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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.

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SUPPORTING FILE 2

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

55
name = lig-Water-frame_1

C	-2.198607	1.568041	4.926534	68.74
H	-3.079733	2.208545	4.958801	27.81
C	-1.030583	-0.158197	3.582042	26.00
H	-0.923779	-1.139969	3.119489	25.44
C	0.152070	0.135536	4.314626	-21.36
O	1.361538	-0.340155	3.941577	162.02
C	1.360230	-1.725600	3.252629	116.01
H	2.358296	-1.736269	3.133364	29.82
H	0.758135	-1.763518	2.431069	32.30
H	1.067728	-2.713775	3.890848	26.64
C	0.180397	1.137275	5.326291	-1.93
O	1.362458	1.639792	5.752322	255.38
H	1.570692	2.518829	5.352244	27.06
C	-1.082419	1.776972	5.651866	62.20
H	-1.064766	2.663335	6.426726	22.29
C	-2.247162	0.670788	3.834354	-18.78
C	-3.419993	0.257013	3.042589	90.04
H	-4.266626	0.896085	3.367612	28.55
O	-3.982037	-1.131981	3.398372	181.76
H	-5.013269	-1.053399	3.584934	20.86
C	-3.387271	0.415628	1.533264	90.28
H	-2.678000	1.367957	1.388672	25.92
C	-4.623525	0.650627	0.793813	111.42
O	-5.763523	-0.177639	1.254849	262.80
H	-5.554700	-1.062060	0.912875	27.42
H	-4.422244	0.397000	-0.202628	27.43
H	-4.923246	1.763088	0.940719	26.13
C	0.291322	0.682746	-1.009292	41.10
H	0.568273	1.658464	-1.297063	24.17
C	0.433907	-1.781937	-0.835021	48.09
H	0.785228	-2.811665	-1.089802	22.69
C	-0.876042	-1.857280	-0.228461	18.56
O	-1.398768	-3.050774	0.229439	184.69
C	-1.032513	-4.214196	-0.369381	98.84
H	-1.581579	-5.048629	0.183152	24.71
H	-1.036202	-4.157805	-1.629062	26.02
H	0.137239	-4.338680	-0.157612	24.99
C	-1.394277	-0.640637	0.153039	4.94

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 O      -2.568469    -0.712640     1.043641      51.13
 C      -0.945254     0.627594    -0.380716      61.17
 H      -1.421676     1.598762    -0.285925      25.41
 C       0.985428    -0.581323    -1.386747      36.73
 C       2.327905    -0.716030    -1.827736      82.79
 H       2.428052    -1.977651    -2.255794      23.14
 O       2.919175     0.206730    -2.764473     170.76
 H       3.055681     1.071098    -2.198092      25.33
 C       3.409538    -0.821444    -0.690101      71.92
 H       2.890699    -1.777881     0.034673      25.91
 O       4.740516    -1.125224    -1.199247     188.67
 H       4.894978    -0.648440    -2.034899      27.31
 C       3.452515     0.414147     0.199491     127.24
 O       3.813532     1.583909    -0.566266     222.74
 H       3.605562     2.401445    -0.046712      27.50
 H       4.198299     0.339853     0.923337      30.03
 H       2.524636     0.491237     0.503631      32.77
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name = lig-Water-frame_2
 C      -2.258342     1.538466     4.939942      43.68
 H      -3.002052     2.377546     4.938263      22.83
 C      -0.995050    -0.176542     3.546920      36.87
 H      -0.933037    -1.077485     2.914957      26.70
 C       0.152813     0.105770     4.294210      -5.08
 O       1.362764    -0.400707     3.881127     167.38
 C       1.398537    -1.743080     3.320550     103.78
 H       2.538367    -1.588655     2.954892      25.70
 H       0.745204    -1.721143     2.315471      29.13
 H       0.879208    -2.501930     4.056786      25.94
 C       0.126793     1.134452     5.314114      13.01
 O       1.408423     1.650304     5.755213     264.61
 H       1.505869     2.462981     5.182204      30.45
 C      -1.091986     1.790250     5.630126      43.14
 H      -1.309866     2.659095     6.270108      16.50
 C      -2.238772     0.613901     3.828101     -53.53
 C      -3.459795     0.228216     3.052907      85.21
 H      -4.278192     0.922258     3.623172      24.33
 O      -3.942830    -1.131502     3.395078     234.37
 H      -4.861965    -1.111848     3.675447      24.25
 C      -3.317383     0.497726     1.494384      83.46
 H      -2.788978     1.369082     1.214989      26.09
 C      -4.607374     0.688896     0.782224      87.25
 O      -5.800545    -0.203398     1.266337     223.84
 H      -5.516861    -1.198819     1.236070      24.81
 H      -4.415634     0.388944    -0.324986      24.21
 H      -4.878454     1.764779     1.087856      25.68
 C       0.311177     0.587148    -1.027331      49.37
 H       0.822419     1.578097    -1.272825      23.86
 C       0.438530    -1.792094    -0.904652      72.00
 H       0.924167    -2.736768    -1.060340      23.72
 C      -0.821236    -1.856679    -0.249612      -7.09
 O      -1.448221    -3.045340     0.255524     179.93
 C      -0.977248    -4.198950    -0.384292     123.58
 H      -1.838991    -4.718769     0.172275      21.65
 H      -1.004418    -4.166249    -1.368146      32.07
 H       0.003198    -4.498919    -0.257158      29.30
 C      -1.464527    -0.646506     0.135653      -1.42
 O      -2.531979    -0.725964     1.002541      67.87
 C      -0.942851     0.609988    -0.385305      63.48
 H      -1.403188     1.621021    -0.242211      25.65
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 C       0.944967    -0.544846    -1.337207      61.93
 C       2.384203    -0.782593    -1.771775      92.89
 H       2.204196    -1.557151    -2.296194      28.77
 O       2.867759     0.252224    -2.807722     199.62
 H       2.923346     1.009169    -2.236026      30.00
 C       3.397801    -0.812251    -0.628164     115.15
 H       3.116111    -1.549956    -0.084729      32.25
 O       4.729734    -1.132433    -1.241151     205.07
 H       4.870008    -0.555645    -2.063799      26.04
 C       3.486883     0.424790     0.171045     110.02
 O       3.800830     1.566188    -0.571359     206.07
 H       3.671980     2.401017    -0.090431      27.62
 H       4.185180     0.079857     1.101140      26.94
 H       2.369467     0.589259     0.774025      27.81
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name = lig-Water-frame_4
 C      -2.311289     1.454024     4.825090      61.96
 H      -3.320288     1.956729     5.036809      26.23
 C      -1.039113    -0.186396     3.540963      90.58
 H      -1.077047    -0.599110     2.623104      28.56
 C       0.152613     0.108316     4.248449       0.24
 O       1.402742    -0.435978     3.858808     170.57
 C       1.464926    -1.752201     3.325387     117.92
 H       2.490565    -2.317864     3.220363      26.19
 H       0.812064    -1.950611     2.406038      29.10
 H       1.172358    -2.556553     4.182023      26.61
 C       0.129656     1.154799     5.260744     -34.16
 O       1.420864     1.647074     5.749743     274.57
 H       1.774002     2.335458     5.106859      26.62
 C      -1.116281     1.829187     5.578892      24.61
 H      -0.779571     2.641928     6.361580      18.09
 C      -2.211845     0.444779     3.882918      33.25
 C      -3.517045     0.253193     3.095493      94.14
 H      -4.449849     1.079094     3.232794      23.90
 O      -3.865079    -1.105315     3.375206     236.43
 H      -4.829645    -1.072407     3.679677      26.75
 C      -3.205652     0.523024     1.473722      85.86
 H      -2.614559     1.352258     1.415689      27.61
 C      -4.702032     0.634599     0.768719      94.03
 O      -5.791834    -0.173335     1.273739     321.43
 H      -5.495810    -1.092150     1.309781      28.73
 H      -4.695421     0.752711    -0.364211      25.40
 H      -5.177675     1.718226     0.955781      24.38
 C       0.299258     0.601340    -1.060708      71.84
 H       0.843505     1.553972    -1.259805      30.03
 C       0.351329    -1.879823    -1.013303      75.45
 H       1.029068    -2.713215    -1.168394      26.36
 C      -0.798606    -1.822442    -0.197721       7.63
 O      -1.461943    -2.904816     0.275298     123.70
 C      -0.991258    -4.308107    -0.357935      91.50
 H      -1.597402    -5.293078    -0.348486      25.02
 H      -1.012071    -4.034844    -1.365007      28.09
 H      -0.104837    -4.576263     0.091340      27.74
 C      -1.519887    -0.576708     0.021339      33.24
 O      -2.549487    -0.730639     0.953039     100.61
 C      -0.948496     0.570926    -0.368467      62.95
 H      -1.444031     1.535010    -0.072759      24.63
 C       1.015779    -0.667647    -1.235158      -8.26
 C       2.405080    -0.748280    -1.836281      93.61
 H       2.768862    -1.609505    -2.296093      27.60
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 O       2.736276     0.308802    -2.842308     139.52
 H       2.986707     1.215889    -2.470109      26.52
 C       3.480128    -0.865119    -0.641773     105.02
 H       3.369169    -1.583932    -0.015865      32.76
 O       4.691554    -1.137929    -1.279418     209.90
 H       4.805467    -0.543425    -2.043095      23.77
 C       3.491233     0.416749     0.311717      91.91
 O       3.779753     1.599904    -0.587373     173.80
 H       3.473809     2.330000    -0.042437      29.47
 H       4.498299     0.384921     1.010488      26.58
 H       2.437887     0.674231     0.938315      26.51
55
name = lig-Water-frame_5
 C      -2.263692     1.454492     4.851650      56.00
 H      -3.304175     1.575092     5.020915      17.18
 C      -1.036977    -0.196099     3.537388      58.70
 H      -0.849013    -0.763383     2.484504      23.64
 C       0.168127     0.117451     4.222652      -2.48
 O       1.443539    -0.398428     3.876656     133.20
 C       1.477138    -1.860674     3.327779      96.85
 H       2.583902    -2.003572     3.349590      26.42
 H       0.783479    -2.059274     2.461016      26.01
 H       1.048935    -2.614408     4.164626      26.02
 C       0.179775     1.171767     5.201852      -8.33
 O       1.380707     1.626928     5.742043     315.52
 H       1.853183     2.253047     5.137190      28.38
 C      -1.099709     1.822516     5.524953      50.23
 H      -0.938481     2.534463     6.236498      24.77
 C      -2.309854     0.440847     3.924154      19.14
 C      -3.468458     0.285693     3.041210     127.11
 H      -4.229685     0.899334     3.245999      27.10
 O      -3.880922    -1.091206     3.369412     251.21
 H      -4.831249    -1.121513     3.557862      29.55
 C      -3.277140     0.452696     1.483477      78.22
 H      -2.465124     1.376377     1.566318      23.27
 C      -4.753274     0.668035     0.771597      93.25
 O      -5.758831    -0.145519     1.277784     297.75
 H      -5.575797    -1.151239     1.056665      24.56
 H      -4.657718     0.476337    -0.365390      25.02
 H      -5.086705     1.640598     1.043067      25.49
 C       0.321608     0.592453    -1.059025      51.83
 H       0.614023     1.639970    -1.281858      27.90
 C       0.334693    -1.923815    -1.021492      60.30
 H       0.698258    -2.958144    -1.200516      24.96
 C      -0.845318    -1.805824    -0.187402       5.74
 O      -1.462581    -2.922978     0.281252     124.43
 C      -1.030416    -4.343082    -0.344083      72.54
 H      -1.702285    -5.130067    -0.146366      23.70
 H      -0.626017    -3.948603    -1.444252      23.51
 H       0.042009    -4.382031     0.162366      24.49
 C      -1.496291    -0.627496    -0.017420      29.46
 O      -2.596976    -0.698179     0.940526      85.66
 C      -0.923700     0.640551    -0.389542      42.60
 H      -1.383657     1.568654    -0.142956      23.60
 C       1.051352    -0.692710    -1.252617     -17.95
 C       2.395495    -0.696965    -1.873941      88.70
 H       2.851615    -1.773366    -2.268187      23.45
 O       2.677118     0.328233    -2.842914     168.09
 H       2.995026     1.102954    -2.373738      27.58
 C       3.513784    -0.842502    -0.647102      64.89
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 H       3.122343    -1.915453     0.036986      26.03
 O       4.710862    -1.134027    -1.288529     182.56
 H       4.890956    -0.571715    -2.108730      21.38
 C       3.542583     0.427246     0.363329     110.15
 O       3.742783     1.626916    -0.570262     190.52
 H       3.391590     2.459368    -0.112799      25.70
 H       4.355233     0.500471     0.938684      30.46
 H       2.635260     0.464512     0.862074      30.60
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name = lig-Water-frame_6
 C      -2.248595     1.439516     4.904953      68.34
 H      -3.268869     1.743773     5.327299      18.22
 C      -1.025676    -0.201565     3.521922      64.86
 H      -0.860504    -0.873382     2.787281      28.32
 C       0.183937     0.136660     4.197425      -1.32
 O       1.471566    -0.391186     3.883684     112.66
 C       1.491738    -1.934753     3.377489      88.88
 H       2.586677    -1.854237     3.219795      26.09
 H       0.969548    -2.061737     2.408584      28.06
 H       0.863298    -2.544324     4.186396      24.80
 C       0.190085     1.201416     5.123453       1.99
 O       1.342892     1.601893     5.745292     294.59
 H       1.781319     2.230652     5.112716      30.80
 C      -1.018204     1.788742     5.463940      41.22
 H      -1.295573     2.652438     6.290463      22.50
 C      -2.293583     0.428219     3.900248       9.41
 C      -3.435803     0.253792     2.969019     111.54
 H      -4.308519     1.033102     3.483346      18.64
 O      -3.913759    -1.097774     3.360798     241.13
 H      -4.958743    -1.052114     3.437645      26.13
 C      -3.337631     0.411966     1.502371     101.29
 H      -2.782871     1.252278     1.384634      27.77
 C      -4.741176     0.696611     0.768149      85.84
 O      -5.746873    -0.155752     1.289288     311.22
 H      -5.718154    -1.014642     0.853022      27.20
 H      -4.553346     0.414971    -0.272710      26.82
 H      -4.964935     1.873487     1.044707      23.81
 C       0.348555     0.564115    -1.045178      59.13
 H       0.691877     1.521560    -1.407135      27.81
 C       0.322689    -1.922041    -0.987740      72.12
 H       0.513661    -2.958908    -1.300776      26.59
 C      -0.859700    -1.850169    -0.236345     -21.37
 O      -1.484540    -2.996174     0.287007     168.00
 C      -0.996479    -4.274944    -0.321404      99.07
 H      -1.893175    -4.861959     0.031379      21.16
 H      -0.618567    -4.326901    -1.366293      27.13
 H      -0.093051    -4.527148     0.235641      27.67
 C      -1.524338    -0.591316     0.017349      -9.28
 O      -2.635085    -0.681319     0.904014      72.49
 C      -0.890175     0.663644    -0.422664      49.06
 H      -1.374185     1.656406    -0.253276      24.12
 C       1.021072    -0.689595    -1.306922     -14.76
 C       2.441413    -0.697706    -1.866841     100.92
 H       2.394919    -1.630903    -2.442840      25.45
 O       2.630382     0.342560    -2.837849     154.91
 H       2.999193     1.036639    -2.186296      26.09
 C       3.495280    -0.804536    -0.626072     100.81
 H       3.139827    -1.624485    -0.284302      32.33
 O       4.769842    -1.137846    -1.292228     203.65
 H       4.914685    -0.625985    -2.100449      25.26
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 C       3.605366     0.431286     0.330651      99.67
 O       3.686580     1.649367    -0.544335     204.06
 H       3.360478     2.517067    -0.094769      24.26
 H       4.484251     0.434627     1.205923      26.29
 H       2.574212     0.371128     0.968922      27.75
55
name = lig-Water-frame_7
 C      -2.266554     1.386188     4.943258      48.11
 H      -2.936543     2.041544     5.500997      15.98
 C      -1.006549    -0.188462     3.545235      73.69
 H      -1.058172    -1.156865     2.846449      28.15
 C       0.206289     0.153803     4.157996      12.50
 O       1.474727    -0.418634     3.880266     152.43
 C       1.489089    -1.928653     3.441311      90.72
 H       2.654782    -2.138616     3.192564      25.76
 H       1.160800    -1.970881     2.311642      27.75
 H       0.999965    -2.554048     4.203965      26.76
 C       0.188398     1.231941     5.054486       4.80
 O       1.331260     1.586471     5.750822     324.82
 H       1.737770     2.285657     5.152584      26.77
 C      -0.994476     1.799019     5.448796      52.99
 H      -1.143029     2.479370     6.156212      24.32
 C      -2.193052     0.432305     3.838396     -10.26
 C      -3.481654     0.208602     2.995423      98.77
 H      -4.080164     0.915479     3.297328      29.89
 O      -3.969644    -1.120081     3.343151     275.33
 H      -4.924868    -0.981436     3.395515      25.47
 C      -3.397949     0.410062     1.481856      88.27
 H      -2.913566     1.473068     1.097251      24.57
 C      -4.687627     0.721845     0.796751      99.51
 O      -5.765736    -0.160718     1.300479     278.46
 H      -5.802412    -0.971596     0.748736      26.02
 H      -4.459908     0.602212    -0.369626      25.36
 H      -4.929181     1.709405     0.841591      28.63
 C       0.386082     0.528313    -1.044661      55.82
 H       0.983844     1.351666    -1.545316      21.90
 C       0.313128    -1.886702    -0.952818      72.41
 H       0.704409    -2.790513    -1.413989      21.86
 C      -0.899195    -1.877293    -0.278083     -24.60
 O      -1.494372    -3.053657     0.259313     196.76
 C      -0.980927    -4.226080    -0.233927     116.11
 H      -1.890425    -4.838632    -0.075048      24.96
 H      -0.860528    -4.508498    -1.445554      25.67
 H      -0.172096    -4.779183     0.405495      26.26
 C      -1.548866    -0.513155     0.081616     -23.49
 O      -2.662759    -0.694955     0.847474      87.59
 C      -0.896882     0.633629    -0.436029      81.86
 H      -1.329110     1.631638    -0.382948      27.73
 C       0.953957    -0.678408    -1.352652      31.69
 C       2.436300    -0.715402    -1.843735      87.69
 H       2.328797    -1.628377    -2.555576      26.48
 O       2.614719     0.368242    -2.804043     133.59
 H       2.977478     1.136609    -2.269624      25.99
 C       3.507474    -0.719431    -0.688686      83.45
 H       3.108357    -1.819771    -0.089568      25.12
 O       4.836832    -1.148625    -1.277242     179.50
 H       4.920391    -0.640325    -2.113084      27.32
 C       3.639709     0.437644     0.316227     116.74
 O       3.627456     1.661545    -0.508679     310.76
 H       3.380425     2.403415     0.071154      26.80
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 H       4.380524     0.265777     0.996551      29.83
 H       2.737239     0.458134     0.920903      30.06
55
name = lig-Water-frame_8
 C      -2.230428     1.337653     4.955117      48.54
 H      -3.006660     2.057914     5.312813      23.58
 C      -0.965392    -0.231872     3.540228      67.70
 H      -1.217745    -1.122722     3.027517      27.67
 C       0.247814     0.157266     4.104972      32.36
 O       1.469820    -0.477246     3.875014     167.78
 C       1.525336    -1.860557     3.455149     118.36
 H       2.505098    -2.328615     3.509111      26.64
 H       1.081266    -1.950512     2.532110      30.72
 H       1.110094    -2.746817     4.263149      24.69
 C       0.205971     1.250607     5.008598      15.55
 O       1.346802     1.588089     5.747449     259.35
 H       1.788990     2.359457     5.307208      26.47
 C      -1.024331     1.792897     5.427120      47.79
 H      -0.751958     2.582288     6.357661      20.60
 C      -2.155463     0.485503     3.797464      -9.73
 C      -3.483437     0.141524     3.045466      71.68
 H      -4.288876     1.111132     3.308535      24.41
 O      -4.023649    -1.145854     3.314510     228.82
 H      -5.026455    -1.053127     3.525347      21.33
 C      -3.398833     0.470350     1.426282      92.77
 H      -2.866078     1.316493     1.233797      28.42
 C      -4.661353     0.683183     0.787486     103.00
 O      -5.795777    -0.144351     1.294705     268.67
 H      -5.826181    -1.016239     0.752451      25.13
 H      -4.507417     0.696769    -0.275915      26.64
 H      -5.113200     1.840785     0.840176      24.54
 C       0.414917     0.520508    -1.068304      54.33
 H       0.989072     1.320456    -1.434893      24.12
 C       0.305000    -1.858032    -0.945240      60.12
 H       0.937886    -2.707542    -1.328040      21.47
 C      -0.957677    -1.846286    -0.282165      -3.47
 O      -1.497103    -3.038703     0.213505     163.43
 C      -0.994762    -4.294067    -0.154365     126.47
 H      -1.825323    -5.055737    -0.111352      26.98
 H      -0.994529    -4.273215    -1.268697      26.62
 H      -0.190348    -4.797278     0.427321      26.73
 C      -1.527149    -0.506497     0.119435      -2.45
 O      -2.703707    -0.710463     0.793928     100.30
 C      -0.913227     0.608147    -0.443694      77.80
 H      -1.332660     1.610060    -0.409333      26.63
 C       0.913530    -0.688786    -1.365395      47.46
 C       2.375398    -0.723309    -1.836710      81.92
 H       2.756712    -1.674684    -2.439762      27.15
 O       2.624786     0.404258    -2.764138     177.30
 H       2.946291     1.221485    -2.409453      28.00
 C       3.522278    -0.740750    -0.753959      99.28
 H       3.386612    -1.399413    -0.036296      30.99
 O       4.883229    -1.147668    -1.256160     174.10
 H       5.022813    -0.670786    -2.136981      26.11
 C       3.621784     0.441958     0.256589      86.35
 O       3.584791     1.670481    -0.461629     280.38
 H       3.411132     2.424913     0.246421      24.70
 H       4.681824     0.176253     0.856824      24.66
 H       2.682391     0.504893     0.966649      27.27
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name = lig-Water-frame_9
 C      -2.202169     1.339393     4.928859      53.85
 H      -3.260335     1.708392     4.954816      27.55
 C      -0.955997    -0.275656     3.528627      49.53
 H      -1.098124    -1.242286     2.963386      27.90
 C       0.294402     0.146571     4.053779      26.50
 O       1.479418    -0.531884     3.885307     192.92
 C       1.549022    -1.826392     3.491394     122.79
 H       2.641624    -2.253604     3.727234      24.87
 H       0.878062    -2.094848     2.531929      27.84
 H       0.981555    -2.538745     4.192728      26.45
 C       0.234760     1.256430     4.978301      -6.38
 O       1.378132     1.597709     5.739576     226.44
 H       1.824153     2.408817     5.383212      25.37
 C      -0.989860     1.805950     5.454247      51.45
 H      -0.711850     2.408327     6.238828      20.55
 C      -2.172196     0.527793     3.790017     -45.58
 C      -3.500837     0.157917     3.069275      79.96
 H      -4.194634     0.760296     3.392539      31.41
 O      -4.072957    -1.179649     3.283059     206.13
 H      -4.983413    -1.112659     3.792817      19.20
 C      -3.342841     0.486541     1.429581      74.46
 H      -2.531914     1.388590     1.441625      27.66
 C      -4.740994     0.684400     0.759243     103.60
 O      -5.822403    -0.123914     1.265393     300.28
 H      -5.778805    -1.012005     0.917885      28.00
 H      -4.628500     0.565281    -0.435026      24.64
 H      -5.043757     1.596173     1.048547      28.82
 C       0.371727     0.554220    -1.080625      32.21
 H       0.843517     1.576844    -1.260427      25.40
 C       0.284793    -1.866076    -0.950243      62.39
 H       0.836636    -2.790274    -0.988886      25.53
 C      -0.963211    -1.806565    -0.275894      29.08
 O      -1.523172    -2.985432     0.191666     139.73
 C      -1.038745    -4.397049    -0.105789      96.46
 H      -1.838033    -5.146297     0.106944      25.95
 H      -0.729430    -4.171259    -1.325042      22.41
 H      -0.017175    -4.614969     0.425323      24.98
 C      -1.495862    -0.585170     0.116750     -15.89
 O      -2.755360    -0.707681     0.750132     100.84
 C      -0.898130     0.611407    -0.458272      57.06
 H      -1.394087     1.604240    -0.312979      26.17
 C       0.939142    -0.717382    -1.367410      35.38
 C       2.370185    -0.720012    -1.843911      96.51
 H       2.821528    -1.656143    -2.352729      28.48
 O       2.637949     0.427146    -2.749088     147.88
 H       2.975146     1.258954    -2.237831      25.74
 C       3.550695    -0.750821    -0.791200      79.78
 H       3.431700    -1.600729     0.168677      27.07
 O       4.902323    -1.134478    -1.251589     160.00
 H       5.191539    -0.726488    -2.082132      27.51
 C       3.610892     0.436928     0.196653     116.40
 O       3.559217     1.703507    -0.408855     290.68
 H       3.433401     2.505036     0.155153      26.69
 H       4.562845     0.341999     0.554698      30.72
 H       2.847582     0.301571     1.019274      31.28
55
name = lig-Water-frame_10
 C      -2.208249     1.377132     4.854637      52.28
 H      -3.275070     1.517822     5.007896      29.82
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 C      -0.975339    -0.300997     3.512187      43.16
 H      -0.844111    -1.217140     2.844489      30.43
 C       0.301708     0.132141     4.015543     -54.84
 O       1.504065    -0.521498     3.912135     195.25
 C       1.547549    -1.893271     3.521832     106.02
 H       2.572013    -2.038746     3.545751      27.74
 H       1.194495    -2.127817     2.567221      30.98
 H       0.700450    -2.278652     4.295103      21.44
 C       0.269518     1.251559     4.963725     -21.81
 O       1.418675     1.604633     5.728401     209.26
 H       1.798639     2.421466     5.273255      24.12
 C      -0.925107     1.789948     5.462844      39.26
 H      -0.916371     2.523182     6.424796      20.23
 C      -2.167239     0.477307     3.784093     -30.66
 C      -3.496782     0.163911     3.045966      79.06
 H      -4.427725     0.847210     3.593387      24.62
 O      -4.096507    -1.221717     3.260093     205.68
 H      -4.881386    -1.062178     3.869632      19.32
 C      -3.273031     0.471829     1.472697      84.93
 H      -2.596643     1.265456     1.478573      30.95
 C      -4.813508     0.681625     0.713569      87.35
 O      -5.852976    -0.107069     1.233963     283.22
 H      -5.682784    -1.081301     1.077732      27.18
 H      -4.763060     0.543995    -0.304937      27.76
 H      -5.055779     1.801369     1.198056      25.04
 C       0.302919     0.604393    -1.089559      33.92
 H       0.684321     1.596220    -1.190560      29.42
 C       0.269474    -1.891876    -0.951985      64.48
 H       0.668850    -2.920339    -0.723786      28.24
 C      -0.918180    -1.823335    -0.269582      16.13
 O      -1.577375    -2.952757     0.193598     139.44
 C      -1.047678    -4.436677    -0.104603     106.30
 H      -1.806314    -5.051028     0.268431      25.04
 H      -0.531142    -4.515168    -1.082852      25.80
 H      -0.066745    -4.334609     0.459629      26.58
 C      -1.504958    -0.632458     0.084229       5.31
 O      -2.789919    -0.688625     0.715302      78.00
 C      -0.898560     0.603408    -0.443362      65.44
 H      -1.388281     1.516715    -0.209762      29.12
 C       0.993399    -0.709580    -1.355550     -75.49
 C       2.438114    -0.714750    -1.860379      96.92
 H       2.462374    -1.709837    -2.545386      23.95
 O       2.658412     0.449677    -2.740857     184.05
 H       2.926747     1.055867    -2.008852      29.06
 C       3.571021    -0.779397    -0.742940     102.23
 H       3.333583    -1.646745    -0.278698      31.72
 O       4.909453    -1.124821    -1.260130     147.89
 H       5.225799    -0.668942    -2.073956      25.34
 C       3.610405     0.426049     0.150688     109.70
 O       3.537224     1.752521    -0.402501     269.14
 H       3.340685     2.595768     0.212965      23.68
 H       4.737321     0.403513     0.634046      26.60
 H       2.938594     0.152950     1.030912      30.58
55
name = lig-Water-frame_11
 C      -2.180473     1.414493     4.770169      20.14
 H      -3.100585     1.724630     5.391874      15.91
 C      -0.953606    -0.313007     3.483132      89.53
 H      -0.887940    -1.066232     2.758759      28.43
 C       0.269222     0.138319     4.014250     -20.26
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 O       1.527366    -0.462891     3.925770     157.56
 C       1.496626    -1.963599     3.573857      84.29
 H       2.717428    -2.169454     3.526732      23.64
 H       1.417555    -2.098285     2.370190      24.97
 H       0.861889    -2.453468     4.263955      26.58
 C       0.304217     1.238819     4.982631     -35.86
 O       1.466633     1.611652     5.699484     223.50
 H       1.796639     2.374649     5.134279      23.52
 C      -0.915571     1.771206     5.461721      28.61
 H      -1.153546     2.443704     6.309282      29.66
 C      -2.161993     0.365349     3.774876       5.26
 C      -3.520407     0.158319     3.029052     107.03
 H      -4.168136     0.854583     3.337134      27.68
 O      -4.077821    -1.250545     3.234702     250.06
 H      -4.964480    -1.062727     3.789696      23.38
 C      -3.294813     0.417782     1.505695      77.08
 H      -2.627423     1.389043     1.345136      26.03
 C      -4.842014     0.736144     0.753204      82.88
 O      -5.896936    -0.106110     1.209349     301.45
 H      -5.573014    -1.065888     1.214688      26.59
 H      -4.738851     0.674770    -0.471145      24.15
 H      -5.088162     1.707134     0.886028      27.20
 C       0.274188     0.596815    -1.107427      56.08
 H       0.735192     1.583201    -1.351631      28.39
 C       0.311075    -1.910829    -0.950440      66.59
 H       0.770175    -2.884764    -0.861783      27.25
 C      -0.903457    -1.877480    -0.247263      -4.67
 O      -1.639456    -2.962233     0.184588     140.96
 C      -1.009349    -4.378400    -0.072346      85.62
 H      -1.852744    -5.085130     0.397060      23.28
 H      -0.734608    -4.734866    -1.207853      24.81
 H      -0.222012    -4.417907     0.713907      26.64
 C      -1.554118    -0.606586     0.037814      32.05
 O      -2.790092    -0.670982     0.688399     115.43
 C      -0.951967     0.555773    -0.384606      63.68
 H      -1.411342     1.551664    -0.127235      24.85
 C       1.017523    -0.661073    -1.311588     -57.38
 C       2.490485    -0.727566    -1.909665      99.63
 H       2.391869    -1.572007    -2.601429      23.16
 O       2.688409     0.462861    -2.717330     200.47
 H       2.880758     1.141072    -2.027118      28.47
 C       3.585081    -0.802530    -0.761860      92.36
 H       3.185104    -1.891507    -0.309435      25.61
 O       4.921614    -1.123271    -1.277855     164.99
 H       5.062938    -0.511237    -2.073725      24.62
 C       3.673607     0.422203     0.185192     108.00
 O       3.508468     1.790979    -0.434869     272.61
 H       3.249969     2.439941     0.294473      25.94
 H       4.586285     0.362264     0.708128      28.65
 H       2.875625     0.240985     1.018116      27.78
55
name = lig-Water-frame_12
 C      -2.115872     1.426468     4.724263      51.33
 H      -2.803203     1.905319     5.380940      20.11
 C      -0.922271    -0.307463     3.449092      49.20
 H      -1.031797    -1.079352     2.555607      23.96
 C       0.257450     0.165835     4.064879       3.69
 O       1.529873    -0.429582     3.914547     135.93
 C       1.526904    -1.980393     3.568580      82.45
 H       2.429296    -2.360526     3.840791      25.51
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 H       1.268281    -2.044820     2.580183      29.12
 H       0.988548    -2.903967     4.223867      23.87
 C       0.306243     1.222088     5.033411      -5.07
 O       1.517092     1.615476     5.650306     300.27
 H       1.893017     2.359787     5.068401      24.86
 C      -0.964148     1.731048     5.403360      37.46
 H      -1.048359     2.440895     6.275867      30.15
 C      -2.188984     0.285375     3.790575     -11.81
 C      -3.486381     0.089683     2.988298      91.04
 H      -4.223366     1.092082     3.247661      21.84
 O      -4.053960    -1.248107     3.218625     285.42
 H      -4.975060    -1.184629     3.548342      27.71
 C      -3.384368     0.401008     1.482459      86.44
 H      -2.861521     1.327854     1.285723      23.79
 C      -4.817308     0.765110     0.769353      79.70
 O      -5.939722    -0.105952     1.190508     349.15
 H      -5.557520    -0.973264     1.250865      28.33
 H      -4.604052     0.715331    -0.228819      26.73
 H      -5.240792     1.930041     0.794119      23.47
 C       0.281950     0.541454    -1.115532      62.78
 H       0.729369     1.458222    -1.539350      26.96
 C       0.380425    -1.901254    -0.931009      56.15
 H       1.018667    -2.801984    -1.217507      24.73
 C      -0.919085    -1.903300    -0.227598     -10.80
 O      -1.681053    -3.011064     0.151133     173.23
 C      -0.998257    -4.300498    -0.000115     116.98
 H      -1.746609    -4.945733     0.292611      26.43
 H      -1.188230    -4.577575    -1.092836      24.14
 H      -0.217119    -4.633723     0.777231      25.30
 C      -1.612269    -0.605702    -0.002196      26.66
 O      -2.779289    -0.668619     0.677358     138.40
 C      -0.993008     0.553694    -0.340054      67.70
 H      -1.422435     1.501698    -0.130927      22.77
 C       1.005780    -0.615694    -1.255002      -0.43
 C       2.493510    -0.696005    -1.930818      87.03
 H       2.635698    -1.644113    -2.760455      22.77
 O       2.731110     0.478326    -2.698581     182.77
 H       2.810323     1.357226    -2.184495      25.11
 C       3.577255    -0.868947    -0.811973     102.52
 H       3.316852    -1.642972    -0.130833      28.33
 O       4.928190    -1.115260    -1.309207     190.67
 H       4.958030    -0.468295    -2.017508      27.70
 C       3.693800     0.421120     0.244054      81.14
 O       3.489167     1.772852    -0.483133     249.23
 H       3.275137     2.417151     0.265307      25.80
 H       4.725508     0.360507     0.845735      24.59
 H       2.832804     0.427059     0.931400      25.73
55
name = lig-Water-frame_13
 C      -2.078615     1.389274     4.690227      72.96
 H      -3.042085     1.970441     5.000026      23.70
 C      -0.936291    -0.295457     3.405217      43.60
 H      -0.907176    -0.994774     2.676780      26.39
 C       0.284555     0.168020     4.128013      -4.94
 O       1.514104    -0.447957     3.889400     137.11
 C       1.549138    -1.989275     3.596629      71.33
 H       2.611793    -2.393915     4.028695      21.50
 H       1.112858    -2.094322     2.506023      24.27
 H       0.880303    -2.645004     4.081047      26.46
 C       0.289173     1.196086     5.081708       5.58
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 O       1.558379     1.610088     5.597782     299.94
 H       1.874314     2.379837     5.011689      24.60
 C      -0.954051     1.711109     5.355278      54.68
 H      -0.799075     2.500899     6.208605      25.54
 C      -2.197994     0.267705     3.813106      12.09
 C      -3.468170     0.050549     2.952178     106.39
 H      -4.112090     0.776577     3.298010      23.70
 O      -4.020659    -1.236865     3.203571     290.71
 H      -5.052889    -1.180454     3.402710      27.19
 C      -3.502616     0.410041     1.421466      75.85
 H      -2.898736     1.391806     1.343340      21.52
 C      -4.805628     0.794558     0.805865      85.17
 O      -5.967890    -0.084820     1.164533     293.30
 H      -5.618532    -1.027060     1.212818      25.43
 H      -4.457120     0.575338    -0.353057      22.33
 H      -5.154373     1.742995     1.011673      25.22
 C       0.263603     0.508739    -1.092700      62.48
 H       0.613940     1.402108    -1.567581      26.21
 C       0.429636    -1.877885    -0.883696      62.24
 H       0.977713    -2.656875    -1.397604      21.95
 C      -0.913788    -1.903041    -0.243134     -15.00
 O      -1.690425    -3.046025     0.117740     184.36
 C      -1.046202    -4.254853     0.078340     107.15
 H      -1.907194    -4.992213     0.399153      21.45
 H      -1.024979    -4.431294    -1.101733      23.45
 H      -0.042378    -4.514511     0.499377      26.21
 C      -1.638715    -0.648171    -0.026723       8.04
 O      -2.798200    -0.690001     0.685792      85.05
 C      -0.968307     0.586718    -0.358411      51.55
 H      -1.487553     1.557325    -0.162551      19.79
 C       1.007939    -0.641369    -1.225346      22.35
 C       2.470634    -0.657484    -1.925969      94.68
 H       2.704971    -1.465763    -2.599825      25.89
 O       2.781245     0.507870    -2.715367     224.28
 H       2.747865     1.296484    -2.150934      25.94
 C       3.580819    -0.874812    -0.814146      91.48
 H       3.412243    -1.688862     0.049964      25.39
 O       4.920537    -1.107081    -1.350041     191.14
 H       5.048928    -0.462250    -2.093106      27.01
 C       3.692235     0.423042     0.265612      78.52
 O       3.491362     1.716812    -0.525888     241.71
 H       3.406919     2.527326     0.097585      25.33
 H       4.655627     0.432952     0.808504      25.41
 H       2.745408     0.484827     0.975214      23.81
55
name = lig-Water-frame_14
 C      -2.147112     1.345142     4.666851      48.84
 H      -3.078276     1.835355     4.491065      18.35
 C      -0.933573    -0.249611     3.429131      39.65
 H      -0.699759    -1.123725     2.659264      26.93
 C       0.294749     0.101995     4.145073     -43.04
 O       1.501146    -0.499631     3.859811     152.82
 C       1.569106    -1.977661     3.617528      84.49
 H       2.547395    -2.177510     3.771869      24.98
 H       1.447786    -2.204351     2.553862      27.46
 H       0.514229    -2.190666     4.245519      23.61
 C       0.310175     1.141939     5.099393      -3.99
 O       1.578771     1.595699     5.556595     371.99
 H       1.698335     2.433090     4.936139      24.30
 C      -0.890977     1.756339     5.366160      57.75
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 H      -0.866570     2.559025     6.027823      26.81
 C      -2.160232     0.277303     3.780445       4.81
 C      -3.457224     0.023153     2.929091      81.22
 H      -4.304486     0.749138     3.537353      22.20
 O      -3.999098    -1.252310     3.190633     278.27
 H      -4.918958    -1.056598     3.406980      27.69
 C      -3.534919     0.438893     1.389611      78.34
 H      -2.867554     1.338918     1.408358      23.68
 C      -4.818700     0.742206     0.793005      96.12
 O      -5.978580    -0.056810     1.134524     320.24
 H      -5.780627    -1.047191     1.066222      27.26
 H      -4.681695     0.704428    -0.221397      27.14
 H      -5.067874     1.847192     1.218965      23.97
 C       0.233147     0.522357    -1.052619      59.02
 H       0.565454     1.506376    -1.514916      26.52
 C       0.425749    -1.861547    -0.823992      76.90
 H       0.808043    -2.809016    -1.254072      23.87
 C      -0.901325    -1.891533    -0.280579      -6.18
 O      -1.683703    -3.007828     0.099352     204.82
 C      -1.116140    -4.305601     0.086013     114.51
 H      -1.712386    -5.022815     0.551300      24.04
 H      -0.605008    -4.497715    -0.931244      24.69
 H       0.018750    -4.112600     0.333123      24.51
 C      -1.612352    -0.663312    -0.035435     -11.14
 O      -2.845948    -0.730763     0.699564      30.87
 C      -0.950939     0.589628    -0.402697      48.56
 H      -1.459331     1.542412    -0.274990      22.39
 C       1.036647    -0.685211    -1.232698      14.84
 C       2.440519    -0.604801    -1.866172      83.81
 H       2.581987    -1.616316    -2.634175      23.71
 O       2.822674     0.534158    -2.746850     208.99
 H       2.776685     1.215408    -2.016049      26.30
 C       3.599778    -0.816401    -0.739618      91.09
 H       3.459157    -1.799696    -0.198376      27.92
 O       4.901842    -1.099891    -1.396635     156.17
 H       5.141840    -0.514888    -2.177584      25.41
 C       3.632141     0.439898     0.239656     116.96
 O       3.515509     1.656623    -0.563638     222.59
 H       3.529588     2.462444    -0.025586      26.84
 H       4.645579     0.476978     0.810104      28.27
 H       2.887879     0.326933     0.997535      28.84
55
name = lig-Water-frame_15
 C      -2.190926     1.319116     4.662248      22.33
 H      -3.086744     1.989493     4.459253      19.80
 C      -0.851312    -0.260686     3.462451      89.55
 H      -0.751727    -1.028362     2.757832      30.20
 C       0.278768     0.009115     4.130211      21.91
 O       1.507985    -0.537805     3.821121     166.21
 C       1.514813    -1.926755     3.636803     114.43
 H       2.669156    -2.236180     3.882107      24.99
 H       1.593813    -2.288041     2.518479      27.36
 H       0.794364    -2.245255     4.257227      29.91
 C       0.347105     1.075297     5.100876       3.41
 O       1.579130     1.582086     5.520238     318.42
 H       1.663590     2.440289     4.985817      28.37
 C      -0.895330     1.801553     5.359019       6.13
 H      -1.056937     2.854774     5.963103      17.54
 C      -2.124427     0.294676     3.690356      -8.77
 C      -3.485756     0.052891     2.948973      97.79
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 H      -4.160970     0.663440     3.449084      27.37
 O      -3.980901    -1.295372     3.180393     248.69
 H      -4.924312    -1.102767     3.526990      25.19
 C      -3.459901     0.429308     1.414174      76.09
 H      -2.829100     1.333168     1.279499      25.72
 C      -4.886424     0.715526     0.786384      96.20
 O      -5.994158    -0.040728     1.109654     314.67
 H      -5.885562    -0.957426     0.884124      28.35
 H      -4.921678     1.001083    -0.412081      23.40
 H      -5.000320     1.710698     1.206206      26.40
 C       0.277085     0.548293    -1.044753      64.43
 H       0.626161     1.485269    -1.361092      26.98
 C       0.394445    -1.892284    -0.782557      87.31
 H       0.721779    -2.951530    -0.879498      23.76
 C      -0.918603    -1.865911    -0.304405       2.81
 O      -1.686110    -2.942152     0.077272     173.03
 C      -1.061165    -4.332412     0.049148      93.26
 H      -1.546834    -5.167265     0.701395      23.97
 H      -0.783549    -4.750856    -0.951831      25.60
 H      -0.219166    -4.039390     0.709570      25.90
 C      -1.585363    -0.636705    -0.014458     -39.92
 O      -2.882159    -0.776175     0.695660      28.30
 C      -0.999706     0.545841    -0.431715      81.42
 H      -1.451371     1.534541    -0.370711      28.02
 C       1.042129    -0.659053    -1.249453       1.33
 C       2.440689    -0.612770    -1.824010      98.18
 H       2.430294    -1.460464    -2.416954      28.80
