     3.008276     0.959616      22.24
 C      -0.160238    -1.828199    -1.094812      51.17
 H      -0.539352    -2.919208    -1.127930      20.50
 C       0.281696    -0.015345    -2.695838      63.67
 H       0.590054     0.025155    -3.797198      19.98
 C       0.952171     0.742929    -1.632139       9.00
 O       1.260083     2.037505    -1.693905     190.24
 C       0.901499     2.811158    -2.976425      76.67
 H       1.647520     3.736199    -3.035839      23.73
 H       1.424611     2.364042    -3.867318      24.06
 H      -0.255403     3.077025    -2.987067      23.85
 C       1.099131     0.160998    -0.293260      14.29
 O       1.579329     0.571791     0.941342     182.05
 C       0.467382    -1.059895    -0.151911      55.68
 H       0.704294    -1.533408     0.742077      22.21
 C      -0.287008    -1.256466    -2.413726      23.75
 C      -1.148521    -1.996620    -3.604101      78.10
 H      -1.292111    -1.215321    -4.340038      24.85
 O      -0.309668    -3.021916    -4.358049     247.04
 H       0.419679    -3.062605    -3.908006      32.46
 C      -2.422595    -2.702070    -3.158781      89.15
 H      -2.286284    -3.508220    -2.405521      22.57
 O      -3.425961    -1.552319    -2.809517     276.20
 H      -4.234482    -1.743884    -2.983173      28.42
 C      -3.144020    -3.288132    -4.300257      92.72
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 O      -4.568332    -3.593498    -4.009999     227.82
 H      -4.858430    -4.538996    -4.804692      21.99
 H      -2.532658    -4.266286    -4.651904      21.52
 H      -3.124447    -2.553690    -5.064636      24.45
55
name = lig-ACN-frame_1030
 C       4.888091     0.822936     0.421583      31.22
 H       4.359704     1.557363    -0.128418      20.28
 C       5.293583    -0.008458     2.652827      84.27
 H       5.235552    -0.385892     3.732275      21.55
 C       6.416858    -0.721293     2.219301     -17.80
 O       7.362958    -1.399805     3.041930     316.61
 C       7.740679    -0.598623     4.256717     100.79
 H       7.396853    -1.366191     4.968294      27.37
 H       7.320962     0.292525     4.099541      35.94
 H       8.865870    -0.446046     4.419440      26.53
 C       6.772429    -0.753150     0.886975      14.15
 O       7.809789    -1.620040     0.425136     208.81
 H       8.412999    -1.767732     1.180591      23.49
 C       6.035979    -0.050888    -0.107906      49.75
 H       6.289245    -0.049071    -1.204306      27.01
 C       4.460292     0.649955     1.758174      41.32
 C       3.145319     1.516483     2.347233     101.21
 H       3.432350     2.317530     2.900486      25.89
 O       2.607274     0.897576     3.500533     260.53
 H       2.189635    -0.162280     3.548040      20.10
 C       1.983020     1.909182     1.224517     101.04
 H       2.629118     2.511952     0.548544      21.49
 C       0.789648     2.755899     1.775909     100.00
 O       0.977697     4.000322     2.505265     271.69
 H       1.306551     4.862973     1.759982      23.63
 H       0.092113     2.187433     2.498725      22.47
 H       0.117348     2.696240     0.976148      24.25
 C      -0.180495    -1.790732    -1.219466      34.55
 H      -0.441444    -2.877175    -0.737783      19.04
 C       0.410184    -0.119075    -2.718321      50.76
 H       0.326153     0.586004    -3.602618      19.47
 C       0.856041     0.664796    -1.570117       2.89
 O       1.217217     2.079075    -1.789398     231.81
 C       1.061429     2.807343    -2.929973      89.30
 H       1.613040     3.909271    -2.701662      21.64
 H       1.050007     2.227932    -3.853334      23.66
 H      -0.086058     3.134030    -3.005724      24.84
 C       1.039424     0.111059    -0.273416       6.36
 O       1.643536     0.503001     0.880412     184.29
 C       0.431535    -1.179977    -0.048254      29.35
 H       0.299778    -1.605582     0.966322      19.37
 C      -0.443309    -1.276127    -2.523133      39.28
 C      -1.099933    -1.940688    -3.665218      93.23
 H      -1.423458    -1.250756    -4.354865      27.29
 O      -0.417143    -3.040065    -4.326006     171.64
 H       0.618146    -3.014376    -4.044546      26.77
 C      -2.496009    -2.680774    -3.117868      82.93
 H      -2.345726    -3.346093    -2.188141      22.71
 O      -3.267373    -1.532560    -2.779774     276.06
 H      -4.205933    -1.968613    -2.793477      23.66