 O       2.837390     0.541196    -2.754365     186.14
 H       2.951666     1.317405    -2.103631      25.65
 C       3.621021    -0.736784    -0.703356     101.30
 H       3.397385    -1.790088    -0.303161      28.52
 O       4.882990    -1.091615    -1.434401     154.49
 H       5.022762    -0.538261    -2.208537      28.01
 C       3.599858     0.440272     0.202354     126.42
 O       3.546500     1.600770    -0.598920     210.12
 H       3.554653     2.386142     0.035437      26.06
 H       4.606547     0.480484     0.762005      29.66
 H       2.821758     0.193862     1.090259      27.88
55
name = lig-Water-frame_16
 C      -2.168636     1.337325     4.659374      30.41
 H      -2.936273     2.098483     4.865875      22.45
 C      -0.824471    -0.327390     3.456529      71.66
 H      -0.830628    -1.110251     2.640419      29.35
 C       0.311356    -0.030907     4.160960       4.00
 O       1.526761    -0.541010     3.778958     205.32
 C       1.545728    -1.920563     3.627954     135.05
 H       2.352996    -2.325687     4.163990      27.42
 H       1.361628    -2.294904     2.584043      28.23
 H       0.902733    -2.777294     4.329696      24.88
 C       0.320426     1.052636     5.102159      -0.44
 O       1.571385     1.555182     5.498069     289.96
 H       1.783409     2.465042     5.025257      26.59
 C      -0.957950     1.822489     5.314054      20.57
 H      -1.007157     2.689066     5.783785      21.62
 C      -2.103708     0.337384     3.616964     -32.92
 C      -3.474538     0.071447     2.953459      84.51
 H      -4.253338     0.899529     3.444414      24.54
 O      -3.979502    -1.334609     3.180064     220.05
 H      -4.899347    -1.312457     3.622186      24.67
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 C      -3.385858     0.371268     1.421850      76.73
 H      -2.814052     1.317246     1.077589      25.15
 C      -4.921222     0.740903     0.745653      89.18
 O      -6.034070    -0.043488     1.097802     274.62
 H      -5.894664    -0.972993     0.698782      26.10
 H      -4.903641     1.072819    -0.217281      27.72
 H      -5.178961     1.784380     1.281126      26.20
 C       0.336743     0.545713    -1.042677      47.88
 H       0.817289     1.557357    -1.275046      25.05
 C       0.369214    -1.921402    -0.766276      68.00
 H       0.888738    -2.865630    -0.626381      24.94
 C      -0.950905    -1.831510    -0.304112      16.36
 O      -1.706488    -2.920252     0.046470     122.72
 C      -0.958992    -4.324004     0.051157      99.54
 H      -1.656576    -4.984350     0.638738      26.98
 H      -1.111797    -4.864377    -0.978392      24.88
 H      -0.245348    -4.308538     0.942966      23.53
 C      -1.613511    -0.612212     0.033803     -12.41
 O      -2.881466    -0.806698     0.675606      88.29
 C      -1.046506     0.522931    -0.469692      93.53
 H      -1.543750     1.513190    -0.367823      30.56
 C       1.006410    -0.609438    -1.235135      15.70
 C       2.473185    -0.591672    -1.778052      75.38
 H       2.512028    -1.671288    -2.513209      24.56
 O       2.829763     0.520706    -2.747379     190.51
 H       3.093074     1.335468    -2.347043      29.17
 C       3.618269    -0.717821    -0.752336     103.66
 H       3.303864    -1.661546    -0.084109      27.68
 O       4.861850    -1.073482    -1.453152     186.29
 H       4.815678    -0.502222    -2.266660      26.42
 C       3.603781     0.404524     0.216523     125.13
 O       3.574322     1.586132    -0.613070     230.65
 H       3.492078     2.339936     0.034247      27.58
 H       4.591927     0.427699     0.773887      29.33
 H       2.767232     0.357481     0.842938      30.12
55
name = lig-Water-frame_17
 C      -2.097305     1.391007     4.655727      62.93
 H      -2.961389     1.914526     5.118016      26.74
 C      -0.888895    -0.409768     3.413728      33.95
 H      -0.805843    -1.187550     2.588120      28.60
 C       0.343339    -0.020541     4.212150     -67.59
 O       1.550638    -0.534819     3.754761     182.85
 C       1.561414    -2.033107     3.648915     112.34
 H       2.563154    -2.397283     4.160784      25.28
 H       1.305330    -2.283671     2.593027      28.04
 H       0.842087    -2.571851     4.097994      28.99
 C       0.250200     1.084900     5.087923      17.82
 O       1.559610     1.521214     5.494773     261.14
 H       1.774104     2.370473     5.000737      25.31
 C      -0.979642     1.753039     5.227969      57.89
 H      -0.879633     2.766123     5.911910      22.84
 C      -2.087066     0.387915     3.607058     -18.57
 C      -3.456803     0.085787     2.948467      91.98
 H      -4.184588     0.849030     3.262751      28.05
 O      -3.978951    -1.351224     3.191625     231.32
 H      -4.856852    -1.271099     3.581080      26.27
 C      -3.390923     0.313415     1.374421      86.30
 H      -2.803464     1.157553     1.158391      27.68
 C      -4.916068     0.814075     0.778258      76.66
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 O      -6.080504    -0.074546     1.076568     243.97
 H      -5.914767    -0.949519     0.636095      27.25
 H      -4.730430     1.014063    -0.423477      24.58
 H      -5.283635     1.689830     1.334598      27.00
 C       0.328977     0.578411    -1.023637      47.32
 H       0.866776     1.470724    -1.219194      26.06
 C       0.360844    -1.883378    -0.769109      73.66
 H       1.109019    -2.703846    -0.595807      24.34
 C      -0.968492    -1.823631    -0.283483      20.41
 O      -1.712998    -2.956336     0.019304     134.90
 C      -0.936057    -4.300219     0.096876     115.70
 H      -1.905863    -4.748515     0.507053      24.41
 H      -0.923217    -4.685823    -0.871217      29.51
 H       0.046938    -4.502771     0.597660      26.96
 C      -1.667682    -0.611354     0.062945      -2.95
 O      -2.857667    -0.816158     0.654096     118.41
 C      -1.050415     0.559441    -0.518754      82.25
 H      -1.591584     1.465613    -0.346295      30.18
 C       0.996490    -0.629295    -1.196475      15.23
 C       2.499163    -0.597788    -1.784724     100.72
 H       2.663685    -1.404376    -2.366872      30.57
 O       2.804243     0.462086    -2.757498     189.52
 H       3.166088     1.300659    -2.336889      26.41
 C       3.589492    -0.769293    -0.798713     110.96
 H       3.352631    -1.577424    -0.015268      28.23
 O       4.828280    -1.039005    -1.461667     209.23
 H       4.719161    -0.554895    -2.337815      26.22
 C       3.645553     0.382782     0.219940      99.17
 O       3.609703     1.615520    -0.605132     208.60
 H       3.432907     2.388668    -0.046892      28.49
 H       4.561677     0.306547     0.983279      26.77
 H       2.574169     0.516097     0.724300      26.67
55
name = lig-Water-frame_18
 C      -2.099962     1.422491     4.609209      62.19
 H      -3.114064     1.591821     5.028870      17.41
 C      -0.945989    -0.439815     3.409530      30.23
 H      -0.823473    -1.187788     2.672173      24.84
 C       0.297091    -0.026941     4.191008     -73.45
 O       1.574391    -0.545511     3.760099     143.64
 C       1.597952    -2.149270     3.663189      71.27
 H       2.653202    -2.401832     3.757697      24.17
 H       1.574630    -2.297375     2.493045      25.42
 H       0.483446    -2.328736     4.217772      21.03
 C       0.246370     1.098132     5.033451      30.19
 O       1.525725     1.489146     5.510352     302.31
 H       1.744058     2.329491     4.960591      24.41
 C      -0.894550     1.753255     5.226005      72.65
 H      -0.891403     2.464795     5.957339      27.66
 C      -2.079689     0.395583     3.629676      -5.76
 C      -3.421960     0.057983     2.901695      98.37
 H      -4.256012     0.822585     3.289155      23.37
 O      -3.966897    -1.330135     3.214077     214.02
 H      -4.946623    -1.065132     3.502906      22.42
 C      -3.474444     0.280735     1.332147      81.91
 H      -2.682062     1.180136     1.318178      23.86
 C      -4.888526     0.842119     0.804707      89.97
 O      -6.106147    -0.101564     1.038991     264.46
 H      -5.930322    -0.957561     0.657784      27.98
 H      -4.715796     0.886739    -0.205280      26.29
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 H      -5.177715     1.800420     1.333833      25.45
 C       0.269595     0.598236    -0.994889      41.09
 H       0.800680     1.547843    -1.257123      21.57
 C       0.381140    -1.798018    -0.774285      71.53
 H       1.024560    -2.655740    -0.753879      24.60
 C      -0.972996    -1.839304    -0.248912      21.12
 O      -1.679069    -3.006271     0.004876     186.10
 C      -0.972496    -4.272242     0.138513     109.24
 H      -1.886896    -4.916172     0.475997      22.38
 H      -0.595962    -4.480732    -1.028557      24.18
 H       0.118922    -4.418853     0.304776      24.71
 C      -1.653207    -0.615217     0.010383     -16.02
 O      -2.856534    -0.816502     0.643892     126.89
 C      -1.046978     0.603088    -0.537951      70.64
 H      -1.569882     1.587847    -0.380738      26.45
 C       1.015110    -0.663944    -1.157499      19.05
 C       2.469382    -0.601163    -1.798429      86.09
 H       2.676414    -1.654962    -2.562647      23.70
 O       2.774597     0.403313    -2.778641     205.40
 H       3.118998     1.136012    -2.159529      24.87
 C       3.571707    -0.806866    -0.776003      98.14
 H       3.425419    -1.806893    -0.108195      25.58
 O       4.796656    -1.004212    -1.475385     219.68
 H       4.784295    -0.676386    -2.369633      28.65
 C       3.649225     0.397393     0.220398     105.45
 O       3.672281     1.665036    -0.589191     250.70
 H       3.410341     2.470094    -0.031710      25.82
 H       4.401151     0.275991     1.019359      27.19
 H       2.757136     0.367074     0.735068      29.46
55
name = lig-Water-frame_19
 C      -2.129718     1.413389     4.549751      52.13
 H      -3.148177     1.589028     4.864227      17.97
 C      -0.947128    -0.406643     3.463393      63.61
 H      -0.932451    -1.301467     2.676738      23.59
 C       0.229149    -0.076320     4.079960      -3.98
 O       1.580636    -0.574869     3.790422      99.01
 C       1.595754    -2.192327     3.622147     101.31
 H       2.633432    -2.558112     3.829645      24.94
 H       1.567661    -2.411972     2.583158      27.12
 H       0.818873    -2.442527     4.271810      27.64
 C       0.339413     1.059721     4.943844     -12.52
 O       1.481109     1.474119     5.532395     346.99
 H       1.818109     2.294240     5.044428      26.98
 C      -0.860711     1.793241     5.265142      27.80
 H      -0.912788     2.479953     6.233978      20.15
 C      -2.099725     0.349969     3.632319      22.13
 C      -3.415832     0.018277     2.853342     117.96
 H      -4.171766     0.704983     3.379575      22.28
 O      -3.964493    -1.275538     3.249414     279.63
 H      -4.903975    -1.074629     3.421938      26.72
 C      -3.532711     0.310647     1.343582      90.01
 H      -2.903837     1.117084     1.273455      24.63
 C      -4.866081     0.788763     0.850646      85.36
 O      -6.107579    -0.095712     1.002308     266.13
 H      -5.839883    -1.034141     0.671354      25.74
 H      -4.798206     0.956267    -0.332341      22.49
 H      -4.988474     1.900376     1.231708      23.67
 C       0.243192     0.594058    -0.987211      51.43
 H       0.590779     1.581671    -1.335755      21.12
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 C       0.382132    -1.765773    -0.757929      75.28
 H       0.799577    -2.789003    -1.011146      22.98
 C      -0.942096    -1.848698    -0.226084      -4.68
 O      -1.632696    -3.035300     0.018267     204.93
 C      -0.986736    -4.268775     0.067221     117.55
 H      -1.504936    -5.189811     0.455603      24.83
 H      -0.755386    -4.448756    -0.914802      28.24
 H      -0.017172    -4.136450     0.685587      26.89
 C      -1.610762    -0.617704    -0.085064     -22.53
 O      -2.880380    -0.812607     0.629589     101.03
 C      -1.068169     0.638331    -0.513377      60.99
 H      -1.497422     1.612112    -0.456070      23.38
 C       1.038185    -0.594921    -1.143693      19.84
 C       2.406764    -0.706221    -1.849255     103.53
 H       2.386441    -1.561631    -2.366027      28.11
 O       2.745249     0.363383    -2.777772     239.15
 H       3.013072     1.070295    -2.187073      28.39
 C       3.574685    -0.823850    -0.738153     104.88
 H       3.405011    -1.852970    -0.261253      26.84
 O       4.792615    -0.983706    -1.482842     234.41
 H       4.779810    -0.734416    -2.440779      27.28
 C       3.626611     0.416190     0.200627      93.15
 O       3.748886     1.711381    -0.559412     245.07
 H       3.454982     2.428088     0.059805      25.60
 H       4.535835     0.346583     1.023900      24.74
 H       2.673363     0.251547     0.911754      24.96
55
name = lig-Water-frame_20
 C      -2.115138     1.399070     4.531150      43.53
 H      -3.094181     1.945231     4.776377      23.55
 C      -0.949017    -0.418524     3.468877      82.38
 H      -1.040440    -1.216366     2.880225      28.08
 C       0.263609    -0.102079     3.978102      12.92
 O       1.560198    -0.650050     3.818380     158.77
 C       1.633254    -2.167197     3.575044      89.08
 H       2.506342    -2.618484     4.171033      22.20
 H       1.230748    -2.599834     2.487860      24.13
 H       0.943853    -2.838431     4.383605      23.72
 C       0.363275     1.044789     4.858241     -43.45
 O       1.470817     1.465133     5.563950     327.46
 H       1.874331     2.265240     5.142911      25.90
 C      -0.890915     1.800788     5.284312      20.39
 H      -0.857825     2.395981     6.215098      20.92
 C      -2.144704     0.297304     3.611882      29.80
 C      -3.433483    -0.009124     2.857607     109.76
 H      -4.119960     0.792515     3.356655      22.76
 O      -3.956352    -1.235021     3.281762     280.43
 H      -4.949985    -1.192228     3.476902      26.06
 C      -3.540223     0.329906     1.376029      67.27
 H      -2.979816     1.365507     1.078482      22.47
 C      -4.879016     0.722587     0.826343     109.01
 O      -6.081664    -0.074064     0.974883     303.46
 H      -5.775688    -0.976041     0.739659      28.24
 H      -4.826844     1.011560    -0.193391      26.26
 H      -5.038804     1.703661     1.254645      26.18
 C       0.250314     0.609478    -1.007225      66.28
 H       0.530622     1.561230    -1.419232      26.70
 C       0.374312    -1.803393    -0.746427      88.05
 H       0.657948    -2.721961    -1.227617      23.17
 C      -0.880451    -1.848848    -0.226643     -22.60
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 O      -1.631011    -3.027877     0.056814     156.28
 C      -0.925379    -4.274909     0.004874      99.47
 H      -1.292212    -5.289069     0.514489      23.70
 H      -0.698004    -4.676789    -1.143232      22.92
 H      -0.317340    -4.011441     0.891133      26.42
 C      -1.638454    -0.607628    -0.136235     -12.09
 O      -2.900347    -0.803039     0.594926      49.97
 C      -1.083813     0.629625    -0.471844      60.36
 H      -1.606511     1.615860    -0.458411      22.45
 C       1.028940    -0.497995    -1.139604      11.20
 C       2.343800    -0.771649    -1.846635      76.19
 H       2.115017    -1.916635    -2.450750      22.71
 O       2.710421     0.317916    -2.773849     168.90
 H       2.938577     1.183615    -2.249793      26.80
 C       3.573957    -0.813414    -0.760877     102.55
 H       3.337903    -1.846405    -0.153894      25.93
 O       4.817360    -0.974368    -1.483499     206.93
 H       4.625491    -0.723113    -2.439051      27.57
 C       3.603286     0.414675     0.219209     112.37
 O       3.815969     1.734997    -0.512528     237.94
 H       3.542299     2.403885     0.159633      27.60
 H       4.513026     0.387954     0.773140      28.07
 H       2.761380     0.451918     0.826363      29.87
55
name = lig-Water-frame_21
 C      -2.089138     1.411918     4.550988      52.34
 H      -2.831231     2.171482     4.648186      25.54
 C      -0.979283    -0.463833     3.432669      40.22
 H      -1.082630    -1.512468     2.828585      27.95
 C       0.373730    -0.063087     3.941822       5.08
 O       1.527790    -0.777749     3.829137     255.14
 C       1.618595    -2.174676     3.583956     118.25
 H       2.605542    -2.425825     3.960287      25.69
 H       1.304157    -2.488609     2.686413      32.30
 H       0.996876    -2.793140     4.163595      28.44
 C       0.292668     1.082799     4.814664     -11.81
 O       1.485604     1.446698     5.597809     255.81
 H       1.856218     2.290673     5.125674      21.09
 C      -0.914554     1.713567     5.218888      44.20
 H      -0.830521     2.412411     6.085292      25.98
 C      -2.169633     0.290146     3.614639      11.26
 C      -3.472259     0.024827     2.910004      93.66
 H      -4.114224     0.957611     3.221138      23.90
 O      -3.956254    -1.241193     3.312276     283.25
 H      -4.951649    -1.190660     3.609643      23.05
 C      -3.492056     0.351400     1.365466      73.77
 H      -3.048832     1.235809     1.149377      27.35
 C      -4.919995     0.682813     0.786410      86.94
 O      -6.047132    -0.066364     0.959545     277.95
 H      -5.871624    -0.997143     0.768051      28.32
 H      -4.712127     0.996048    -0.333159      23.84
 H      -5.295637     1.599419     1.504616      22.69
 C       0.244247     0.673914    -1.033879      70.99
 H       0.650856     1.629930    -1.504760      27.42
 C       0.393799    -1.817703    -0.771876      77.88
 H       0.807974    -2.693334    -1.298867      24.91
 C      -0.872450    -1.840268    -0.225495     -33.42
 O      -1.664910    -3.004140     0.086723     140.51
 C      -0.833408    -4.311087    -0.037129     108.25
 H      -1.562521    -5.046227     0.409070      25.05
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 H      -0.427205    -4.564307    -0.907553      28.74
 H       0.024337    -4.160932     0.686293      28.18
 C      -1.714694    -0.606045    -0.113532       2.40
 O      -2.906918    -0.782964     0.543308      53.33
 C      -1.086749     0.602562    -0.442537      45.80
 H      -1.730106     1.476903    -0.402539      23.63
 C       0.984227    -0.505893    -1.130229       8.24
 C       2.295732    -0.806171    -1.821963     103.91
 H       2.264160    -1.598103    -2.333862      30.41
 O       2.673314     0.268715    -2.783790     202.35
 H       2.845405     1.067155    -2.260928      30.40
 C       3.542101    -0.814099    -0.803568     100.88
 H       3.400023    -1.657545    -0.038993      27.84
 O       4.836941    -0.966361    -1.483891     222.23
 H       4.565784    -0.683181    -2.354513      30.07
 C       3.599235     0.421014     0.200379      88.34
 O       3.866606     1.743799    -0.462175     184.73
 H       3.651192     2.472549     0.209091      27.27
 H       4.685360     0.195504     0.801769      24.71
 H       2.683449     0.649069     0.872107      26.65
55
name = lig-Water-frame_22
 C      -2.080838     1.413833     4.539511      62.35
 H      -2.834668     2.251400     4.563951      24.96
 C      -0.976293    -0.537783     3.381433      23.02
 H      -1.021367    -1.450570     2.937993      29.68
 C       0.388743    -0.024138     3.921906     -25.54
 O       1.501845    -0.871428     3.843933     154.61
 C       1.608402    -2.207374     3.622230      97.67
 H       2.790379    -2.293031     3.455820      23.78
 H       1.500261    -2.376674     2.339632      26.08
 H       0.786780    -2.747319     4.309460      24.02
 C       0.272933     1.104193     4.813237       1.23
 O       1.487204     1.436180     5.608060     171.74
 H       1.770776     2.238625     5.120155      24.34
 C      -0.901079     1.611230     5.142694      59.97
 H      -0.832526     2.553612     5.837569      26.91
 C      -2.148477     0.320668     3.645567      -5.74
 C      -3.506555     0.104538     2.948366      81.93
 H      -4.229557     0.918773     3.268889      25.81
 O      -3.974992    -1.268632     3.345418     266.49
 H      -4.870091    -1.096415     3.713281      23.09
 C      -3.475341     0.320379     1.342000      63.83
 H      -2.797010     1.325763     1.263015      27.33
 C      -4.933073     0.719320     0.763942     104.60
 O      -6.043732    -0.110623     0.951261     276.61
 H      -6.015086    -1.104793     0.697963      26.28
 H      -4.706691     0.957139    -0.273058      26.96
 H      -5.230194     1.531166     1.326966      27.47
 C       0.225317     0.732336    -1.052795      85.14
 H       0.663489     1.610504    -1.417632      30.15
 C       0.405352    -1.798890    -0.815782      63.90
 H       1.019632    -2.676679    -1.101773      27.53
 C      -0.942465    -1.826936    -0.221856     -24.88
 O      -1.659653    -2.989541     0.096470     114.62
 C      -0.754923    -4.318126     0.000924      83.99
 H      -1.810643    -4.835687     0.112789      19.72
 H      -0.208733    -4.380316    -1.119789      23.44
 H       0.269585    -4.422302     0.432674      24.82
 C      -1.726276    -0.632025    -0.061056      33.82
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 O      -2.926873    -0.752884     0.499579      59.92
 C      -1.087408     0.586329    -0.439388      27.00
 H      -1.745426     1.454382    -0.352356      25.06
 C       0.921121    -0.579940    -1.129636       4.72
 C       2.298908    -0.738394    -1.760753      79.35
 H       2.443596    -1.822502    -2.540799      23.39
 O       2.633015     0.217756    -2.803250     178.95
 H       2.813042     1.003623    -2.248162      33.28
 C       3.493399    -0.797714    -0.822580      93.33
 H       3.519919    -1.609130     0.079420      27.83
 O       4.824764    -0.959476    -1.482557     164.55
 H       4.711935    -0.595685    -2.408544      26.94
 C       3.638716     0.444587     0.184942     119.97
 O       3.910120     1.746523    -0.417815     195.15
 H       3.727752     2.480000     0.205616      27.54
 H       4.386257     0.065204     0.831402      30.92
 H       2.792050     0.540880     0.862896      31.28
55
name = lig-Water-frame_23
 C      -2.112720     1.402530     4.477157      58.25
 H      -2.940878     2.073145     4.586649      23.02
 C      -0.934706    -0.523880     3.384713      38.68
 H      -0.998747    -1.577397     2.857167      27.03
 C       0.298605    -0.064115     3.892903     -11.47
 O       1.486048    -0.858355     3.882092     192.80
 C       1.608340    -2.274010     3.553628     121.83
 H       2.601810    -2.485202     3.502124      28.41
 H       1.378382    -2.379885     2.574399      31.40
 H       1.015138    -2.842054     4.298214      27.18
 C       0.376233     1.043279     4.821694     -42.12
 O       1.461685     1.434237     5.592310     265.80
 H       1.809137     2.293125     5.127227      20.52
 C      -0.878538     1.622767     5.125715      51.19
 H      -0.826749     2.482501     5.652043      33.32
 C      -2.123250     0.327962     3.646949      14.13
 C      -3.511196     0.141709     2.956589      78.85
 H      -4.401979     0.783462     3.439513      22.91
 O      -3.987330    -1.277300     3.373285     219.77
 H      -4.950801    -1.116497     3.796474      20.59
 C      -3.480399     0.323201     1.336302      85.83
 H      -2.792002     1.085005     1.305697      28.60
 C      -4.890792     0.742136     0.748393      85.37
 O      -6.071469    -0.184195     0.954011     241.18
 H      -5.914880    -1.066752     0.546718      25.88
 H      -4.805797     0.976220    -0.367443      24.88
 H      -5.147435     1.904713     1.166165      23.94
 C       0.183405     0.690146    -1.037192      42.74
 H       0.638215     1.715439    -1.307101      27.30
 C       0.339278    -1.801100    -0.820149      55.27
 H       1.023668    -2.640418    -0.775303      29.33
 C      -1.004169    -1.826296    -0.236946      29.64
 O      -1.596415    -2.993056     0.107750     160.35
 C      -0.715747    -4.290446    -0.039091     110.99
 H      -1.430182    -5.058328    -0.053627      30.00
 H      -0.573593    -4.175300    -1.031348      27.34
 H       0.138949    -4.612374     0.659314      26.92
 C      -1.647190    -0.649526    -0.023589      12.13
 O      -2.980783    -0.725193     0.482188     119.39
 C      -1.084000     0.600168    -0.460403      35.36
 H      -1.653164     1.544370    -0.329292      26.04
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 C       0.887075    -0.587447    -1.167820     -41.51
 C       2.334990    -0.730526    -1.765882     112.60
 H       2.387531    -1.581206    -2.172785      28.21
 O       2.594182     0.190572    -2.813101     179.40
 H       2.844007     1.108462    -2.422197      29.57
 C       3.492629    -0.745871    -0.783897      99.22
 H       3.439586    -1.649391    -0.127589      29.70
 O       4.784084    -0.955697    -1.490017     176.84
 H       4.895996    -0.519501    -2.379747      26.38
 C       3.664742     0.463939     0.164802     115.80
 O       3.955523     1.740548    -0.386121     198.01
 H       3.704368     2.453225     0.281751      26.49
 H       4.423206     0.015154     1.054836      26.92
 H       2.713377     0.413596     0.803308      29.58
55
name = lig-Water-frame_24
 C      -2.103315     1.395155     4.432997      22.73
 H      -3.080788     1.881872     4.685877      18.42
 C      -0.931261    -0.486210     3.391121      89.13
 H      -1.013685    -1.409283     2.840459      27.56
 C       0.243882    -0.156647     3.905084      15.19
 O       1.482819    -0.811989     3.919839     142.73
 C       1.598137    -2.312002     3.488007      81.66
 H       2.707113    -2.719437     3.793368      21.17
 H       0.875164    -2.580826     2.456200      23.03
 H       1.169621    -3.071961     4.250696      24.33
 C       0.416396     0.964467     4.826233     -37.87
 O       1.454669     1.444088     5.563010     331.87
 H       1.826628     2.284323     5.155764      27.06
 C      -0.839525     1.674196     5.101592      34.99
 H      -0.770355     2.643079     5.854249      26.57
 C      -2.130349     0.286490     3.584794      26.43
 C      -3.522257     0.090238     2.961049     101.28
 H      -4.217408     0.756772     3.403572      24.83
 O      -3.992166    -1.268246     3.398411     272.72
 H      -4.934401    -1.227169     3.658036      26.37
 C      -3.524925     0.335820     1.353936      81.25
 H      -2.754754     1.232537     1.203171      22.80
 C      -4.857282     0.793167     0.727005      96.52
 O      -6.080782    -0.231306     0.963544     225.64
 H      -5.716361    -0.986921     0.456642      25.56
 H      -4.860049     0.841012    -0.393260      24.28
 H      -5.115833     1.700901     1.026257      27.66
 C       0.164395     0.612881    -1.019864      60.48
 H       0.534561     1.578656    -1.195547      25.44
 C       0.240961    -1.799781    -0.791927      34.19
 H       0.881915    -2.672782    -0.539359      25.32
 C      -0.992943    -1.856742    -0.273333      18.21
 O      -1.531444    -3.043917     0.150804     190.40
 C      -0.730140    -4.247268    -0.088793      99.87
 H      -1.161573    -5.400051    -0.028129      25.47
 H      -0.481716    -4.089802    -1.254194      21.65
 H      -0.097996    -4.400013     0.782061      26.25
 C      -1.613679    -0.605641     0.013529     -48.76
 O      -3.023520    -0.718469     0.474433     130.46
 C      -1.093463     0.622856    -0.473365      71.89
 H      -1.567476     1.564630    -0.313895      24.35
 C       0.891341    -0.549096    -1.225976      11.03
 C       2.346999    -0.686566    -1.748939      76.88
 H       2.317087    -1.961209    -2.157686      21.77
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 O       2.565257     0.193466    -2.839311     200.79
 H       2.817495     1.087176    -2.627049      29.96
 C       3.546514    -0.663029    -0.743602     101.38
 H       3.261129    -1.768419    -0.315693      25.74
 O       4.748720    -0.962956    -1.500951     198.64
 H       4.817550    -0.409286    -2.276460      28.30
 C       3.675499     0.432865     0.222999     122.12
 O       3.992720     1.736177    -0.358617     229.30
 H       3.648260     2.383529     0.322401      27.43
 H       4.440470     0.273970     0.906082      28.26
 H       2.631734     0.500452     0.619058      27.67
55
name = lig-Water-frame_25
 C      -2.047711     1.388827     4.424859      59.48
 H      -3.013130     1.748731     4.799021      16.17
 C      -1.002204    -0.471818     3.357508      56.77
 H      -1.053456    -1.382116     2.732351      27.84
 C       0.295900    -0.210853     4.007098       9.53
 O       1.492598    -0.826851     3.927132     187.18
 C       1.561094    -2.356969     3.450174      79.25
 H       2.584315    -2.525924     3.511821      24.49
 H       1.039060    -2.580059     2.683685      30.77
 H       1.050597    -2.989195     4.258402      23.01
 C       0.316346     0.939893     4.829606     -25.53
 O       1.483559     1.439427     5.540432     410.17
 H       1.778242     2.281195     5.031507      27.64
 C      -0.800980     1.742920     5.069382      29.72
 H      -0.742841     2.352466     5.850204      12.50
 C      -2.152463     0.259330     3.516333      -1.08
 C      -3.519898    -0.026490     2.940402      76.30
 H      -4.078994     1.008313     3.368968      20.05
 O      -3.973158    -1.262591     3.408931     252.70
 H      -5.029360    -1.189466     3.495130      24.27
 C      -3.556336     0.377915     1.365644      86.35
 H      -3.009201     1.278223     1.209382      22.97
 C      -4.864665     0.777252     0.693875      79.01
 O      -6.051476    -0.239916     0.974052     232.33
 H      -5.663329    -1.047591     0.458771      25.38
 H      -4.721788     0.737326    -0.385124      23.99
 H      -5.334496     1.854640     1.177102      22.44
 C       0.179247     0.563633    -1.020160      59.26
 H       0.618420     1.574963    -1.261966      20.50
 C       0.244405    -1.769941    -0.782156      66.09
 H       0.788150    -2.673920    -0.625578      22.47
 C      -1.008146    -1.868435    -0.280159      -1.13
 O      -1.510972    -3.114054     0.212454     206.81
 C      -0.753046    -4.239815    -0.168614     121.12
 H      -1.283210    -5.077785    -0.022515      27.81
 H      -0.045591    -4.249652    -0.974575      26.77
 H       0.058046    -4.016069     0.645906      24.94
 C      -1.678263    -0.559230     0.041264     -25.77
 O      -3.027864    -0.724090     0.475604     146.03
 C      -1.129825     0.614439    -0.451557      50.42
 H      -1.594011     1.623821    -0.293280      20.97
 C       0.899580    -0.568765    -1.255757      50.51
 C       2.332255    -0.680727    -1.738687      96.98
 H       2.420932    -1.539251    -2.127052      29.71
 O       2.543197     0.192204    -2.895450     211.03
 H       2.771711     1.096273    -2.610316      28.22
 C       3.583875    -0.655399    -0.748678     112.87
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 H       3.348773    -1.524624    -0.168077      27.84
 O       4.727007    -0.971787    -1.510819     210.31
 H       4.654587    -0.256717    -2.207609      27.43
 C       3.653853     0.426053     0.293999     101.65
 O       4.008396     1.735946    -0.337613     218.78
 H       3.635504     2.418046     0.270367      26.01
 H       4.611084     0.361239     1.092344      22.68
 H       2.670266     0.599223     0.713094      24.89
55
name = lig-Water-frame_26
 C      -1.988651     1.368804     4.431945      75.67
 H      -2.879993     1.817278     4.865048      27.72
 C      -1.015135    -0.509921     3.313919      16.17
 H      -1.049739    -1.404958     2.580214      22.89
 C       0.302716    -0.230363     4.115989     -12.35
 O       1.512576    -0.901073     3.904329     132.10
 C       1.518484    -2.348568     3.498246      54.41
 H       2.660960    -2.385796     3.107877      20.51
 H       1.027717    -2.528679     2.257600      21.57
 H       0.974931    -2.815270     4.309220      23.85
 C       0.240459     0.956414     4.853998       1.06
 O       1.507136     1.412106     5.509734     309.17
 H       1.770271     2.204567     4.915031      24.18
 C      -0.823765     1.761918     5.000919      39.69
 H      -0.752074     2.379749     6.036034      13.54
 C      -2.156570     0.285283     3.492872      16.85
 C      -3.502989    -0.052769     2.896320      99.26
 H      -4.053269     0.745737     3.266884      27.10
 O      -3.973746    -1.273647     3.411758     269.49
 H      -4.947360    -1.114560     3.450981      27.04
 C      -3.601633     0.390553     1.373320      74.09
 H      -3.005215     1.389226     1.323546      21.05
 C      -4.949793     0.747972     0.704217      99.61
 O      -5.984577    -0.228989     0.973035     288.74
 H      -5.858688    -1.118437     0.614132      28.95
 H      -4.585704     0.831644    -0.401336      23.47
 H      -5.303595     1.584639     1.036213      27.60
 C       0.190519     0.588513    -1.027665      48.31
 H       0.682369     1.496747    -1.388882      17.21
 C       0.307196    -1.756031    -0.788576      70.03
 H       0.906117    -2.687855    -0.958706      20.12
 C      -1.067312    -1.832025    -0.239474      -4.82
 O      -1.531219    -3.125402     0.240302     174.84
 C      -0.689955    -4.223508    -0.179734     105.95
 H      -1.592133    -5.037075     0.013502      21.74
 H       0.052957    -4.332861    -1.046368      23.86
 H       0.200873    -4.212595     0.464540      26.55
 C      -1.788269    -0.587386     0.037000       6.35
 O      -3.012843    -0.719237     0.496840     154.62
 C      -1.148135     0.609995    -0.417986      47.27
 H      -1.620203     1.560109    -0.309463      20.88
 C       0.901090    -0.630432    -1.242681      34.82
 C       2.320623    -0.628657    -1.728694      60.16
 H       2.585679    -1.770543    -2.381010      21.67
 O       2.536138     0.197206    -2.947438     189.82
 H       2.662366     1.133130    -2.531790      26.14
 C       3.567350    -0.682374    -0.738618      89.18
 H       3.508258    -1.492271     0.190066      22.95
 O       4.717761    -0.962125    -1.531612     205.84
 H       4.694607    -0.222893    -2.208861      27.41
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 C       3.681558     0.480220     0.371208      97.69
 O       3.999841     1.734450    -0.319455     252.15
 H       3.643629     2.547132     0.199915      22.99
 H       4.308683     0.166234     1.113065      26.06
 H       2.714369     0.555897     1.029664      23.12
55
name = lig-Water-frame_27
 C      -2.013789     1.349172     4.425437      52.41
 H      -2.873808     1.978578     4.781811      26.56
 C      -0.955596    -0.561882     3.297083      34.83
 H      -0.975457    -1.328133     2.610092      24.55
 C       0.230396    -0.265903     4.150363     -17.97
 O       1.516593    -0.966510     3.879853     171.22
 C       1.482802    -2.287686     3.458985      91.02
 H       2.488783    -2.548299     3.164175      26.43
 H       1.026354    -2.353621     2.626650      35.05
 H       1.061847    -2.994862     4.320839      23.63
 C       0.300186     0.958784     4.891832      -5.12
 O       1.496498     1.361356     5.470382     330.16
 H       1.890534     2.159671     4.953079      23.80
 C      -0.862964     1.786433     4.997575      51.85
 H      -0.886690     2.467696     5.803630      21.77
 C      -2.109341     0.313193     3.496993      20.15
 C      -3.467593    -0.007448     2.839905      87.08
 H      -4.385526     0.661802     3.387938      23.10
 O      -3.974995    -1.308005     3.403233     201.17
 H      -4.976833    -1.149371     3.589633      24.51
 C      -3.631696     0.386084     1.375018      84.23
 H      -2.968700     1.265100     1.412294      23.58
 C      -4.994720     0.663283     0.698962     104.97
 O      -5.941472    -0.218620     0.976356     312.91
 H      -5.864833    -1.156425     0.652167      27.18
 H      -4.768946     0.916567    -0.313729      25.57
 H      -5.445219     1.819026     1.063957      23.06
 C       0.170687     0.616703    -1.027211      46.32
 H       0.604915     1.526235    -1.439238      20.78
 C       0.316734    -1.811998    -0.777396      53.38
 H       0.872675    -2.629526    -1.219703      18.86
 C      -1.068344    -1.794855    -0.191971      -0.39
 O      -1.545870    -3.071905     0.227527     147.33
 C      -0.619258    -4.255737    -0.149988     104.42
 H      -1.282935    -5.030608    -0.101569      28.09
 H      -0.559827    -4.200762    -1.312805      23.60
 H       0.156467    -4.655909     0.596311      26.31
 C      -1.823791    -0.647917    -0.019680      34.72
 O      -3.039503    -0.702666     0.550856     100.20
 C      -1.118992     0.598407    -0.403105      56.88
 H      -1.685964     1.559896    -0.318827      19.54
 C       0.901741    -0.623047    -1.209570      -0.10
 C       2.343149    -0.677563    -1.782318      89.21
 H       2.466656    -1.534460    -2.161865      28.75
 O       2.542699     0.226687    -2.951038     221.35
 H       2.536573     1.135019    -2.669304      30.28
 C       3.521002    -0.697735    -0.655757      86.07
 H       3.515930    -1.556195    -0.066425      28.25
 O       4.716657    -0.937088    -1.546247     228.72
 H       4.834895    -0.297052    -2.236607      28.80
 C       3.678798     0.545874     0.413673     106.89
 O       3.977960     1.733968    -0.289525     253.51
 H       3.652905     2.530258     0.208296      23.89
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 H       4.434876    -0.040523     1.234910      24.13
 H       2.808118     0.541042     1.017011      27.42
55
name = lig-Water-frame_28
 C      -2.099043     1.362834     4.412998      40.07
 H      -2.972897     1.976544     4.487501      23.88
 C      -0.890998    -0.555948     3.344527      65.21
 H      -0.867824    -1.444161     2.547765      26.08
 C       0.171719    -0.316107     4.116831      -7.38
 O       1.489765    -0.963774     3.890001     182.24
 C       1.454889    -2.273486     3.452866      97.58
 H       2.537925    -2.704327     3.335765      24.86
 H       0.524273    -2.360272     2.482384      26.81
 H       1.211901    -3.073602     4.099045      27.17
 C       0.356244     0.954004     4.907511      -3.01
 O       1.491188     1.297073     5.446196     357.29
 H       1.905980     2.138298     5.048147      25.25
 C      -0.850995     1.767590     5.022255      38.48
 H      -0.977094     2.709704     5.679952      21.56
 C      -2.050440     0.293579     3.487668       5.27
 C      -3.505039     0.065241     2.861385      80.48
 H      -4.158883     0.670070     3.289149      28.22
 O      -3.965955    -1.350407     3.381689     190.84
 H      -4.924477    -1.215221     3.691964      24.48
 C      -3.630547     0.367828     1.365291      89.86
 H      -2.964945     1.274212     1.266162      24.92
 C      -4.989584     0.689715     0.713410     110.59
 O      -5.973658    -0.258957     0.996931     294.74
 H      -5.622783    -1.121335     0.552124      25.40
 H      -4.986006     0.853452    -0.461091      23.46
 H      -5.347342     1.529219     1.079883      27.15
 C       0.142566     0.619402    -1.016954      76.94
 H       0.444679     1.646844    -1.396270      26.74
 C       0.279711    -1.840013    -0.774696      55.86
 H       0.674292    -2.781623    -1.180680      23.75
 C      -0.985758    -1.830919    -0.166717     -11.44
 O      -1.539939    -3.017100     0.213388     132.38
 C      -0.603593    -4.287284    -0.146545      84.91
 H      -1.320297    -5.311331    -0.104486      25.16
 H      -0.820594    -4.056016    -1.145604      23.30
 H       0.160391    -4.637081     0.515126      25.62
 C      -1.792377    -0.648243    -0.088471      21.22
 O      -3.085161    -0.702299     0.609296      70.91
 C      -1.098699     0.576199    -0.405054      26.57
 H      -1.673588     1.489915    -0.320804      22.16
 C       0.899735    -0.568537    -1.169045      -7.22
 C       2.342369    -0.688745    -1.798779      65.27
 H       2.428323    -1.933089    -2.274580      22.59
 O       2.558729     0.252149    -2.928668     182.66
 H       2.441177     1.196319    -2.697946      30.71
 C       3.488090    -0.653919    -0.619010      81.34
 H       3.370255    -1.849542    -0.318830      24.79
 O       4.720274    -0.915433    -1.526317     152.93
 H       4.834186    -0.246255    -2.264988      26.79
 C       3.689475     0.514543     0.443426     114.35
 O       3.960434     1.730792    -0.257746     232.95
 H       3.601096     2.482447     0.355104      25.09
 H       4.528180     0.303237     0.996477      28.83
 H       2.651694     0.673058     0.997730      25.50
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name = lig-Water-frame_29
 C      -2.125130     1.374435     4.384981      24.18
 H      -3.077059     1.976488     4.261457      23.89
 C      -0.903798    -0.558485     3.359702      73.66
 H      -0.849392    -1.331788     2.731219      32.60
 C       0.233427    -0.312450     4.109708      -5.36
 O       1.433678    -0.925734     3.930035     191.68
 C       1.397489    -2.317658     3.391223     104.20
 H       2.509814    -2.501845     3.139538      28.03
 H       0.809054    -2.479054     2.693935      37.23
 H       1.001000    -3.089442     4.244607      26.32
 C       0.282539     0.928280     4.875961      -6.67
 O       1.535817     1.233076     5.456620     314.44
 H       1.765241     2.140259     5.064214      24.08
 C      -0.846733     1.717236     5.057999      54.73
 H      -0.862424     2.756407     5.525182      23.32
 C      -2.051479     0.264918     3.478668     -22.56
 C      -3.517364     0.073757     2.909451      43.80
 H      -4.133055     1.054821     3.458858      22.15
 O      -3.944620    -1.363659     3.355610     189.86
 H      -4.893820    -1.232441     3.573904      22.55
 C      -3.600584     0.369148     1.333265      78.89
 H      -3.046293     1.322148     1.057156      25.61
 C      -4.974887     0.725861     0.706276      83.62
 O      -6.026491    -0.338186     1.013336     246.78
 H      -5.607793    -1.097197     0.599577      27.33
 H      -4.942981     0.752987    -0.333896      25.37
 H      -5.390454     1.765878     1.317037      22.20
 C       0.143333     0.626410    -1.011565      82.68
 H       0.401426     1.603011    -1.284498      29.66
 C       0.263515    -1.804229    -0.800976      79.94
 H       0.606625    -2.829010    -0.951491      26.60
 C      -0.913547    -1.873183    -0.157939     -20.54
 O      -1.527246    -3.010699     0.227782     141.54
 C      -0.706282    -4.337028    -0.143525      85.21
 H      -1.334356    -5.126624     0.094979      26.38
 H      -0.431626    -4.125596    -1.317959      24.28
 H       0.382918    -4.239308     0.318030      25.02
 C      -1.755354    -0.619551    -0.105557       9.07
 O      -3.082183    -0.743293     0.628000      49.29
 C      -1.136747     0.542226    -0.408196      43.85
 H      -1.656727     1.497028    -0.303302      24.46
 C       0.900857    -0.551051    -1.144602      15.62
 C       2.311689    -0.706602    -1.794444      98.50
 H       2.435959    -1.550546    -2.242292      29.62
 O       2.581891     0.264482    -2.897552     191.54
 H       2.350858     1.182417    -2.494261      30.45
 C       3.473690    -0.662196    -0.668707     108.16
 H       3.284031    -1.545976    -0.237649      31.77
 O       4.729373    -0.883581    -1.476666     194.83
 H       4.649703    -0.165638    -2.168843      28.06
 C       3.651710     0.449953     0.435223     113.32
 O       3.943080     1.733095    -0.240556     229.87
 H       3.575764     2.456826     0.379694      26.25
 H       4.695120     0.481957     1.064207      25.46
 H       2.822162     0.618768     1.020142      29.56
55
name = lig-Water-frame_30
 C      -2.072183     1.372343     4.341949      50.48
 H      -2.905171     2.041501     4.358075      23.89
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 C      -0.951032    -0.554980     3.377336      30.75
 H      -0.958580    -1.503295     2.669823      31.99
 C       0.292556    -0.246531     4.110349      23.25
 O       1.387898    -0.915030     3.966557     153.39
 C       1.381092    -2.362226     3.408799      88.06
 H       2.368205    -2.374230     2.947342      28.38
 H       0.700046    -2.606692     2.230239      26.96
 H       0.970227    -2.828883     4.213394      29.10
 C       0.212570     0.879656     4.856167       9.38
 O       1.568385     1.182086     5.469279     200.07
 H       1.708940     2.107879     5.088028      24.86
 C      -0.904975     1.673832     5.061739      88.25
 H      -0.695042     2.507307     5.607170      34.17
 C      -2.116928     0.259284     3.496623      19.97
 C      -3.505617     0.078678     2.954674      80.86
 H      -4.063002     0.742683     3.385772      29.22
 O      -3.923226    -1.323367     3.326681     235.57
 H      -4.972556    -1.265501     3.351704      21.05
 C      -3.584606     0.389148     1.303293      67.90
 H      -3.018050     1.292022     1.078424      27.44
 C      -5.008316     0.746421     0.769058      90.62
 O      -6.063316    -0.385347     1.023496     192.07
 H      -5.747172    -1.320322     0.647454      22.97
 H      -4.818818     0.863201    -0.389950      23.94
 H      -5.303743     1.641060     1.182614      26.72
 C       0.153390     0.615028    -0.994896      58.34
 H       0.583980     1.661475    -1.244414      27.31
 C       0.294503    -1.761994    -0.833461      71.43
 H       0.942913    -2.647889    -0.855162      27.35
 C      -0.939462    -1.847843    -0.152798     -32.22
 O      -1.504801    -3.058964     0.244388     148.56
 C      -0.769958    -4.298373    -0.170901     105.28
 H      -1.446308    -5.140681     0.343728      22.82
 H      -0.365246    -4.524347    -1.143506      29.24
 H       0.162612    -4.018013     0.212608      27.17
 C      -1.748075    -0.660518    -0.044284      28.38
 O      -3.020922    -0.808343     0.604497      36.29
 C      -1.184875     0.555152    -0.428595      47.65
 H      -1.683847     1.528229    -0.265463      26.09
 C       0.907927    -0.560118    -1.154232      11.91
 C       2.278213    -0.636700    -1.752464      89.21
 H       2.472385    -1.759390    -2.426829      23.12
 O       2.596825     0.287295    -2.844387     218.01
 H       2.393023     1.088125    -2.373608      33.60
 C       3.482676    -0.675315    -0.744682      93.47
 H       3.264004    -1.562385     0.140264      27.21
 O       4.719697    -0.836645    -1.410130     228.49
 H       4.573854    -0.165583    -2.076170      30.48
 C       3.664649     0.414657     0.395344     105.54
 O       3.921839     1.722040    -0.251116     232.55
 H       3.554172     2.527439     0.305931      24.13
 H       4.403128     0.112054     1.071164      30.24
 H       2.790037     0.421295     1.237908      28.37
55
name = lig-Water-frame_31
 C      -2.012582     1.395190     4.311184      62.04
 H      -2.807333     2.139299     4.561608      18.63
 C      -0.995645    -0.568089     3.389535      61.93
 H      -1.116208    -1.456373     2.816197      28.93
 C       0.215910    -0.205530     4.040658      18.23
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 O       1.394553    -0.951315     3.978281     172.57
 C       1.330286    -2.350527     3.356065      82.94
 H       2.498950    -2.487183     2.995469      24.33
 H       0.813548    -2.449783     2.588891      33.48
 H       0.999104    -3.007306     4.302200      23.44
 C       0.233721     0.861195     4.900612      16.98
 O       1.547715     1.148886     5.474404     258.44
 H       1.836362     2.039137     5.108342      27.72
 C      -0.944265     1.630836     5.052670      21.15
 H      -0.682668     2.405284     5.959733      28.28
 C      -2.163166     0.252891     3.530824      27.41
 C      -3.470497     0.023925     2.925111      92.58
 H      -4.396982     0.713242     3.505618      20.92
 O      -3.922711    -1.258276     3.290431     292.63
 H      -4.877426    -1.286353     3.217148      26.34
 C      -3.587995     0.381596     1.312526      54.54
 H      -2.858146     1.273859     1.197550      22.43
 C      -5.025306     0.668716     0.793196      97.20
 O      -6.079320    -0.395023     1.026658     213.24
 H      -5.843922    -1.269120     0.651754      25.45
 H      -4.926648     0.972493    -0.209267      25.51
 H      -5.459106     1.748570     1.251914      23.04
 C       0.150272     0.625878    -0.966563      56.50
 H       0.652680     1.514899    -1.178082      23.49
 C       0.333002    -1.757955    -0.831214      47.03
 H       1.184826    -2.456316    -0.870172      22.24
 C      -0.983848    -1.823612    -0.176633      16.37
 O      -1.493239    -3.103284     0.231096     162.79
 C      -0.822779    -4.249678    -0.162014     130.47
 H      -1.223372    -5.040943     0.541740      25.46
 H      -0.812439    -4.801499    -1.228617      27.32
 H       0.159138    -4.209822     0.492017      24.89
 C      -1.756247    -0.711120     0.049327      17.21
 O      -2.949510    -0.860618     0.572377      75.26
 C      -1.194677     0.590909    -0.461138      71.63
 H      -1.730408     1.501102    -0.274477      27.14
 C       0.901630    -0.544795    -1.184335      14.61
 C       2.299101    -0.633248    -1.750584     112.14
 H       2.294040    -1.519900    -2.194465      28.66
 O       2.602665     0.325752    -2.774853     228.40
 H       2.539225     1.242001    -2.411547      30.17
 C       3.467493    -0.708608    -0.713134     119.56
 H       3.385361    -1.502947    -0.122142      31.04
 O       4.703258    -0.792887    -1.352655     212.72
 H       4.723022    -0.181707    -2.154177      28.59
 C       3.636378     0.400375     0.356236     104.16
 O       3.904886     1.687331    -0.269687     253.78
 H       3.538312     2.456589     0.280438      24.32
 H       4.447614    -0.270345     1.008896      25.69
 H       2.823896     0.337081     0.981783      30.27
55
name = lig-Water-frame_32
 C      -2.031251     1.453111     4.295855      45.96
 H      -2.892325     2.067082     4.597078      20.74
 C      -1.066219    -0.574518     3.404673      87.54
 H      -1.185307    -1.542537     2.882073      25.29
 C       0.135417    -0.227588     3.951467      -0.77
 O       1.396768    -1.001344     3.964803     173.21
 C       1.348298    -2.315753     3.391284      94.63
 H       2.314252    -2.608771     3.212599      25.35
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 H       0.406581    -2.329070     2.389824      22.92
 H       1.126428    -3.136959     3.999565      24.99
 C       0.294607     0.872870     4.954237       8.68
 O       1.496776     1.127490     5.484662     346.61
 H       1.874645     1.946646     5.047749      28.11
 C      -0.849312     1.619543     5.127321      31.38
 H      -1.041403     2.233465     5.923692      25.81
 C      -2.160846     0.258806     3.564023      31.59
 C      -3.523973     0.011199     2.876816     116.65
 H      -4.146357     0.659962     3.272965      27.57
 O      -3.922550    -1.238680     3.248137     301.82
 H      -4.939814    -1.222395     3.254323      23.97
 C      -3.577562     0.341677     1.365661      67.04
 H      -2.946840     1.152564     1.232256      23.35
 C      -5.047071     0.595657     0.822268     101.90
 O      -6.081375    -0.368509     1.026737     252.57
 H      -5.772849    -1.180005     0.512405      24.58
 H      -5.112107     0.921892    -0.297919      22.86
 H      -5.479049     1.406384     1.407491      24.65
 C       0.127119     0.641368    -0.934554      59.89
 H       0.627304     1.643006    -1.167738      19.82
 C       0.352331    -1.759348    -0.795364      50.88
 H       1.013045    -2.645567    -0.857654      21.58
 C      -0.958467    -1.869618    -0.231625      14.69
 O      -1.513031    -3.093826     0.197975     153.63
 C      -0.813620    -4.277642    -0.099353     135.11
 H      -1.284925    -5.077434     0.650609      24.96
 H      -1.204173    -4.522725    -1.046649      28.65
 H       0.180835    -4.494183     0.226601      26.53
 C      -1.706989    -0.678715     0.087183     -23.42
 O      -2.942768    -0.890197     0.572909      88.57
 C      -1.181977     0.582557    -0.469609      79.85
 H      -1.775435     1.524934    -0.337854      25.69
 C       0.874871    -0.511599    -1.205317      30.45
 C       2.327660    -0.601899    -1.728854      78.74
 H       2.262270    -1.754248    -2.340457      21.94
 O       2.607840     0.379465    -2.719616     227.92
 H       2.754832     1.349116    -2.429036      26.61
 C       3.435604    -0.699665    -0.673434      93.79
 H       3.378673    -1.907988    -0.242507      22.83
 O       4.718115    -0.763484    -1.330312     205.59
 H       4.820565    -0.256041    -2.174236      29.00
 C       3.616511     0.348832     0.324719     109.98
 O       3.897401     1.629533    -0.290177     248.56
 H       3.531171     2.334591     0.341633      25.06
 H       4.486700     0.036361     0.796307      26.37
 H       2.569432     0.479352     0.894186      24.59
55
name = lig-Water-frame_33
 C      -2.041293     1.487902     4.324885      39.17
 H      -2.999605     1.982674     4.510073      18.74
 C      -1.131337    -0.611962     3.405575      76.55
 H      -1.249007    -1.652555     2.923938      25.27
 C       0.148748    -0.255321     3.940339      -5.26
 O       1.362071    -1.035133     3.945718     197.88
 C       1.312623    -2.286707     3.379282      86.16
 H       2.465143    -2.633457     3.030787      23.09
 H       0.731746    -2.289621     2.626425      33.86
 H       0.881638    -3.190273     4.027048      23.13
 C       0.307713     0.847306     4.925899       2.29
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 O       1.481252     1.116995     5.518433     278.17
 H       1.810132     1.894359     4.970310      27.74
 C      -0.793801     1.628124     5.193546      21.87
 H      -1.188609     2.326236     6.050374      21.76
 C      -2.185731     0.315173     3.571220      20.39
 C      -3.534210     0.034528     2.825879      87.73
 H      -4.212590     1.045747     3.267840      22.28
 O      -3.958968    -1.280825     3.209791     261.54
 H      -4.950847    -1.217544     3.468781      19.36
 C      -3.584062     0.248664     1.393490      79.13
 H      -3.019318     1.260820     1.124297      23.56
 C      -5.054932     0.545844     0.832173      84.37
 O      -6.075050    -0.363160     1.014453     251.59
 H      -5.839665    -1.176634     0.423501      23.84
 H      -5.093198     0.806747    -0.201228      24.49
 H      -5.412303     1.422400     1.616998      23.29
 C       0.131969     0.681510    -0.929247      64.03
 H       0.422314     1.688803    -1.174800      21.94
 C       0.349090    -1.774542    -0.753575      80.95
 H       0.707131    -2.795362    -0.902206      22.33
 C      -0.909971    -1.908061    -0.272982       9.30
 O      -1.532169    -3.036463     0.177199     140.84
 C      -0.823608    -4.379903    -0.015766     109.61
 H      -1.480239    -5.053226     0.619202      23.53
 H      -1.299598    -4.431117    -1.089604      24.63
 H       0.340464    -4.455365    -0.213774      23.18
 C      -1.620855    -0.635261     0.056090     -29.14
 O      -2.977250    -0.890813     0.603795      67.71
 C      -1.192676     0.554474    -0.431797      92.04
 H      -1.742196     1.467299    -0.403445      27.83
 C       0.863890    -0.500199    -1.199203      30.70
 C       2.319931    -0.598704    -1.729226     106.42
 H       2.461291    -1.395376    -2.360096      28.26
 O       2.621411     0.446363    -2.697334     246.86
 H       2.907571     1.224596    -2.221931      28.85
 C       3.418485    -0.765544    -0.674756     118.37
 H       3.289265    -1.684788    -0.326376      30.91
 O       4.760664    -0.753263    -1.327290     220.46
 H       4.682376    -0.295942    -2.157308      32.30
 C       3.548798     0.325962     0.333763     108.75
 O       3.890070     1.576796    -0.324051     221.11
 H       3.545230     2.306125     0.301568      25.24
 H       4.554143     0.307499     1.017321      24.26
 H       2.708996     0.537158     0.919347      28.04
55
name = lig-Water-frame_34
 C      -2.013754     1.483601     4.398792      39.32
 H      -2.968712     2.080250     4.503455      20.10
 C      -1.146416    -0.654126     3.417641      31.84
 H      -1.333160    -1.562399     2.965378      29.03
 C       0.182096    -0.293166     3.982224       9.18
 O       1.310172    -1.025997     3.939596     202.14
 C       1.328517    -2.340725     3.378267      93.49
 H       2.211519    -2.457089     2.994182      28.39
 H       0.639403    -2.311906     2.127160      25.90
 H       0.753934    -2.863794     4.090094      25.19
 C       0.258357     0.805186     4.854813      -8.61
 O       1.509010     1.115191     5.560988     298.84
 H       1.843668     1.891623     5.023093      26.55
 C      -0.867827     1.663216     5.221337      39.53
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 H      -0.729344     2.340176     6.083417      23.95
 C      -2.218499     0.370460     3.541559      12.35
 C      -3.533971     0.113644     2.860974      97.42
 H      -4.174434     0.813391     3.151063      27.79
 O      -4.022511    -1.327660     3.189688     276.07
 H      -4.902646    -1.291088     3.568631      17.64
 C      -3.595353     0.179104     1.328335     100.35
 H      -3.194771     1.101600     1.103675      27.63
 C      -5.040274     0.539996     0.872454      98.40
 O      -6.086831    -0.395688     0.987492     255.78
 H      -5.987953    -1.216561     0.526871      25.21
 H      -4.882441     0.910165    -0.207724      24.09
 H      -5.190058     1.481043     1.469771      24.90
 C       0.142557     0.700059    -0.945919      55.40
 H       0.389522     1.721308    -1.275633      18.73
 C       0.354320    -1.799593    -0.745517     110.79
 H       0.804840    -2.749959    -1.112381      24.42
 C      -0.915311    -1.870466    -0.254243      28.50
 O      -1.530964    -2.987688     0.174577     124.04
 C      -0.876852    -4.462293    -0.017219     112.07
 H      -1.384300    -5.126882     0.682821      24.66
 H      -1.134613    -4.771600    -0.999160      28.82
 H       0.154778    -4.278580    -0.241050      26.04
 C      -1.607103    -0.676163     0.020835     -12.54
 O      -2.987089    -0.871233     0.634149      87.65
 C      -1.179572     0.559759    -0.386600      75.70
 H      -1.825802     1.466763    -0.349959      27.43
 C       0.884386    -0.510421    -1.169106      24.79
 C       2.297795    -0.555081    -1.748388      94.65
 H       2.511380    -1.550359    -2.545386      24.73
 O       2.641356     0.526026    -2.678792     217.09
 H       3.022218     1.170906    -1.984448      24.87
 C       3.445041    -0.800894    -0.701929      90.17
 H       3.195912    -1.890189    -0.078896      25.63
 O       4.792316    -0.759267    -1.333374     197.98
 H       4.486120    -0.330571    -2.204503      30.50
 C       3.531345     0.338897     0.394342     102.36
 O       3.871599     1.548579    -0.376186     222.77
 H       3.566847     2.344676     0.103452      26.47
 H       4.190277     0.140997     1.218098      28.53
 H       2.607284     0.478772     1.119929      26.78
55
name = lig-Water-frame_35
 C      -2.030542     1.479020     4.482609      56.73
 H      -2.763859     2.236539     4.607091      27.11
 C      -1.138333    -0.620450     3.459708      37.03
 H      -1.407559    -1.625116     2.859732      30.03
 C       0.140586    -0.341902     4.030469      23.79
 O       1.288751    -1.006875     3.926126     212.07
 C       1.250238    -2.362432     3.295800      80.16
 H       2.493661    -2.579751     3.079580      23.95
 H       0.882982    -2.395961     2.463221      36.78
 H       0.743489    -2.984954     4.113005      24.68
 C       0.201247     0.820093     4.837294       7.61
 O       1.521913     1.107766     5.582964     219.04
 H       1.931994     1.908641     5.130442      24.61
 C      -0.906305     1.660105     5.207296      36.60
 H      -0.403451     2.343801     5.947655      20.04
 C      -2.185988     0.376878     3.517485      16.86
 C      -3.527106     0.123786     2.900053      62.55
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 H      -4.487816     0.827726     3.318415      21.78
 O      -4.068383    -1.354999     3.183496     161.12
 H      -5.032934    -1.278390     3.566784      17.59
 C      -3.617472     0.147878     1.272784      93.27
 H      -3.082045     1.182963     1.015041      25.04
 C      -4.990858     0.531545     0.857159      97.06
 O      -6.122556    -0.410945     0.963549     223.53
 H      -5.883216    -1.350111     0.561317      22.63
 H      -4.820325     0.944099    -0.139010      24.35
 H      -5.265336     1.558106     1.418275      22.98
 C       0.138352     0.687872    -0.966414      80.75
 H       0.543296     1.643152    -1.413682      24.63
 C       0.391399    -1.797556    -0.791839      63.86
 H       1.025628    -2.547657    -1.234780      21.11
 C      -0.930655    -1.832465    -0.203185      22.87
 O      -1.534984    -3.010132     0.177930     136.46
 C      -0.953071    -4.472962    -0.072604      87.97
 H      -1.055957    -5.163182     0.964577      25.12
 H      -1.221070    -5.141549    -0.985794      25.20
 H       0.154120    -4.279104     0.157513      26.26
 C      -1.690293    -0.714835     0.015831      27.64
 O      -2.953826    -0.874453     0.636606      81.67
 C      -1.138067     0.595053    -0.354574      39.12
 H      -1.846087     1.400454    -0.201644      20.11
 C       0.914221    -0.524274    -1.129243       9.82
 C       2.303152    -0.560890    -1.820807     100.09
 H       2.225212    -1.450696    -2.369663      28.35
 O       2.666394     0.614602    -2.633589     206.07
 H       3.091383     1.258965    -1.969998      24.84
 C       3.481246    -0.831023    -0.668839     104.20
 H       3.310121    -1.697834    -0.156246      30.68
 O       4.780569    -0.773525    -1.354433     206.69
 H       4.548223    -0.461272    -2.265845      30.83
 C       3.483223     0.347957     0.470995      88.67
 O       3.849785     1.527147    -0.421447     187.33
 H       3.524904     2.409946    -0.005864      25.42
 H       4.215305    -0.092580     1.329763      25.36
 H       2.485749     0.426725     0.884603      28.42
55
name = lig-Water-frame_36
 C      -2.102773     1.468645     4.527251      63.38
 H      -2.797598     2.370544     4.661054      24.40
 C      -1.149603    -0.583240     3.475268      66.42
 H      -1.279310    -1.403021     2.928072      31.37
 C       0.057534    -0.356407     4.092262      24.10
 O       1.293846    -1.016786     3.893086     168.56
 C       1.250870    -2.373100     3.294698      94.36
 H       2.173471    -2.704313     3.418597      27.48
 H       0.626021    -2.454679     2.034307      25.10
 H       0.863256    -3.222924     3.874505      26.62
 C       0.199789     0.851910     4.877883      15.81
 O       1.496019     1.091575     5.579087     238.11
 H       1.921667     1.880941     5.141487      25.26
 C      -0.835619     1.620618     5.186865      42.41
 H      -0.537586     2.581932     5.791568      23.01
 C      -2.141821     0.380395     3.552536      10.67
 C      -3.574419     0.088434     2.915676      77.84
 H      -4.290487     0.676307     3.404229      26.57
 O      -4.100157    -1.360921     3.198480     183.99
 H      -5.062420    -1.203109     3.365671      21.59
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 C      -3.602367     0.217271     1.297254      93.13
 H      -3.034403     1.037314     1.047636      25.93
 C      -4.974242     0.530875     0.797775      98.95
 O      -6.144869    -0.420102     0.928310     225.43
 H      -5.702895    -1.241188     0.607168      27.32
 H      -4.987597     0.834901    -0.295300      25.04
 H      -5.464938     1.373190     1.421139      23.62
 C       0.141598     0.655145    -0.985047      78.64
 H       0.606914     1.499509    -1.407537      27.40
 C       0.409925    -1.750039    -0.843717      67.71
 H       1.050496    -2.624737    -1.162029      23.42
 C      -0.894889    -1.865209    -0.176067     -13.40
 O      -1.555169    -3.096747     0.177339     176.29
 C      -0.971537    -4.451500    -0.071794     127.75
 H      -1.120348    -4.924783     0.857737      27.52
 H      -1.353421    -5.082002    -0.826500      26.88
 H       0.078810    -4.418111     0.213260      27.24
 C      -1.766664    -0.669681     0.015498      23.48
 O      -2.916042    -0.917732     0.620597      60.78
 C      -1.112447     0.592719    -0.322626      57.63
 H      -1.708577     1.492708    -0.116860      22.37
 C       0.938106    -0.509058    -1.103797      29.06
 C       2.318553    -0.540927    -1.833330      68.80
 H       2.142243    -1.550843    -2.598027      23.90
 O       2.685715     0.682829    -2.584698     197.18
 H       3.104971     1.291483    -1.975785      26.46
 C       3.509884    -0.781512    -0.653264      82.85
 H       3.405449    -1.956568    -0.144935      24.96
 O       4.750754    -0.799097    -1.375046     202.57
 H       4.697721    -0.607272    -2.300759      31.24
 C       3.440043     0.317917     0.484769      94.85
 O       3.827738     1.513954    -0.429962     214.15
 H       3.497685     2.313889     0.053348      27.90
 H       4.248001     0.097765     1.187710      26.50
 H       2.360608     0.487620     0.718035      26.27
55
name = lig-Water-frame_37
 C      -2.141726     1.456587     4.548199      42.76
 H      -2.911474     2.173428     4.612415      17.04
 C      -1.151491    -0.543537     3.482983      32.58
 H      -1.209872    -1.499830     2.772582      26.19
 C       0.040470    -0.336194     4.172425      33.01
 O       1.273924    -1.053691     3.855738     193.37
 C       1.209982    -2.390221     3.256880      85.41
 H       2.377634    -2.775329     3.408815      23.33
 H       0.903717    -2.378984     2.382545      36.53
 H       0.597891    -3.172878     3.776941      25.01
 C       0.290752     0.822753     4.942801      15.19
 O       1.448949     1.070179     5.556127     328.70
 H       1.831532     1.860055     5.060967      29.80
 C      -0.816741     1.656305     5.167795      57.91
 H      -0.838679     2.587153     5.655222      23.60
 C      -2.197928     0.404553     3.629731      -6.58
 C      -3.578489    -0.000992     2.902534      79.83
 H      -4.299276     0.816645     3.479674      25.94
 O      -4.113525    -1.341539     3.219634     228.22
 H      -5.095510    -1.197807     3.245934      21.35
 C      -3.581473     0.285268     1.370504      58.00
 H      -2.906478     1.194330     1.111586      23.55
 C      -5.029371     0.539361     0.711965      97.11
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 O      -6.128423    -0.435833     0.891921     227.98
 H      -5.768800    -1.279790     0.525727      27.91
 H      -5.092608     0.704368    -0.385778      25.65
 H      -5.442149     1.374982     1.361990      24.81
 C       0.154733     0.607117    -0.983380      55.63
 H       0.569437     1.633462    -1.337600      22.99
 C       0.376622    -1.746853    -0.853003      68.62
 H       0.843174    -2.702680    -0.954146      23.21
 C      -0.859092    -1.907010    -0.185166     -18.49
 O      -1.566258    -3.167640     0.154446     164.08
 C      -0.954586    -4.404649    -0.010300     112.19
 H      -1.609821    -4.948064     0.924858      20.47
 H      -1.459809    -4.884812    -0.937117      24.82
 H       0.187801    -4.481795    -0.189616      24.80
 C      -1.715911    -0.638158    -0.009895      16.52
 O      -2.930001    -0.959469     0.628494      -7.45
 C      -1.121279     0.575942    -0.293880      75.04
 H      -1.458606     1.618546    -0.143525      22.56
 C       0.968119    -0.471844    -1.124810      43.04
 C       2.336064    -0.520920    -1.806801      86.21
 H       2.423824    -1.171340    -2.659722      27.38
 O       2.686439     0.715436    -2.551755     213.66
 H       3.150680     1.298141    -1.804870      20.46
 C       3.498351    -0.778342    -0.670777     116.33
 H       3.449597    -1.749865    -0.333072      28.38
 O       4.744785    -0.825719    -1.377246     202.58
 H       4.661728    -0.710145    -2.377733      29.62
 C       3.413931     0.296758     0.391937      98.15
 O       3.805456     1.510657    -0.397682     245.81
 H       3.518280     2.265146     0.185279      26.42
 H       4.192975     0.342438     1.256086      24.79
 H       2.362056     0.487969     0.845728      24.47
55
name = lig-Water-frame_38
 C      -2.114695     1.432028     4.557215      30.43
 H      -3.084931     2.031652     4.672594      19.10
 C      -1.147190    -0.519361     3.483296      25.86
 H      -1.207971    -1.311944     2.799045      25.15
 C       0.092144    -0.339869     4.214216      25.22
 O       1.230655    -1.086731     3.835607     179.92
 C       1.218285    -2.423671     3.301312      80.62
 H       2.229774    -2.714906     3.177360      24.37
 H       0.993985    -2.267389     1.882476      23.97
 H       0.328593    -2.879883     3.789505      23.84
 C       0.299827     0.783372     5.007263      20.99
 O       1.457399     1.064329     5.541800     362.37
 H       1.795825     1.883504     5.058393      31.04
 C      -0.871610     1.707100     5.125703      70.63
 H      -0.899055     2.734938     5.799370      21.93
 C      -2.307692     0.357655     3.686406      -6.97
 C      -3.579235    -0.036547     2.917307      97.63
 H      -4.263408     0.767349     3.228032      26.89
 O      -4.112029    -1.312907     3.239592     238.79
 H      -5.149821    -1.260094     3.317439      19.75
 C      -3.575299     0.320781     1.408245      44.97
 H      -2.992875     1.222547     1.277753      25.75
 C      -5.093249     0.541815     0.646102      90.51
 O      -6.090798    -0.466059     0.867799     224.79
 H      -5.949667    -1.336092     0.325388      24.03
 H      -4.943158     0.752058    -0.416433      25.78
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 H      -5.374745     1.625681     1.137091      23.64
 C       0.167934     0.617372    -0.965437      51.19
 H       0.417418     1.597813    -1.167949      24.28
 C       0.322979    -1.786817    -0.818888      75.25
 H       0.872256    -2.765067    -0.909274      25.06
 C      -0.879487    -1.910473    -0.216002       2.52
 O      -1.554730    -3.138730     0.118499     224.63
 C      -0.972006    -4.428474     0.042085     152.44
 H      -1.387114    -5.085277     0.649935      27.03
 H      -1.379603    -4.652479    -0.948369      26.29
 H       0.040958    -4.509241    -0.350784      26.84
 C      -1.635329    -0.694910    -0.009806       5.76
 O      -2.952946    -0.957931     0.650026     -80.36
 C      -1.104518     0.578874    -0.295936      69.90
 H      -1.453027     1.584522    -0.134118      22.93
 C       0.989953    -0.494522    -1.184209      33.39
 C       2.379281    -0.448817    -1.762193      83.93
 H       2.580082    -1.274160    -2.683780      24.78
 O       2.685524     0.744344    -2.505840     232.57
 H       3.072837     1.303692    -1.832517      25.38
 C       3.458948    -0.783885    -0.744002     102.10
 H       3.255147    -1.918047    -0.224658      25.24
 O       4.771439    -0.844550    -1.380848     171.72
 H       4.510826    -0.754048    -2.331655      30.55
 C       3.419774     0.315863     0.303383     120.56
 O       3.778999     1.528117    -0.342575     277.19
 H       3.584167     2.323661     0.270360      25.82
 H       3.997026     0.305903     1.284345      26.95
 H       2.478533     0.337301     0.849239      27.40
55
name = lig-Water-frame_39
 C      -2.128964     1.414208     4.548446      53.12
 H      -2.984363     1.972570     4.882687      24.40
 C      -1.150188    -0.470613     3.515194      55.04
 H      -1.223901    -1.288892     2.729513      27.44
 C       0.123261    -0.376678     4.187688       9.89
 O       1.209572    -1.096071     3.839551     206.50
 C       1.162514    -2.399260     3.244994     107.51
 H       2.227316    -2.876651     3.277425      25.58
 H       1.070501    -2.335861     2.337659      36.18
 H       0.338231    -2.924254     3.709935      26.68
 C       0.177227     0.783631     5.050653     -16.56
 O       1.532803     1.079652     5.551633     293.18
 H       1.811198     1.950358     5.128957      25.31
 C      -0.906950     1.758037     5.117121      54.06
 H      -0.722224     2.497185     5.756445      22.90
 C      -2.351630     0.231231     3.717575      19.49
 C      -3.596345    -0.008698     2.924145      87.82
 H      -4.464377     0.828543     3.208872      23.99
 O      -4.114418    -1.303892     3.266130     258.65
 H      -5.060838    -1.269948     3.466243      25.29
 C      -3.604290     0.286835     1.395925      68.35
 H      -3.042782     1.259782     1.315633      25.51
 C      -5.097841     0.562860     0.609687      91.79
 O      -6.060895    -0.489017     0.849468     243.27
 H      -5.911754    -1.177894     0.198157      26.34
 H      -4.705589     0.743176    -0.455053      24.70
 H      -5.494427     1.556837     0.889976      25.84
 C       0.178028     0.637159    -0.932509      48.27
 H       0.521336     1.723863    -1.147834      21.08
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 C       0.352422    -1.828719    -0.803581      84.70
 H       0.976559    -2.674476    -0.996956      26.77
 C      -0.949550    -1.908865    -0.244083      53.71
 O      -1.542858    -3.049158     0.106284     169.37
 C      -0.987579    -4.447912    -0.020781     111.55
 H      -1.118662    -5.473445     0.790329      23.77
 H      -1.403401    -4.798744    -0.995372      28.60
 H       0.134861    -4.456990    -0.061710      26.62
 C      -1.622273    -0.759202     0.039386      -1.19
 O      -2.946990    -0.908907     0.667583      21.21
 C      -1.064392     0.552455    -0.318815      53.29
 H      -1.714319     1.433043    -0.058285      23.58
 C       0.950327    -0.570125    -1.233520      -8.98
 C       2.425431    -0.414365    -1.788395     102.52
 H       2.444182    -1.350979    -2.347324      26.79
 O       2.679158     0.774182    -2.466577     253.87
 H       3.031447     1.498192    -1.860548      23.63
 C       3.440219    -0.821867    -0.777205     102.07
 H       3.032691    -1.647489    -0.244326      29.40
 O       4.787926    -0.864361    -1.387554     203.69
 H       4.601397    -0.782299    -2.314405      32.23
 C       3.435579     0.332551     0.280044      99.39
 O       3.758225     1.581012    -0.286480     284.66
 H       3.599689     2.341935     0.317930      27.40
 H       4.126727     0.001456     1.183586      26.15
 H       2.313329     0.216424     0.643499      26.36
55
name = lig-Water-frame_40
 C      -2.188336     1.386555     4.539247      40.29
 H      -2.979672     2.031288     4.986424      23.45
 C      -1.146269    -0.488605     3.521233      83.51
 H      -1.188367    -1.264151     2.708463      29.50
 C       0.080383    -0.366407     4.153378       2.05
 O       1.223604    -1.086089     3.862352     148.58
 C       1.118495    -2.381470     3.233586     100.34
 H       1.985840    -2.955417     3.724978      24.95
 H       0.882466    -2.319948     1.853293      25.82
 H       0.402649    -3.172624     3.635223      25.60
 C       0.101945     0.793967     5.064217     -26.44
 O       1.583759     1.094332     5.568344     203.55
 H       1.780726     1.997004     5.115544      25.08
 C      -0.901495     1.727825     5.111932      34.03
 H      -0.581952     2.626193     5.908693      19.87
 C      -2.332211     0.170296     3.767200      26.40
 C      -3.670707     0.052031     2.926822      86.98
 H      -4.410264     0.749541     3.355588      27.21
 O      -4.107433    -1.315970     3.295611     237.88
 H      -5.120599    -1.235485     3.566155      23.03
 C      -3.645788     0.240764     1.356940     100.94
 H      -3.080004     1.204378     1.217774      27.70
 C      -5.018318     0.563308     0.589357      97.17
 O      -6.035792    -0.481658     0.822645     256.66
 H      -5.774972    -1.168139     0.146815      26.76
 H      -4.708681     0.549532    -0.430782      26.32
 H      -5.750897     1.541430     0.797707      23.59
 C       0.206693     0.656217    -0.911289      61.36
 H       0.693349     1.555719    -1.188727      23.50
 C       0.418634    -1.832997    -0.821376      58.76
 H       1.012776    -2.741398    -1.086852      23.15
 C      -0.955559    -1.914086    -0.288632      22.93
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 O      -1.566630    -3.031530     0.132413     122.66
 C      -0.962004    -4.489457    -0.102328     110.17
 H      -1.138613    -5.018621     0.720436      29.02
 H      -1.356647    -5.049847    -0.978013      26.65
 H       0.086375    -4.287997     0.175621      25.01
 C      -1.664440    -0.732706     0.103807       8.26
 O      -2.924098    -0.838069     0.680523      96.25
 C      -1.066146     0.484195    -0.320995      65.87
 H      -1.793416     1.234822    -0.087802      27.97
 C       0.879565    -0.610837    -1.246297       5.31
 C       2.407387    -0.428654    -1.818863      74.59
 H       2.379939    -1.398532    -2.611587      24.95
 O       2.669632     0.806094    -2.459874     232.46
 H       2.978210     1.531958    -1.789740      23.29
 C       3.458406    -0.771318    -0.778391      80.56
 H       3.008870    -1.784484    -0.206103      26.79
 O       4.787474    -0.899833    -1.384733     180.42
 H       4.833449    -0.821899    -2.396701      28.13
 C       3.434156     0.301237     0.306115     109.04
 O       3.753794     1.643527    -0.237975     260.34
 H       3.519953     2.378642     0.469612      25.80
 H       4.234087    -0.174565     0.936446      27.51
 H       2.426238     0.320454     0.549249      29.42
55
name = lig-Water-frame_41
 C      -2.229767     1.366913     4.569261      28.12
 H      -3.106876     2.017412     4.822804      21.95
 C      -1.144281    -0.582348     3.479534      84.50
 H      -1.159808    -1.306759     2.726080      30.58
 C       0.023283    -0.302031     4.153051     -19.49
 O       1.229926    -1.072471     3.892936     164.11
 C       1.064902    -2.400166     3.194049     134.44
 H       1.953659    -2.849950     3.678496      27.39
 H       1.025876    -2.336208     2.272766      34.30
 H       0.246859    -2.985425     3.553411      29.28
 C       0.160342     0.778281     5.045286       1.98
 O       1.568814     1.101799     5.580994     324.71
 H       1.782207     1.941107     5.045444      27.41
 C      -0.900849     1.692420     5.149951      37.09
 H      -0.815695     2.531306     5.676291      23.58
 C      -2.330946     0.224206     3.799211     -60.51
 C      -3.720315     0.061207     2.947068      74.74
 H      -4.428177     0.863571     3.489820      22.44
 O      -4.114083    -1.326497     3.325514     248.50
 H      -5.092565    -1.331807     3.481858      22.99
 C      -3.672082     0.250537     1.328028     113.66
 H      -3.098038     1.152184     1.144844      29.83
 C      -4.957434     0.538193     0.584297     111.60
 O      -6.006522    -0.462190     0.780161     226.05
 H      -5.731928    -1.329765     0.300490      25.99
 H      -4.773861     0.444174    -0.559435      25.50
 H      -5.426387     1.433802     0.807545      28.52
 C       0.224909     0.601654    -0.901022      65.39
 H       0.751405     1.528405    -1.247343      25.26
 C       0.427930    -1.853688    -0.846748      41.14
 H       0.911015    -2.783777    -1.126115      23.58
 C      -0.913946    -1.907949    -0.321673      -2.14
 O      -1.609659    -3.092601     0.159005      66.85
 C      -0.918184    -4.465687    -0.154103      99.31
 H      -1.547389    -4.749025     0.919673      20.81
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 H      -1.177951    -5.098272    -1.000683      26.14
 H       0.148106    -4.264914    -0.058579      25.45
 C      -1.669689    -0.690325     0.126845       7.36
 O      -2.916413    -0.786377     0.697004      91.73
 C      -1.094908     0.438517    -0.305073      77.18
 H      -1.682919     1.388749    -0.193823      29.96
 C       0.866968    -0.562681    -1.245493      31.82
 C       2.332006    -0.501417    -1.875835      88.99
 H       2.482601    -0.951989    -2.849196      29.14
 O       2.652769     0.838941    -2.470568     229.83
 H       2.924042     1.336383    -1.717415      29.71
 C       3.456397    -0.726329    -0.799124     102.81
 H       3.391131    -1.721057    -0.380175      28.94
 O       4.789153    -0.941926    -1.368444     184.70
 H       4.888707    -0.863274    -2.351264      28.38
 C       3.466127     0.269321     0.310138     112.01
 O       3.765000     1.686962    -0.183892     235.86
 H       3.438780     2.364833     0.482907      27.46
 H       4.255900    -0.029227     1.064876      30.06
 H       2.397873     0.404237     0.912717      28.28
55
name = lig-Water-frame_42
 C      -2.220305     1.363267     4.632010      46.29
 H      -3.119294     1.953374     4.630173      21.36
 C      -1.193480    -0.642739     3.456821      16.85
 H      -1.198152    -1.524018     2.653093      28.26
 C       0.026671    -0.279729     4.143388      -7.02
 O       1.205606    -1.051362     3.922596     112.64
 C       1.023237    -2.403996     3.255665      85.11
 H       2.109924    -2.932053     3.384879      24.31
 H       1.241495    -2.233841     1.874905      28.64
 H      -0.030022    -2.711074     3.549254      23.13
 C       0.271474     0.800571     5.029461      30.03
 O       1.494230     1.094927     5.581620     338.32
 H       1.864637     1.881013     5.030959      27.94
 C      -0.942468     1.621365     5.181008      27.12
 H      -0.971591     2.730661     5.688492      20.96
 C      -2.344963     0.281243     3.744295     -67.30
 C      -3.731327     0.037979     2.994279      82.64
 H      -4.435546     0.864688     3.388478      26.43
 O      -4.119901    -1.325401     3.344976     228.62
 H      -5.143589    -1.399594     3.380469      18.03
 C      -3.656797     0.305619     1.335669      84.55
 H      -3.060905     1.294549     1.200438      28.61
 C      -4.918763     0.453033     0.533088     112.57
 O      -5.987946    -0.447233     0.747989     248.77
 H      -5.716028    -1.328472     0.511470      27.25
 H      -4.719484     0.580780    -0.497729      26.86
 H      -5.087290     1.663591     0.947482      24.00
 C       0.207423     0.535510    -0.895870      53.55
 H       0.530603     1.547056    -1.217692      25.40
 C       0.361118    -1.870542    -0.874143      47.88
 H       0.872320    -2.783182    -1.181365      24.28
 C      -0.903572    -1.915195    -0.296316      11.60
 O      -1.620806    -3.144870     0.133964     137.97
 C      -0.916859    -4.402778    -0.110790     120.02
 H      -1.391711    -5.026027     0.539468      25.77
 H      -1.154336    -4.951159    -1.092814      26.03
 H       0.201622    -4.427492    -0.221055      26.17
 C      -1.643931    -0.703237     0.111066     -18.91
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 O      -2.917612    -0.786619     0.713342       8.29
 C      -1.095506     0.508416    -0.303038      77.25
 H      -1.471390     1.520259    -0.266327      30.78
 C       0.936572    -0.543760    -1.255347      28.42
 C       2.265549    -0.510869    -1.943249      90.03
 H       2.461590    -1.064351    -2.958810      27.16
 O       2.622553     0.866390    -2.478802     188.58
 H       2.946320     1.364463    -1.603674      25.77
 C       3.451778    -0.725424    -0.860360      89.94
 H       3.414025    -1.812069    -0.314761      27.13
 O       4.809572    -0.973431    -1.353414     174.56
 H       4.785822    -0.807706    -2.287432      31.00
 C       3.486534     0.300126     0.357553     122.45
 O       3.786823     1.678293    -0.143534     251.13
 H       3.412848     2.444985     0.468174      25.96
 H       4.254588     0.196058     1.206174      30.14
 H       2.712414     0.247684     1.012833      32.48
55
name = lig-Water-frame_43
 C      -2.190801     1.326314     4.659168      40.38
 H      -3.055336     2.092575     4.674830      20.72
 C      -1.262875    -0.638915     3.465904      46.75
 H      -1.320249    -1.422594     2.851462      31.48
 C       0.056784    -0.312288     4.106435      -4.17
 O       1.179128    -1.048593     3.942627     197.07
 C       1.030022    -2.350640     3.247648     128.54
 H       1.785125    -3.015602     3.429214      30.74
 H       1.062726    -2.191761     2.306506      35.37
 H       0.051530    -2.724692     3.473681      29.51
 C       0.270405     0.854860     4.993938       8.68