 C      -3.204851    -3.329461    -4.327745      91.47
 O      -4.582643    -3.575794    -4.045832     292.11
 H      -4.792101    -4.644813    -4.386629      24.14
 H      -2.671346    -4.387097    -4.680174      21.44
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 H      -3.119623    -2.658151    -5.150564      24.82
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name = lig-ACN-frame_1031
 C       4.931079     0.822432     0.446294      47.02
 H       4.444018     1.443706    -0.285482      24.13
 C       5.402029     0.010269     2.740704      47.03
 H       4.932488     0.295328     3.730077      22.53
 C       6.421392    -0.828570     2.277157       5.06
 O       7.342974    -1.373184     3.099861     280.01
 C       7.655966    -0.626069     4.253121     116.68
 H       7.289685    -0.777454     5.290321      28.06
 H       7.358629     0.363789     4.214022      33.56
 H       8.739397    -0.672056     4.207976      27.45
 C       6.778188    -0.724482     0.830524      10.41
 O       7.768051    -1.635817     0.488414     199.25
 H       8.437186    -1.607199     1.180256      25.91
 C       5.960020    -0.009178    -0.070445      60.00
 H       6.334071    -0.130335    -1.104036      25.90
 C       4.440280     0.659066     1.769879      13.69
 C       3.176621     1.568606     2.366464     102.46
 H       3.657535     2.432887     2.500628      25.03
 O       2.577293     0.921811     3.469527     270.35
 H       2.338390    -0.094767     2.869889      17.04
 C       2.162604     1.979909     1.361023      52.39
 H       2.496863     2.524624     0.370572      19.11
 C       0.829687     2.709650     1.835397      89.89
 O       0.976554     4.022053     2.484175     245.06
 H       1.598253     4.563312     1.692702      24.94
 H       0.317700     1.910453     2.566684      20.39
 H       0.404003     3.064150     0.965391      20.41
 C      -0.299016    -1.900288    -1.218392      44.98
 H      -1.076250    -2.838175    -1.222195      19.72
 C       0.365040    -0.045949    -2.688690      64.40
 H      -0.008374     0.477259    -3.572088      22.19
 C       0.845812     0.691646    -1.602299       3.75
 O       1.248882     1.980314    -1.692534     185.46
 C       1.041121     2.830745    -2.985090      93.56
 H       2.054753     3.599886    -2.862453      23.07
 H       1.526692     2.425761    -3.844211      26.70
 H       0.030211     3.312377    -3.079300      25.24
 C       0.885368     0.009371    -0.268223       6.23
 O       1.675315     0.533115     0.792957     117.55
 C       0.360649    -1.266031    -0.164764      57.73
 H       0.399109    -1.703358     0.911539      20.17
 C      -0.285889    -1.291910    -2.494448      20.92
 C      -1.202432    -2.031519    -3.644881      99.82
 H      -1.416076    -1.303133    -4.360066      27.39
 O      -0.449902    -3.061822    -4.279628     104.77
 H       0.749691    -3.223001    -4.048460      22.49
 C      -2.444432    -2.554397    -3.200437      87.12
 H      -2.194021    -3.339827    -2.348374      22.28
 O      -3.223811    -1.463214    -2.681801     211.73
 H      -4.307340    -1.862747    -2.478577      21.48
 C      -3.216986    -3.411935    -4.431748      82.02
 O      -4.603509    -3.535711    -3.994123     290.10
 H      -4.996444    -4.297418    -4.564306      27.04
 H      -2.643742    -4.527743    -4.540323      22.07
 H      -3.153066    -2.852224    -5.360976      25.14
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name = lig-ACN-frame_1032
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 C       4.871966     0.740865     0.437810      60.60
 H       4.273694     1.274706    -0.327302      21.20
 C       5.212333     0.092972     2.742772      52.94
 H       5.280065     0.179900     3.830176      23.55
 C       6.355048    -0.690859     2.238495      16.39
 O       7.335473    -1.438879     3.182004     276.82
 C       7.685071    -0.549840     4.349386     117.35
 H       6.974313    -1.021798     5.079738      27.69
 H       7.625459     0.436976     4.025244      31.08
 H       8.681247    -0.726624     4.641184      27.92
 C       6.695691    -0.861317     0.885261      18.99
 O       7.742985    -1.604403     0.450635     211.56
 H       8.164021    -1.970507     1.327388      26.36
 C       6.009720     0.013634     0.024441      55.09
 H       6.175610     0.187760    -1.017103      20.07