 O       1.427717     1.085856     5.584473     310.61
 H       1.889377     1.861608     5.144816      25.65
 C      -0.966713     1.595254     5.239469      49.48
 H      -0.872443     2.522999     5.723719      27.99
 C      -2.346586     0.278586     3.635174     -29.24
 C      -3.702291     0.017887     3.016524      87.51
 H      -4.528397     0.778821     3.346519      27.17
 O      -4.126787    -1.319661     3.353469     214.66
 H      -5.160791    -1.307482     3.368665      18.14
 C      -3.590548     0.354208     1.374365      71.41
 H      -3.096891     1.277325     1.319213      27.32
 C      -4.880848     0.447477     0.508584     111.58
 O      -5.987415    -0.421607     0.738649     268.21
 H      -5.633222    -1.367890     0.531564      24.21
 H      -4.575884     0.693100    -0.582714      25.14
 H      -5.182995     1.362064     0.854029      27.47
 C       0.166452     0.526582    -0.904266      42.64
 H       0.401824     1.529489    -1.185511      26.47
 C       0.295564    -1.853374    -0.923851      67.85
 H       0.842256    -2.773377    -1.221747      29.31
 C      -0.943833    -1.936980    -0.224961      12.84
 O      -1.595272    -3.162973     0.084747     172.01
 C      -0.918693    -4.369464    -0.114834     109.64
 H      -1.162085    -5.532743     0.490227      22.97
 H      -1.263209    -4.560329    -1.132406      27.15
 H       0.166399    -4.436549    -0.015262      27.51
 C      -1.632904    -0.712395     0.081797      -4.34
 O      -2.895338    -0.828913     0.724698      15.34
 C      -1.060791     0.589016    -0.307414      65.98
 H      -1.510273     1.583081    -0.167176      25.53
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 C       0.990545    -0.619431    -1.256926     -14.85
 C       2.280259    -0.455568    -2.017855     104.32
 H       2.244999    -1.413330    -2.673020      24.12
 O       2.583809     0.886547    -2.472103     242.23
 H       2.908133     1.443075    -1.750283      28.27
 C       3.457986    -0.791986    -0.869790      76.34
 H       3.016793    -1.623859    -0.267078      29.51
 O       4.829953    -0.989474    -1.356207     185.85
 H       4.777908    -0.679429    -2.321025      28.03
 C       3.543300     0.361670     0.405015      92.51
 O       3.802226     1.647153    -0.119465     255.31
 H       3.491027     2.436006     0.427019      26.75
 H       4.425270     0.100348     1.064519      28.59
 H       2.507608     0.119304     1.052305      27.27
55
name = lig-Water-frame_44
 C      -2.192556     1.280590     4.618564      66.55
 H      -2.841519     2.060889     4.883054      25.93
 C      -1.279374    -0.573487     3.514131      50.65
 H      -1.477327    -1.559183     2.867257      27.98
 C       0.039357    -0.317124     4.077829      12.79
 O       1.177896    -1.076342     3.957670     183.12
 C       1.020309    -2.275693     3.270919     102.46
 H       1.686249    -3.199958     3.803154      24.28
 H       0.841729    -1.986034     1.939492      26.13
 H       0.089302    -2.902393     3.502311      26.80
 C       0.138174     0.863892     4.905794       7.53
 O       1.404248     1.079049     5.609297     220.06
 H       1.802215     1.930225     5.236305      23.00
 C      -0.944269     1.570511     5.293544      43.92
 H      -0.746848     2.480561     6.001723      22.94
 C      -2.334154     0.283177     3.585517      19.66
 C      -3.664259     0.019991     2.984637     102.81
 H      -4.537247     0.692538     3.415409      24.64
 O      -4.137703    -1.316880     3.352060     224.66
 H      -5.107460    -1.216255     3.464019      21.70
 C      -3.539737     0.325485     1.418652      71.93
 H      -2.941109     1.349537     1.363470      24.14
 C      -4.826584     0.498054     0.500043      89.80
 O      -5.975794    -0.415822     0.735612     213.96
 H      -5.695136    -1.325941     0.403771      26.26
 H      -4.530067     0.529158    -0.533204      25.63
 H      -5.635714     1.459350     0.787013      21.00
 C       0.172836     0.548150    -0.946266      50.49
 H       0.619222     1.564137    -1.269414      24.95
 C       0.264547    -1.839087    -0.982070      68.70
 H       0.715386    -2.778425    -1.228950      26.42
 C      -0.974882    -1.939954    -0.167672      -4.83
 O      -1.582176    -3.145662     0.076318     183.36
 C      -0.908976    -4.425216    -0.152736     114.93
 H      -1.141921    -5.238885     0.370676      28.96
 H      -1.108798    -4.449382    -1.263286      25.94
 H       0.158946    -4.195690     0.143897      25.91
 C      -1.648368    -0.688670     0.064498      15.73
 O      -2.847167    -0.873598     0.738689      54.88
 C      -1.057522     0.591656    -0.287620      67.58
 H      -1.633382     1.489560    -0.005836      23.69
 C       0.943734    -0.670140    -1.233094       8.12
 C       2.348304    -0.417310    -2.004213      91.09
 H       2.283821    -1.319367    -2.675151      25.11
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 O       2.530685     0.886556    -2.502804     270.19
 H       2.875491     1.411230    -1.736082      26.78
 C       3.447801    -0.813478    -0.836005      68.32
 H       2.883025    -1.697998    -0.299654      27.03
 O       4.826196    -1.005869    -1.372475     174.44
 H       4.903149    -0.605747    -2.278413      29.04
 C       3.576351     0.362225     0.441756      96.12
 O       3.815654     1.626265    -0.118693     275.81
 H       3.551604     2.375542     0.510430      27.35
 H       4.510810    -0.164172     0.841751      26.85
 H       2.675563     0.318145     0.848075      28.96
55
name = lig-Water-frame_45
 C      -2.176696     1.281304     4.585465      68.06
 H      -3.022532     1.962967     5.006861      27.16
 C      -1.227042    -0.572844     3.519324      52.52
 H      -1.471414    -1.465637     3.064198      28.69
 C      -0.025050    -0.287258     4.057251      22.43
 O       1.176194    -1.097588     3.984556     204.80
 C       0.980790    -2.279300     3.253221     135.91
 H       1.741575    -2.804898     3.666336      29.25
 H       0.995073    -2.123558     2.289331      33.04
 H       0.041172    -2.730318     3.537658      30.00
 C       0.076197     0.824345     4.838939       1.95
 O       1.373084     1.068946     5.624565     261.44
 H       1.624832     1.963908     5.243632      22.53
 C      -0.961065     1.565603     5.317965      43.18
 H      -0.816830     2.206373     6.240758      16.37
 C      -2.328820     0.337857     3.629824      21.86
 C      -3.650814     0.024294     2.926630     116.42
 H      -4.343695     0.774424     3.398201      26.23
 O      -4.138545    -1.317179     3.341976     218.09
 H      -5.169055    -1.180181     3.558538      20.49
 C      -3.512887     0.281515     1.436624      91.50
 H      -2.880360     1.083501     1.357823      25.93
 C      -4.840869     0.589462     0.539979     100.04
 O      -5.948034    -0.429471     0.732998     231.64
 H      -5.761060    -1.273421     0.279695      27.19
 H      -4.506091     0.383293    -0.533128      23.96
 H      -5.310666     1.457999     0.586977      27.22
 C       0.216811     0.590932    -0.997324      61.70
 H       0.776708     1.410279    -1.286126      23.24
 C       0.216170    -1.869611    -0.999732      60.26
 H       0.655485    -2.852937    -1.307295      20.84
 C      -0.950747    -1.904255    -0.180927       1.59
 O      -1.611963    -3.121331     0.108355     143.15
 C      -0.848759    -4.408896    -0.244338      76.29
 H      -1.526538    -5.246294     0.554503      21.24
 H      -0.681674    -4.728768    -1.303057      26.26
 H       0.135999    -4.125504     0.099977      26.37
 C      -1.657412    -0.674558     0.064504      28.46
 O      -2.810360    -0.893115     0.772512      60.79
 C      -1.072464     0.535804    -0.261608      70.10
 H      -1.614104     1.414334     0.035828      23.52
 C       0.861163    -0.622560    -1.227504      17.51
 C       2.401949    -0.437453    -1.902827      75.62
 H       2.587206    -0.948202    -2.985497      22.00
 O       2.479088     0.881710    -2.546261     262.52
 H       2.851746     1.394172    -1.721544      23.43
 C       3.415399    -0.769962    -0.802007      91.31
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 H       3.219346    -1.869248    -0.464684      25.13
 O       4.807476    -1.030178    -1.379065     186.41
 H       4.921943    -0.593282    -2.212001      31.66
 C       3.629749     0.276606     0.393879      89.55
 O       3.841404     1.628518    -0.132211     273.05
 H       3.594365     2.306283     0.568401      27.24
 H       4.435600    -0.178531     0.955085      26.46
 H       2.584626     0.448373     1.084793      23.22
55
name = lig-Water-frame_46
 C      -2.195760     1.380810     4.630299      38.45
 H      -3.182427     1.676730     4.860413       9.74
 C      -1.222144    -0.583897     3.482555      58.50
 H      -1.399729    -1.608303     3.029074      26.25
 C      -0.015463    -0.285778     4.036382      17.52
 O       1.141016    -1.069877     4.020307     170.75
 C       0.931322    -2.315605     3.282422      98.33
 H       2.090653    -2.790870     3.428195      23.02
 H       1.246517    -2.219148     1.942018      24.28
 H      -0.063655    -2.702390     3.556328      26.29
 C       0.117892     0.821004     4.877434      -5.00
 O       1.314339     1.053541     5.610992     291.93
 H       1.559105     1.944067     5.234418      25.89
 C      -1.017725     1.542245     5.311031      65.63
 H      -0.993547     2.016672     6.276446      24.24
 C      -2.307205     0.344677     3.680539     -32.84
 C      -3.638967     0.021941     2.905611      91.91
 H      -4.269349     1.001822     3.275763      22.06
 O      -4.148433    -1.303183     3.330435     231.05
 H      -5.102086    -1.220758     3.461227      22.43
 C      -3.521996     0.219830     1.407300      81.03
 H      -2.728808     1.092930     1.311154      25.21
 C      -4.838778     0.584230     0.567223      96.03
 O      -5.920402    -0.415442     0.748455     216.84
 H      -5.644555    -1.228406     0.134535      23.75
 H      -4.469005     0.409955    -0.450931      24.97
 H      -5.004435     1.886967     0.545149      22.41
 C       0.215093     0.607729    -1.003892      60.90
 H       0.809879     1.568827    -1.274348      22.29
 C       0.179354    -1.906487    -0.990295      63.96
 H       0.647480    -2.769056    -1.397430      21.54
 C      -0.927273    -1.882670    -0.248566      11.93
 O      -1.643327    -3.098585     0.122862     115.99
 C      -0.804348    -4.390405    -0.283339     110.72
 H      -1.504841    -4.904707     0.241206      24.04
 H      -0.542607    -4.888114    -1.235528      27.49
 H       0.202168    -4.350110     0.210085      26.95
 C      -1.644190    -0.693130     0.082665      29.08
 O      -2.804299    -0.899230     0.826356      14.12
 C      -1.052898     0.502427    -0.268766      62.52
 H      -1.516513     1.482432    -0.011123      24.23
 C       0.824094    -0.574754    -1.271835      17.08
 C       2.396351    -0.467388    -1.847076      85.03
 H       2.729721    -0.950854    -2.733860      24.75
 O       2.447097     0.889214    -2.547214     267.73
 H       2.779090     1.560916    -1.968905      28.36
 C       3.431914    -0.730868    -0.785630     107.68
 H       3.359840    -1.797599    -0.445134      25.97
 O       4.784495    -1.051754    -1.374873     156.37
 H       4.869952    -0.534763    -2.241814      30.06
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 C       3.616577     0.185972     0.350029     114.68
 O       3.882395     1.622515    -0.152574     282.11
 H       3.610656     2.278439     0.526981      28.74
 H       4.419148    -0.013124     1.183774      26.61
 H       2.938314     0.243991     1.081416      29.36
55
name = lig-Water-frame_47
 C      -2.267901     1.448389     4.646784      43.18
 H      -3.330245     1.736432     4.898764      10.21
 C      -1.265348    -0.596184     3.428508      82.91
 H      -1.348877    -1.573882     2.875963      25.20
 C       0.042855    -0.274642     4.040912       3.32
 O       1.097270    -1.053978     4.031808     176.88
 C       0.987988    -2.347343     3.257457     130.25
 H       1.751568    -2.951425     3.430748      30.39
 H       0.980487    -2.190717     2.244662      30.14
 H       0.089857    -2.960551     3.490328      27.20
 C       0.145815     0.841252     4.966489      23.08
 O       1.262580     1.042670     5.588503     257.39
 H       1.663201     1.912077     5.269949      26.69
 C      -1.052272     1.518705     5.308323      61.37
 H      -1.112020     2.051168     6.390458      27.11
 C      -2.281655     0.295931     3.695453     -14.78
 C      -3.619718     0.052999     2.934464      97.95
 H      -4.344898     0.868172     3.137981      25.41
 O      -4.152995    -1.272457     3.317438     228.48
 H      -5.207669    -1.216651     3.309731      18.98
 C      -3.511439     0.202869     1.362094     101.70
 H      -2.947394     1.076865     1.287598      28.96
 C      -4.789506     0.575636     0.574541     117.59
 O      -5.890335    -0.370998     0.766475     224.86
 H      -5.598726    -1.060646     0.187134      27.72
 H      -4.456490     0.523752    -0.496351      26.61
 H      -4.940321     1.516891     0.745284      29.44
 C       0.182740     0.625164    -0.978159      63.97
 H       0.509348     1.607716    -1.145486      21.15
 C       0.224908    -1.868756    -1.013777      98.74
 H       0.682663    -2.789966    -1.442132      23.99
 C      -0.989255    -1.910419    -0.300399      -5.83
 O      -1.628029    -3.072705     0.091082     189.54
 C      -0.752215    -4.350944    -0.281639      94.29
 H      -1.607989    -5.205450     0.227826      22.81
 H      -0.720582    -4.630928    -1.382785      27.48
 H       0.088086    -4.554456     0.417426      27.28
 C      -1.619120    -0.712742     0.111495       1.05
 O      -2.807273    -0.921423     0.872492     100.92
 C      -1.019050     0.528421    -0.296902      67.25
 H      -1.442392     1.486519    -0.062833      26.95
 C       0.852123    -0.598401    -1.347733      36.28
 C       2.328054    -0.438999    -1.819158      76.43
 H       2.658619    -1.470977    -2.492057      22.47
 O       2.425098     0.886335    -2.538106     241.63
 H       2.771752     1.700426    -2.072878      26.49
 C       3.499861    -0.739525    -0.777155      82.09
 H       3.077585    -1.727586    -0.174203      25.47
 O       4.766436    -1.056359    -1.387273     189.40
 H       4.844542    -0.526539    -2.224249      30.90
 C       3.646094     0.177506     0.361412      90.68
 O       3.921705     1.591988    -0.174720     260.82
 H       3.578952     2.282803     0.476633      27.70
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 H       4.513403    -0.012570     0.924812      27.10
 H       2.638032     0.034214     1.113751      25.41
55
name = lig-Water-frame_48
 C      -2.344153     1.415070     4.610261      30.05
 H      -3.170241     2.009535     5.031088      10.93
 C      -1.236024    -0.590208     3.406472      71.98
 H      -1.406530    -1.387376     2.739388      27.56
 C       0.013778    -0.230005     4.060476       9.18
 O       1.099386    -1.101731     4.019279     131.81
 C       1.025032    -2.370109     3.260245      96.14
 H       1.882753    -3.175175     3.637310      24.20
 H       0.604633    -1.944135     2.069081      24.37
 H       0.214241    -3.058630     3.545819      27.46
 C       0.064642     0.827245     4.993762      14.49
 O       1.287154     1.049233     5.607505     275.70
 H       1.718029     1.872558     5.268889      25.64
 C      -1.094129     1.537722     5.363338      51.31
 H      -1.026296     2.118913     6.194309      27.35
 C      -2.324011     0.283077     3.692561     -17.76
 C      -3.603951     0.079035     2.955806      94.36
 H      -4.575287     0.763121     3.228693      22.59
 O      -4.170940    -1.239207     3.304640     244.03
 H      -5.151488    -1.134879     3.241108      22.78
 C      -3.495414     0.209221     1.356092      97.25
 H      -2.956440     1.245561     1.204279      26.79
 C      -4.704156     0.508732     0.563855      90.70
 O      -5.864404    -0.304532     0.785101     188.78
 H      -5.695828    -1.130398     0.215374      26.45
 H      -4.548889     0.698694    -0.549482      25.51
 H      -5.232702     1.589435     1.136462      22.93
 C       0.157738     0.598730    -0.957775      54.80
 H       0.406669     1.687341    -1.134501      21.60
 C       0.298515    -1.802352    -1.062727      98.24
 H       0.716271    -2.757038    -1.345079      24.13
 C      -1.048320    -1.927918    -0.350812      -0.11
 O      -1.577720    -3.087087     0.040496     162.93
 C      -0.802126    -4.351875    -0.230014      97.50
 H      -1.321060    -5.268761    -0.120828      27.76
 H      -0.751141    -4.145555    -1.301897      28.43
 H       0.069684    -4.472605     0.422330      28.35
 C      -1.596997    -0.716009     0.131040      16.05
 O      -2.793309    -0.955143     0.890440      93.75
 C      -1.031312     0.550367    -0.301386      70.17
 H      -1.513701     1.501944    -0.012155      27.73
 C       0.890989    -0.609635    -1.394875      33.50
 C       2.277270    -0.430148    -1.814822     103.40
 H       2.334832    -1.345311    -2.378399      27.08
 O       2.405682     0.850967    -2.546315     262.03
 H       2.846624     1.508483    -1.889890      25.86
 C       3.519666    -0.777531    -0.753918      79.64
 H       3.022412    -1.623388    -0.191715      27.87
 O       4.750005    -1.059802    -1.410308     222.59
 H       4.794538    -0.574703    -2.223606      31.72
 C       3.661916     0.237104     0.413137      97.75
 O       3.944147     1.552839    -0.184525     257.10
 H       3.581849     2.254548     0.399935      28.55
 H       4.695806    -0.181004     0.796826      24.82
 H       2.738253     0.082537     0.775652      28.93
55
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name = lig-Water-frame_49
 C      -2.344962     1.337686     4.607904      40.27
 H      -3.049843     2.124791     4.892295      21.87
 C      -1.190100    -0.528567     3.428501      53.08
 H      -1.401521    -1.296464     2.564407      29.28
 C      -0.056893    -0.242656     4.064458      18.51
 O       1.124055    -1.164285     4.008818     141.28
 C       1.017614    -2.391862     3.250703     129.76
 H       2.008962    -2.730871     3.407478      28.27
 H       0.833337    -2.159922     2.294064      31.85
 H       0.140629    -2.912352     3.712541      28.26
 C      -0.026140     0.814143     5.010441     -30.93
 O       1.332782     1.055310     5.647803     213.26
 H       1.622498     1.889521     5.149971      24.04
 C      -1.158664     1.552689     5.382824      37.70
 H      -0.899566     2.479013     6.168647      21.70
 C      -2.402529     0.316671     3.688737     -18.61
 C      -3.663572     0.096617     2.942251     111.93
 H      -4.352197     0.781037     3.352028      27.16
 O      -4.180321    -1.219687     3.289207     233.63
 H      -5.169405    -1.090188     3.325801      24.85
 C      -3.445184     0.251008     1.389969     101.75
 H      -2.838770     1.101856     1.177063      28.05
 C      -4.696678     0.526120     0.584749     124.47
 O      -5.848202    -0.272216     0.787757     226.90
 H      -5.916417    -1.154956     0.304980      26.97
 H      -4.580458     0.821094    -0.444135      28.37
 H      -5.044873     1.264537     1.074337      30.77
 C       0.156339     0.578411    -0.963435      58.59
 H       0.570693     1.554853    -1.260307      22.29
 C       0.304601    -1.781975    -1.088683     102.86
 H       0.879594    -2.704703    -1.259101      24.63
 C      -1.006654    -1.894619    -0.427203      10.92
 O      -1.553540    -3.136196     0.022497     175.14
 C      -0.847758    -4.319793    -0.221315      90.17
 H      -1.451255    -5.365775    -0.259253      23.60
 H      -0.368312    -4.041454    -1.231720      26.33
 H       0.160733    -4.232126     0.293477      27.95
 C      -1.595875    -0.726913     0.127648      13.18
 O      -2.761907    -0.977194     0.889496      66.01
 C      -1.097149     0.540098    -0.267226      72.76
 H      -1.581223     1.461874     0.049353      27.64
 C       0.877580    -0.541165    -1.363865      35.70
 C       2.278096    -0.431126    -1.822465      83.80
 H       2.287792    -1.205483    -2.813777      23.71
 O       2.407011     0.800494    -2.545281     294.16
 H       2.861889     1.194114    -1.821777      28.68
 C       3.477621    -0.774995    -0.744074      78.04
 H       3.174506    -1.877821    -0.279748      25.85
 O       4.736794    -1.075039    -1.432876     199.15
 H       4.697720    -0.622882    -2.337778      29.62
 C       3.738897     0.275917     0.394519     107.35
 O       3.958093     1.526392    -0.187225     253.12
 H       3.625421     2.261240     0.372379      28.01
 H       4.486606    -0.156603     1.032560      27.92
 H       2.646014     0.319525     0.989968      25.99
55
name = lig-Water-frame_50
 C      -2.321686     1.298621     4.662167      39.92
 H      -3.176220     2.044319     4.543668      22.20
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 C      -1.255167    -0.453209     3.408731      69.90
 H      -1.196059    -1.163892     2.690370      29.44
 C      -0.050261    -0.309953     4.099679     -32.29
 O       1.125056    -1.169413     4.007280     121.59
 C       0.990619    -2.390017     3.285935     101.48
 H       2.161879    -2.611491     3.192410      22.09
 H       1.032140    -2.420806     1.925572      22.92
 H       0.208966    -2.974811     3.775479      24.09
 C      -0.043735     0.805512     5.068945     -78.86
 O       1.336172     1.065799     5.667719     232.40
 H       1.560208     1.854821     5.079269      23.44
 C      -1.172793     1.588380     5.393552      57.09
 H      -1.060229     2.443197     5.865197      25.98
 C      -2.427760     0.328521     3.675280       6.01
 C      -3.723891     0.097153     2.904252      90.12
 H      -4.289043     1.085940     3.399870      24.41
 O      -4.197314    -1.209680     3.272556     207.10
 H      -5.220603    -1.122734     3.488727      22.61
 C      -3.399280     0.261326     1.419687      80.52
 H      -2.645217     1.072791     1.287889      26.06
 C      -4.703073     0.545741     0.610990      90.80
 O      -5.867132    -0.273232     0.792227     252.31
 H      -5.856968    -1.061602     0.262604      30.00
 H      -4.476349     0.866684    -0.494003      25.51
 H      -4.974080     1.727297     1.192324      24.02
 C       0.132014     0.605543    -0.968386      48.50
 H       0.671324     1.475492    -1.318951      19.72
 C       0.269803    -1.801733    -1.088655      91.74
 H       1.010179    -2.598007    -1.224753      22.47
 C      -0.915845    -1.884606    -0.487351       9.02
 O      -1.567330    -3.144647     0.020513     179.92
 C      -0.798348    -4.273375    -0.280754     124.13
 H      -1.550019    -5.178238    -0.240711      23.44
 H      -0.220606    -4.442375    -1.201785      29.12
 H       0.029517    -4.314942     0.424434      28.28
 C      -1.619554    -0.745035     0.097133      14.70
 O      -2.724464    -0.983925     0.886403      58.27
 C      -1.139979     0.512191    -0.238006      71.05
 H      -1.584865     1.449791     0.056821      25.65
 C       0.839182    -0.487150    -1.285177      42.34
 C       2.292193    -0.483612    -1.901491      83.96
 H       2.470598    -1.089594    -2.748357      26.57
 O       2.438687     0.763463    -2.526164     274.80
 H       2.975631     1.392422    -1.884885      23.94
 C       3.421567    -0.795583    -0.756370      98.57
 H       3.276137    -1.802158    -0.336693      26.38
 O       4.721395    -1.083796    -1.464624     208.98
 H       4.624215    -0.766818    -2.397740      31.36
 C       3.724855     0.263077     0.388095     113.98
 O       3.989557     1.533738    -0.204482     265.04
 H       3.697449     2.272985     0.417053      27.30
 H       4.416559    -0.015216     1.303361      25.46
 H       3.028810     0.515153     1.112792      26.99
55
name = lig-Water-frame_51
 C      -2.350433     1.299663     4.696107      58.86
 H      -3.204306     1.893623     4.538948      22.01
 C      -1.310722    -0.402939     3.387070      40.05
 H      -1.156954    -1.254178     2.607108      28.20
 C      -0.033720    -0.344205     4.190766     -38.01
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 O       1.084873    -1.124801     3.998459     161.23
 C       1.022150    -2.396102     3.252732     121.68
 H       2.006252    -2.895670     3.339208      26.24
 H       0.805464    -2.403092     2.218538      29.86
 H       0.420566    -3.217833     3.699859      26.93
 C       0.020900     0.762652     5.142438     -26.21
 O       1.289964     1.081109     5.664594     294.63
 H       1.681230     1.841450     5.126236      27.07
 C      -1.147772     1.591664     5.366157      40.04
 H      -1.178475     2.701306     5.902390      18.83
 C      -2.411889     0.310377     3.664566      -3.27
 C      -3.738717     0.131808     2.903515      97.38
 H      -4.403069     0.895436     3.063844      29.08
 O      -4.240696    -1.200795     3.265840     252.00
 H      -5.160102    -1.135841     3.490306      26.03
 C      -3.389316     0.243418     1.418207      76.89
 H      -2.654583     1.104625     1.482441      26.38
 C      -4.703220     0.660247     0.652141     114.09
 O      -5.887796    -0.268892     0.798196     258.70
 H      -5.607023    -0.982441     0.104420      26.92
 H      -4.467102     0.706079    -0.374588      28.21
 H      -4.913651     1.544119     0.909670      30.48
 C       0.080576     0.668945    -0.956783      49.69
 H       0.547583     1.676965    -1.249837      21.87
 C       0.299200    -1.804226    -1.095898      74.14
 H       0.949674    -2.650415    -1.259022      24.84
 C      -0.922411    -1.920934    -0.455675      13.24
 O      -1.570239    -3.097108    -0.017860     173.36
 C      -0.710571    -4.275051    -0.324711     119.24
 H      -1.514912    -5.079282    -0.144793      24.47
 H      -0.345898    -4.630658    -1.332608      26.99
 H      -0.179469    -4.584020     0.662989      25.35
 C      -1.636320    -0.764104     0.033592      29.70
 O      -2.700068    -0.986667     0.890103      11.87
 C      -1.130861     0.505938    -0.241526      63.55
 H      -1.609742     1.461811     0.048520      24.39
 C       0.833376    -0.524555    -1.233249      15.08
 C       2.289660    -0.506260    -1.924723      67.82
 H       2.598544    -1.482274    -2.690776      22.62
 O       2.504458     0.770063    -2.506201     263.35
 H       2.962051     1.528110    -2.108716      27.39
 C       3.393855    -0.808495    -0.789341      78.00
 H       3.116628    -1.867305    -0.150627      24.92
 O       4.699938    -1.085420    -1.496939     171.60
 H       4.600316    -0.916425    -2.424567      31.66
 C       3.694360     0.238842     0.416442      93.86
 O       4.041444     1.569157    -0.236484     228.37
 H       3.803470     2.237284     0.425405      28.94
 H       4.591467     0.005196     0.988028      26.24
 H       2.786166     0.492635     1.182979      24.82
55
name = lig-Water-frame_52
 C      -2.378657     1.296219     4.695783      47.34
 H      -3.292756     2.002992     4.938300      24.11
 C      -1.238355    -0.440359     3.381051      40.46
 H      -1.399453    -1.164867     2.602694      31.06
 C      -0.092775    -0.331837     4.279133     -14.05
 O       1.039144    -1.088891     3.979614     137.76
 C       1.067328    -2.440589     3.253891      97.72
 H       2.049890    -2.967696     3.444584      24.85
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 H       0.364825    -2.111393     2.185834      27.07
 H       0.450941    -3.232817     3.742644      27.66
 C       0.081432     0.721284     5.192623       9.74
 O       1.249111     1.099720     5.669850     334.36
 H       1.708377     1.825178     5.158630      26.35
 C      -1.119540     1.614428     5.333180      28.22
 H      -1.067488     2.465424     5.917482      19.99
 C      -2.429069     0.319197     3.687445     -23.41
 C      -3.700914     0.118348     2.907501      85.14
 H      -4.724164     0.815688     2.902794      21.96
 O      -4.278030    -1.193335     3.265171     208.97
 H      -5.317257    -1.073556     3.394941      22.19
 C      -3.409789     0.226150     1.412085      85.06
 H      -2.780692     1.094677     1.432840      29.72
 C      -4.680687     0.711331     0.665103      78.64
 O      -5.877333    -0.250813     0.788228     179.40
 H      -5.544496    -0.936486     0.134690      26.91
 H      -4.462705     0.541811    -0.485487      25.30
 H      -5.136511     1.941453     0.893035      23.08
 C       0.064492     0.709453    -0.948398      73.90
 H       0.278140     1.722121    -1.092570      27.57
 C       0.335790    -1.811184    -1.083759      72.35
 H       0.822323    -2.771640    -1.352062      28.06
 C      -0.986099    -1.942991    -0.378181      15.31
 O      -1.536362    -3.059356    -0.089954     137.50
 C      -0.675798    -4.349044    -0.308754      97.79
 H      -1.626792    -5.096487    -0.153140      23.92
 H      -0.400819    -4.392848    -1.343909      27.02
 H      -0.085663    -4.605349     0.558273      27.40
 C      -1.638228    -0.774048    -0.037348      40.13
 O      -2.703801    -0.978375     0.896330     -45.89
 C      -1.107310     0.531597    -0.268893      48.09
 H      -1.675886     1.378548     0.041924      27.07
 C       0.865275    -0.546231    -1.242044     -16.47
 C       2.300980    -0.514417    -1.874877      94.53
 H       2.366363    -1.379400    -2.506245      26.95
 O       2.565420     0.774049    -2.533610     237.64
 H       3.041086     1.394091    -1.960613      28.82
 C       3.384764    -0.828610    -0.795125      85.10
 H       3.005555    -1.715294    -0.229204      29.71
 O       4.670647    -1.087537    -1.506418     148.64
 H       4.545411    -1.031297    -2.506181      27.45
 C       3.653059     0.246326     0.411909     100.98
 O       4.089785     1.597877    -0.260908     171.54
 H       3.911135     2.293114     0.424301      28.38
 H       4.678722    -0.171597     0.681014      26.49
 H       2.725503     0.188887     0.922112      29.17
55
name = lig-Water-frame_53
 C      -2.386371     1.331896     4.719369      52.27
 H      -3.111902     1.863583     5.227436      24.96
 C      -1.192259    -0.468950     3.429826      43.18
 H      -1.415055    -1.186860     2.640313      29.51
 C      -0.161168    -0.351930     4.296691      -1.11
 O       1.022051    -1.081230     3.968131     140.03
 C       1.028225    -2.455324     3.265092     105.92
 H       2.203640    -2.644788     3.173339      26.68
 H       0.632767    -2.220065     2.392884      34.11
 H       0.329774    -3.033593     3.864143      28.64
 C       0.018514     0.736718     5.201885       5.84
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 O       1.267893     1.119166     5.709761     333.96
 H       1.566969     1.850104     5.055789      25.35
 C      -1.083741     1.574960     5.287839      40.14
 H      -0.884581     2.438232     6.093664      16.51
 C      -2.440517     0.338974     3.726540     -25.23
 C      -3.715072     0.075436     2.896815     107.07
 H      -4.402770     0.771361     3.162741      28.75
 O      -4.320586    -1.195346     3.273413     261.70
 H      -5.302064    -1.029741     3.224706      26.17
 C      -3.446178     0.229855     1.410387      84.79
 H      -2.746554     1.150354     1.229741      29.46
 C      -4.692516     0.741445     0.617235     116.82
 O      -5.842497    -0.209912     0.775091     220.64
 H      -5.702030    -1.020870     0.278245      28.68
 H      -4.455874     0.725339    -0.385625      29.73
 H      -5.022987     1.608195     0.836556      31.21
 C       0.099145     0.687657    -0.947010      75.43
 H       0.334654     1.817632    -1.092252      26.73
 C       0.306148    -1.822205    -1.030903      68.64
 H       0.778363    -2.714342    -1.418081      28.96
 C      -0.951375    -1.896219    -0.363797      -2.79
 O      -1.511675    -3.112371    -0.142670     161.58
 C      -0.735064    -4.426229    -0.277911     102.19
 H      -1.507484    -5.135227    -0.282996      25.69
 H      -0.283799    -4.192763    -1.301285      27.21
 H       0.254560    -4.446491     0.378729      26.43
 C      -1.658044    -0.743100    -0.065805       7.72
 O      -2.734870    -0.956042     0.890266     -85.75
 C      -1.117028     0.530186    -0.300832      43.82
 H      -1.743939     1.385648     0.014184      27.03
 C       0.902608    -0.505186    -1.279270     -61.73
 C       2.304902    -0.466078    -1.780461      94.80
 H       2.113616    -1.296305    -2.706055      23.10
 O       2.626689     0.759882    -2.573546     185.07
 H       3.098238     1.116007    -1.718696      27.97
 C       3.394208    -0.804861    -0.810944      92.10
 H       2.943939    -1.832570    -0.256241      27.81
 O       4.638428    -1.096116    -1.500608     147.23
 H       4.459994    -1.111740    -2.476945      27.12
 C       3.660788     0.239208     0.295855     117.05
 O       4.114354     1.604291    -0.259248     116.65
 H       3.994150     2.362638     0.401329      25.96
 H       4.512340    -0.307262     0.829162      29.69
 H       2.727559     0.125883     0.967909      29.76
55
name = lig-Water-frame_54
 C      -2.338994     1.357948     4.753763      52.82
 H      -3.243813     1.824221     5.315372      19.26
 C      -1.276651    -0.461371     3.495840      50.12
 H      -1.167135    -1.324019     2.713577      26.54
 C      -0.141460    -0.403313     4.274200      -7.79
 O       1.024739    -1.081219     3.970991     160.00
 C       0.992162    -2.404500     3.322137      99.57
 H       1.995129    -2.505070     3.077424      28.49
 H       0.763216    -2.437080     1.966998      26.30
 H       0.355619    -3.088386     3.978381      26.54
 C      -0.062604     0.749122     5.174240     -13.24
 O       1.298705     1.137421     5.747630     313.43
 H       1.495951     1.846385     5.070042      25.36
 C      -1.064594     1.563578     5.298965      64.51
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 H      -0.867208     2.320293     6.068756      21.19
 C      -2.423218     0.333306     3.754843     -10.01
 C      -3.714787     0.027746     2.914950      87.94
 H      -4.226304     1.024190     3.468666      20.81
 O      -4.352295    -1.207552     3.275803     257.86
 H      -5.351999    -1.112680     3.194405      25.64
 C      -3.471994     0.280140     1.385258      87.84
 H      -2.790292     1.040201     1.284624      31.33
 C      -4.700044     0.657571     0.547948      92.61
 O      -5.814169    -0.148835     0.765321     207.61
 H      -5.775420    -1.105368     0.373024      25.89
 H      -4.381081     0.982652    -0.582331      25.09
 H      -5.070154     1.839199     1.062284      24.07
 C       0.168436     0.660937    -0.954570     111.70
 H       0.617015     1.576265    -1.189233      29.11
 C       0.286254    -1.769940    -0.985992      84.63
 H       0.828482    -2.628455    -1.386296      26.27
 C      -0.876562    -1.879734    -0.390511     -43.00
 O      -1.514341    -3.198738    -0.162092     215.76
 C      -0.750772    -4.411409    -0.280114     110.11
 H      -1.408878    -5.507951    -0.333320      20.97
 H      -0.282920    -4.415178    -1.265164      27.29
 H       0.172950    -4.364996     0.247568      28.86
 C      -1.705526    -0.694785    -0.031183     -49.97
 O      -2.780474    -0.929841     0.859380     -10.72
 C      -1.155358     0.518437    -0.340217      62.42
 H      -1.650882     1.453521    -0.116554      30.32
 C       0.883158    -0.447472    -1.278744      -6.84
 C       2.268974    -0.427549    -1.798324     105.40
 H       2.262442    -1.128324    -2.586560      29.42
 O       2.698657     0.731169    -2.567279     221.48
 H       3.154157     1.335531    -1.923286      30.28
 C       3.400506    -0.800951    -0.831209     119.45
 H       3.094747    -1.737183    -0.287886      30.13
 O       4.612746    -1.111114    -1.491910     192.68
 H       4.424623    -1.153140    -2.416580      29.77
 C       3.681870     0.216533     0.195151     140.15
 O       4.122310     1.580245    -0.243965     136.14
 H       3.962321     2.261719     0.422853      28.05
 H       4.372732    -0.169237     1.024416      30.27
 H       2.910963     0.449001     0.969852      30.45
55
name = lig-Water-frame_55
 C      -2.316731     1.356691     4.778595      24.24
 H      -3.239446     1.809295     5.040853      18.31
 C      -1.357424    -0.498755     3.550503      54.63
 H      -1.225248    -1.230150     2.863843      24.21
 C      -0.093762    -0.402391     4.259589      20.87
 O       1.029094    -1.087986     3.971207     236.09
 C       0.939561    -2.337667     3.321165     103.01
 H       2.130306    -2.734017     3.293342      24.14
 H       0.614219    -2.483562     2.328082      29.40
 H       0.561282    -3.176828     3.857695      26.28
 C      -0.010127     0.685388     5.119713     -18.39
 O       1.293196     1.139990     5.767404     360.10
 H       1.650065     1.894456     5.168700      26.18
 C      -1.106558     1.613341     5.366658      36.23
 H      -0.966245     2.431722     6.100367      20.74
 C      -2.411615     0.305761     3.774712      16.28
 C      -3.716822     0.055512     2.984429      88.28
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 H      -4.289922     0.859632     3.250641      25.40
 O      -4.369272    -1.224969     3.274143     231.03
 H      -5.421344    -1.178359     3.284574      21.32
 C      -3.501001     0.312988     1.367740      64.61
 H      -2.698702     1.199646     1.434033      23.26
 C      -4.695056     0.660810     0.490326     131.47
 O      -5.820423    -0.104511     0.749034     251.67
 H      -5.658422    -0.987546     0.366793      26.62
 H      -4.505546     0.938604    -0.471754      27.89
 H      -4.905687     1.444230     1.001522      30.07
 C       0.194797     0.651052    -0.949933      59.44
 H       0.806137     1.565126    -1.264355      24.86
 C       0.351690    -1.686028    -0.993387      76.95
 H       0.897846    -2.605483    -1.260633      23.61
 C      -0.911799    -1.919535    -0.382153     -40.84
 O      -1.533752    -3.247029    -0.168436     162.78
 C      -0.738402    -4.414399    -0.340546     117.92
 H      -1.193291    -5.270430    -0.109640      26.14
 H      -0.394917    -4.665288    -1.404054      25.78
 H       0.085485    -4.436452     0.531644      25.08
 C      -1.733187    -0.694921     0.031242     -31.85
 O      -2.828634    -0.907614     0.805305      60.83
 C      -1.164649     0.548908    -0.400105      66.64
 H      -1.591647     1.538066    -0.232610      27.48
 C       0.852968    -0.444302    -1.254132      67.44
 C       2.254764    -0.385518    -1.862537      81.60
 H       2.494119    -1.356595    -2.633041      24.96
 O       2.770963     0.724379    -2.554369     254.85
 H       3.109684     1.542251    -2.200640      30.01
 C       3.386143    -0.802953    -0.849316      98.22
 H       3.131271    -1.779172    -0.120862      26.57
 O       4.610903    -1.133876    -1.494571     168.13
 H       4.489864    -1.150773    -2.495334      27.89
 C       3.711942     0.249836     0.198571     128.54
 O       4.134099     1.541695    -0.247003     171.33
 H       3.860310     2.115921     0.516053      28.37
 H       4.466523    -0.045297     0.994185      28.82
 H       2.783759     0.606822     0.750076      27.39
55
name = lig-Water-frame_56
 C      -2.328607     1.328803     4.765365      -0.93
 H      -3.240856     1.997591     4.825412      18.25
 C      -1.347855    -0.578379     3.616863      48.23
 H      -1.577035    -1.375101     2.713766      20.52
 C      -0.090182    -0.354409     4.244130      25.05
 O       1.039753    -1.097695     3.968067     242.56
 C       0.979770    -2.344719     3.339848      98.98
 H       1.890318    -2.720382     3.388393      26.46
 H       0.154100    -2.287023     2.280837      21.31
 H       0.505705    -3.199864     3.976699      24.73
 C       0.086829     0.698185     5.111011       3.33
 O       1.268332     1.122838     5.769114     341.07
 H       1.701494     1.826146     5.216763      28.46
 C      -1.122894     1.630375     5.442786      24.57
 H      -1.053413     2.589187     6.143911      21.87
 C      -2.441558     0.289654     3.807217      26.42
 C      -3.735518     0.085206     3.015035      85.66
 H      -4.671808     0.889267     3.133844      22.31
 O      -4.371340    -1.244849     3.279787     230.35
 H      -5.340653    -1.080179     3.328304      24.27
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 C      -3.479005     0.328499     1.379938      84.02
 H      -2.861894     1.139946     1.404106      22.37
 C      -4.665674     0.689585     0.488877      79.86
 O      -5.857338    -0.092470     0.718602     249.88
 H      -5.612318    -0.944777     0.305650      25.88
 H      -4.524222     0.814985    -0.715436      20.55
 H      -4.983651     1.848528     1.072889      20.96
 C       0.157004     0.710692    -0.935706      46.32
 H       0.580228     1.673468    -1.195814      20.78
 C       0.375154    -1.698494    -0.985689      73.15
 H       0.999898    -2.554727    -1.163916      22.65
 C      -0.988606    -1.950550    -0.362019      -6.58
 O      -1.555744    -3.239116    -0.181027     130.44
 C      -0.666283    -4.426622    -0.386811      85.68
 H      -1.495516    -5.220249     0.275449      21.27
 H      -0.438504    -4.674270    -1.421618      25.26
 H      -0.008917    -4.436558     0.453021      25.67
 C      -1.690363    -0.729588     0.056628     -14.07
 O      -2.881371    -0.883304     0.750926      92.02
 C      -1.143858     0.595453    -0.454157      51.72
 H      -1.690216     1.548526    -0.275442      22.39
 C       0.901618    -0.471095    -1.266245      33.61
 C       2.309988    -0.405996    -1.917449      97.20
 H       2.342374    -1.196483    -2.580344      27.06
 O       2.827667     0.727973    -2.591753     237.90
 H       2.934890     1.650615    -2.070931      25.60
 C       3.372175    -0.812878    -0.823238      81.83
 H       3.030796    -1.678809    -0.192952      26.41
 O       4.629749    -1.166006    -1.514343     210.83
 H       4.607351    -1.078581    -2.503278      27.73
 C       3.711305     0.301676     0.261544     114.18
 O       4.156615     1.530443    -0.266470     199.05
 H       3.880500     2.158991     0.471854      26.63
 H       4.510023    -0.131413     0.906152      27.42
 H       2.601227     0.334669     0.551430      24.97
55
name = lig-Water-frame_57
 C      -2.352069     1.327628     4.751718      31.19
 H      -3.065178     2.175458     4.737000      20.13
 C      -1.355363    -0.672936     3.643163      51.32
 H      -1.647135    -1.366024     3.002356      27.04
 C      -0.096248    -0.325933     4.212258      14.36
 O       1.060545    -1.091252     3.973351     220.29
 C       0.929450    -2.398994     3.353496      86.66
 H       2.147947    -2.747984     3.063804      22.94
 H       0.369589    -2.218476     2.506339      29.17
 H       0.340876    -2.920545     4.067692      27.18
 C       0.096892     0.829236     5.163312       4.93
 O       1.259739     1.086256     5.767966     324.50
 H       1.662157     1.764630     5.108500      25.66
 C      -1.103170     1.588897     5.478596      34.61
 H      -1.050666     2.438275     6.067060      24.33
 C      -2.478420     0.271165     3.851085      10.56
 C      -3.801165     0.111535     2.991752      95.89
 H      -4.592115     0.773989     3.216872      25.99
 O      -4.344941    -1.254543     3.291362     225.41
 H      -5.387667    -1.050212     3.261768      22.19
 C      -3.466033     0.308718     1.403632      84.04
 H      -2.721506     1.241961     1.281779      21.23
 C      -4.679081     0.804138     0.525221     100.90
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 O      -5.888988    -0.086756     0.676930     270.64
 H      -5.681426    -1.005503     0.239299      25.21
 H      -4.403256     0.671766    -0.463050      25.16
 H      -4.948976     1.730594     0.605617      26.70
 C       0.122524     0.760364    -0.946799      45.64
 H       0.316956     1.841454    -1.143789      19.82
 C       0.329540    -1.775734    -0.946529      56.79
 H       1.046568    -2.613351    -1.135536      21.66
 C      -1.015360    -1.940211    -0.363496      27.97
 O      -1.567192    -3.192231    -0.203752     139.78
 C      -0.682551    -4.468378    -0.346708     100.54
 H      -1.387782    -5.016968    -0.018956      27.65
 H      -0.411827    -4.643459    -1.409621      26.55
 H       0.343684    -4.348333     0.258669      25.13
 C      -1.614819    -0.749971     0.032727      -4.43
 O      -2.921420    -0.859075     0.701909     123.91
 C      -1.150255     0.600399    -0.458037      52.95
 H      -1.809748     1.422123    -0.295187      21.99
 C       0.957812    -0.440797    -1.286448      -7.88
 C       2.387142    -0.431196    -1.908226      89.11
 H       2.159442    -1.227296    -2.868542      22.42
 O       2.867693     0.760050    -2.652146     250.13
 H       2.703567     1.323852    -1.895125      29.39
 C       3.411635    -0.795973    -0.821874      79.75
 H       2.853368    -1.763420    -0.275286      23.98
 O       4.657645    -1.208818    -1.521912     198.21
 H       4.634027    -0.950304    -2.437633      29.79
 C       3.660435     0.288869     0.291081     116.94
 O       4.170282     1.550599    -0.274337     187.78
 H       4.039105     2.337684     0.277235      26.34
 H       4.396665    -0.267017     1.009173      27.25
 H       2.700893     0.246615     0.800699      27.42
55
name = lig-Water-frame_58
 C      -2.338492     1.351610     4.746147      54.74
 H      -2.994883     2.195456     4.787655      24.21
 C      -1.390374    -0.686975     3.700797      43.31
 H      -1.526073    -1.750889     3.088909      24.16
 C      -0.098030    -0.305992     4.194199     -26.40
 O       1.086868    -1.058043     3.986713     155.43
 C       0.920755    -2.446557     3.387054      96.13
 H       1.744787    -2.721682     2.987005      29.27
 H       0.408694    -2.230713     2.158112      26.44
 H       0.254002    -2.981109     4.141294      24.29
 C      -0.004456     0.917838     5.182891      -9.15
 O       1.294378     1.065398     5.763247     274.91
 H       1.725825     1.701749     5.113612      25.41
 C      -1.089449     1.510465     5.459228      73.32
 H      -1.008444     2.474715     6.210350      24.64
 C      -2.514552     0.241417     3.883585      -8.16
 C      -3.810917     0.086095     2.952530      92.94
 H      -4.564385     0.938887     3.355487      23.78
 O      -4.327581    -1.245294     3.299349     270.29
 H      -5.287414    -1.249681     3.150897      25.88
 C      -3.464128     0.334700     1.419528      87.42
 H      -2.701378     1.027350     1.355813      26.29
 C      -4.704827     0.833623     0.562211      69.46
 O      -5.908420    -0.069163     0.631072     220.74
 H      -5.649578    -0.901044     0.224615      28.79
 H      -4.158788     0.586648    -0.480310      21.97
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 H      -5.101272     2.069256     0.406571      20.89
 C       0.126444     0.778573    -0.993688      45.17
 H       0.289679     1.865827    -1.213190      20.40
 C       0.305184    -1.793014    -0.920537      74.69
 H       0.856034    -2.692212    -1.129941      24.63
 C      -0.956802    -1.925171    -0.395764      31.09
 O      -1.571170    -3.146151    -0.221541     146.13
 C      -0.677020    -4.441681    -0.302924      90.14
 H      -1.488996    -5.447978    -0.082708      21.83
 H      -0.476866    -4.552871    -1.428586      25.30
 H       0.369148    -4.331435    -0.027037      25.47
 C      -1.602158    -0.706288     0.002475      -5.17
 O      -2.927585    -0.842052     0.654642     107.93
 C      -1.184228     0.525687    -0.413007      53.63
 H      -1.918424     1.373524    -0.316763      23.32
 C       0.944952    -0.401443    -1.272681     -17.81
 C       2.423452    -0.477413    -1.945057     100.45
 H       2.375808    -1.142522    -2.669799      29.41
 O       2.876691     0.782758    -2.687095     237.15
 H       2.704434     1.364241    -1.921277      28.82
 C       3.461342    -0.801503    -0.857206     113.59
 H       3.037889    -1.683834    -0.359101      28.89
 O       4.685429    -1.256063    -1.501169     203.42
 H       4.638413    -0.758380    -2.386789      28.82
 C       3.613083     0.233947     0.309859     108.67
 O       4.167537     1.561643    -0.270411     158.85
 H       4.104051     2.409805     0.263331      26.04
 H       4.307876    -0.175911     1.038280      29.10
 H       2.819507     0.507110     1.143151      26.11
55
name = lig-Water-frame_59
 C      -2.312266     1.351598     4.727308      44.32
 H      -3.131639     2.152233     4.901157      20.72
 C      -1.413006    -0.692954     3.755716      67.20
 H      -1.352828    -1.664588     3.417364      27.14
 C      -0.118860    -0.278158     4.206007     -30.57
 O       1.094572    -1.030283     3.992822     152.13
 C       0.842404    -2.420461     3.387437     105.13
 H       1.981618    -2.983598     3.094356      25.62
 H       0.364831    -2.389456     2.416393      32.50
 H       0.376626    -3.189852     3.984695      27.68
 C       0.009416     0.839042     5.122958     -40.52
 O       1.320678     1.058214     5.751192     243.95
 H       1.806796     1.705909     5.157602      25.69
 C      -1.175236     1.549846     5.482675      62.51
 H      -1.056492     2.235908     6.175099      30.21
 C      -2.541900     0.214584     3.893916       2.41
 C      -3.783743     0.049335     2.952557     100.96
 H      -4.406495     0.930225     3.257108      28.14
 O      -4.305151    -1.237795     3.298592     253.47
 H      -5.294781    -1.297628     3.061216      24.09
 C      -3.500028     0.362977     1.439631      60.02
 H      -2.599258     1.112271     1.532492      27.35
 C      -4.727048     0.846647     0.529474     104.18
 O      -5.903790    -0.026364     0.586957     236.15
 H      -5.522617    -0.872002     0.161326      26.48
 H      -4.254174     0.706159    -0.392994      27.14
 H      -5.038032     1.784144     0.618210      27.87
 C       0.125190     0.744859    -1.044516      97.43
 H       0.468366     1.709882    -1.360079      28.32
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 C       0.345412    -1.728715    -0.933007      80.72
 H       0.764237    -2.706950    -1.219204      26.41
 C      -0.894061    -1.898564    -0.415724     -35.00
 O      -1.567171    -3.130696    -0.217964     158.93
 C      -0.731461    -4.417426    -0.328820     101.32
 H      -1.042275    -5.275766     0.023417      28.13
 H      -0.652901    -4.483368    -1.389409      25.46
 H       0.305679    -4.340878     0.165574      26.33
 C      -1.677446    -0.688973    -0.005884     -21.37
 O      -2.906897    -0.833922     0.615429      73.03
 C      -1.186132     0.492310    -0.380457      77.64
 H      -1.843680     1.314235    -0.328826      28.95
 C       0.900788    -0.392506    -1.250897     -16.57
 C       2.419992    -0.460001    -1.960570      72.75
 H       2.647535    -1.482758    -2.739724      24.11
 O       2.857425     0.778691    -2.692639     179.75
 H       2.938948     1.686512    -2.146075      27.81
 C       3.486801    -0.810160    -0.884962      95.24
 H       3.216222    -1.858250    -0.243108      27.88
 O       4.713274    -1.282139    -1.479172     170.98
 H       4.860587    -0.653208    -2.243433      27.26
 C       3.594512     0.229361     0.348203     104.15
 O       4.151549     1.554764    -0.261453     149.35
 H       3.991313     2.217150     0.480449      29.59
 H       4.533417    -0.110023     0.991496      27.80
 H       2.826550     0.625072     0.937223      28.89
55
name = lig-Water-frame_60
 C      -2.349953     1.349527     4.703244      48.80
 H      -3.194708     1.902087     4.921366      19.78
 C      -1.409037    -0.659141     3.827822      64.05
 H      -1.473455    -1.765099     3.452201      27.03
 C      -0.131213    -0.265366     4.242143      37.95
 O       1.059154    -1.038413     3.981999     162.72
 C       0.855882    -2.400194     3.392997     106.80
 H       1.747787    -2.785304     3.433526      30.48
 H       0.036713    -2.453912     2.357965      29.22
 H       0.424607    -3.193578     4.070622      28.10
 C       0.067968     0.736061     5.069703     -38.98
 O       1.316112     1.047917     5.729244     236.79
 H       1.730486     1.779714     5.131691      25.55
 C      -1.211540     1.576079     5.482425     -13.87
 H      -1.168210     2.369775     6.428240      23.55
 C      -2.528197     0.187090     3.881766      23.53
 C      -3.725188     0.011683     2.974531      95.69
 H      -4.487413     0.896353     3.181277      25.79
 O      -4.293827    -1.247438     3.287563     268.04
 H      -5.272764    -1.117659     3.085287      26.35
 C      -3.519642     0.389325     1.450869      49.93
 H      -2.820261     1.205841     1.570919      28.82
 C      -4.719960     0.811527     0.508913      87.65
 O      -5.868019     0.007504     0.536375     185.41
 H      -5.583276    -0.896845     0.132183      26.28
 H      -4.377644     0.901837    -0.646512      23.58
 H      -5.080985     1.980071     0.977135      23.03
 C       0.098781     0.671954    -1.071718     107.03
 H       0.600472     1.616172    -1.489575      30.04
 C       0.415625    -1.654012    -0.972999      75.54
 H       0.936885    -2.533049    -1.370694      28.78
 C      -0.898265    -1.854407    -0.393238     -27.98
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 O      -1.554244    -3.134407    -0.190315     141.56
 C      -0.752241    -4.330738    -0.378946      89.27
 H      -1.164844    -5.331872     0.361339      21.52
 H      -0.657875    -4.577227    -1.530524      23.57
 H       0.134595    -4.186803     0.306112      26.44
 C      -1.748588    -0.742497    -0.016852      10.63
 O      -2.896527    -0.828612     0.606086     -31.54
 C      -1.133582     0.546981    -0.393872      27.35
 H      -1.778188     1.465170    -0.272628      25.20
 C       0.903716    -0.434615    -1.267877      27.02
 C       2.410981    -0.438686    -1.962330      90.52
 H       2.529240    -1.165418    -2.585707      31.83
 O       2.827005     0.759594    -2.702425     232.10
 H       3.128926     1.536174    -2.280103      32.15
 C       3.478485    -0.845953    -0.838593      94.19
 H       3.190186    -1.739043    -0.329209      31.15
 O       4.752113    -1.278367    -1.461348     184.01
 H       5.167854    -0.677621    -2.076000      28.37
 C       3.672507     0.252717     0.337757     108.97
 O       4.116226     1.542286    -0.229936     201.71
 H       3.912661     2.060935     0.557181      30.93
 H       4.437130    -0.099284     0.932137      31.81
 H       2.536382     0.442060     0.725610      29.59
55
name = lig-Water-frame_61
 C      -2.395595     1.338024     4.701470      11.03
 H      -3.417143     1.851507     4.930668      16.98
 C      -1.411048    -0.665832     3.866613     102.29
 H      -1.719610    -1.623404     3.364238      29.87
 C      -0.109250    -0.337981     4.256496       7.34
 O       0.990160    -1.070826     3.954094     222.22
 C       0.818098    -2.380748     3.417955     105.12
 H       2.082363    -2.707608     3.342685      24.06
 H       0.262756    -2.396435     2.528002      29.48
 H       0.299982    -2.860961     4.267169      26.85
 C       0.072913     0.776430     5.131434      -6.99
 O       1.294722     1.035029     5.688840     306.38
 H       1.582447     1.823526     5.131054      26.73
 C      -1.164642     1.570788     5.465095      34.20
 H      -1.278440     2.232340     6.222837      26.69
 C      -2.474316     0.188515     3.863859      -2.95
 C      -3.687346     0.000994     2.991752     105.22
 H      -4.535638     0.725877     3.248716      22.74
 O      -4.302378    -1.269286     3.264559     285.54
 H      -5.252579    -1.042571     3.277880      23.74
 C      -3.527069     0.380086     1.424132      57.44
 H      -2.901262     1.349098     1.407202      25.19
 C      -4.697074     0.843273     0.504905     115.07
 O      -5.834401     0.008012     0.484372     238.43
 H      -5.676070    -0.860150     0.119172      26.61
 H      -4.490256     1.217954    -0.471351      25.89
 H      -4.967566     1.638253     1.069268      27.27
 C       0.091601     0.632654    -1.093037     100.12
 H       0.425503     1.560297    -1.431553      32.04
 C       0.430898    -1.664252    -1.001636      77.47
 H       1.091622    -2.424039    -1.378952      23.41
 C      -0.924136    -1.827841    -0.365867       2.54
 O      -1.541689    -3.121134    -0.159556     196.03
 C      -0.771936    -4.287652    -0.379407     136.57
 H      -1.410856    -4.854532     0.118182      26.74
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 H      -0.551353    -4.639991    -1.323809      30.47
 H       0.214053    -4.040236     0.086140      28.63
 C      -1.711276    -0.739077    -0.066649      14.83
 O      -2.924218    -0.826704     0.640482     -33.82
 C      -1.108749     0.604889    -0.416095      43.96
 H      -1.594354     1.544332    -0.205082      23.27
 C       0.975924    -0.455200    -1.330886      17.99
 C       2.396619    -0.368154    -1.892318      79.09
 H       2.284420    -1.234107    -2.882362      23.80
 O       2.788603     0.719160    -2.732515     202.44
 H       3.239365     1.335404    -2.071127      29.30
 C       3.493238    -0.824486    -0.797279      71.26
 H       2.935204    -1.863943    -0.302780      26.01
 O       4.790704    -1.280349    -1.431993     147.08
 H       5.321723    -0.599729    -1.969254      25.33
 C       3.707779     0.255158     0.260420     125.53
 O       4.071432     1.526506    -0.183542     204.21
 H       3.912912     2.271720     0.528757      24.70
 H       4.341925    -0.188093     1.218007      27.80
 H       2.748081     0.113179     0.616344      32.02
55
name = lig-Water-frame_62
 C      -2.416834     1.318086     4.730662      58.98
 H      -3.259268     1.907699     4.903311      22.66
 C      -1.412461    -0.721252     3.850383      71.24
 H      -1.665529    -1.580595     3.237353      28.58
 C      -0.107277    -0.400767     4.296302      -2.54
 O       0.946204    -1.079428     3.922005     186.03
 C       0.845707    -2.385293     3.503531     111.88
 H       1.728927    -2.697882     3.142622      28.83
 H       0.368021    -2.387089     2.265341      26.13
 H       0.209107    -2.839898     4.258252      26.90
 C      -0.007069     0.842333     5.207869      21.12
 O       1.284000     1.033484     5.650815     295.13
 H       1.628078     1.886221     5.194486      24.44
 C      -1.126068     1.522317     5.389835      62.16
 H      -1.186550     2.347971     6.245110      24.19
 C      -2.438806     0.251220     3.859443       6.71
 C      -3.694054     0.004038     2.985198      91.12
 H      -4.425964     0.753303     3.393852      23.94
 O      -4.315180    -1.300608     3.233076     242.61
 H      -5.292210    -1.141363     3.529768      20.42
 C      -3.496779     0.352671     1.359540      74.70
 H      -2.832204     1.237917     1.241274      25.67
 C      -4.679509     0.861534     0.549978      87.06
 O      -5.822925     0.000731     0.435799     198.32
 H      -5.556952    -0.948287    -0.003814      20.31
 H      -4.329156     1.434811    -0.432244      22.23
 H      -5.115010     1.836841     1.280178      21.65
 C       0.125212     0.636089    -1.117681      86.39
 H       0.318556     1.745988    -1.369423      28.38
 C       0.399418    -1.724687    -1.012137      77.70
 H       1.009274    -2.645759    -1.215454      21.95
 C      -0.909992    -1.847397    -0.379711     -12.47
 O      -1.536915    -3.046597    -0.143232     225.23
 C      -0.761836    -4.235697    -0.348693     111.57
 H      -1.620966    -5.019347     0.105390      21.65
 H      -0.552457    -4.621398    -1.485753      26.87
 H       0.370997    -4.173976    -0.051713      26.77
 C      -1.655444    -0.633956    -0.096348     -19.75
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 O      -2.939960    -0.825312     0.685474      15.56
 C      -1.116667     0.598542    -0.431690      70.57
 H      -1.506464     1.587902    -0.155162      24.12
 C       1.014348    -0.427831    -1.375970       9.35
 C       2.381973    -0.383021    -1.893735     111.72
 H       2.270271    -1.102274    -2.518062      30.00
 O       2.760508     0.704902    -2.739678     226.66
 H       3.284182     1.216848    -2.005802      27.36
 C       3.525683    -0.811530    -0.811396     103.89
 H       3.092418    -1.608350    -0.360184      31.23
 O       4.819232    -1.293338    -1.393089     193.62
 H       5.171131    -0.500961    -1.866305      28.36
 C       3.729207     0.188787     0.248440     122.88
 O       4.034568     1.538355    -0.145497     246.06
 H       3.851488     2.304172     0.432777      25.45
 H       4.232481    -0.085033     1.072021      30.97
 H       2.639353     0.153215     0.800527      28.18
55
name = lig-Water-frame_63
 C      -2.378961     1.297208     4.770609      64.70
 H      -3.149830     2.118463     4.920862      20.47
 C      -1.400949    -0.767415     3.810004      52.11
 H      -1.420474    -1.674606     3.027037      27.22
 C      -0.189819    -0.398197     4.371639      -3.61
 O       0.969109    -1.055889     3.903533     202.08
 C       0.818776    -2.408416     3.518663     102.70
 H       1.902189    -2.959097     3.215037      25.60
 H       0.319433    -2.435683     2.514757      29.18
 H       0.220493    -3.175800     4.096996      26.77
 C      -0.044803     0.785098     5.200063      22.13
 O       1.284483     1.051839     5.633574     272.58
 H       1.691402     1.873032     5.243260      25.00
 C      -1.173269     1.555062     5.369430      60.14
 H      -0.926163     2.380499     6.037408      27.50
 C      -2.443498     0.279186     3.840627     -24.14
 C      -3.723843     0.021094     2.961414      75.38
 H      -4.351139     0.933536     3.419833      23.71
 O      -4.323481    -1.324131     3.203741     235.59
 H      -5.215855    -1.250500     3.580820      20.17
 C      -3.455929     0.317692     1.317763      83.79
 H      -2.634726     1.075757     1.283765      26.11
 C      -4.698156     0.927178     0.631596     113.49
 O      -5.801726    -0.015056     0.371183     230.45
 H      -5.417956    -0.802518    -0.006036      24.64
 H      -4.245128     1.347371    -0.264041      24.16
 H      -5.104816     1.707636     1.172343      27.10
 C       0.177304     0.702312    -1.141101     108.20
 H       0.472005     1.698839    -1.329000      29.21
 C       0.365740    -1.772968    -1.013179      92.74
 H       0.762896    -2.755447    -1.048927      19.70
 C      -0.866966    -1.825607    -0.429981     -41.62
 O      -1.528411    -2.960942    -0.129988     228.70
 C      -0.765748    -4.248501    -0.347831     120.41
 H      -1.159184    -5.129132     0.056585      27.24
 H      -0.817262    -4.276280    -1.371336      31.13
 H       0.190667    -4.342260     0.123238      29.77
 C      -1.645066    -0.564266    -0.077272     -40.77
 O      -2.908936    -0.825025     0.705969      51.57
 C      -1.113069     0.588445    -0.457753      95.13
 H      -1.546325     1.553559    -0.136464      27.90
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 C       0.954544    -0.418123    -1.359049      19.30
 C       2.403125    -0.430520    -1.907631      87.83
 H       2.482012    -1.579101    -2.576626      25.26
 O       2.753114     0.712842    -2.719443     232.02
 H       3.233915     1.366226    -2.248230      31.03
 C       3.568179    -0.785169    -0.878835      88.34
 H       3.161455    -1.807366    -0.162683      25.90
 O       4.827879    -1.293024    -1.355660     209.29
 H       5.087033    -0.534271    -1.877613      30.67
 C       3.664541     0.158556     0.314483      97.17
 O       4.014895     1.551579    -0.148886     227.68
 H       3.689628     2.201884     0.606975      25.57
 H       4.600631    -0.175016     1.086263      24.70
 H       2.778413     0.352372     0.775286      28.51
55
name = lig-Water-frame_64
 C      -2.362793     1.310540     4.793807      41.48
 H      -3.087479     2.138892     4.856123      21.47
 C      -1.418161    -0.769256     3.740633      83.13
 H      -1.322590    -1.509075     3.083248      32.11
 C      -0.252808    -0.404266     4.432317       6.67
 O       1.006865    -1.029974     3.917238     139.02
 C       0.831241    -2.487439     3.488432     104.58
 H       1.811617    -2.876470     3.597149      28.36
 H       0.062762    -2.504007     2.493595      28.30
 H       0.360269    -3.181039     4.183565      28.43
 C      -0.029803     0.683397     5.152527      20.80
 O       1.270856     1.062294     5.637519     251.69
 H       1.590649     1.907169     5.104272      24.41
 C      -1.166939     1.620026     5.398918      36.67
 H      -0.910208     2.573127     5.924979      24.49
 C      -2.471193     0.205675     3.799692     -71.48
 C      -3.745261     0.059537     2.938423      78.01
 H      -4.427583     0.814286     3.166684      27.03
 O      -4.311257    -1.324242     3.174846     211.69
 H      -5.253952    -1.234309     3.468534      18.09
 C      -3.428257     0.304598     1.361337      81.76
 H      -2.559389     1.032632     1.491355      27.44
 C      -4.701443     0.944336     0.683044      95.33
 O      -5.765701     0.007559     0.314417     206.52
 H      -5.351271    -0.885737    -0.072760      20.69
 H      -4.317629     1.323003    -0.353677      22.95
 H      -5.147654     1.859305     1.334049      24.36
 C       0.212440     0.762345    -1.137889      83.13
 H       0.771191     1.718657    -1.369403      25.56
 C       0.352642    -1.759622    -1.015456      75.32
 H       0.840209    -2.755423    -1.128706      24.44
 C      -0.879791    -1.738431    -0.460482      -7.80
 O      -1.524972    -2.921114    -0.091097     120.51
 C      -0.778622    -4.249583    -0.357961      77.53
 H      -1.219155    -5.272731     0.134429      24.17
 H      -0.835781    -4.119104    -1.522184      26.56
 H       0.231576    -4.236319     0.291138      26.18
 C      -1.657857    -0.609280    -0.040850     -16.53
 O      -2.838511    -0.834600     0.686817      52.26
 C      -1.082706     0.647286    -0.496248      45.96
 H      -1.624894     1.525533    -0.205675      31.81
 C       0.899158    -0.473739    -1.330597       3.12
 C       2.454565    -0.544046    -1.947922      89.73
 H       2.611730    -1.274429    -2.544041      31.35
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 O       2.742988     0.708465    -2.714812     231.33
 H       3.182979     1.505927    -2.284874      27.48
 C       3.551673    -0.817740    -0.857412     105.93
 H       3.237404    -1.645537    -0.378192      32.18
 O       4.827891    -1.267946    -1.333438     204.50
 H       5.237974    -0.688006    -2.076913      27.76
 C       3.671364     0.173094     0.390422      94.88
 O       3.996671     1.555499    -0.159204     256.53
 H       3.753592     2.118863     0.633610      26.69
 H       4.481419    -0.215139     0.817362      29.88
 H       2.629008     0.313021     0.970034      27.58
55
name = lig-Water-frame_65
 C      -2.358712     1.321083     4.763385      -1.78
 H      -3.199133     2.004642     4.779902      24.36
 C      -1.463442    -0.701088     3.694768      65.38
 H      -1.401895    -1.627629     2.889345      35.98
 C      -0.237255    -0.490216     4.416679     -23.23
 O       1.011310    -1.035325     3.948306     103.36
 C       0.822943    -2.535767     3.477412     101.22
 H       2.007309    -2.830884     3.513172      27.07
 H       0.299024    -2.661809     2.546966      31.79
 H       0.325551    -2.919904     4.437408      25.63
 C      -0.020507     0.700326     5.173899     -17.47
 O       1.243707     1.067853     5.633659     272.56
 H       1.453162     1.819075     5.028248      29.72
 C      -1.088425     1.636655     5.425583      31.25
 H      -1.040773     2.724393     5.846797      19.43
 C      -2.517814     0.131754     3.798069     -14.47
 C      -3.734901     0.044605     2.903714      79.22
 H      -4.732621     0.782464     3.018387      23.93
 O      -4.297360    -1.300984     3.152028     223.23
 H      -5.317134    -1.187980     3.201108      16.80
 C      -3.406972     0.320799     1.459615      76.12
 H      -2.692634     1.127519     1.546953      32.96
 C      -4.671690     0.938736     0.675610      96.35
 O      -5.723386     0.049829     0.277012     215.55
 H      -5.476975    -0.860137    -0.076087      21.37
 H      -4.461179     1.455130    -0.278832      26.26
 H      -5.016769     1.761672     1.399441      27.45
 C       0.241729     0.774410    -1.110766      61.21
 H       0.876375     1.632607    -1.380017      27.02
 C       0.367581    -1.705150    -1.030422      72.04
 H       0.992287    -2.528140    -1.321828      29.79
 C      -0.958548    -1.700413    -0.444351      48.84
 O      -1.525049    -2.924111    -0.037163     106.78
 C      -0.791208    -4.225835    -0.355240     128.89
 H      -1.565186    -4.920842    -0.028456      28.65
 H      -0.529239    -4.390856    -1.372354      31.71
 H       0.146724    -4.055616     0.036081      31.82
 C      -1.625789    -0.616838    -0.046520       7.35
 O      -2.772746    -0.845663     0.658095      27.19
 C      -1.059373     0.709164    -0.516485      26.25
 H      -1.690333     1.634884    -0.340012      31.88
 C       0.922143    -0.537813    -1.334322     -11.21
 C       2.491680    -0.565280    -1.940301      69.28
 H       2.612727    -1.369989    -2.996145      25.05
 O       2.730954     0.690887    -2.731526     188.93
 H       3.076798     1.350323    -2.015532      28.09
 C       3.507058    -0.818051    -0.803476      73.50
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 H       3.035152    -1.959704    -0.368153      28.00
 O       4.844505    -1.233806    -1.327464     161.38
 H       5.218855    -0.930922    -2.187933      27.10
 C       3.650039     0.221373     0.390728     106.39
 O       3.977302     1.522658    -0.165558     224.09
 H       3.959793     2.346965     0.535028      22.58
 H       4.594112    -0.301424     1.017314      28.22
 H       2.860788     0.045670     1.072268      33.19
55
name = lig-Water-frame_66
 C      -2.330618     1.297558     4.696175      12.80
 H      -3.313116     1.889544     4.817528      18.16
 C      -1.449851    -0.693912     3.634847      58.11
 H      -1.612414    -1.418901     2.972257      31.91
 C      -0.190591    -0.546220     4.362901     -64.52
 O       0.984019    -1.075366     3.967809     116.12
 C       0.871691    -2.538268     3.553630     103.55
 H       1.898837    -2.830871     3.241977      28.50
 H       0.471375    -2.858801     2.390941      28.63
 H       0.273454    -2.828910     4.391251      25.44
 C      -0.035538     0.749296     5.223248     -30.46
 O       1.220581     1.064025     5.623819     312.70
 H       1.564029     1.875471     5.070556      24.78
 C      -1.074587     1.621518     5.396680      59.91
 H      -0.993583     2.540865     5.860438      26.08
 C      -2.583957     0.163313     3.870330      54.22
 C      -3.765170    -0.004191     2.890131     104.04
 H      -4.466696     0.656720     3.148430      34.85
 O      -4.303757    -1.278657     3.129855     309.39
 H      -5.245495    -1.240473     2.955684      24.91
 C      -3.395759     0.348277     1.490277      69.01
 H      -2.732155     1.308057     1.451920      31.45
 C      -4.609165     0.911609     0.645258      93.72
 O      -5.707058     0.104481     0.266015     243.07
 H      -5.421947    -0.793839    -0.097319      22.01
 H      -4.299518     1.626877    -0.210651      26.11
 H      -5.045352     1.660485     1.433343      26.06
 C       0.276554     0.715469    -1.072641      40.91
 H       0.734937     1.652324    -1.358958      29.35
 C       0.341497    -1.670449    -1.037509      58.15
 H       0.925442    -2.511189    -1.417334      30.20
 C      -0.973727    -1.769544    -0.437616      33.61
 O      -1.516635    -2.940180    -0.009799     125.60
 C      -0.833816    -4.154486    -0.356402     117.09
 H      -1.686804    -4.800584    -0.036124      26.75
 H      -0.448733    -4.559334    -1.398846      27.65
 H       0.302719    -4.122417     0.164161      28.18
 C      -1.575076    -0.509878    -0.083052     -37.40
 O      -2.741828    -0.829012     0.658295      14.84
 C      -1.042340     0.749489    -0.519114      98.58
 H      -1.589450     1.647689    -0.475441      33.47
 C       1.015565    -0.497911    -1.368902       7.61
 C       2.483589    -0.560773    -1.989943     111.02
 H       2.471136    -1.250176    -2.653511      32.91
 O       2.728939     0.669448    -2.717875     243.74
 H       2.956544     1.161594    -1.962255      32.61
 C       3.459285    -0.866661    -0.764324      97.86
 H       3.078385    -1.664617    -0.344984      33.82
 O       4.864187    -1.211343    -1.308383     163.37
 H       4.927361    -1.012049    -2.256637      29.87
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 C       3.688962     0.210544     0.378726     125.43
 O       3.954967     1.483729    -0.173134     238.14
 H       4.027172     2.293875     0.374059      26.04
 H       4.440974    -0.052352     1.009195      34.35
 H       2.826417     0.059038     1.171083      33.09
55
name = lig-Water-frame_67
 C      -2.334402     1.283967     4.646313      66.92
 H      -3.111204     1.905940     4.939044      23.25
 C      -1.408792    -0.680665     3.629639      18.98
 H      -1.688506    -1.529027     2.830709      27.30
 C      -0.198903    -0.496363     4.307332     -28.16
 O       0.971566    -1.146579     3.965493     194.13
 C       0.925109    -2.517931     3.588683     127.49
 H       2.003811    -2.928769     3.430942      28.83
 H       0.396441    -2.687951     2.670541      31.29
 H       0.297207    -3.195193     4.321035      27.27
 C      -0.053359     0.728412     5.216771     -14.55
 O       1.233399     1.067999     5.619303     266.83
 H       1.592635     1.899874     5.217615      24.90
 C      -1.138705     1.578322     5.320426      55.30
 H      -0.875001     2.497768     6.075195      21.88
 C      -2.587800     0.201487     3.939786      24.15
 C      -3.761593    -0.046510     2.928703      81.76
 H      -4.444425     0.895985     3.412908      25.06
 O      -4.324064    -1.292657     3.106026     291.83
 H      -5.273734    -1.340426     2.796933      23.39
 C      -3.386109     0.386817     1.420573      81.48
 H      -2.711763     1.187215     1.462767      31.81
 C      -4.543642     0.918395     0.628921      96.46
 O      -5.695761     0.150274     0.259710     266.13
 H      -5.334748    -0.720732    -0.180135      23.11
 H      -4.033016     1.592073    -0.117052      26.47
 H      -5.120135     1.585122     1.411233      23.52
 C       0.329804     0.658463    -1.048380      60.27
 H       0.553339     1.737896    -1.338823      28.59
 C       0.308546    -1.673242    -1.055103      58.00
 H       0.659342    -2.676445    -1.370713      30.98
 C      -0.905803    -1.787254    -0.451653     -31.85
 O      -1.502179    -2.940680    -0.020762     181.53
 C      -0.837400    -4.119618    -0.332544     120.16
 H      -1.463293    -5.015898     0.087344      26.58
 H      -0.752416    -4.272525    -1.406670      27.79
 H      -0.073524    -4.337041     0.326078      29.88
 C      -1.550513    -0.436714    -0.114951     -76.57
 O      -2.724212    -0.763080     0.681564      51.37
 C      -1.005286     0.742101    -0.516511     122.06
 H      -1.510112     1.746787    -0.487636      31.84
 C       1.079625    -0.414280    -1.387891      31.68
 C       2.427219    -0.510313    -1.978556      96.28
 H       2.419739    -1.666365    -2.671256      25.15
 O       2.742493     0.639051    -2.694143     170.65
 H       2.972110     1.382656    -1.968416      27.33
 C       3.471597    -0.868236    -0.769109      75.54
 H       2.994128    -1.859502    -0.033380      29.35
 O       4.864610    -1.194355    -1.281686     147.08
 H       4.597111    -1.070265    -2.258947      27.43
 C       3.690193     0.170143     0.381166     112.25
 O       3.934738     1.440668    -0.230411     180.26
 H       3.878773     2.164981     0.560644      25.47
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 H       4.692526    -0.047569     1.064466      28.42
 H       2.779006     0.367572     0.933797      30.49
55
name = lig-Water-frame_68
 C      -2.367151     1.339702     4.666241      27.11
 H      -3.130643     2.149032     5.010509      20.49
 C      -1.415566    -0.670795     3.645790      93.70
 H      -1.442537    -1.481645     2.946355      25.27
 C      -0.210267    -0.400150     4.258615      -9.08
 O       0.977980    -1.206456     3.979504     197.42
 C       0.967162    -2.543521     3.627627     116.37
 H       2.058318    -2.912329     3.747565      25.30
 H       0.198435    -2.456515     2.654469      25.52
 H       0.568226    -3.368908     4.228494      27.47
 C      -0.055269     0.666095     5.139722       3.15
 O       1.256350     1.059723     5.633422     295.08
 H       1.418292     1.973317     5.207920      27.92
 C      -1.160119     1.548816     5.284066      48.51
 H      -1.056639     2.268470     5.958231      22.49
 C      -2.528923     0.125698     3.903576     -13.91
 C      -3.751864     0.005125     3.008134      85.42
 H      -4.420661     0.692729     3.230920      28.55
 O      -4.353963    -1.338536     3.085370     313.99
 H      -5.304722    -1.353666     2.741807      26.42
 C      -3.376249     0.382127     1.366279      77.44
 H      -2.527512     1.179135     1.572285      29.79
 C      -4.512614     0.974540     0.637236     105.75
 O      -5.660286     0.175646     0.237078     261.94
 H      -5.456444    -0.637916    -0.223212      27.43
 H      -4.034887     1.490781    -0.267449      25.23
 H      -4.950947     1.721470     1.320969      26.39
 C       0.364123     0.708137    -1.044126      87.67
 H       0.693370     1.658782    -1.315760      28.84
 C       0.333015    -1.691419    -1.107599      77.16
 H       0.625574    -2.687793    -1.327387      29.58
 C      -0.846680    -1.698433    -0.445945     -29.45
 O      -1.499239    -2.905933    -0.039779     166.82
 C      -0.868202    -4.160756    -0.293468     100.98
 H      -1.442796    -5.039878     0.013167      25.72
 H      -0.851799    -4.079815    -1.387060      24.84
 H       0.069084    -4.423708     0.477285      24.44
 C      -1.572142    -0.480054    -0.110943     -24.21
 O      -2.699306    -0.668239     0.700379      30.67
 C      -0.958287     0.724043    -0.510997      87.65
 H      -1.385834     1.693611    -0.345180      33.47
 C       1.054794    -0.424674    -1.371227      14.86
 C       2.390413    -0.529232    -1.937079     109.77
 H       2.466764    -1.298213    -2.495102      31.68
 O       2.780059     0.625805    -2.679742     201.07
 H       2.974564     1.427703    -2.171492      30.71
 C       3.494008    -0.902317    -0.714936     105.74
 H       3.143268    -1.690543    -0.272226      33.88
 O       4.816915    -1.177607    -1.268341     176.05
 H       4.697949    -1.199070    -2.240829      28.36
 C       3.698968     0.137467     0.375342     131.64
 O       3.923260     1.427850    -0.296268     224.66
 H       3.757029     2.026484     0.445009      29.62
 H       4.504073    -0.194738     0.948229      33.03
 H       2.733977     0.378316     0.883363      29.38
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name = lig-Water-frame_69
 C      -2.421652     1.386070     4.702104      35.05
 H      -3.177816     2.091542     4.830788      24.85
 C      -1.420030    -0.678620     3.669963     102.66
 H      -1.334195    -1.552797     2.988938      27.11
 C      -0.155988    -0.366688     4.207429      21.56
 O       0.984458    -1.206346     4.039747     205.43
 C       0.974337    -2.601412     3.630439     112.15
 H       2.117848    -2.790435     3.554475      26.33
 H       0.557776    -2.700157     2.655835      28.27
 H       0.509366    -3.285549     4.421832      26.27
 C      -0.022921     0.650957     5.061020      29.88
 O       1.252630     1.046466     5.643941     262.75
 H       1.304773     1.927700     5.182029      30.80
 C      -1.142063     1.502178     5.266084      38.14
 H      -1.162125     2.433028     6.054980      17.45
 C      -2.505580     0.088130     3.835091     -17.41
 C      -3.736052     0.010615     3.023140      80.42
 H      -4.706485     0.768316     3.178128      21.22
 O      -4.376413    -1.379811     3.068721     311.12
 H      -5.303985    -1.244019     2.857382      26.24
 C      -3.317919     0.396736     1.401336      92.81
 H      -2.662034     1.184351     1.566654      31.18
 C      -4.499004     1.045800     0.608370      98.56
 O      -5.627058     0.210703     0.224970     218.06
 H      -5.441479    -0.701211    -0.244922      23.74
 H      -4.218856     1.353654    -0.447181      25.14
 H      -4.762316     2.094094     1.205240      25.26
 C       0.372733     0.793403    -1.046423      64.12
 H       1.031948     1.710061    -1.308803      24.07
 C       0.391876    -1.686633    -1.165656      75.16
 H       0.907792    -2.643227    -1.392196      26.44
 C      -0.847232    -1.624916    -0.412615      -7.04
 O      -1.504305    -2.839880    -0.043177     146.60
 C      -0.870231    -4.220949    -0.237059     102.37
 H      -1.810836    -4.951989    -0.114975      21.46
 H      -0.555620    -4.272372    -1.364193      24.88
 H       0.085097    -4.229291     0.135278      27.24
 C      -1.583176    -0.530754    -0.093871      64.73
 O      -2.674657    -0.605062     0.702267      60.71
 C      -0.913851     0.697399    -0.486487      55.63
 H      -1.358378     1.649040    -0.149783      29.61
 C       0.976937    -0.508553    -1.339153       5.40
 C       2.419752    -0.500453    -1.831636      73.13
 H       2.544617    -1.433238    -2.808941      24.96
 O       2.826446     0.609925    -2.699711     170.87
 H       2.976764     1.364246    -2.142251      30.67
 C       3.504836    -0.899378    -0.696182      90.23
 H       3.054468    -2.067732    -0.301940      27.43
 O       4.768608    -1.169011    -1.266452     163.05
 H       4.934709    -1.271994    -2.203268      26.86
 C       3.661060     0.131303     0.330576     126.14
 O       3.920667     1.411387    -0.359477     171.94
 H       3.821516     2.242248     0.274420      23.52
 H       4.495385    -0.307797     1.105149      29.28
 H       2.774642     0.064115     1.046215      30.52
55
name = lig-Water-frame_70
 C      -2.423779     1.319643     4.688804      64.07
 H      -3.299584     2.026056     4.714435      26.34
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 C      -1.378482    -0.729142     3.670172      38.56
 H      -1.482951    -1.697035     3.003405      31.55
 C      -0.079001    -0.423582     4.147430       2.75
 O       0.994925    -1.182769     4.104326     184.39
 C       0.992441    -2.658509     3.647125      94.65
 H       2.112249    -2.718371     3.344980      25.50
 H       0.791420    -3.125605     2.502292      25.93
 H       0.430775    -3.063918     4.506041      24.66
 C       0.027906     0.719070     5.033520      -8.60
 O       1.218264     1.030978     5.641473     256.87
 H       1.518054     1.904999     5.238901      26.23
 C      -1.149799     1.515075     5.293926      60.57
 H      -0.963536     2.321305     5.909908      24.81
 C      -2.547130     0.173394     3.816023     -49.72
 C      -3.780624    -0.027524     2.950910      98.26
 H      -4.478382     0.664573     3.283248      27.17
 O      -4.384559    -1.387401     3.053996     278.67
 H      -5.387020    -1.180353     3.108757      21.75
 C      -3.292704     0.459662     1.475547      75.65
 H      -2.636150     1.432659     1.589587      28.89
 C      -4.472489     1.117396     0.538837     105.94
 O      -5.620416     0.246380     0.233508     204.75
 H      -5.235755    -0.608345    -0.078932      25.59
 H      -4.082158     1.391336    -0.461205      27.47
 H      -4.774177     2.034850     0.970954      29.29
 C       0.388169     0.819861    -1.054544      97.14
 H       1.022567     1.652761    -1.169462      29.49
 C       0.385440    -1.712055    -1.170758      91.07
 H       1.072553    -2.493665    -1.418560      29.37
 C      -0.846488    -1.679301    -0.404978      -0.28
 O      -1.504819    -2.789396    -0.042840     118.99
 C      -0.902732    -4.237592    -0.250547     103.09