 C       4.522420     0.801214     1.821232      38.54
 C       3.397598     1.613508     2.311845     103.29
 H       3.607210     2.443440     2.841788      24.95
 O       2.563964     0.924643     3.454986     213.87
 H       2.156930    -0.075416     3.177093      17.18
 C       2.198927     1.937869     1.304863      57.75
 H       2.714816     2.609528     0.389123      18.75
 C       0.891870     2.700765     1.810624      87.93
 O       1.036838     3.957006     2.504224     302.37
 H       1.353194     4.703722     1.907275      28.00
 H       0.289713     2.040030     2.669955      20.16
 H       0.188107     2.485368     1.034098      23.43
 C      -0.425496    -1.987951    -1.252156      39.19
 H      -1.016505    -2.978291    -0.989436      21.08
 C       0.144289     0.013892    -2.695670      78.75
 H       0.391398     0.327685    -3.687437      22.48
 C       0.807549     0.647988    -1.601314       2.65
 O       1.306544     1.991030    -1.622812     209.73
 C       1.164315     2.783403    -2.964119      84.19
 H       1.693815     3.876428    -2.644985      21.66
 H       1.307067     2.152908    -3.778486      25.81
 H       0.124829     3.053109    -3.115379      26.97
 C       0.877477     0.072783    -0.333649      -7.01
 O       1.680888     0.560897     0.740295     141.28
 C       0.263013    -1.333126    -0.206577      25.60
 H       0.499310    -1.957970     0.775245      18.47
 C      -0.225844    -1.386128    -2.519384      41.28
 C      -1.025900    -1.903396    -3.643023      87.40
 H      -1.132456    -1.213131    -4.377740      26.11
 O      -0.429882    -3.177813    -4.282265      89.51
 H       0.388262    -3.086670    -3.399330      20.31
 C      -2.524736    -2.612488    -3.314158      59.60
 H      -2.459467    -3.494384    -2.495614      20.25
 O      -3.258834    -1.388604    -2.593030     158.84
 H      -4.336451    -1.739241    -2.462635      22.20
 C      -3.208600    -3.373940    -4.397643      92.41
 O      -4.613316    -3.517109    -3.948842     347.51
 H      -5.017311    -3.807796    -4.632904      34.60
 H      -2.693948    -4.529466    -4.365859      22.02
 H      -3.124738    -3.042505    -5.451816      24.61
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name = lig-ACN-frame_1033
 C       4.806374     0.693603     0.469642      65.69
 H       4.198464     1.296863    -0.274339      20.61
 C       5.291300     0.055984     2.772724      49.12
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H	4.832543	0.075694	3.738406	24.84
C	6.384619	-0.683428	2.397788	18.90
O	7.235389	-1.387160	3.168274	246.26
C	7.681533	-0.568201	4.424088	111.72
H	6.898005	-0.397606	5.228507	29.57
H	7.794564	0.477551	4.169486	31.29
H	8.519068	-0.970617	4.828069	28.00
C	6.594632	-0.872597	0.951157	7.65
O	7.748396	-1.614409	0.440444	220.72
H	7.906482	-2.445134	0.971757	29.62
C	6.004457	0.006669	0.016748	47.53
H	6.522374	-0.084747	-0.902345	21.25
C	4.540963	0.954120	1.808512	13.58
C	3.231128	1.621228	2.372301	97.38
H	3.615943	2.498057	2.736096	24.43
O	2.631330	0.944775	3.443289	344.82
H	2.472129	0.028683	3.186868	25.20
C	2.171400	1.927009	1.134857	72.99
H	2.666329	2.567384	0.167354	18.40
C	0.950257	2.582261	1.821793	91.90
O	1.103189	3.891109	2.488628	308.50
H	1.185525	4.502866	1.855672	32.45
H	0.810558	1.774010	2.781868	17.19
H	0.176450	2.865575	1.138420	21.96
C	-0.353007	-1.935389	-1.232800	57.05
H	-0.566965	-3.016760	-1.085687	22.95
C	0.095811	-0.057590	-2.651910	51.30
H	0.116801	0.402252	-3.629058	21.20
C	0.724756	0.724793	-1.597904	1.74
O	1.366083	2.017820	-1.653313	223.06
C	1.171707	2.648675	-2.827095	127.81
H	1.829786	3.683914	-2.856822	22.88
H	1.779382	2.289305	-3.619192	27.21
H	0.160015	2.788939	-3.020543	28.10
C	0.897913	-0.006877	-0.319891	8.49
O	1.678771	0.527925	0.715082	141.81
C	0.279321	-1.233330	-0.152526	50.21
H	0.284773	-1.690340	0.928905	20.39
C	-0.426704	-1.373832	-2.543532	35.66
C	-1.067380	-2.020290	-3.786997	85.55
H	-1.061566	-1.327239	-4.538478	26.12
O	-0.307109	-3.222135	-4.214776	226.75
H	0.273772	-3.894412	-3.782686	26.72
C	-2.510179	-2.432621	-3.245050	75.69
H	-2.187419	-3.133406	-2.293443	21.39
O	-3.288456	-1.424317	-2.624894	300.69
H	-4.148634	-1.767683	-2.750491	27.51
C	-3.273556	-3.329358	-4.362094	85.12
O	-4.605500	-3.456754	-3.922641	266.99
H	-5.188745	-4.004571	-4.633637	26.64
H	-2.665216	-4.423414	-4.450625	21.58
H	-3.250406	-2.745216	-5.345907	23.59