 H      -1.723951    -4.771962    -0.027303      26.25
 H      -0.519607    -4.510530    -1.212655      27.20
 H       0.216137    -4.207340     0.266817      25.01
 C      -1.539776    -0.487346    -0.086798      49.39
 O      -2.667415    -0.599673     0.699826      47.47
 C      -0.882576     0.711626    -0.435904      55.05
 H      -1.394920     1.594296    -0.000521      31.06
 C       0.965515    -0.486849    -1.336206     -24.29
 C       2.484111    -0.524921    -1.806233     108.12
 H       2.491414    -1.218098    -2.449372      34.29
 O       2.869780     0.589887    -2.716216     150.23
 H       3.030524     1.358233    -2.021611      26.77
 C       3.455263    -0.956377    -0.742530     126.03
 H       3.080882    -1.722494    -0.301559      35.18
 O       4.764656    -1.167705    -1.256006     180.39
 H       4.932359    -1.263787    -2.260121      24.93
 C       3.631654     0.120195     0.348090     122.73
 O       3.911597     1.396550    -0.398193     130.63
 H       3.980711     2.236295     0.151582      24.79
 H       4.459302    -0.056286     1.003357      34.50
 H       2.788457     0.012459     1.022523      33.62
55
name = lig-Water-frame_71
 C      -2.405159     1.217658     4.648301      81.24
 H      -3.227764     1.929646     4.794467      24.25
 C      -1.364214    -0.775570     3.648688      44.73
 H      -1.614335    -1.635469     3.140657      34.94
 C      -0.071899    -0.454245     4.128810      -5.06
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 O       1.045250    -1.197998     4.130377     170.18
 C       1.037888    -2.690549     3.629907     102.58
 H       2.143531    -2.869077     3.678844      28.39
 H       0.555384    -3.057082     2.772069      30.71
 H       0.528638    -3.201945     4.467660      28.02
 C       0.020773     0.799031     4.994854     -43.33
 O       1.201058     1.029589     5.639729     245.43
 H       1.747797     1.817169     5.329142      23.39
 C      -1.138285     1.521797     5.306895      40.80
 H      -0.806600     2.447047     5.965130      28.56
 C      -2.547161     0.228960     3.814151      -5.74
 C      -3.791257    -0.077098     2.858745      94.38
 H      -4.504430     0.754011     3.360231      25.13
 O      -4.403443    -1.355204     3.034693     275.59
 H      -5.328032    -1.297817     3.422948      21.65
 C      -3.314685     0.569282     1.513574      67.41
 H      -2.617099     1.332369     1.700942      31.20
 C      -4.424910     1.146937     0.459928      87.73
 O      -5.604862     0.290057     0.254432     197.43
 H      -5.172126    -0.552168     0.042463      26.94
 H      -3.719678     1.442896    -0.425668      26.75
 H      -5.036823     2.140565     0.922455      24.55
 C       0.393896     0.767022    -1.046230      93.64
 H       0.893185     1.781667    -1.063900      31.66
 C       0.338178    -1.717406    -1.130025      80.37
 H       0.969946    -2.562608    -1.365241      31.57
 C      -0.825475    -1.760287    -0.439129      12.82
 O      -1.512570    -2.811594    -0.046023     191.27
 C      -0.880046    -4.179377    -0.251315     114.36
 H      -1.695980    -4.899685     0.342177      25.71
 H      -0.736120    -4.593735    -1.361800      26.11
 H      -0.226325    -4.346277     0.540203      29.47
 C      -1.454752    -0.422305    -0.080781     -20.89
 O      -2.673139    -0.612227     0.705643      14.59
 C      -0.866120     0.770995    -0.363208      87.47
 H      -1.346090     1.647216     0.000830      34.55
 C       1.029248    -0.377271    -1.357424      -5.84
 C       2.495106    -0.518032    -1.823694      93.90
 H       2.449089    -1.662497    -2.589424      25.65
 O       2.912585     0.570089    -2.700737     165.83
 H       3.153918     1.305822    -2.121434      30.61
 C       3.434825    -0.942548    -0.786949      96.57
 H       2.919330    -1.919075    -0.060699      29.24
 O       4.798028    -1.186276    -1.253061     154.65
 H       4.680396    -1.177590    -2.225736      29.51
 C       3.614650     0.127753     0.360072     101.25
 O       3.894758     1.380759    -0.424666     147.82
 H       3.979312     2.058813     0.287700      28.25
 H       4.616571     0.056329     0.972238      29.80
 H       2.609038     0.306332     0.936304      32.63
55
name = lig-Water-frame_72
 C      -2.367547     1.209399     4.672754      59.42
 H      -3.180046     1.860673     4.929423      20.22
 C      -1.376974    -0.758942     3.637596      35.76
 H      -1.694909    -1.833300     3.141745      31.55
 C      -0.122341    -0.440882     4.153946     -31.81
 O       1.114473    -1.252948     4.123394     148.89
 C       1.095710    -2.689531     3.669188     103.66
 H       2.146896    -3.143505     3.962357      26.37
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 H       0.240536    -2.699596     2.794336      29.80
 H       0.630593    -3.426100     4.451340      27.71
 C      -0.012649     0.832150     4.927268     -42.28
 O       1.214538     1.030332     5.652039     180.43
 H       1.667168     1.822401     5.236576      20.02
 C      -1.101637     1.536451     5.305098      77.55
 H      -1.032332     2.437678     5.938389      35.32
 C      -2.495789     0.123251     3.747849      -9.95
 C      -3.789445    -0.034966     2.840129      98.79
 H      -4.564403     0.686038     3.170433      26.57
 O      -4.423375    -1.319779     3.007022     306.69
 H      -5.194311    -1.294766     3.575217      23.70
 C      -3.384667     0.623791     1.482528      60.58
 H      -2.513706     1.306010     1.847511      30.58
 C      -4.382578     1.203981     0.435901     110.73
 O      -5.553214     0.335855     0.264487     201.65
 H      -5.320531    -0.655662     0.032774      23.72
 H      -3.755455     1.392278    -0.412539      28.69
 H      -4.819255     2.032475     0.747022      30.87
 C       0.397838     0.771583    -1.008966      93.95
 H       0.760670     1.803191    -1.112491      35.27
 C       0.356429    -1.661045    -1.100692      61.87
 H       0.730782    -2.698702    -1.306798      32.03
 C      -0.828457    -1.740584    -0.470189     -15.25
 O      -1.534915    -2.898269    -0.053187     188.00
 C      -0.927175    -4.150279    -0.206901     124.93
 H      -1.573604    -4.804872     0.214185      30.80
 H      -0.881540    -4.376284    -1.176070      29.82
 H      -0.165924    -4.377916     0.697854      27.45
 C      -1.409979    -0.425373    -0.038778     -73.11
 O      -2.664840    -0.608297     0.708470     -15.59
 C      -0.846595     0.826380    -0.296245      69.26
 H      -1.249731     1.862666    -0.055019      30.19
 C       1.095726    -0.356498    -1.381915      -8.34
 C       2.451541    -0.561495    -1.937695     122.10
 H       2.467561    -1.343318    -2.446448      30.69
 O       2.957607     0.532522    -2.689734     214.03
 H       3.286707     1.256413    -2.148307      32.53
 C       3.443176    -0.939531    -0.703854     112.00
 H       3.071991    -1.759474    -0.364891      35.64
 O       4.813382    -1.217398    -1.264357     177.39
 H       4.621672    -1.119170    -2.197922      30.05
 C       3.598661     0.164258     0.338957     126.77
 O       3.879133     1.379732    -0.428710     154.10
 H       3.875261     2.028116     0.385956      27.31
 H       4.468261    -0.110698     1.016911      31.93
 H       2.746896     0.466287     0.836893      34.91
55
name = lig-Water-frame_73
 C      -2.319662     1.216943     4.697508      56.77
 H      -3.274112     1.780500     5.006056      16.86
 C      -1.403273    -0.786150     3.604464      78.76
 H      -1.457020    -1.693328     3.233213      32.64
 C      -0.137814    -0.427810     4.206274     -43.62
 O       1.159323    -1.298982     4.117373     125.72
 C       1.093753    -2.687863     3.754873     131.33
 H       2.120550    -3.093468     3.607811      30.31
 H       0.644717    -2.588726     2.831830      34.17
 H       0.511147    -3.291378     4.425937      28.38
 C       0.021693     0.788036     4.875055     -24.05
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 O       1.228986     1.040377     5.646747     202.43
 H       1.477618     1.885625     5.135208      22.48
 C      -1.128718     1.559446     5.271612     101.01
 H      -1.188202     2.419629     5.966130      32.35
 C      -2.458092     0.028451     3.703192     -10.48
 C      -3.786595     0.046654     2.865766      99.43
 H      -4.618421     0.793706     3.169937      22.89
 O      -4.429489    -1.289185     2.958178     272.87
 H      -5.155438    -1.138579     3.654990      22.63
 C      -3.411770     0.614774     1.421276      77.20
 H      -2.654388     1.312042     1.740673      30.73
 C      -4.335321     1.209960     0.442166      97.40
 O      -5.496333     0.372035     0.263000     227.41
 H      -5.371474    -0.530017    -0.041984      26.90
 H      -3.893022     1.309496    -0.667485      24.79
 H      -4.673010     2.424724     0.749389      24.31
 C       0.408691     0.829749    -0.960909      39.42
 H       0.852309     1.773167    -1.297633      28.63
 C       0.427788    -1.602159    -1.094321      28.62
 H       0.712639    -2.589123    -1.352895      28.57
 C      -0.882591    -1.651168    -0.456268      -6.08
 O      -1.568065    -2.934413    -0.064713      74.39
 C      -0.959235    -4.157333    -0.095922     119.26
 H      -1.889673    -4.952111     0.049190      23.25
 H      -0.659758    -4.319883    -1.289454      23.39
 H       0.064462    -4.196725     0.270210      28.55
 C      -1.443213    -0.456540     0.045663     -34.13
 O      -2.641957    -0.585932     0.707485      31.81
 C      -0.811307     0.848218    -0.249160      59.15
 H      -1.183343     1.815943    -0.076662      30.41
 C       1.088512    -0.418276    -1.388278      30.28
 C       2.439660    -0.550510    -1.989454      77.64
 H       2.480537    -1.606814    -2.859668      23.97
 O       3.004239     0.493671    -2.717488     180.48
 H       3.397902     1.163987    -1.986192      26.37
 C       3.471099    -0.905719    -0.655168      72.06
 H       3.036140    -2.061137    -0.332219      29.77
 O       4.804662    -1.251793    -1.272512     125.12
 H       4.810288    -1.056291    -2.286173      25.42
 C       3.592423     0.191473     0.296166     128.12
 O       3.880202     1.408081    -0.400002     200.52
 H       3.793539     2.201572     0.169518      28.57
 H       4.322281    -0.206874     1.102360      30.73
 H       2.639425     0.377637     1.001864      33.70
55
name = lig-Water-frame_74
 C      -2.331072     1.181911     4.665302      74.76
 H      -3.229194     1.619962     4.938390      27.66
 C      -1.361718    -0.835207     3.584845       5.25
 H      -1.236829    -1.915604     3.005769      23.38
 C      -0.100178    -0.464621     4.246458     -23.12
 O       1.171265    -1.290719     4.134674     141.02
 C       1.080428    -2.674434     3.823576     112.91
 H       2.097599    -2.916157     3.306919      24.09
 H       0.879844    -2.823550     2.562004      27.00
 H       0.286013    -3.220708     4.493410      21.95
 C       0.080390     0.732282     4.897036     -24.55
 O       1.230277     1.064908     5.605887     260.05
 H       1.533134     1.970503     5.213989      22.46
 C      -1.153568     1.569921     5.213579      22.67
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 H      -1.080232     2.394626     6.055751      19.02
 C      -2.486178     0.060558     3.723767      -1.43
 C      -3.784632     0.110177     2.880956     100.91
 H      -4.457657     0.938845     3.373138      25.36
 O      -4.436423    -1.233635     2.908560     257.99
 H      -5.146987    -1.092403     3.575051      26.42
 C      -3.365320     0.558817     1.372876      91.28
 H      -2.665370     1.459982     1.530357      27.09
 C      -4.322137     1.236424     0.401359     121.93
 O      -5.474515     0.422035     0.264575     268.55
 H      -5.131684    -0.434547    -0.136291      27.91
 H      -3.919945     1.295457    -0.545344      29.14
 H      -4.497522     2.139017     0.693148      31.05
 C       0.448740     0.860526    -0.933247      46.82
 H       0.959072     1.736637    -1.440360      20.97
 C       0.425776    -1.585200    -1.064977      50.43
 H       0.961095    -2.494261    -1.499121      22.57
 C      -0.909865    -1.591623    -0.422703      10.08
 O      -1.615425    -2.871281    -0.077072     112.30
 C      -0.964176    -4.220455    -0.089065     125.82
 H      -1.671535    -4.936105     0.064572      27.37
 H      -0.594400    -4.381811    -1.025817      28.55
 H       0.131365    -4.137795     0.199596      26.98
 C      -1.488637    -0.437050     0.127092      16.59
 O      -2.644593    -0.555906     0.726547     120.94
 C      -0.758995     0.812097    -0.221286      56.08
 H      -1.305586     1.774636     0.041565      26.95
 C       1.032057    -0.435123    -1.383328      16.94
 C       2.471265    -0.611050    -2.032288      90.76
 H       2.439982    -1.299743    -2.658584      32.60
 O       3.058975     0.483181    -2.751870     225.29
 H       3.395359     0.988249    -2.039246      28.94
 C       3.471717    -0.952031    -0.724151      92.42
 H       3.114267    -1.700688    -0.113819      31.03
 O       4.792788    -1.284425    -1.276523     183.32
 H       4.958123    -0.975432    -2.177398      29.08
 C       3.559601     0.216560     0.329485     107.06
 O       3.894812     1.454298    -0.373666     267.76
 H       3.714598     2.321259     0.123670      26.70
 H       4.376328    -0.049039     1.115284      28.11
 H       2.666985     0.153267     0.853518      34.12
55
name = lig-Water-frame_75
 C      -2.374855     1.121394     4.600593      63.87
 H      -3.350081     1.679934     4.894024      28.29
 C      -1.286074    -0.891163     3.577215      59.93
 H      -1.258724    -1.649328     2.885212      25.14
 C      -0.040646    -0.556497     4.249555     -11.90
 O       1.148106    -1.246258     4.160993     206.67
 C       1.059618    -2.658754     3.778143     113.64
 H       2.131689    -2.966179     3.826161      26.77
 H       0.616424    -2.936143     2.871483      29.10
 H       0.477712    -3.253352     4.407399      27.94
 C       0.076478     0.727353     4.978430     -12.37
 O       1.243290     1.096397     5.559450     299.92
 H       1.632300     1.946281     5.233703      24.90
 C      -1.099932     1.543236     5.164317      52.43
 H      -0.946162     2.260849     5.892023      15.93
 C      -2.490188     0.100957     3.754340       0.47
 C      -3.755151     0.146857     2.878547     100.09
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 H      -4.301848     0.921536     3.380842      28.46
 O      -4.446401    -1.144930     2.862611     274.71
 H      -5.229342    -1.162375     3.424462      27.42
 C      -3.274505     0.542233     1.359007     107.66
 H      -2.581060     1.394162     1.417365      27.75
 C      -4.312850     1.201585     0.359128      76.92
 O      -5.484186     0.457808     0.252097     236.09
 H      -5.026652    -0.375991    -0.135124      26.51
 H      -3.638462     1.395226    -0.661579      24.34
 H      -4.610089     2.349535     0.883224      24.72
 C       0.507831     0.838000    -0.943085      60.70
 H       0.892175     1.755868    -1.296785      19.89
 C       0.349505    -1.626443    -1.025859      45.22
 H       0.944107    -2.404568    -1.414581      21.20
 C      -0.896480    -1.622421    -0.378035      13.99
 O      -1.655554    -2.773430    -0.098380     102.10
 C      -0.902592    -4.222966    -0.130586      74.58
 H      -1.581491    -5.106656     0.391096      23.90
 H      -0.707047    -4.521748    -1.268617      22.37
 H      -0.112938    -4.218604     0.701633      25.32
 C      -1.452086    -0.375069     0.147718     -11.15
 O      -2.693807    -0.534784     0.775833     145.18
 C      -0.737801     0.778928    -0.185447      81.60
 H      -1.274023     1.646222     0.134660      27.94
 C       1.007181    -0.362030    -1.381408     -30.16
 C       2.499574    -0.631972    -1.982684      60.99
 H       2.393620    -1.689179    -2.847075      22.57
 O       3.107263     0.471742    -2.789049     171.98
 H       3.493160     1.142704    -2.073253      24.00
 C       3.481979    -0.950306    -0.841931      86.89
 H       3.093647    -1.765434     0.065530      25.88
 O       4.788209    -1.331549    -1.266338     191.36
 H       4.951729    -0.856105    -2.103095      26.82
 C       3.557691     0.229358     0.347049      84.11
 O       3.902477     1.507104    -0.352395     258.03
 H       3.677172     2.244970     0.331408      25.70
 H       4.433201     0.112291     1.035386      26.65
 H       2.441276     0.175324     0.771536      29.59
55
name = lig-Water-frame_76
 C      -2.397773     1.134806     4.600401      52.91
 H      -3.211033     1.773637     4.767278      25.04
 C      -1.228794    -0.860608     3.605473      67.99
 H      -1.360788    -1.594760     2.701573      26.79
 C      -0.023936    -0.604145     4.246964       4.96
 O       1.119533    -1.220400     4.178521     191.01
 C       1.085858    -2.651197     3.739317     100.64
 H       1.985461    -3.060183     4.317039      22.38
 H       0.276786    -2.875668     2.858562      22.96
 H       0.570951    -3.284143     4.661475      23.85
 C       0.014379     0.709994     5.040386       6.54
 O       1.280594     1.109827     5.540783     343.48
 H       1.586037     1.978888     4.977636      24.22
 C      -1.042975     1.459515     5.108307      62.76
 H      -0.909949     2.456446     5.813500      18.33
 C      -2.435628     0.042550     3.731024     -24.96
 C      -3.691712     0.145874     2.853177      87.36
 H      -4.429656     1.056759     3.273511      23.27
 O      -4.454090    -1.052845     2.810673     249.43
 H      -5.356307    -1.092108     3.279071      23.73
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 C      -3.229455     0.607589     1.387236      95.79
 H      -2.388827     1.328537     1.554003      27.58
 C      -4.270328     1.234247     0.361737     113.89
 O      -5.492748     0.467169     0.208873     206.91
 H      -5.347707    -0.459543    -0.023769      27.15
 H      -3.767214     1.443986    -0.489950      28.05
 H      -4.609006     2.048683     0.747460      30.62
 C       0.519099     0.819906    -0.943895      75.03
 H       0.879906     1.905263    -1.046895      28.40
 C       0.283430    -1.622172    -1.008053      51.94
 H       0.744146    -2.639651    -1.227616      28.75
 C      -0.879418    -1.680534    -0.317029     -22.08
 O      -1.677712    -2.711760    -0.124604     120.49
 C      -0.862512    -4.215703    -0.143996      76.20
 H      -1.562118    -4.794372     0.407018      24.75
 H      -0.750271    -4.511416    -1.143060      22.80
 H      -0.295713    -4.137993     0.763282      25.33
 C      -1.391834    -0.363727     0.129527     -62.34
 O      -2.707149    -0.555715     0.803346      72.82
 C      -0.725198     0.773761    -0.149682      65.45
 H      -1.101895     1.761712     0.180900      29.67
 C       1.032344    -0.349535    -1.383676     -76.31
 C       2.498147    -0.664532    -1.965832      99.49
 H       2.459143    -1.423955    -2.502389      27.49
 O       3.150683     0.450211    -2.805885     225.91
 H       3.447401     1.229211    -2.255483      29.13
 C       3.487957    -0.936361    -0.849111     105.94
 H       3.144160    -1.822130    -0.390759      30.47
 O       4.788228    -1.385383    -1.266893     179.27
 H       5.002219    -0.775509    -2.068443      25.21
 C       3.541465     0.237390     0.291569     103.17
 O       3.891215     1.557782    -0.318931     261.46
 H       3.820213     2.225990     0.414514      27.09
 H       4.412012     0.033406     1.095106      27.78
 H       2.617035     0.398168     0.734705      31.40
55
name = lig-Water-frame_77
 C      -2.337861     1.151995     4.613600      31.38
 H      -3.151260     1.944872     4.670187      20.68
 C      -1.237916    -0.810341     3.599465      75.40
 H      -1.325570    -1.565991     2.781722      25.96
 C      -0.066808    -0.550237     4.280415      15.58
 O       1.129277    -1.242456     4.177581     232.31
 C       1.067915    -2.670501     3.804587     106.39
 H       2.063041    -3.109621     3.966343      26.51
 H       0.617269    -2.807530     2.913442      31.13
 H       0.421904    -2.954770     4.590637      26.19
 C       0.033393     0.602136     5.059375      11.31
 O       1.311398     1.117773     5.523051     365.41
 H       1.481642     1.900037     4.888015      27.94
 C      -1.093797     1.464163     5.107271      68.64
 H      -0.975314     2.367767     5.487205      28.80
 C      -2.366416    -0.015366     3.716934     -19.02
 C      -3.651555     0.167390     2.817814      94.87
 H      -4.259715     0.916405     3.116417      28.53
 O      -4.473186    -0.993536     2.749569     264.31
 H      -5.333127    -0.763801     3.164665      26.60
 C      -3.214511     0.694204     1.433647      84.94
 H      -2.330691     1.328223     1.732932      25.31
 C      -4.226783     1.226315     0.416094      87.54
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 O      -5.508130     0.464209     0.152920     123.05
 H      -5.502396    -0.553904     0.126123      25.30
 H      -3.796428     1.493503    -0.718084      23.42
 H      -4.747695     2.335849     0.827961      23.74
 C       0.482878     0.846485    -0.911232      62.46
 H       1.004313     1.769326    -0.904186      30.53
 C       0.298160    -1.610972    -1.031331      66.14
 H       0.552982    -2.654598    -1.120423      29.62
 C      -0.876810    -1.652634    -0.257988      -5.40
 O      -1.690755    -2.727519    -0.146619     127.52
 C      -0.895126    -4.148662    -0.101828      67.10
 H      -1.889932    -4.693806     0.214963      21.80
 H      -0.535781    -4.496205    -1.129285      24.33
 H       0.093269    -3.914683     0.533880      25.14
 C      -1.395005    -0.428462     0.126638      10.45
 O      -2.656124    -0.590686     0.794947      28.98
 C      -0.690889     0.818153    -0.132620      27.77
 H      -0.926818     1.843151     0.219326      25.57
 C       1.083786    -0.432284    -1.383638     -56.86
 C       2.495241    -0.588318    -1.928986      76.75
 H       2.483809    -1.694302    -2.720968      20.22
 O       3.176532     0.411580    -2.822326     206.35
 H       3.325743     1.180485    -2.285546      32.17
 C       3.492969    -0.903871    -0.797182      83.21
 H       2.990816    -2.013367    -0.455622      26.39
 O       4.796407    -1.418750    -1.291390     155.48
 H       5.136253    -0.878266    -2.009166      25.77
 C       3.565139     0.249636     0.213472     117.60
 O       3.881465     1.584958    -0.297012     238.97
 H       3.989515     2.363605     0.425394      22.73
 H       4.210396    -0.136959     1.013957      29.99
 H       2.589653     0.455217     0.846218      28.59
55
name = lig-Water-frame_78
 C      -2.277358     1.140486     4.586341      39.82
 H      -3.043329     1.909467     4.560207      22.87
 C      -1.278712    -0.790521     3.558878      54.79
 H      -1.185249    -1.640442     2.907121      21.01
 C      -0.070864    -0.511763     4.324273      16.79
 O       1.159126    -1.264547     4.158618     219.96
 C       1.053132    -2.672774     3.912345      82.28
 H       2.083595    -3.075717     3.554787      21.61
 H       0.894186    -2.842354     2.653393      23.87
 H       0.093487    -3.038152     4.538164      21.81
 C       0.075382     0.550963     5.085679      10.12
 O       1.307420     1.091132     5.509653     313.40
 H       1.531678     1.984900     4.953411      27.11
 C      -1.124170     1.472887     5.139452      76.62
 H      -0.944660     2.645299     5.453259      23.23
 C      -2.364277     0.013098     3.734713      32.02
 C      -3.593150     0.164315     2.772616      80.13
 H      -4.220618     1.125793     3.353053      23.55
 O      -4.508071    -0.952673     2.684213     262.42
 H      -5.283379    -0.567257     3.086629      26.13
 C      -3.183376     0.720006     1.459512      71.22
 H      -2.437813     1.475524     1.656037      24.98
 C      -4.235971     1.267012     0.450493     116.80
 O      -5.524564     0.458958     0.106933     146.50
 H      -5.215136    -0.489203     0.245460      26.69
 H      -3.832935     1.390094    -0.444698      27.95
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 H      -4.550919     2.145300     0.750852      30.26
 C       0.476417     0.814175    -0.880020      72.73
 H       1.205759     1.678133    -0.929209      28.40
 C       0.345750    -1.608837    -1.056134      98.75
 H       0.735404    -2.612578    -1.342820      29.45
 C      -0.859659    -1.585766    -0.250949       1.29
 O      -1.681150    -2.788418    -0.165611     175.17
 C      -0.946827    -4.035768    -0.064718     121.40
 H      -1.780166    -4.802431     0.064494      24.23
 H      -0.443102    -4.349368    -1.020491      25.86
 H      -0.007199    -3.956910     0.345791      28.27
 C      -1.440671    -0.440373     0.156136      30.05
 O      -2.582033    -0.593405     0.779237      27.26
 C      -0.665335     0.850004    -0.118655      27.57
 H      -0.975022     1.777797     0.313838      24.37
 C       1.088642    -0.491270    -1.356748     -64.01
 C       2.517447    -0.570296    -1.961541     105.90
 H       2.502913    -1.317517    -2.529916      27.79
 O       3.179396     0.368803    -2.827499     200.61
 H       3.246100     1.227045    -2.230624      27.59
 C       3.480659    -0.905141    -0.770302      83.84
 H       2.977175    -1.692101    -0.181628      28.95
 O       4.801150    -1.441632    -1.305070     155.74
 H       5.185311    -0.950117    -2.065462      23.59
 C       3.570238     0.276154     0.198928     118.84
 O       3.895439     1.597223    -0.300282     245.59
 H       3.901935     2.296463     0.383372      25.16
 H       4.305215    -0.232261     1.024695      27.41
 H       2.612476     0.223039     0.709545      30.37
55
name = lig-Water-frame_79
 C      -2.253839     1.137333     4.537304      48.46
 H      -3.065863     1.859433     4.515009      24.76
 C      -1.269740    -0.795865     3.543375      49.11
 H      -1.135665    -1.830647     2.944196      18.07
 C      -0.046039    -0.571497     4.315802      50.25
 O       1.178947    -1.268815     4.140836     249.44
 C       1.013210    -2.679629     3.914188     104.21
 H       2.046954    -3.108087     3.930959      25.81
 H       0.763585    -2.757312     2.925883      30.99
 H       0.347147    -3.352479     4.329665      26.68
 C       0.073504     0.656243     5.141974       6.75
 O       1.301149     1.056341     5.506576     378.28
 H       1.495729     1.943322     5.098907      28.97
 C      -1.035801     1.504579     5.213296      37.52
 H      -0.950919     2.461891     5.542968      24.39
 C      -2.417485     0.057990     3.727722      46.19
 C      -3.565330     0.194059     2.796090      93.09
 H      -4.011145     0.917282     3.265445      29.61
 O      -4.540284    -0.909383     2.616313     254.10
 H      -5.407792    -0.617394     3.080696      24.73
 C      -3.163757     0.692803     1.438651      69.68
 H      -2.493415     1.634458     1.442302      24.75
 C      -4.277026     1.260863     0.483896      82.82
 O      -5.504683     0.454687     0.088562     159.64
 H      -5.037847    -0.378142     0.188642      28.58
 H      -3.582671     1.359741    -0.557486      23.45
 H      -4.587481     2.424543     0.893068      23.27
 C       0.540520     0.738415    -0.862583     103.67
 H       1.172438     1.616075    -1.005089      31.21
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 C       0.386707    -1.646358    -1.068196      72.19
 H       0.908230    -2.468744    -1.571269      29.02
 C      -0.816494    -1.595677    -0.314967     -51.47
 O      -1.657404    -2.812539    -0.173820     182.20
 C      -0.982730    -3.953818    -0.093879     112.48
 H      -1.526934    -4.910803     0.195317      25.66
 H      -0.624468    -4.180940    -1.128739      25.22
 H      -0.124344    -4.045476     0.825000      26.13
 C      -1.418067    -0.360321     0.164788       0.21
 O      -2.557178    -0.552514     0.796268      69.62
 C      -0.679860     0.831876    -0.091846      60.22
 H      -1.094924     1.761874     0.406276      26.25
 C       1.063708    -0.452856    -1.322673     -63.80
 C       2.543001    -0.571072    -1.958571      86.78
 H       2.486614    -1.668793    -2.757031      22.15
 O       3.166525     0.362596    -2.810911     197.36
 H       3.294715     1.221752    -2.366321      30.52
 C       3.494770    -0.873275    -0.793533      77.87
 H       3.040510    -1.657490     0.108762      26.54
 O       4.789800    -1.464793    -1.294717     118.33
 H       5.035042    -0.971957    -2.162339      21.93
 C       3.601763     0.269787     0.236458     111.99
 O       3.918077     1.582579    -0.327815     237.73
 H       3.702871     2.285698     0.438206      25.10
 H       4.397364     0.044092     0.937094      29.29
 H       2.530069     0.180199     0.642393      30.00
55
name = lig-Water-frame_80
 C      -2.215463     1.185856     4.525695      32.76
 H      -3.099750     1.889684     4.616586      26.27
 C      -1.206810    -0.838823     3.568050      68.31
 H      -1.351605    -1.658639     3.009805      24.85
 C      -0.040320    -0.601107     4.301030      30.52
 O       1.164188    -1.265897     4.148844     212.01
 C       1.020464    -2.706968     3.874734      80.59
 H       2.005295    -3.117798     4.355004      23.61
 H       0.511351    -2.764946     2.766993      25.14
 H       0.433824    -3.521590     4.572667      23.56
 C       0.047092     0.727876     5.142372      20.46
 O       1.322434     1.026097     5.533835     360.50
 H       1.474122     2.008607     5.127343      24.97
 C      -0.980258     1.513352     5.265658      37.16
 H      -0.911131     2.538044     5.871722      23.00
 C      -2.415992     0.046123     3.700610      36.36
 C      -3.572739     0.200994     2.816278      60.86
 H      -4.296985     1.181326     3.286820      22.72
 O      -4.568071    -0.864494     2.553879     251.64
 H      -5.400142    -0.842654     3.069387      27.35
 C      -3.175898     0.663057     1.386024      95.41
 H      -2.502566     1.462159     1.388438      29.37
 C      -4.306597     1.279978     0.472365     118.04
 O      -5.445012     0.467680     0.096483     225.56
 H      -5.140072    -0.523817    -0.045372      24.61
 H      -3.740982     1.464336    -0.331078      29.37
 H      -4.603175     2.183416     0.845213      29.85
 C       0.590692     0.713414    -0.819283      40.05
 H       1.057488     1.669866    -1.047642      23.44
 C       0.414423    -1.685225    -1.080256      43.83
 H       0.863966    -2.533615    -1.565537      24.58
 C      -0.788517    -1.647952    -0.407110     -31.48
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 O      -1.663233    -2.743166    -0.159797     132.95
 C      -0.931689    -3.983600    -0.107232     113.82
 H      -1.583734    -4.870965     0.303043      24.85
 H      -0.555094    -4.172109    -1.169786      21.25
 H      -0.423637    -3.917008     0.776822      26.89
 C      -1.321746    -0.317052     0.129420     -51.09
 O      -2.571044    -0.481531     0.834405     122.27
 C      -0.687404     0.807565    -0.067461     111.90
 H      -0.998254     1.737335     0.292264      28.92
 C       1.077909    -0.404752    -1.319062      36.30
 C       2.535033    -0.662021    -1.957469      96.69
 H       2.498881    -1.445071    -2.494311      33.17
 O       3.149957     0.374498    -2.802749     209.84
 H       3.346581     1.206482    -2.375526      29.46
 C       3.531536    -0.869116    -0.787983     112.59
 H       3.256190    -1.693515    -0.112667      29.24
 O       4.767104    -1.470239    -1.279861     189.00
 H       4.837255    -1.106753    -2.158292      28.47
 C       3.632525     0.265898     0.256214     113.20
 O       3.928632     1.571244    -0.355143     263.61
 H       3.664998     2.287692     0.266689      28.56
 H       4.526151     0.249587     1.068772      26.20
 H       2.631222     0.384870     0.753118      29.46
55
name = lig-Water-frame_81
 C      -2.175251     1.246301     4.543898      32.41
 H      -2.984956     1.888273     4.750612      25.05
 C      -1.188902    -0.856555     3.618746      59.15
 H      -1.521277    -1.752496     2.885604      22.57
 C      -0.045278    -0.548375     4.308849      16.75
 O       1.128306    -1.278086     4.176015     201.51
 C       1.021007    -2.773064     3.853840      86.97
 H       2.067510    -3.046549     4.155300      25.76
 H       0.771362    -2.990302     2.902258      31.85
 H       0.329804    -2.985374     4.646048      26.76
 C       0.080789     0.666028     5.075989      15.26
 O       1.358607     1.029656     5.577050     384.28
 H       1.551957     1.864002     5.149644      29.18
 C      -1.033785     1.578265     5.299806      50.03
 H      -0.910544     2.308084     6.113172      24.37
 C      -2.331049     0.049342     3.720174      11.21
 C      -3.682167     0.254337     2.818116      70.90
 H      -4.200892     0.994404     3.114582      29.66
 O      -4.578472    -0.841319     2.496091     280.41
 H      -5.297589    -0.979690     3.147538      27.88
 C      -3.222517     0.656204     1.355466     101.80
 H      -2.367174     1.437882     1.542082      27.25
 C      -4.317487     1.246110     0.461816      92.74
 O      -5.387652     0.465419     0.106163     221.73
 H      -5.300281    -0.418949    -0.279132      25.95
 H      -3.762728     1.721826    -0.598690      24.53
 H      -4.826693     2.263778     0.990348      24.17
 C       0.596900     0.779333    -0.751240       5.15
 H       1.024689     1.784162    -1.058203      20.46
 C       0.437916    -1.695235    -1.103550      14.98
 H       0.779119    -2.712453    -1.411538      23.60
 C      -0.807803    -1.665888    -0.471637      16.88
 O      -1.677976    -2.648400    -0.144667     108.14
 C      -0.907942    -4.052638    -0.119609      93.76
 H      -1.785416    -4.715443     0.076609      24.91
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 H      -0.303183    -4.345719    -0.956232      23.18
 H      -0.059891    -3.741461     0.742412      24.90
 C      -1.288301    -0.400851     0.106352     -44.94
 O      -2.552239    -0.436574     0.834170      59.45
 C      -0.610354     0.826617    -0.081325      73.81
 H      -0.931334     1.876648     0.200966      27.16
 C       1.144941    -0.448264    -1.348018      24.66
 C       2.520130    -0.670073    -1.888820      64.95
 H       2.495096    -1.785501    -2.647759      23.60
 O       3.126556     0.372272    -2.806996     167.50
 H       3.345543     1.162965    -2.118690      26.12
 C       3.578092    -0.890918    -0.754993      87.20
 H       3.113898    -1.939238    -0.142261      27.07
 O       4.752070    -1.458342    -1.272154     165.56
 H       4.853536    -1.264067    -2.252190      24.52
 C       3.693849     0.308741     0.286684     123.67
 O       3.932876     1.566567    -0.408763     263.03
 H       3.751446     2.344838     0.193300      27.85
 H       4.386274     0.077063     1.041297      30.43
 H       2.783478     0.442228     0.908024      30.39
55
name = lig-Water-frame_82
 C      -2.148355     1.290912     4.574594      28.55
 H      -3.078396     1.928640     4.800597      21.67
 C      -1.281998    -0.860980     3.640015      62.68
 H      -1.218547    -1.700506     3.036362      23.14
 C      -0.015249    -0.493071     4.315894      26.04
 O       1.107573    -1.292207     4.189839     172.40
 C       1.034799    -2.789305     3.899143      78.59
 H       2.113540    -3.142252     3.899371      24.34
 H       0.917525    -3.250943     2.738701      25.58
 H       0.111684    -2.828353     4.594846      19.19
 C       0.112036     0.627929     5.023102      12.00
 O       1.381534     1.028078     5.630084     356.26
 H       1.667148     1.892730     5.048473      22.98
 C      -1.046441     1.571497     5.309293      43.32
 H      -0.985448     2.229496     6.199830      22.30
 C      -2.254579     0.108126     3.758757      12.22
 C      -3.750944     0.247775     2.768397      42.01
 H      -4.376986     1.284804     3.315990      21.41
 O      -4.582871    -0.840009     2.456676     230.59
 H      -5.180862    -1.060718     3.257654      23.79
 C      -3.227541     0.711524     1.371935      98.20
 H      -2.564341     1.471000     1.646674      30.03
 C      -4.289809     1.280981     0.414628     113.96
 O      -5.383609     0.447740     0.100217     219.88
 H      -5.112258    -0.369896    -0.392257      25.45
 H      -3.967820     1.782897    -0.373569      30.19
 H      -4.828607     1.953336     1.036920      28.98
 C       0.650139     0.834363    -0.747593      25.97
 H       1.110652     1.748894    -0.977099      24.94
 C       0.447644    -1.688845    -1.131000      35.99
 H       0.825928    -2.679033    -1.290949      27.04
 C      -0.850781    -1.598034    -0.490397      36.27
 O      -1.674168    -2.623284    -0.150381      86.50
 C      -0.877444    -4.068240    -0.083559      90.38
 H      -1.905463    -4.667404    -0.107793      22.54
 H      -0.180918    -4.475186    -0.934432      23.14
 H      -0.116019    -3.979281     0.545437      27.70
 C      -1.300853    -0.457067     0.101069       1.57
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 O      -2.499801    -0.455190     0.788119      60.91
 C      -0.537631     0.843058    -0.093089      58.06
 H      -0.971514     1.784629     0.181425      29.03
 C       1.180748    -0.500351    -1.343704      -1.26
 C       2.543458    -0.695287    -1.866448     102.06
 H       2.545952    -1.500991    -2.395577      29.61
 O       3.095992     0.364633    -2.775239     237.09
 H       3.296186     0.973981    -2.096545      33.22
 C       3.567891    -0.952750    -0.688372      99.85
 H       2.966664    -1.670225    -0.164997      30.62
 O       4.772498    -1.441977    -1.273976     167.74
 H       4.924783    -1.393737    -2.274934      24.37
 C       3.744159     0.344066     0.306053     104.82
 O       3.942386     1.567213    -0.471199     194.04
 H       3.914444     2.349958     0.217883      25.38
 H       4.599518    -0.149105     1.040894      27.29
 H       2.780886     0.375284     0.967151      30.73
55
name = lig-Water-frame_83
 C      -2.172427     1.327001     4.605869      73.38
 H      -3.070598     1.847375     4.732364      26.87
 C      -1.329702    -0.826706     3.691395      70.91
 H      -1.107894    -1.768222     3.057267      23.23
 C      -0.006578    -0.515395     4.275193     -22.94
 O       1.124502    -1.309974     4.176758     199.30
 C       1.018654    -2.771954     3.919043     103.50
 H       2.043948    -3.282582     4.166256      25.26
 H       0.767754    -3.022701     2.957309      30.37
 H       0.271152    -3.399781     4.435451      23.70
 C       0.142200     0.708355     5.053125      15.82
 O       1.387362     1.037726     5.662841     247.31
 H       1.649682     1.788289     5.119447      25.19
 C      -0.973061     1.496525     5.307270      50.32
 H      -1.020469     2.289841     6.181974      22.43
 C      -2.281558     0.194990     3.760444     -20.90
 C      -3.785628     0.267640     2.731786      84.57
 H      -4.238561     0.940318     3.223403      28.62
 O      -4.586992    -0.854149     2.452476     287.66
 H      -5.125405    -1.107193     3.209517      25.94
 C      -3.208897     0.766049     1.393204      63.68
 H      -2.571452     1.707388     1.637051      27.86
 C      -4.280313     1.305241     0.419238      83.00
 O      -5.400707     0.404508     0.062848     162.67
 H      -4.872737    -0.373108    -0.348318      24.28
 H      -3.833056     2.013383    -0.543395      26.42
 H      -4.814137     2.065985     1.198897      24.95
 C       0.743674     0.810693    -0.805218      45.13
 H       1.374926     1.781182    -0.907548      29.47
 C       0.417690    -1.651994    -1.137416      58.37
 H       0.952021    -2.605517    -1.326502      26.28
 C      -0.859220    -1.534711    -0.494585      12.71
 O      -1.642763    -2.684651    -0.172774     132.15
 C      -0.897739    -4.063926    -0.103131     101.67
 H      -1.657475    -4.749290     0.029063      28.81
 H      -0.467766    -4.296817    -1.045897      27.68
 H      -0.208241    -4.245923     0.984278      24.90
 C      -1.299123    -0.360600     0.099621      27.45
 O      -2.463718    -0.492372     0.742920      49.59
 C      -0.517908     0.804202    -0.091409      60.57
 H      -1.029729     1.714405     0.275090      31.12
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 C       1.171474    -0.497501    -1.295844     -27.09
 C       2.603512    -0.673095    -1.837140     111.14
 H       2.619546    -1.810317    -2.561582      22.15
 O       3.056898     0.338733    -2.723173     199.58
 H       3.352660     1.131545    -2.133174      28.67
 C       3.531440    -0.940793    -0.660714      77.42
 H       2.921643    -1.789248     0.139064      27.49
 O       4.824838    -1.438441    -1.254935     121.13
 H       4.826244    -1.399175    -2.212503      26.71
 C       3.798444     0.300172     0.320413     112.47
 O       3.964462     1.568628    -0.505963     178.60
 H       4.011202     2.266370     0.138390      29.28
 H       4.681779     0.152595     0.825683      31.83
 H       2.908128     0.391626     0.880797      32.51
55
name = lig-Water-frame_84
 C      -2.195615     1.318477     4.617621      47.25
 H      -3.100589     1.997387     4.794573      24.18
 C      -1.284422    -0.784349     3.746853      65.16
 H      -1.497292    -1.674847     3.069645      26.69
 C      -0.027045    -0.528443     4.249267      -5.63
 O       1.144148    -1.342311     4.165687     196.83
 C       1.000278    -2.776024     3.957231      97.97
 H       1.927805    -3.160221     4.378866      25.83
 H       0.639675    -2.724599     2.780378      24.99
 H       0.475277    -3.643520     4.481349      24.49
 C       0.189415     0.754738     5.089577       8.78
 O       1.381100     1.044915     5.688908     279.45
 H       1.722986     1.910629     5.210573      24.21
 C      -0.924542     1.461380     5.324880      59.99
 H      -0.841801     2.248072     5.976745      28.37
 C      -2.390801     0.260416     3.721580     -24.75
 C      -3.723809     0.244236     2.700341      66.95
 H      -4.473372     1.114164     3.367085      21.67
 O      -4.578593    -0.884120     2.458912     247.25
 H      -5.211908    -1.096673     3.183523      22.92
 C      -3.182776     0.812104     1.388020      66.06
 H      -2.499426     1.627328     1.509769      28.22
 C      -4.302937     1.366349     0.440930     110.66
 O      -5.378474     0.370351     0.005865     158.92
 H      -4.956965    -0.482604    -0.211530      25.01
 H      -3.842325     1.807198    -0.326898      29.09
 H      -4.713220     2.197447     1.043089      27.83
 C       0.809355     0.758760    -0.854092      98.68
 H       1.466028     1.559250    -0.835796      31.67
 C       0.364712    -1.607268    -1.121468      79.59
 H       0.880406    -2.512905    -1.426934      27.27
 C      -0.829771    -1.553384    -0.491642     -12.67
 O      -1.593929    -2.774197    -0.191693     179.68
 C      -0.925406    -4.035989    -0.083665     108.66
 H      -1.691068    -4.968461     0.185970      25.25
 H      -0.548464    -4.084575    -1.176873      24.00
 H      -0.491469    -4.198083     0.772104      29.99
 C      -1.274079    -0.242926     0.072076      10.71
 O      -2.476071    -0.491677     0.734549      55.23
 C      -0.490571     0.795401    -0.099912      73.99
 H      -0.862869     1.727642     0.373589      29.84
 C       1.184654    -0.444812    -1.253485       8.66
 C       2.631396    -0.710185    -1.829093     128.69
 H       2.668013    -1.518243    -2.375424      30.99
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 O       3.028991     0.329240    -2.667666     219.26
 H       3.377699     1.197860    -2.269064      26.38
 C       3.516773    -0.927432    -0.621259     109.00
 H       3.342269    -1.702206     0.054667      31.47
 O       4.871544    -1.435594    -1.200917     124.20
 H       4.725891    -1.381145    -2.192349      27.57
 C       3.845472     0.247246     0.268900     102.44
 O       3.993891     1.556182    -0.533233     162.08
 H       3.999623     2.336172     0.148637      26.37
 H       4.887010     0.427891     0.856039      26.33
 H       2.939593     0.490475     1.037029      28.09
55
name = lig-Water-frame_85
 C      -2.226090     1.301726     4.625430      43.10
 H      -2.857901     2.134993     4.902529      26.78
 C      -1.296193    -0.720049     3.751225      45.90
 H      -1.682392    -1.541887     3.215255      23.78
 C      -0.004607    -0.501722     4.275867      16.93
 O       1.131172    -1.358025     4.186970     214.62
 C       0.982364    -2.804636     3.948072      87.39
 H       2.154318    -2.980649     4.147139      23.32
 H       0.873011    -2.844914     2.917999      28.75
 H       0.232244    -3.255323     4.665387      25.88
 C       0.223058     0.697600     5.074692      -0.16
 O       1.396941     1.066576     5.709545     268.88
 H       1.724966     1.980743     5.397433      25.55
 C      -0.947028     1.470685     5.328366      47.84
 H      -0.635949     2.490012     5.957968      20.93
 C      -2.481215     0.270978     3.694682      17.87
 C      -3.662549     0.270199     2.755407      99.01
 H      -4.287986     0.947601     3.014658      29.13
 O      -4.546046    -0.926080     2.468386     250.38
 H      -5.304026    -0.930084     3.160619      24.41
 C      -3.184823     0.803494     1.349223      78.26
 H      -2.323567     1.522051     1.483422      26.32
 C      -4.333865     1.372856     0.479405      96.50
 O      -5.337701     0.372199    -0.045027     146.60
 H      -5.022275    -0.587655    -0.072261      25.40
 H      -3.725179     1.736899    -0.573414      25.05
 H      -4.881540     2.311057     0.940400      25.66
 C       0.798001     0.748774    -0.835735      62.37
 H       1.571822     1.583419    -0.797994      25.08
 C       0.356684    -1.572040    -1.117757      66.11
 H       0.678593    -2.536551    -1.523581      26.25
 C      -0.825688    -1.611167    -0.450388      -7.79
 O      -1.572113    -2.804525    -0.193263     203.54
 C      -0.995749    -4.045902    -0.118765     113.95
 H      -1.747965    -4.711547    -0.050205      25.79
 H      -0.343074    -4.285563    -0.946707      27.41
 H      -0.086059    -3.985453     0.857017      24.46
 C      -1.287755    -0.269962     0.029415     -10.40
 O      -2.510492    -0.429294     0.745218      81.56
 C      -0.409622     0.881304    -0.121940      63.58
 H      -0.557027     1.815588     0.378247      25.45
 C       1.237942    -0.464540    -1.260263      29.39
 C       2.600017    -0.699364    -1.759253      99.25
 H       2.640661    -1.799806    -2.532028      23.58
 O       3.022746     0.344532    -2.653788     206.11
 H       3.338809     1.054055    -2.122787      29.40
 C       3.610289    -0.911888    -0.597139      94.57
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 H       3.353372    -1.909565     0.136206      25.96
 O       4.901226    -1.426214    -1.144774     128.29
 H       4.871996    -1.384142    -2.154133      27.12
 C       3.895811     0.293023     0.249263     131.72
 O       4.024487     1.548488    -0.556719     228.39
 H       3.883592     2.289423     0.100027      27.14
 H       4.722767     0.142654     0.839247      31.90
 H       3.202161     0.403400     0.990232      31.23
55
name = lig-Water-frame_86
 C      -2.226930     1.318780     4.657334      65.46
 H      -2.839157     2.208576     4.877013      23.62
 C      -1.372492    -0.624590     3.715498      37.56
 H      -1.539628    -1.772697     3.284424      21.28
 C       0.033667    -0.482341     4.320180      19.93
 O       1.096791    -1.341744     4.219295     198.76
 C       1.011453    -2.803220     3.959665      91.06
 H       2.006729    -3.127242     3.964259      25.41
 H       0.856106    -3.234115     2.770397      24.88
 H       0.146810    -2.921781     4.634868      23.43
 C       0.196344     0.645295     5.057374       3.81
 O       1.429496     1.081879     5.731046     247.32
 H       1.578363     1.967989     5.422057      26.49
 C      -0.955085     1.508166     5.308454      46.87
 H      -0.797662     2.359053     5.777962      22.46
 C      -2.477655     0.247632     3.738727      45.46
 C      -3.602761     0.280628     2.773348      76.36
 H      -4.437229     1.251445     3.012171      23.41
 O      -4.494101    -0.963800     2.498600     255.98
 H      -5.258843    -0.783830     3.041552      25.64
 C      -3.177535     0.758186     1.322520      95.27
 H      -2.373574     1.505337     1.500974      26.53
 C      -4.327820     1.355843     0.445239     116.44
 O      -5.303507     0.395924    -0.079869     186.72
 H      -4.921682    -0.532334     0.055443      28.51
 H      -3.884911     1.662317    -0.408007      28.79
 H      -5.029088     2.184394     0.786229      26.79
 C       0.802697     0.785934    -0.782463      61.91
 H       1.461944     1.634769    -0.817823      27.49
 C       0.392477    -1.589139    -1.136433      64.44
 H       0.586858    -2.568527    -1.612530      27.17
 C      -0.851471    -1.626121    -0.382010       7.57
 O      -1.585970    -2.754261    -0.198850     174.31
 C      -0.951152    -4.072033    -0.120807     104.34
 H      -2.000472    -4.722718    -0.134025      21.63
 H      -0.199529    -4.548942    -0.854349      25.11
 H      -0.270026    -3.970326     0.549008      30.51
 C      -1.309045    -0.344895     0.002369     -22.98
 O      -2.544552    -0.338780     0.743260     111.67
 C      -0.363138     0.944852    -0.136100      34.49
 H      -0.423659     1.962935     0.378341      23.47
 C       1.254266    -0.534776    -1.276071      33.96
 C       2.589664    -0.740665    -1.736117     106.78
 H       2.562284    -1.581169    -2.254407      29.76
 O       3.027363     0.361366    -2.657807     190.59
 H       3.341234     1.004503    -1.905252      24.21
 C       3.731807    -0.948807    -0.581533     107.11
 H       3.135073    -1.636947     0.027034      30.31
 O       4.934410    -1.413607    -1.103287     188.15
 H       5.093582    -1.359511    -2.045329      26.09
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 C       3.948660     0.359598     0.238054     107.86
 O       4.059864     1.540666    -0.562756     203.45
 H       3.813519     2.274552     0.025119      28.06
 H       4.865626    -0.159873     0.869227      27.46
 H       3.048012     0.397534     1.073848      28.04
55
name = lig-Water-frame_87
 C      -2.201523     1.371016     4.700503      54.59
 H      -3.043697     2.114607     4.719823      20.02
 C      -1.384963    -0.624749     3.668803      53.54
 H      -1.355128    -1.538305     3.316467      24.85
 C      -0.009834    -0.494476     4.331130      17.92
 O       1.087071    -1.318253     4.227339     210.48
 C       1.009758    -2.773359     3.916203      91.59
 H       1.984057    -3.443917     4.275173      23.91
 H       0.572609    -3.218146     3.094928      28.78
 H       0.203758    -3.201800     4.635304      23.57
 C       0.159044     0.677367     5.100380      19.80
 O       1.442728     1.073410     5.739063     241.83
 H       1.470347     2.043742     5.299799      24.91
 C      -0.961879     1.502309     5.237175      53.43
 H      -0.927084     2.556383     5.890102      24.40
 C      -2.428508     0.239705     3.830190      37.58
 C      -3.630930     0.324874     2.749142      89.62
 H      -4.169325     1.043615     3.162726      27.83
 O      -4.416803    -0.976212     2.547156     275.38
 H      -5.291590    -0.789809     2.990162      25.56
 C      -3.167258     0.748013     1.342790      96.99
 H      -2.554166     1.663481     1.496486      25.28
 C      -4.332457     1.316161     0.397871      94.62
 O      -5.280133     0.403992    -0.098525     199.09
 H      -4.849648    -0.449119     0.015473      27.96
 H      -3.738433     1.881429    -0.594802      24.27
 H      -4.940221     2.125317     0.887434      26.98
 C       0.853028     0.783749    -0.748343      62.73
 H       1.428160     1.717662    -0.883196      26.66
 C       0.396582    -1.665857    -1.144357      70.11
 H       0.695240    -2.577291    -1.638770      30.43
 C      -0.837440    -1.581293    -0.346161      -4.77
 O      -1.618821    -2.693936    -0.217790     114.98
 C      -0.932798    -4.131523    -0.162341      85.08
 H      -1.722019    -4.723612     0.074179      26.10
 H      -0.434915    -4.471036    -1.067145      24.77
 H      -0.316626    -4.122779     1.020386      24.20
 C      -1.320479    -0.340859     0.020642      -1.02
 O      -2.555128    -0.289240     0.701872     127.67
 C      -0.396654     0.943751    -0.119696      18.32
 H      -0.650489     1.874916     0.311007      25.32
 C       1.214599    -0.544084    -1.249277       5.32
 C       2.652103    -0.747269    -1.734632      77.24
 H       2.615905    -1.918780    -2.410980      25.06
 O       3.035082     0.366299    -2.646200     174.87
 H       3.367742     1.097464    -2.031803      24.90
 C       3.762837    -0.922441    -0.614012      99.69
 H       3.139621    -1.660867     0.164923      28.67
 O       4.997046    -1.425488    -1.066388     151.64
 H       5.193898    -1.230337    -2.059398      24.10
 C       3.982768     0.349408     0.286258     121.82
 O       4.110134     1.537367    -0.550039     226.17
 H       3.827328     2.381912    -0.009445      27.08
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 H       4.865038     0.200849     0.839248      31.35
 H       3.163240     0.508893     0.830602      31.98
55
name = lig-Water-frame_88
 C      -2.226040     1.394004     4.682798      41.83
 H      -3.076021     2.015892     4.746552      21.86
 C      -1.287769    -0.663924     3.667774      43.92
 H      -1.437334    -1.680765     2.892860      21.19
 C      -0.106888    -0.492867     4.337648      10.49
 O       1.095706    -1.313257     4.212098     209.29
 C       0.977975    -2.781341     3.956734     103.60
 H       1.790115    -3.194938     4.365204      26.22
 H       0.384764    -2.965034     2.897425      24.97
 H       0.363687    -3.386001     4.682041      25.02
 C       0.143278     0.711046     5.160028       1.45
 O       1.414054     1.076246     5.716488     319.03
 H       1.630005     1.930144     5.283104      29.10
 C      -0.953871     1.583556     5.225374      63.55
 H      -0.847639     2.359229     5.857390      25.74
 C      -2.401939     0.259968     3.887419      13.52
 C      -3.637964     0.305031     2.746784      72.91
 H      -4.356312     1.151285     3.380311      20.71
 O      -4.335205    -0.955721     2.611044     271.48
 H      -5.296986    -0.945907     2.934464      26.32
 C      -3.185460     0.811909     1.371863      75.99
 H      -2.642904     1.801303     1.477646      24.80
 C      -4.304133     1.324208     0.326570     102.97
 O      -5.268675     0.391226    -0.112212     227.44
 H      -4.858679    -0.563393    -0.180835      22.58
 H      -3.798193     1.885795    -0.347220      28.37
 H      -4.707313     2.101536     1.119660      26.44
 C       0.870432     0.753944    -0.713670      73.49
 H       1.484550     1.657519    -0.968745      25.69
 C       0.374982    -1.720153    -1.118950      74.82
 H       0.819054    -2.648166    -1.547986      29.42
 C      -0.781157    -1.551315    -0.370556     -65.41
 O      -1.660010    -2.676638    -0.230800     108.06
 C      -0.908041    -4.141134    -0.133305      82.08
 H      -1.789986    -4.918904     0.223644      23.12
 H      -0.585566    -4.246121    -1.195921      22.35
 H      -0.473184    -4.266100     0.704002      27.99
 C      -1.298628    -0.227588     0.077017      -3.68
 O      -2.536198    -0.293991     0.632048     108.95
 C      -0.468018     0.857690    -0.104083      66.46
 H      -1.006697     1.813311     0.233634      25.74
 C       1.205651    -0.524661    -1.207448     -67.54
 C       2.726956    -0.771162    -1.779978     110.53
 H       2.817458    -1.589016    -2.335628      29.36
 O       3.042789     0.352902    -2.639830     244.44
 H       3.406040     1.105468    -2.191101      27.61
 C       3.717152    -0.875335    -0.617798      97.22
 H       3.602995    -1.697347     0.121261      29.28
 O       5.077044    -1.453587    -1.055392     128.41
 H       5.164546    -1.111644    -1.981543      27.80
 C       4.010316     0.337936     0.299718     102.01
 O       4.169462     1.560901    -0.538718     230.50
 H       3.978260     2.336810     0.002950      29.35
 H       4.950801     0.510567     1.029817      26.27
 H       2.981767     0.582156     0.942761      27.47
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name = lig-Water-frame_89
 C      -2.255429     1.384052     4.636230      64.16
 H      -3.086862     2.120622     4.935432      25.84
 C      -1.243749    -0.736478     3.641169      61.15
 H      -1.453122    -1.293582     2.896076      26.37
 C      -0.112816    -0.486279     4.378017       3.00
 O       1.081352    -1.311676     4.200696     175.94
 C       0.878819    -2.774969     3.998630      87.14
 H       2.154598    -2.986492     4.072423      23.02
 H       0.747545    -2.725696     2.933780      27.84
 H       0.212467    -3.280587     4.776586      25.79
 C       0.107235     0.722520     5.181007       4.67
 O       1.369523     1.073723     5.681937     314.19
 H       1.739282     1.882492     5.208878      29.60
 C      -0.932877     1.674424     5.252082      32.95
 H      -0.688052     2.573811     6.022467      20.08
 C      -2.380456     0.253566     3.854382       9.34
 C      -3.649755     0.294953     2.831281      95.09
 H      -4.382674     0.972507     3.116690      26.54
 O      -4.261437    -0.938811     2.673471     299.66
 H      -5.180534    -0.991923     2.901113      28.70
 C      -3.221485     0.892758     1.359620      66.41
 H      -2.531666     1.715658     1.517363      26.53
 C      -4.267624     1.336948     0.367335      92.50
 O      -5.263971     0.362338    -0.131358     169.11
 H      -4.895027    -0.537845    -0.331620      23.39
 H      -3.714371     1.991475    -0.569633      24.90
 H      -4.780939     2.049397     1.004922      28.20
 C       0.829698     0.707030    -0.682630      83.28
 H       1.473389     1.513546    -0.914787      29.02
 C       0.396856    -1.711687    -1.078848      76.99
 H       0.773888    -2.687735    -1.334360      31.75
 C      -0.769362    -1.558323    -0.406008     -86.71
 O      -1.688340    -2.684234    -0.220809     112.33
 C      -0.991007    -4.122055    -0.132692      73.93
 H      -1.781382    -4.799824    -0.066097      25.21
 H      -0.524497    -4.212737    -1.151688      22.73
 H       0.051947    -4.205703     0.741694      23.47
 C      -1.255095    -0.196222     0.125541     -33.65
 O      -2.516761    -0.301271     0.576922      73.73
 C      -0.513782     0.826775    -0.098288     127.53
 H      -1.016167     1.748436     0.048039      31.50
 C       1.253989    -0.535774    -1.178311     -63.20
 C       2.756858    -0.708489    -1.776830      94.17
 H       2.958347    -1.776066    -2.577068      20.90
 O       3.051862     0.325993    -2.663950     208.35
 H       3.512567     1.128964    -2.116002      23.91
 C       3.750806    -0.851966    -0.571795      79.30
 H       3.578764    -1.757178     0.130863      28.51
 O       5.134492    -1.467723    -1.069226      90.09
 H       5.318324    -1.126836    -1.963728      26.06
 C       3.995144     0.395006     0.322643     122.12
 O       4.230119     1.592747    -0.535580     222.12
 H       4.114266     2.346249     0.136100      26.69
 H       4.769718     0.319002     1.109725      30.18
 H       3.173031     0.437316     0.913384      31.43
55
name = lig-Water-frame_90
 C      -2.231741     1.407921     4.638754      49.29
 H      -3.011466     2.052750     4.925167      25.64
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 C      -1.288031    -0.711025     3.655206      29.69
 H      -1.369557    -1.437683     2.615840      23.16
 C      -0.037712    -0.496812     4.420698      -6.46
 O       1.039830    -1.282959     4.216945     205.23
 C       0.880433    -2.725570     4.033741     109.65
 H       1.801728    -3.009294     3.847739      28.47
 H       0.753296    -2.911710     2.845585      26.23
 H       0.120199    -3.146732     4.667122      28.23
 C       0.049744     0.744984     5.165776      12.91
 O       1.337609     1.062826     5.649326     305.62
 H       1.603255     1.891718     5.042267      24.29
 C      -0.937205     1.740998     5.298317      44.38
 H      -0.724714     2.644444     5.854635      23.43
 C      -2.364413     0.234157     3.763389       7.21
 C      -3.622250     0.289580     2.893472      86.37
 H      -4.519555     1.131641     3.163261      22.82
 O      -4.195483    -0.962276     2.727840     266.70
 H      -5.177034    -0.917286     2.914774      26.67
 C      -3.221069     0.911571     1.343006      64.38
 H      -2.348165     1.616707     1.569560      24.24
 C      -4.237989     1.373067     0.403386     100.13
 O      -5.256309     0.346166    -0.149285     167.64
 H      -4.779939    -0.538651    -0.280990      25.11
 H      -3.873664     1.742061    -0.489445      25.95
 H      -5.117159     2.132420     0.707006      23.25
 C       0.768818     0.644236    -0.668419      39.41
 H       1.432109     1.584206    -0.763991      26.30
 C       0.465229    -1.674411    -1.029137      57.05
 H       0.736052    -2.725547    -1.231549      26.70
 C      -0.823964    -1.579579    -0.408542      16.09
 O      -1.687144    -2.701042    -0.193203     140.55
 C      -1.019133    -4.046846    -0.140250     118.92
 H      -1.919473    -4.798680    -0.132555      23.92
 H      -0.488906    -4.305783    -1.068655      25.57
 H      -0.201683    -4.019540     0.334955      31.04
 C      -1.249424    -0.341612     0.145974     -46.01
 O      -2.526657    -0.287938     0.557402      61.58
 C      -0.468775     0.899484    -0.124071      49.79
 H      -0.841509     1.950319    -0.049731      23.27
 C       1.330085    -0.576826    -1.160102      31.09
 C       2.758767    -0.691447    -1.766871     104.76
 H       2.821283    -1.542361    -2.274103      25.70
 O       3.081639     0.332902    -2.695828     261.48
 H       3.476018     0.986301    -2.153135      30.42
 C       3.859750    -0.860638    -0.526774      76.74
 H       3.191849    -1.624049     0.094057      27.34
 O       5.159729    -1.465021    -1.079505     108.63
 H       5.483149    -1.231414    -2.042025      23.29
 C       3.984193     0.438807     0.314464      99.84
 O       4.280802     1.626501    -0.503328     179.84
 H       4.218374     2.415761     0.161193      25.40
 H       4.824049     0.048815     1.091467      27.20
 H       2.955333     0.504832     0.973331      27.85
55
name = lig-Water-frame_91
 C      -2.151865     1.424245     4.657203      45.85
 H      -3.116160     2.029040     4.771668      23.47
 C      -1.332533    -0.668253     3.644572      59.02
 H      -1.144540    -1.428626     3.000085      24.86
 C      -0.053086    -0.482419     4.427230     -39.23
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 O       1.021839    -1.253709     4.249023     234.70
 C       0.878909    -2.642979     3.974979     104.80
 H       1.952654    -3.370080     4.116364      23.36
 H       0.311989    -3.054812     3.122220      24.77
 H       0.062318    -3.177395     4.658063      24.15
 C       0.026294     0.758088     5.143613      -9.72
 O       1.319343     1.068473     5.602979     305.40
 H       1.463173     1.851385     5.075266      26.32
 C      -0.999710     1.735911     5.294088      46.54
 H      -0.813740     2.740582     5.773470      24.57
 C      -2.344508     0.271058     3.710195      24.05
 C      -3.600240     0.322319     2.891907     100.48
 H      -4.215857     1.057705     3.379318      26.80
 O      -4.157867    -1.011685     2.785651     285.97
 H      -5.154747    -0.889558     2.868935      27.25
 C      -3.151414     0.871726     1.371463      75.63
 H      -2.406991     1.602649     1.515492      26.20
 C      -4.315359     1.409063     0.406220      90.95
 O      -5.232070     0.330213    -0.154315     214.85
 H      -4.711434    -0.544939    -0.145279      24.46
 H      -3.701464     1.752181    -0.620228      23.43
 H      -4.968357     2.156735     0.633645      26.81
 C       0.776380     0.633798    -0.680245      46.40
 H       1.316759     1.522396    -0.697006      26.67
 C       0.518395    -1.673146    -0.963820      50.98
 H       0.827892    -2.667160    -1.303679      23.16
 C      -0.859392    -1.612636    -0.396836      50.11
 O      -1.672391    -2.715783    -0.168886     150.64
 C      -1.083354    -3.963588    -0.231262      95.92
 H      -1.828493    -4.753847     0.185196      24.45
 H      -0.670651    -4.340921    -1.223468      24.54
 H      -0.133799    -3.933509     0.729555      22.53
 C      -1.252240    -0.419955     0.133039     -39.42
 O      -2.578262    -0.270568     0.569509     102.01
 C      -0.442795     0.912222    -0.146503      42.02
 H      -0.644947     1.991368     0.000470      22.04
 C       1.385213    -0.606152    -1.131084      54.99
 C       2.761799    -0.663299    -1.698512      72.80
 H       2.709029    -1.871201    -2.292300      22.21
 O       3.115035     0.344920    -2.731573     200.40
 H       3.502452     1.114650    -2.199077      26.59
 C       3.919669    -0.856121    -0.557662      94.24
 H       3.314877    -1.524380     0.076904      27.54
 O       5.166756    -1.455146    -1.066247     175.37
 H       5.289450    -1.347736    -2.045429      23.66
 C       3.980134     0.438900     0.327602     114.67
 O       4.324856     1.654851    -0.443161     193.40
 H       4.221227     2.433958     0.121897      28.60
 H       4.826324     0.147211     0.983247      27.54
 H       3.073477     0.685079     0.748216      28.64
55
name = lig-Water-frame_92
 C      -2.156203     1.414477     4.618885      39.66
 H      -3.019575     2.052946     4.614403      23.36
 C      -1.301595    -0.620648     3.675713      76.50
 H      -1.216795    -1.656247     3.067476      24.15
 C      -0.179674    -0.415992     4.413695     -18.86
 O       1.042154    -1.237961     4.276825     222.48
 C       0.860878    -2.650810     3.945141     129.06
 H       1.631169    -3.108231     4.291673      27.55
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 H       0.176047    -2.847162     3.090388      27.28
 H       0.268682    -3.014249     4.803730      25.66
 C       0.041946     0.754913     5.127711     -12.26
 O       1.305036     1.081552     5.556633     408.62
 H       1.559107     2.044172     5.127177      25.62
 C      -1.032443     1.697222     5.280040      61.59
 H      -0.895305     2.741021     5.792932      21.99
 C      -2.309898     0.354361     3.718534      25.33
 C      -3.532471     0.328219     2.838668      94.67
 H      -4.207985     1.105971     3.493936      24.85
 O      -4.144416    -1.048717     2.846890     295.47
 H      -5.090936    -0.997945     2.792368      28.60
 C      -3.112595     0.811124     1.400266      76.53
 H      -2.426313     1.749585     1.457614      24.28
 C      -4.363283     1.399718     0.337901      91.08
 O      -5.196552     0.329270    -0.131233     252.10
 H      -4.737378    -0.530956    -0.130881      25.20
 H      -3.626533     1.789158    -0.325613      26.00
 H      -4.861698     2.400727     0.875266      24.56
 C       0.841552     0.657045    -0.705329      42.34
 H       1.483638     1.606422    -0.830426      24.16
 C       0.537138    -1.724081    -0.901650      68.33
 H       0.939414    -2.618687    -1.376898      22.90
 C      -0.818533    -1.645952    -0.389719     -10.74
 O      -1.683068    -2.699891    -0.159466     182.43
 C      -1.075074    -3.947404    -0.252858     134.84
 H      -1.771363    -4.631427     0.313680      25.21
 H      -0.883177    -4.216209    -1.267500      26.62
 H      -0.495887    -4.011651     0.490035      30.38
 C      -1.288140    -0.336791     0.114602     -53.58
 O      -2.634020    -0.266344     0.599321     123.56
 C      -0.452816     0.814403    -0.152405      60.64
 H      -0.690983     1.814411     0.173159      25.49
 C       1.380890    -0.587236    -1.072294      26.21
 C       2.802834    -0.706036    -1.666143      99.35
 H       2.759108    -1.552487    -2.178927      29.84
 O       3.146067     0.343952    -2.744947     179.08
 H       3.481812     1.229174    -2.289598      25.12
 C       3.907577    -0.820049    -0.633658      97.25
 H       3.702375    -1.676813     0.236891      25.34
 O       5.151911    -1.436493    -1.036638     192.62
 H       5.114673    -1.407628    -2.034034      24.65
 C       4.030035     0.437872     0.302411     105.05
 O       4.371366     1.671432    -0.398578     171.81
 H       4.109979     2.464717     0.272820      23.83
 H       4.848921     0.378287     1.168203      26.19
 H       2.968640     0.690262     0.794475      24.96
55
name = lig-Water-frame_93
 C      -2.233854     1.422700     4.543012      55.21
 H      -2.968718     2.247426     4.578836      23.76
 C      -1.281263    -0.618888     3.675078      76.96
 H      -1.663613    -1.533763     3.190473      25.93
 C      -0.211650    -0.377710     4.409054      -9.73
 O       1.049321    -1.203235     4.298370     154.80
 C       0.764460    -2.635532     3.975915      82.51
 H       1.996800    -3.076738     4.134288      23.78
 H       0.420477    -2.677566     2.855683      25.82
 H       0.234355    -2.912487     4.944560      25.46
 C       0.047247     0.800833     5.125859      14.30
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 O       1.315819     1.116589     5.513751     478.16
 H       1.547241     1.981625     5.196936      28.88
 C      -0.998799     1.660491     5.288435      68.85
 H      -0.917265     2.526839     5.846613      24.24
 C      -2.279535     0.393089     3.723126      21.99
 C      -3.471537     0.317909     2.801329      92.00
 H      -4.307314     1.011062     3.135631      25.81
 O      -4.120739    -1.065898     2.905223     293.31
 H      -5.109431    -1.053505     2.729974      27.14
 C      -3.144998     0.798719     1.399522      92.22
 H      -2.499615     1.624705     1.458121      28.32
 C      -4.352447     1.388507     0.352603      99.29
 O      -5.178090     0.356028    -0.098361     226.85
 H      -4.671083    -0.529576    -0.225477      23.38
 H      -3.626523     1.896283    -0.475051      26.49
 H      -4.821240     2.091850     0.889223      30.01
 C       0.916753     0.708392    -0.725279      84.05
 H       1.514811     1.543064    -0.970062      28.23
 C       0.541377    -1.780931    -0.854281      76.86
 H       0.949211    -2.701819    -1.315064      23.48
 C      -0.755556    -1.621944    -0.360004     -53.38
 O      -1.710869    -2.641141    -0.157842     175.26
 C      -1.103728    -3.991798    -0.261392      80.90
 H      -2.007740    -4.686699     0.105761      21.82
 H      -0.929623    -4.221003    -1.379474      24.34
 H       0.038591    -4.116448     0.476834      22.85
 C      -1.326750    -0.250104     0.071701     -24.49
 O      -2.646357    -0.283449     0.626472     146.17
 C      -0.460127     0.701589    -0.144261      83.34
 H      -0.876061     1.638548     0.348585      28.07
 C       1.357698    -0.552415    -1.007731     -14.97
 C       2.834168    -0.703979    -1.649679      85.96
 H       2.887552    -1.773931    -2.451237      23.45
 O       3.174627     0.333294    -2.734562     211.75
 H       3.411246     1.104571    -2.297617      32.18
 C       3.899862    -0.801044    -0.608446     105.72
 H       3.685727    -1.526034     0.147512      28.69
 O       5.130436    -1.405362    -1.030824     192.03
 H       5.306452    -1.444728    -2.052082      23.20
 C       4.083055     0.459058     0.289637     128.51
 O       4.406739     1.698283    -0.365325     225.24
 H       4.116781     2.344396     0.306345      27.34
 H       4.673223     0.409046     1.250984      28.86
 H       3.112768     0.401825     0.773043      29.62
55
name = lig-Water-frame_94
 C      -2.264510     1.513305     4.532080      59.84
 H      -2.975830     2.382340     4.544578      24.81
 C      -1.347933    -0.621895     3.655014      70.51
 H      -1.771555    -1.504220     3.224620      28.75
 C      -0.091278    -0.395144     4.410234     -26.19
 O       1.021794    -1.153287     4.318445     205.24
 C       0.758045    -2.592487     4.035912     130.32
 H       1.635085    -2.933671     3.760689      31.08
 H       0.541700    -2.731426     2.994498      30.93
 H       0.038696    -3.100665     4.693125      28.30
 C       0.049004     0.852715     5.114420      15.00
 O       1.350469     1.142708     5.495802     347.27
 H       1.506809     2.093863     5.048540      21.68
 C      -1.019604     1.640026     5.279378      72.64
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 H      -0.883155     2.537354     6.116763      24.67
 C      -2.299144     0.374322     3.679587      14.06
 C      -3.475030     0.274489     2.766393      90.51
 H      -4.372786     1.048228     2.976358      25.64
 O      -4.080593    -1.069196     2.955936     298.20
 H      -5.048239    -1.015174     2.685243      26.59
 C      -3.223225     0.808420     1.343115      99.17
 H      -2.403052     1.611482     1.519400      26.66
 C      -4.242996     1.359535     0.405882     103.53
 O      -5.178978     0.371421    -0.075278     163.13
 H      -4.646199    -0.407911    -0.367255      28.25
 H      -3.989834     1.894360    -0.526848      27.43
 H      -5.095693     2.049627     0.988535      25.64
 C       0.917839     0.730162    -0.718188      93.70
 H       1.473653     1.666526    -1.002240      29.25
 C       0.554896    -1.791127    -0.814940      79.84
 H       0.877118    -2.775315    -1.111349      27.02
 C      -0.748119    -1.570456    -0.305928     -51.30
 O      -1.706663    -2.589168    -0.155060     170.18
 C      -1.118371    -4.061340    -0.260484     114.23
 H      -1.935683    -4.711159    -0.073879      25.48
 H      -0.910864    -4.219524    -1.281056      28.32
 H      -0.209484    -4.133098     0.000748      30.97
 C      -1.363642    -0.311517     0.009124      15.26
 O      -2.604644    -0.321719     0.634385      84.54
 C      -0.424118     0.733044    -0.116425      44.62
 H      -0.834243     1.609861     0.297283      28.24
 C       1.378363    -0.566657    -0.989457     -50.10
 C       2.824836    -0.722328    -1.703328     113.38
 H       2.959507    -1.582858    -2.221326      26.84
 O       3.193539     0.302532    -2.705956     212.35
 H       3.434847     1.135562    -2.141984      28.61
 C       3.939342    -0.780268    -0.548727      80.10
 H       3.238432    -1.514624     0.224391      28.11
 O       5.133539    -1.378776    -1.045417     210.57
 H       5.489743    -1.357407    -1.963371      23.53
 C       4.117100     0.461866     0.290597     117.03
 O       4.429136     1.707408    -0.351495     181.22
 H       4.194344     2.504668     0.367469      22.33
 H       4.811876     0.193986     1.202309      28.87
 H       3.022226     0.428349     0.733641      29.22
55
name = lig-Water-frame_95
 C      -2.232866     1.602770     4.536749      39.24
 H      -3.001850     2.329318     4.514510      23.79
 C      -1.374927    -0.616002     3.678794      47.73
 H      -1.526349    -1.703765     3.153192      24.53
 C      -0.033257    -0.392178     4.377646      -6.00
 O       1.003560    -1.144431     4.342197     228.72
 C       0.756305    -2.522429     4.058776     106.42
 H       1.843348    -3.122217     3.833756      25.90
 H       0.136082    -2.631769     3.004686      27.75
 H      -0.003929    -3.273968     4.476115      24.39
 C       0.075465     0.829891     5.069295     -24.03
 O       1.394952     1.200317     5.490506     302.13
 H       1.537139     2.039808     4.914879      21.62
 C      -1.103828     1.703260     5.301418      48.10
 H      -0.943452     2.361569     6.012081      25.56
 C      -2.361711     0.404464     3.648015      16.74
 C      -3.567601     0.237227     2.736791      95.41
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 H      -4.258289     1.072129     3.155126      26.13
 O      -4.038127    -1.060221     2.989368     324.39
 H      -4.939919    -1.058196     2.689109      27.83
 C      -3.213133     0.812920     1.275279      90.95
 H      -2.485183     1.540464     1.544094      26.87
 C      -4.235482     1.370185     0.472287     113.22
 O      -5.186174     0.360229    -0.069307     137.80
 H      -4.701235    -0.409490    -0.432873      28.25
 H      -3.944524     2.007487    -0.421672      26.67
 H      -4.878317     1.972250     0.979699      30.10
 C       0.858934     0.714331    -0.690932      51.07
 H       1.338298     1.687474    -0.888072      28.50
 C       0.572269    -1.727771    -0.767267      71.70
 H       0.881340    -2.785162    -0.917839      27.20
 C      -0.777051    -1.568310    -0.261678       5.40
 O      -1.672183    -2.591395    -0.144118     128.72
 C      -1.175665    -4.066677    -0.330322      75.34
 H      -1.999431    -4.945536     0.106913      22.67
 H      -1.040173    -4.170478    -1.481278      25.20
 H       0.015189    -4.222839     0.194958      24.21
 C      -1.336127    -0.371790    -0.043536      13.82
 O      -2.545825    -0.376252     0.622101      56.19
 C      -0.393222     0.822623    -0.089936       4.96
 H      -0.701168     1.900838     0.183721      22.43
 C       1.430083    -0.616167    -1.028592     -10.72
 C       2.813756    -0.693775    -1.708709     100.96
 H       2.926899    -1.897717    -2.258698      22.14
 O       3.203618     0.282762    -2.662211     226.38
 H       3.496694     1.087431    -2.090651      27.07
 C       3.931392    -0.784603    -0.529381      93.10
 H       3.383540    -1.436788     0.119647      30.43
 O       5.155702    -1.367814    -1.024912     175.36
 H       5.380543    -1.161707    -2.041956      21.79
 C       4.115396     0.450241     0.339340     112.82
 O       4.447133     1.711193    -0.343955     204.32
 H       4.299280     2.421669     0.294866      27.96
 H       4.985054     0.041164     0.956661      28.19
 H       3.147749     0.758274     0.765164      26.20
55
name = lig-Water-frame_96
 C      -2.212167     1.626469     4.490481      25.40
 H      -3.131347     2.322870     4.565702      21.31
 C      -1.352926    -0.612615     3.722704      76.20
 H      -1.296706    -1.454702     3.212147      26.13
 C      -0.123990    -0.321008     4.327581       1.10
 O       1.034504    -1.199174     4.373116     218.22
 C       0.760696    -2.524844     3.979703     131.34
 H       1.636765    -2.998678     4.156721      28.41
 H       0.165568    -2.406875     3.142341      28.36
 H       0.165226    -3.031616     4.783300      27.02
 C       0.076801     0.821462     5.030956     -24.08
 O       1.421770     1.265383     5.486801     277.26
 H       1.657599     2.086860     4.903743      23.15
 C      -1.114417     1.735296     5.304476      13.86
 H      -1.002957     2.628904     6.166093      22.63
 C      -2.392700     0.452325     3.647196       7.30
 C      -3.644817     0.254272     2.740597      92.19
 H      -4.373875     1.037751     3.260655      24.28
 O      -4.014998    -1.060484     3.003201     303.08
 H      -4.967486    -1.268804     2.707826      24.02
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 C      -3.126372     0.746010     1.261907      70.50
 H      -2.430425     1.619377     1.504535      24.51
 C      -4.300173     1.388176     0.458233      89.61
 O      -5.194428     0.348183    -0.076138     165.34
 H      -4.701991    -0.527359    -0.322560      24.31
 H      -3.666700     2.080525    -0.235472      25.13
 H      -4.830459     2.166223     1.266777      24.17
 C       0.812652     0.662768    -0.669526      32.23
 H       1.355423     1.594577    -0.787104      27.98
 C       0.591913    -1.660754    -0.718790      77.12
 H       0.984553    -2.661089    -0.821041      28.72
 C      -0.753285    -1.621656    -0.263036     -19.64
 O      -1.639789    -2.665318    -0.117976     159.82
 C      -1.192849    -4.064893    -0.403531     127.27
 H      -1.834349    -4.666329     0.132137      27.72
 H      -1.236107    -4.167025    -1.441851      27.45
 H      -0.474857    -4.237835     0.216388      30.97
 C      -1.268786    -0.290287    -0.037424     -37.90
 O      -2.506062    -0.422423     0.602692      90.90
 C      -0.414165     0.895540    -0.075280      50.76
 H      -0.643093     1.912425     0.039548      21.44
 C       1.439546    -0.619708    -1.076542      12.41
 C       2.832526    -0.735240    -1.682031     128.78
 H       2.783520    -1.651219    -2.160183      26.04
 O       3.207433     0.281305    -2.621620     291.87
 H       3.559584     0.995585    -2.151504      30.08
 C       3.885783    -0.780888    -0.572082      82.73
 H       3.673176    -1.710998     0.275727      25.52
 O       5.182767    -1.349768    -0.994088     189.95
 H       5.140061    -1.161536    -1.938145      27.71
 C       4.124232     0.454595     0.376927     101.29
 O       4.479107     1.682285    -0.367996     213.27
 H       4.277540     2.426520     0.378176      24.14
 H       5.024594     0.145382     0.995541      27.69
 H       3.265424     0.782758     1.074812      26.32
55
name = lig-Water-frame_97
 C      -2.240745     1.611275     4.427047      43.84
 H      -3.023515     2.260689     4.618738      21.59
 C      -1.364635    -0.541963     3.760498      82.10
 H      -1.360083    -1.515676     2.995040      23.85
 C      -0.172073    -0.279118     4.298725     -17.34
 O       1.056778    -1.213024     4.404723     149.13
 C       0.733133    -2.544155     3.965319      91.63
 H       1.801893    -3.092776     4.077426      24.29
 H       0.282784    -2.556574     2.777697      23.56
 H       0.225153    -2.716922     4.947095      22.09
 C       0.058967     0.932187     5.047128     -15.22
 O       1.418770     1.308140     5.481084     211.34
 H       1.624112     2.221271     4.972732      20.49
 C      -1.031963     1.766024     5.315422      49.66
 H      -1.068244     2.569957     5.902940      29.62
 C      -2.379122     0.472439     3.669836      38.84
 C      -3.649437     0.314665     2.777312      91.09
 H      -4.635013     0.942186     3.034094      22.68
 O      -4.019795    -1.093037     3.001218     315.67
 H      -4.939087    -1.395489     2.752850      24.16
 C      -3.074082     0.672447     1.291880      83.61
 H      -2.356663     1.495196     1.372744      26.18
 C      -4.329531     1.406513     0.459304      98.26
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 O      -5.198045     0.350607    -0.095290     215.15
 H      -4.697587    -0.482722    -0.039909      26.87
 H      -3.809109     1.996789    -0.287979      27.53
 H      -4.760620     2.002736     1.206887      27.68
 C       0.836113     0.621408    -0.675932      49.94
 H       1.545562     1.501643    -0.772046      25.14
 C       0.617477    -1.670814    -0.686261      63.75
 H       1.137600    -2.638379    -0.818239      25.41
 C      -0.698012    -1.623041    -0.290462     -41.41
 O      -1.609978    -2.744044    -0.083204     137.44
 C      -1.233062    -4.027703    -0.468000      87.80
 H      -2.230250    -4.597046     0.139997      19.45
 H      -1.240941    -4.324668    -1.585946      24.23
 H      -0.193830    -4.347114     0.251307      22.98
 C      -1.210564    -0.209554     0.022817     -49.57
 O      -2.485217    -0.434581     0.587695     138.90
 C      -0.459094     0.905040    -0.089602      91.71
 H      -0.812425     1.968205     0.047712      23.30
 C       1.382623    -0.540526    -1.083512      46.21
 C       2.842018    -0.753623    -1.616786      79.69
 H       2.806133    -1.858067    -2.354820      22.76
 O       3.200873     0.278236    -2.601581     238.20
 H       3.705464     1.075137    -2.089066      23.01
 C       3.863891    -0.831102    -0.526082     101.57
 H       3.656584    -1.572844     0.159915      28.74
 O       5.190943    -1.311109    -0.960592     167.75
 H       5.271277    -1.361561    -2.007101      25.44
 C       4.136880     0.464842     0.398235     106.50
 O       4.498442     1.650543    -0.378745     246.26
 H       4.248420     2.385851     0.225423      26.89
 H       5.052457     0.264612     1.107308      27.37
 H       3.417951     0.503593     1.287026      27.56
55
name = lig-Water-frame_98
 C      -2.221256     1.592674     4.438066      65.79
 H      -3.043143     2.370167     4.592623      26.86
 C      -1.406986    -0.509928     3.715202      68.59
 H      -1.612192    -1.281271     3.130535      24.95
 C      -0.100185    -0.247234     4.334285     -24.36
 O       1.045405    -1.157337     4.405697     158.48
 C       0.740061    -2.570390     3.973748     114.10
 H       1.637885    -3.097224     3.778924      26.14
 H       0.461872    -2.844002     3.013963      27.45
 H      -0.050563    -2.982398     4.674228      24.76
 C       0.078650     1.056915     5.075807     -24.12
 O       1.389109     1.339806     5.476385     316.75
 H       1.510763     2.266711     5.060594      21.21
 C      -0.998063     1.786971     5.248705      65.27
 H      -0.966266     2.803208     5.882914      29.12
 C      -2.393574     0.482450     3.697423      54.64
 C      -3.614343     0.328795     2.798808      95.79
 H      -4.575939     0.959401     2.868817      23.55
 O      -4.027255    -1.139392     2.991439     296.51
 H      -4.961906    -1.235434     2.769330      27.10
 C      -3.097198     0.643975     1.316037      89.67
 H      -2.268095     1.360333     1.400586      24.89
 C      -4.287557     1.357814     0.468472      88.04
 O      -5.198699     0.368577    -0.112180     180.17
 H      -4.756218    -0.491792     0.129746      27.06
 H      -4.122057     1.978390    -0.564181      23.78
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 H      -4.964024     2.020299     1.211174      24.39
 C       0.884453     0.697752    -0.680705      59.27
 H       1.575358     1.469764    -0.810464      22.23
 C       0.658919    -1.745069    -0.686996      59.66
 H       1.182307    -2.689413    -0.860463      22.19
 C      -0.659989    -1.576438    -0.307389      -7.58
 O      -1.566976    -2.746128    -0.052598     156.07
 C      -1.272759    -4.071920    -0.469987     143.09
 H      -2.105826    -4.606669    -0.263568      26.96
 H      -1.147049    -4.270389    -1.507439      27.51
 H      -0.368726    -4.405411    -0.258640      27.88
 C      -1.202871    -0.258269     0.104308      -4.17
 O      -2.473681    -0.423521     0.580697     164.37
 C      -0.467693     0.916666    -0.135115      70.25
 H      -0.928732     1.866126     0.123638      23.68
 C       1.335464    -0.511643    -1.063295      35.92
 C       2.817923    -0.771002    -1.597906      81.89
 H       2.929624    -1.634835    -2.164912      26.85
 O       3.197377     0.284162    -2.577269     259.91
 H       3.720540     0.945030    -2.087203      25.79
 C       3.902812    -0.860596    -0.443588      75.45
 H       3.282724    -1.698307     0.362445      23.29
 O       5.198070    -1.270315    -0.945983     159.82
 H       5.426294    -1.579946    -1.867272      25.44
 C       4.178354     0.435531     0.429342     109.96
 O       4.487792     1.613139    -0.380702     246.05
 H       4.226354     2.449016     0.139027      25.55
 H       5.083304     0.184215     0.996146      27.46
 H       3.328933     0.496451     1.146625      26.66
55
name = lig-Water-frame_99
 C      -2.189995     1.632963     4.527516      49.24
 H      -2.945215     2.393403     4.464815      32.48
 C      -1.376385    -0.468907     3.687416      23.57
 H      -1.738447    -1.471391     3.132337      23.62
 C      -0.039056    -0.214237     4.382912      -0.86
 O       0.999367    -1.098560     4.376747     165.44
 C       0.736030    -2.589253     4.006514      88.61
 H       1.772908    -3.144368     3.961057      24.78
 H       0.247343    -2.760939     2.839526      24.70
 H      -0.049849    -3.293458     4.380527      25.23
 C       0.145574     1.053129     5.055501     -35.53
 O       1.356145     1.377420     5.489409     443.66
 H       1.582036     2.352082     5.100480      20.84
 C      -1.052544     1.895901     5.173116      50.36
 H      -0.799179     2.795301     5.713773      22.50
 C      -2.436582     0.489602     3.725374      20.37
 C      -3.557364     0.264903     2.791299      77.44
 H      -4.420760     1.137620     2.971522      24.57
 O      -4.042587    -1.162846     2.972255     247.87
 H      -5.046364    -1.030043     2.810637      25.41
 C      -3.140847     0.675218     1.311313      87.62
 H      -2.323012     1.412697     1.597745      24.52
 C      -4.257919     1.316914     0.462068     113.33
 O      -5.196966     0.367557    -0.113181     196.61
 H      -4.970871    -0.617272     0.011367      27.03
 H      -4.071672     1.928710    -0.345545      27.93
 H      -4.926127     1.972698     1.030452      27.32
 C       0.885782     0.833559    -0.672440      29.22
 H       1.570164     1.739024    -0.904352      20.97
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 C       0.694891    -1.790045    -0.721573      53.52
 H       1.103223    -2.780084    -0.927343      22.68
 C      -0.647503    -1.571570    -0.291648       7.83
 O      -1.518277    -2.693071    -0.019797      87.84
 C      -1.289111    -4.111481    -0.522107      87.20
 H      -2.240153    -4.997441    -0.417227      21.90
 H      -1.193950    -3.918383    -1.697346      24.03
 H      -0.201477    -4.677615    -0.265365      22.33
 C      -1.189920    -0.359562     0.158065      -3.93
 O      -2.485903    -0.417384     0.586295     143.58
 C      -0.445448     0.896939    -0.183153      52.00
 H      -0.888252     1.835444     0.143610      25.84
 C       1.354592    -0.577891    -1.030908      11.50
 C       2.798710    -0.707174    -1.560962      62.11
 H       2.932128    -1.891119    -2.185949      23.31
 O       3.188159     0.280307    -2.550389     234.38
 H       3.731033     0.905240    -2.047349      27.14
 C       3.907839    -0.891580    -0.360524      90.46
 H       3.439663    -1.579609     0.291660      28.75
 O       5.221310    -1.242290    -0.905692     127.43
 H       5.174635    -1.622424    -1.845645      23.76
 C       4.214753     0.375000     0.451390     104.54
 O       4.459300     1.576571    -0.384466     158.81
 H       4.210313     2.400303     0.206120      25.25
 H       5.199124     0.039573     1.051384      26.07
 H       3.216101     0.717861     0.921963      23.77
55
name = lig-Water-frame_100
 C      -2.238566     1.684082     4.576868      50.40
 H      -2.958376     2.501248     4.467547      21.89
 C      -1.310658    -0.427864     3.688118      37.04
 H      -1.444441    -1.475063     3.368291      27.32
 C      -0.070708    -0.189222     4.400120      15.15
 O       0.955857    -1.096988     4.341135     171.80
 C       0.728008    -2.607552     3.961127     107.09
 H       1.735943    -2.917109     4.323019      27.10
 H       0.412597    -2.374583     2.996669      30.83
 H       0.038497    -3.255006     4.599303      27.22
 C       0.121428     1.005424     4.992789      -1.97
 O       1.367365     1.436707     5.530867     467.97
 H       1.601091     2.274086     5.078686      26.99
 C      -0.997582     1.990980     5.117894      49.97
 H      -0.812167     2.955765     5.612027      22.13
 C      -2.412139     0.475043     3.775769     -16.84
 C      -3.524688     0.196626     2.776565      86.22
 H      -4.274648     1.018069     3.157933      27.36
 O      -4.080368    -1.142478     2.941954     265.51
 H      -5.072080    -1.095243     2.898208      26.23
 C      -3.154394     0.724517     1.316897      79.37
 H      -2.537560     1.559409     1.595268      27.51
 C      -4.253117     1.262395     0.455814     101.03
 O      -5.210610     0.340785    -0.115178     156.91
 H      -4.967690    -0.599870    -0.226257      26.07
 H      -3.567324     2.007008    -0.311322      24.81
 H      -4.844469     2.007065     1.134968      26.76
 C       0.874076     0.892340    -0.684629      13.68
 H       1.333909     1.801720    -0.949097      22.53
 C       0.695580    -1.776811    -0.767532      74.87
 H       1.012785    -2.811060    -1.028759      26.82
 C      -0.635173    -1.644471    -0.250715       2.02
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 O      -1.482569    -2.666132     0.025408     114.41
 C      -1.269030    -4.164566    -0.647697     101.93
 H      -2.025139    -4.723502    -0.372652      28.82
 H      -1.295920    -3.731746    -1.585162      26.61
 H      -0.515955    -4.605077    -0.142556      26.58
 C      -1.151218    -0.398486     0.167990     -19.97
 O      -2.512955    -0.414553     0.601486      88.75
 C      -0.422586     0.842977    -0.199486      50.76
 H      -0.841330     1.850341     0.102649      29.99
 C       1.423897    -0.596874    -0.986226     -11.62
 C       2.813698    -0.694860    -1.533931     108.92
 H       2.781071    -1.620974    -1.939620      30.92
 O       3.172955     0.269848    -2.517460     213.07
 H       3.763857     1.004986    -2.003836      25.41
 C       3.906268    -0.865211    -0.343630      78.36
 H       3.637937    -1.848347     0.471361      28.71
 O       5.237399    -1.235867    -0.864210     137.58
 H       4.948460    -1.458156    -1.785795      26.92
 C       4.222027     0.333213     0.470017     141.31
 O       4.438034     1.542859    -0.389287     145.81
 H       4.253620     2.221679     0.252318      27.50
 H       4.994160     0.139008     1.208214      31.69
 H       3.385485     0.665185     1.031923      30.04
55
name = lig-Water-frame_101
 C      -2.303685     1.718780     4.569913      45.59
 H      -3.075485     2.546469     4.594662      17.19
 C      -1.245535    -0.386821     3.736358      79.56
 H      -1.263968    -1.440738     3.405783      26.60
 C      -0.132434    -0.215398     4.377599      21.45
 O       0.927983    -1.118797     4.326251     183.08
 C       0.729707    -2.574742     3.973760     103.94
 H       1.730807    -2.847461     4.276813      28.22
 H       0.684480    -2.347123     2.721212      27.27
 H       0.032741    -2.932169     4.713852      27.66
 C       0.067931     1.065286     4.971628      11.56
 O       1.385878     1.470393     5.586474     338.80
 H       1.548591     2.348416     4.921854      22.81
 C      -0.896685     2.025695     5.066244      77.70
 H      -0.827740     3.106008     5.517236      22.82
 C      -2.338306     0.449430     3.825020      -4.52
 C      -3.522480     0.165931     2.783635      88.18
 H      -4.367133     0.855423     3.311723      24.59
 O      -4.119987    -1.114504     2.905061     280.03
 H      -5.099105    -1.207376     2.928832      26.52
 C      -3.152554     0.722156     1.359692      67.09
 H      -2.576648     1.740231     1.444569      25.64
 C      -4.233939     1.245072     0.435163     113.05
 O      -5.227646     0.322739    -0.128151     176.34
 H      -4.650052    -0.515546    -0.372450      23.87
 H      -3.602560     1.680582    -0.228824      26.95
 H      -4.746668     1.996385     1.115529      27.04
 C       0.862459     0.807629    -0.714617      30.51
 H       1.250242     1.836258    -1.009762      28.28
 C       0.667731    -1.733818    -0.808875      68.64
 H       1.053925    -2.686233    -1.135041      32.35
 C      -0.608041    -1.709796    -0.197318     -14.09
 O      -1.468956    -2.702412     0.073527     135.80
 C      -1.246314    -4.127782    -0.745438      62.21
 H      -2.381769    -4.527113    -0.231771      19.86
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 H      -1.217310    -3.881654    -1.887836      23.22
 H      -0.337934    -4.586725    -0.110893      22.93
 C      -1.123126    -0.377282     0.150636     -27.56
 O      -2.513896    -0.401384     0.617043      79.10
 C      -0.426282     0.789697    -0.172561      95.43
 H      -0.886609     1.717855     0.005921      29.63
 C       1.481331    -0.515952    -0.932297     -32.36
 C       2.849160    -0.684734    -1.458395     105.54
 H       2.804361    -1.874691    -2.104079      23.73
 O       3.172569     0.275734    -2.481857     214.41
 H       3.594434     0.988567    -2.057860      30.13
 C       3.919653    -0.871608    -0.315412     105.92
 H       3.680980    -1.661706     0.322337      33.74
 O       5.229520    -1.241245    -0.844432     143.54
 H       5.191224    -1.286955    -1.846003      24.51
 C       4.187654     0.337643     0.498071     128.63
 O       4.431727     1.495601    -0.389293     117.23
 H       4.307230     2.323199     0.268080      23.82
 H       5.011969     0.261081     1.384446      29.32
 H       3.333577     0.484088     1.342134      29.46
55
name = lig-Water-frame_102
 C      -2.280850     1.717202     4.538444      45.29
 H      -3.108245     2.341878     4.699884      21.79
 C      -1.256760    -0.410808     3.762473      80.11
 H      -1.393632    -1.413890     3.115187      26.77
 C      -0.078127    -0.214594     4.401665       1.90
 O       0.919350    -1.121301     4.334906     202.60
 C       0.763918    -2.466851     3.963264     115.12
 H       1.769567    -3.079046     4.103595      25.97
 H       0.696699    -2.846622     2.946072      29.94
 H      -0.195313    -2.815405     4.537278      26.29
 C       0.087531     1.144687     5.000509     -55.94
 O       1.386023     1.501739     5.603889     364.66
 H       1.548835     2.302694     5.117863      24.12
 C      -0.919866     2.060825     5.006103      62.36
 H      -0.660527     2.944092     5.409038      23.34
 C      -2.329049     0.474546     3.850245      -0.76
 C      -3.550396     0.192149     2.853927      91.22
 H      -4.394297     0.893965     3.173407      24.82
 O      -4.136278    -1.119103     2.860696     280.64
 H      -5.184512    -1.133315     2.866873      24.39
 C      -3.142285     0.696804     1.410187      79.20
 H      -2.496130     1.522234     1.441045      28.72
 C      -4.238759     1.225011     0.445600      86.32
 O      -5.211888     0.304954    -0.149898     176.63
 H      -4.590729    -0.419289    -0.381147      26.84
 H      -3.692622     1.606454    -0.651604      25.28
 H      -4.796080     2.052668     0.924333      27.68
 C       0.862418     0.682776    -0.746742      87.95
 H       1.308851     1.625327    -1.008676      32.76
 C       0.647465    -1.665227    -0.830189      51.66
 H       1.186992    -2.562771    -1.230331      30.27
 C      -0.574007    -1.698709    -0.144503      13.55
 O      -1.453423    -2.785968     0.086078     140.04
 C      -1.271813    -4.050168    -0.762968     119.94
 H      -2.116156    -4.427358    -0.570012      28.92
 H      -1.106763    -4.185121    -1.815230      27.34
 H      -0.374976    -4.552013    -0.493316      27.33
 C      -1.142083    -0.377630     0.139577      11.57
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 O      -2.473510    -0.381857     0.629492      96.48
 C      -0.441203     0.746997    -0.134789      70.72
 H      -1.036298     1.726494    -0.071718      25.96
 C       1.482423    -0.433215    -0.885045      16.51
 C       2.894247    -0.736902    -1.414209     104.48
 H       2.971541    -1.536241    -1.994480      30.56
 O       3.177434     0.278946    -2.455984     197.02
 H       3.506263     1.101183    -1.972122      27.49
 C       3.965442    -0.861596    -0.323269      92.94
 H       3.407957    -1.793676     0.430468      27.95
 O       5.229018    -1.257537    -0.850867     145.12
 H       5.502155    -1.121601    -1.798962      22.55
 C       4.136960     0.381710     0.601980     120.19
 O       4.422634     1.462408    -0.357100     180.70
 H       4.363173     2.335274     0.055745      27.72
 H       5.055512     0.233674     1.133085      32.01
 H       3.277380     0.439558     1.173650      31.06
55
name = lig-Water-frame_103
 C      -2.193924     1.693663     4.502154      68.25
 H      -3.178379     2.210916     4.778115      28.38
 C      -1.314046    -0.474768     3.754300      34.54
 H      -1.468165    -1.157240     3.050614      25.49
 C      -0.001177    -0.156960     4.447209       4.10
 O       0.967807    -1.097593     4.348634     188.53
 C       0.785119    -2.423329     3.957566     137.89
 H       1.570445    -3.040977     4.296181      28.40
 H       0.451974    -3.033322     2.969927      26.06
 H      -0.115587    -2.866484     4.317923      28.80
 C       0.160468     1.150796     5.030615     -12.62
 O       1.365580     1.513241     5.610383     281.75
 H       1.665673     2.516920     5.275084      20.86
 C      -1.005288     2.076404     4.955285      42.98
 H      -0.573628     3.083025     5.454784      20.69
 C      -2.385243     0.502449     3.841524       1.05
 C      -3.585411     0.244950     2.941600      94.19
 H      -4.436455     1.132420     2.972380      23.97
 O      -4.137699    -1.133143     2.818794     290.93
 H      -5.104483    -1.033323     2.789258      25.82
 C      -3.130501     0.658443     1.426838      71.96
 H      -2.270265     1.436092     1.629329      26.46
 C      -4.233921     1.226064     0.401007     106.39
 O      -5.181924     0.287411    -0.164113     203.27
 H      -4.771011    -0.628667    -0.357122      25.55
 H      -3.822057     1.600502    -0.414360      28.21
 H      -4.883667     2.171631     0.684206      25.69
 C       0.811356     0.684405    -0.737797      64.00
 H       1.441383     1.552756    -0.988054      29.76
 C       0.660609    -1.610727    -0.823353      56.25
 H       1.143920    -2.487675    -1.199710      30.11
 C      -0.558593    -1.663992    -0.114915      17.84
 O      -1.412716    -2.862901     0.049795     157.21
 C      -1.261646    -3.965222    -0.767618     113.92
 H      -2.305598    -4.825792    -0.708601      22.50
 H      -1.137248    -3.885245    -1.922622      25.15
 H      -0.365527    -4.668271    -0.483826      25.26
 C      -1.201190    -0.415322     0.161446      23.13
 O      -2.425214    -0.381746     0.646024     111.99
 C      -0.455573     0.753554    -0.124651      66.23
 H      -0.966661     1.663224    -0.126654      26.00
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 C       1.499669    -0.524462    -0.876486       9.77
 C       2.927577    -0.710104    -1.383790      76.56
 H       3.023437    -1.830396    -2.114243      23.44
 O       3.198945     0.293111    -2.431927     173.11
 H       3.407752     1.142612    -1.843843      24.81
 C       3.980251    -0.864516    -0.311492     105.27
 H       3.562083    -1.651634     0.281679      30.10
 O       5.255875    -1.288638    -0.848067     150.95
 H       5.427900    -0.941706    -1.770221      24.30
 C       4.107225     0.408607     0.657973      96.08
 O       4.410701     1.447257    -0.326875     177.30
 H       4.339305     2.339449     0.064673      27.58
 H       5.164914     0.124441     1.141005      25.49
 H       3.045234     0.624013     1.163452      26.44
55
name = lig-Water-frame_105
 C      -2.206401     1.677196     4.453161      56.31
 H      -2.982249     2.501998     4.609349      15.78
 C      -1.331025    -0.435648     3.824312      92.05
 H      -1.190564    -1.197934     3.238760      26.81
 C      -0.065343    -0.118121     4.391950     -44.79
 O       1.140188    -0.981337     4.375851     111.43
 C       0.712236    -2.512906     3.982302      98.35
 H       1.565975    -2.930725     4.344927      27.85
 H       0.939507    -2.093916     2.945699      24.26
 H      -0.154739    -2.678631     4.505319      24.75
 C       0.149948     1.164398     5.009740       7.20
 O       1.378805     1.552326     5.647703     367.48
 H       1.465566     2.512532     5.213866      28.99
 C      -0.886793     2.048773     5.011517      50.38
 H      -1.111171     3.080785     5.468207      13.03
 C      -2.440016     0.393836     3.807957       6.61
 C      -3.660618     0.302985     2.864774     118.98
 H      -4.546433     0.993788     3.442289      22.05
 O      -4.073985    -1.071285     2.790820     326.92
 H      -5.039994    -1.231069     2.888480      24.63
 C      -3.099234     0.696934     1.413194      82.64
 H      -2.396774     1.637376     1.549934      24.05
 C      -4.155048     1.233410     0.326089      96.54
 O      -5.154936     0.235997    -0.191461     234.28
 H      -4.710788    -0.639336    -0.073451      27.03
 H      -3.573917     1.637915    -0.326894      29.75
 H      -4.855775     1.962818     0.991594      23.53
 C       0.841809     0.726772    -0.659424      12.61
 H       1.212487     1.723971    -0.833082      21.80
 C       0.667852    -1.780095    -0.727339      62.40
 H       0.925299    -2.806499    -0.949727      29.50
 C      -0.627732    -1.680190    -0.154669       0.95
 O      -1.337504    -2.841036     0.047863     186.23
 C      -1.195941    -3.986049    -0.910031      84.54
 H      -2.372357    -4.619812    -0.749250      21.29
 H      -1.172397    -3.403935    -1.864643      23.34
 H      -0.269313    -4.588755    -0.639112      22.54
 C      -1.172715    -0.417950     0.208269      -1.78
 O      -2.489233    -0.469719     0.759501     126.25
 C      -0.497126     0.788679    -0.167480      68.84
 H      -0.926234     1.759826     0.038640      25.58
 C       1.508156    -0.579525    -0.923213     -39.74
 C       2.930603    -0.701069    -1.451219     102.25
 H       2.989085    -1.899182    -2.018386      20.86
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 O       3.263583     0.334223    -2.370974     232.06
 H       3.564193     1.168175    -1.770183      21.30
 C       3.998391    -0.860932    -0.214534      99.03
 H       3.752206    -1.666505     0.385915      29.64
 O       5.308202    -1.302327    -0.833519     181.11
 H       5.272953    -1.028601    -1.801439      25.96
 C       4.113263     0.367115     0.630174     105.76
 O       4.399588     1.515314    -0.248009     275.88
 H       4.235820     2.243784     0.333229      30.01
 H       4.698644     0.355227     1.672560      26.67
 H       3.128742     0.669539     1.274994      25.96
55
name = lig-Water-frame_106
 C      -2.199716     1.660905     4.445201      53.01
 H      -2.881967     2.507424     4.330145      26.45
 C      -1.265310    -0.429678     3.849621      50.68
 H      -1.219549    -1.547672     3.344128      22.60
 C      -0.059456    -0.122414     4.367130     -18.56
 O       1.162130    -0.905342     4.405310     117.38
 C       0.740768    -2.446015     4.018818      92.76
 H       1.688812    -3.232494     4.109602      24.25
 H       0.873928    -2.381023     2.938471      27.08
 H      -0.395004    -2.668926     4.310629      21.13
 C       0.137272     1.169656     5.005503     -48.31
 O       1.383844     1.567595     5.649086     378.77
 H       1.579896     2.468443     5.159931      23.67
 C      -0.946430     2.018539     5.037075      57.76
 H      -0.740550     2.985906     5.633653      18.47
 C      -2.454313     0.424977     3.824323      -0.29
 C      -3.664325     0.277742     2.798861     116.73
 H      -4.385644     0.812579     3.195109      29.82
 O      -4.020268    -1.041667     2.790321     297.16
 H      -5.060631    -1.117315     2.930854      22.84
 C      -3.143327     0.765439     1.377875      96.64
 H      -2.458897     1.558743     1.370281      27.77
 C      -4.128399     1.210080     0.373656      95.22
 O      -5.131100     0.246148    -0.190959     208.02
 H      -4.525160    -0.587624    -0.210165      24.63
 H      -3.598882     1.757320    -0.713742      23.76
 H      -4.635816     1.914385     0.898463      29.10
 C       0.890658     0.679106    -0.622515      41.92
 H       1.279027     1.724419    -0.824281      20.58
 C       0.672088    -1.869125    -0.663835      37.27
 H       1.112303    -2.871673    -0.847628      24.07
 C      -0.642871    -1.704790    -0.205987      10.59
 O      -1.338609    -2.807720     0.098427     146.52
 C      -1.182810    -3.962891    -0.979251      92.61
 H      -2.028923    -4.381475    -0.884455      29.29
 H      -1.092308    -3.798537    -2.091872      24.18
 H      -0.232994    -4.563713    -1.003568      23.24
 C      -1.164874    -0.380522     0.223697     -11.01
 O      -2.521536    -0.522868     0.841474      75.37
 C      -0.512802     0.777604    -0.173558      71.01
 H      -0.944887     1.734739     0.128580      26.61
 C       1.442878    -0.527570    -0.947001      21.12
 C       2.916107    -0.748378    -1.441871      86.57
 H       3.089623    -1.491881    -2.103954      27.59
 O       3.304661     0.361801    -2.350628     236.17
 H       3.738531     1.036603    -1.759226      25.00
 C       4.029851    -0.888602    -0.200730      66.58
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 H       3.496928    -1.790257     0.633360      24.52
 O       5.309017    -1.275221    -0.819047     179.75
 H       5.442235    -1.309103    -1.806197      26.68
 C       4.097464     0.379296     0.660986     103.85
 O       4.405531     1.572973    -0.183455     283.83
 H       4.204421     2.394724     0.407365      26.91
 H       4.835808     0.342327     1.394372      27.41
 H       3.058663     0.378736     0.873017      29.82
55
name = lig-Water-frame_107
 C      -2.195509     1.674594     4.432464      53.25
 H      -2.914891     2.440291     4.158002      30.89
 C      -1.245540    -0.481860     3.829760      15.62
 H      -1.522897    -1.471972     3.546923      23.87
 C       0.034598    -0.088143     4.392884      16.13
 O       1.136529    -0.884467     4.429482     161.31
 C       0.817294    -2.354995     4.016373     131.52
 H       1.391906    -3.143704     4.296453      31.35
 H       0.553330    -2.647526     2.865278      28.55
 H      -0.127647    -2.708199     4.207522      30.97
 C       0.138721     1.156786     5.010118     -73.38
 O       1.373017     1.576293     5.620091     311.19
 H       1.686166     2.385107     5.150885      20.01
 C      -1.009870     1.997161     5.083905      48.45
 H      -0.623642     2.850163     5.626939      14.84
 C      -2.419299     0.474946     3.824694     -16.99
 C      -3.581483     0.269500     2.763290      79.66
 H      -4.622435     1.081758     2.959685      22.90
 O      -3.987373    -1.057564     2.790150     276.48
 H      -4.981243    -0.994989     2.815708      23.14
 C      -3.172284     0.765715     1.334729      85.56
 H      -2.331042     1.554047     1.414589      26.98
 C      -4.133824     1.214404     0.334953     119.60
 O      -5.081443     0.275428    -0.168549     206.55
 H      -4.714472    -0.620472    -0.474081      23.03
 H      -3.779031     1.632687    -0.437389      28.44
 H      -4.698722     2.217496     0.788620      26.58
 C       0.878022     0.668635    -0.594370      30.15
 H       1.523923     1.485835    -0.835324      24.75
 C       0.701480    -1.848173    -0.621393      46.84
 H       1.321074    -2.748681    -0.753777      25.27
 C      -0.611196    -1.685703    -0.233932      -2.79
 O      -1.363984    -2.833085     0.107188     102.02
 C      -1.131520    -3.907844    -1.057652      70.22
 H      -2.226348    -4.671045    -0.848829      22.62
 H      -1.206569    -3.704766    -2.150745      24.99
 H      -0.286118    -4.591668    -0.866332      24.62
 C      -1.214729    -0.394709     0.226202      -9.82
 O      -2.495956    -0.550106     0.903357      42.22
 C      -0.498206     0.752029    -0.151603      80.72
 H      -0.897427     1.773033     0.112151      29.51
 C       1.393898    -0.587311    -0.963299      20.81
 C       2.911951    -0.731108    -1.401750      56.22
 H       3.069736    -1.679470    -2.272135      24.34
 O       3.348781     0.389635    -2.325600     215.52
 H       3.859132     0.986965    -1.759887      27.92
 C       4.036218    -0.936701    -0.238743      90.71
 H       3.644199    -1.671130     0.461551      29.07
 O       5.315688    -1.252838    -0.782101     194.47
 H       5.320584    -1.556678    -1.740913      26.54
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 C       4.074910     0.397582     0.645912      93.07
 O       4.410199     1.633437    -0.111641     246.51
 H       4.148646     2.448860     0.460123      26.95
 H       4.988981     0.230075     1.364304      25.60
 H       2.946505     0.294115     0.872900      28.83
55
name = lig-Water-frame_108
 C      -2.212139     1.735548     4.416151      59.67
 H      -3.033579     2.498670     4.215197      21.35
 C      -1.269302    -0.480843     3.833526      51.80
 H      -1.585807    -1.462938     3.644049      24.74
 C       0.072003    -0.075787     4.405131      -3.79
 O       1.117248    -0.940937     4.435273     205.21
 C       0.865686    -2.258322     3.962592     114.62
 H       1.577048    -2.944629     4.692067      25.48
 H       0.620554    -2.463617     2.968956      29.01
 H      -0.153731    -2.607618     4.586182      26.24
 C       0.129897     1.168138     5.025872     -14.00
 O       1.353231     1.565726     5.582368     179.80
 H       1.681854     2.447088     5.008483      19.01
 C      -1.010482     1.960750     5.140569      57.98
 H      -0.868243     3.077316     5.633127      29.35
 C      -2.327499     0.473780     3.779730      18.02
 C      -3.525244     0.338368     2.765677     109.84
 H      -4.280520     0.928414     2.889413      27.77
 O      -3.967653    -1.084736     2.788857     320.93
 H      -4.999364    -1.142167     2.722289      24.84
 C      -3.121644     0.713615     1.325302      85.15
 H      -2.378926     1.472862     1.530678      25.92
 C      -4.194654     1.257157     0.304268     106.07
 O      -5.067971     0.302577    -0.149932     179.92
 H      -4.809228    -0.583631    -0.459729      24.07
 H      -3.425576     1.775773    -0.698314      24.45
 H      -4.731944     2.048162     0.620106      29.46
 C       0.838746     0.636615    -0.596080      34.27
 H       1.638492     1.403858    -0.797520      23.68
 C       0.759956    -1.756456    -0.611290      60.60
 H       1.297388    -2.694897    -0.669769      26.71
 C      -0.610201    -1.665389    -0.197621     -24.22
 O      -1.381724    -2.885305     0.055090     113.92
 C      -1.166324    -3.906498    -1.084125      87.36
 H      -1.830054    -4.609859    -0.918587      28.09
 H      -1.291213    -3.283185    -1.992269      27.23
 H      -0.289551    -4.460884    -0.610090      21.84
 C      -1.268656    -0.459524     0.199808       1.25
 O      -2.426035    -0.549405     0.921579      80.24
 C      -0.470879     0.750291    -0.102149      59.34
 H      -0.815521     1.733433     0.043554      30.70
 C       1.399082    -0.677995    -0.953744      25.77
 C       2.931669    -0.724606    -1.419411      81.26
 H       2.839404    -1.642139    -1.904117      31.71
 O       3.378245     0.402975    -2.290841     179.97
 H       3.990695     1.068233    -1.703942      23.60
 C       4.016830    -0.914951    -0.325753      84.55
 H       3.770784    -1.890297     0.500631      25.83
 O       5.332464    -1.241332    -0.749125     167.28
 H       5.140634    -1.653665    -1.627333      27.98
 C       4.063702     0.386186     0.606194     114.59
 O       4.406654     1.682693    -0.041993     272.56
 H       4.069688     2.374184     0.568923      28.35
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 H       4.692737     0.170475     1.432394      29.74
 H       3.185379     0.538298     1.270936      28.76
55
name = lig-Water-frame_109
 C      -2.214171     1.780860     4.401272      59.22
 H      -2.954806     2.514845     4.450554      20.56
 C      -1.261702    -0.431425     3.870499      70.84
 H      -1.434709    -1.622507     3.631621      19.16
 C       0.003424    -0.099126     4.388281       7.27
 O       1.121582    -0.978096     4.432426     210.60
 C       0.868178    -2.235533     4.026196     124.74
 H       1.787267    -2.560766     4.456487      25.33
 H       0.884930    -2.257868     2.816459      24.72
 H       0.101363    -2.440215     4.646966      27.08
 C       0.119797     1.178660     5.046040     -26.11
 O       1.354364     1.573131     5.531683     310.11
 H       1.485424     2.335042     5.001476      25.93
 C      -1.028050     1.995604     5.189657      41.43
 H      -1.094755     2.921223     5.574856      24.06
 C      -2.249944     0.495377     3.709798      44.14
 C      -3.455401     0.334072     2.776242     122.43
 H      -4.407003     1.133213     3.238793      20.69
 O      -3.953807    -1.099050     2.786015     336.39
 H      -4.955215    -1.214428     2.769074      24.48
 C      -3.045237     0.656358     1.335999      81.24
 H      -2.336229     1.522489     1.473656      23.46
 C      -4.141529     1.296008     0.225097      98.84
 O      -5.114093     0.321201    -0.152503     202.27
 H      -4.614468    -0.580973    -0.241882      25.05
 H      -3.543562     1.610809    -0.442579      27.66
 H      -4.892491     2.147208     0.690884      23.27
 C       0.826204     0.569809    -0.631109      56.77
 H       1.383161     1.499360    -0.702752      26.76
 C       0.751000    -1.745393    -0.591900      39.80
 H       1.131582    -2.788758    -0.630551      23.84
 C      -0.640248    -1.695815    -0.128638       3.07
 O      -1.390861    -2.918413    -0.009780     148.62
 C      -1.171986    -3.871220    -1.043672      95.52
 H      -2.078650    -4.821036    -1.013856      22.18
 H      -1.163719    -3.136948    -1.900475      25.38
 H      -0.148098    -4.220690    -0.907170      24.52
 C      -1.256100    -0.499380     0.145562      -1.65
 O      -2.365142    -0.533258     0.908636     118.00
 C      -0.445267     0.728622    -0.048014      34.77
 H      -0.860865     1.794769     0.074288      19.53
 C       1.490405    -0.620385    -0.929264      24.32
 C       2.942581    -0.703800    -1.430273     100.22
 H       2.866449    -1.837980    -2.031143      20.96
 O       3.398803     0.403643    -2.251633     242.97
 H       3.868607     0.991019    -1.706740      27.54
 C       3.965999    -0.868247    -0.332090      93.41
 H       3.681753    -1.725648     0.324921      26.70
 O       5.343709    -1.233701    -0.739601     149.91
 H       5.284815    -1.613738    -1.657424      27.18
 C       4.047744     0.372460     0.601099     117.80
 O       4.405093     1.702156     0.017394     243.39
 H       3.968770     2.391455     0.705747      24.13
 H       4.777246     0.092479     1.485415      26.09
 H       3.285587     0.689607     1.351325      24.12
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name = lig-Water-frame_110
 C      -2.162035     1.761750     4.397718      26.56
 H      -2.997133     2.538406     4.580576      23.17
 C      -1.227943    -0.445279     3.894740      66.35
 H      -1.290070    -1.339885     3.541630      19.89
 C      -0.056070    -0.099097     4.404616      20.62
 O       1.118263    -0.897228     4.444161     231.92
 C       0.913317    -2.259664     4.063416     100.77
 H       2.019152    -2.788394     4.117917      23.51
 H       0.958646    -2.274546     2.990893      25.96
 H      -0.044619    -2.846284     4.588128      23.09
 C       0.078505     1.163046     5.057679      -9.60
 O       1.367833     1.577442     5.486785     325.00
 H       1.494475     2.522283     4.907760      22.13
 C      -1.064391     2.022461     5.188186      47.17
 H      -1.061386     3.095951     5.871346      18.17
 C      -2.237753     0.579164     3.654511      66.88
 C      -3.453351     0.299311     2.815175     165.20
 H      -4.073287     0.874966     3.197691      28.82
 O      -3.929482    -1.098806     2.786136     338.77
 H      -4.935692    -1.027788     2.896866      25.22
 C      -2.988742     0.665247     1.345414      84.84
 H      -2.264554     1.511555     1.314390      22.91
 C      -4.107279     1.302593     0.247819      75.05
 O      -5.164150     0.322005    -0.174361     209.43
 H      -4.659338    -0.501773    -0.081312      26.50
 H      -3.395049     1.709594    -0.824244      21.87
 H      -4.556306     2.117276     0.705643      25.95
 C       0.822480     0.568047    -0.658321      58.48
 H       1.158254     1.614678    -0.743862      25.43
 C       0.688927    -1.790123    -0.563664      31.69
 H       1.068106    -2.792508    -0.692435      22.99
 C      -0.626846    -1.783444    -0.092503      12.16
 O      -1.407035    -2.915676    -0.026921     216.38
 C      -1.169451    -3.847213    -1.019648     121.74
 H      -1.933676    -4.518223    -1.178602      26.96
 H      -1.172248    -3.398676    -2.047995      26.75
 H      -0.133927    -4.233285    -1.320617      24.96
 C      -1.194464    -0.462338     0.107721       7.90
 O      -2.341620    -0.523673     0.880812     104.93
 C      -0.440320     0.670232    -0.016504      71.07
 H      -0.837282     1.613655     0.156010      21.34
 C       1.582149    -0.547644    -0.889688      11.62
 C       2.950117    -0.719384    -1.469937     108.72
 H       3.153980    -1.475953    -2.162543      23.67
 O       3.396304     0.387640    -2.238063     243.87
 H       3.793975     1.071686    -1.567293      23.34
 C       3.931614    -0.802507    -0.301957      66.05
 H       3.335804    -1.723298     0.373364      23.43
 O       5.338854    -1.225152    -0.738289     117.68
 H       5.489826    -1.383587    -1.722946      24.19
 C       4.066321     0.381677     0.671008     111.75
 O       4.401969     1.700143     0.071788     258.37
 H       4.025054     2.406776     0.621261      26.90
 H       4.961420     0.065346     1.169375      26.79
 H       3.041958     0.486351     1.145120      23.94
55
name = lig-Water-frame_111
 C      -2.143142     1.757564     4.412462      36.80
 H      -3.001386     2.355387     4.423349      21.14
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 C      -1.260243    -0.432034     3.868692      36.78
 H      -1.322186    -1.462744     3.191775      16.44
 C      -0.031433    -0.064197     4.480587      20.38
 O       1.099142    -0.805660     4.470769     194.21
 C       0.992405    -2.327763     4.094357      98.49
 H       1.819002    -2.965068     4.098941      27.79
 H       0.679223    -2.369656     2.896403      24.84
 H       0.295010    -3.042707     4.308812      28.98
 C       0.028251     1.175726     5.077595      18.45
 O       1.377298     1.602981     5.429252     238.04
 H       1.580044     2.402059     4.958085      26.06
 C      -1.044937     2.070971     5.207406      34.64
 H      -0.908505     2.768319     5.850841      20.47
 C      -2.222649     0.611673     3.642853      31.90
 C      -3.414425     0.229622     2.807745     127.00
 H      -4.393760     1.037650     3.207611      24.26
 O      -3.907513    -1.081512     2.795477     302.12
 H      -4.885104    -0.951809     3.010575      23.10
 C      -2.974050     0.718782     1.317034      90.07
 H      -2.213800     1.486169     1.365445      23.30
 C      -4.020968     1.267197     0.246768      86.41
 O      -5.194206     0.346525    -0.184975     226.02
 H      -4.896956    -0.606539    -0.105225      25.92
 H      -3.684199     1.562494    -0.591382      29.20
 H      -4.373556     2.294082     0.791986      24.50
 C       0.838414     0.648673    -0.669619      48.43
 H       1.212581     1.650638    -0.983888      24.51
 C       0.683221    -1.819168    -0.555780      48.57
 H       1.186352    -2.774180    -0.825123      22.62
 C      -0.580866    -1.824015    -0.094154      14.28
 O      -1.427103    -2.897466    -0.008448     216.00
 C      -1.121513    -3.821259    -1.110034     105.28
 H      -2.086295    -4.661577    -1.104615      23.05
 H      -1.430824    -3.450820    -2.125105      24.99
 H      -0.225384    -4.458835    -1.131688      25.20
 C      -1.155304    -0.471060     0.131065      16.37
 O      -2.341749    -0.524087     0.836598     115.84
 C      -0.416908     0.605693    -0.026199      76.02
 H      -0.842888     1.605315     0.276052      20.39
 C       1.565114    -0.572565    -0.838128      -7.22
 C       2.989034    -0.691713    -1.495114      90.50
 H       3.228633    -1.577227    -2.322664      20.84
 O       3.397465     0.409776    -2.245802     230.27
 H       3.584037     1.181637    -1.573051      23.84
 C       3.914312    -0.786015    -0.277958      75.49
 H       3.419163    -1.603004     0.415889      25.28
 O       5.316755    -1.213976    -0.722168     108.67
 H       5.369770    -1.061407    -1.711796      26.93
 C       4.077451     0.398715     0.727945     106.16
 O       4.404286     1.671361     0.098965     254.75
 H       4.015480     2.486643     0.679369      23.23
 H       5.027255     0.070906     1.256103      25.19
 H       3.087523     0.240023     1.139701      25.87
55
name = lig-Water-frame_112
 C      -2.161589     1.778945     4.434990      70.37
 H      -3.097132     2.374086     4.287157      21.89
 C      -1.285057    -0.421978     3.799044      57.63
 H      -1.332045    -1.223679     3.152363      19.23
 C      -0.045870    -0.057933     4.540997       3.42
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 O       1.099385    -0.793409     4.502638     113.07
 C       1.053098    -2.363965     4.029587      67.65
 H       2.097880    -2.879247     4.280773      22.70
 H       0.567411    -2.292363     3.099865      26.25
 H       0.203091    -3.079995     4.623835      23.37
 C       0.040994     1.225376     5.110736      24.60
 O       1.372693     1.608858     5.394687     323.60
 H       1.575462     2.490714     4.760849      19.85
 C      -1.005783     2.071831     5.198876      44.30
 H      -0.803933     2.977344     6.066962      19.29
 C      -2.201762     0.557307     3.669261      18.87
 C      -3.423484     0.266683     2.776260     132.47
 H      -4.233337     0.800615     2.886490      25.96
 O      -3.888019    -1.071068     2.817267     316.91
 H      -4.848463    -1.127928     3.015411      27.27
 C      -2.984335     0.745050     1.264245      74.62
 H      -2.198382     1.542768     1.558703      21.78
 C      -3.978927     1.211285     0.311524      85.43
 O      -5.207282     0.390362    -0.170451     193.23
 H      -5.086334    -0.621382    -0.204147      25.73
 H      -3.531316     1.543730    -0.894119      21.41
 H      -4.385899     2.129562     0.706834      25.13
 C       0.895797     0.708753    -0.685557      46.27
 H       1.353349     1.565650    -1.147051      20.19
 C       0.789905    -1.825974    -0.583768      73.30
 H       1.284524    -2.730599    -0.910507      25.63
 C      -0.560927    -1.786893    -0.103314      10.83
 O      -1.433190    -2.894784    -0.000475     156.70
 C      -1.162763    -3.872339    -1.228884      97.03
 H      -1.840632    -4.570848    -0.779152      24.62
 H      -1.439305    -3.269567    -2.084162      25.34
 H      -0.283149    -4.466641    -0.806847      22.80
 C      -1.144120    -0.577638     0.205250      21.45
 O      -2.353992    -0.526925     0.780893     123.42
 C      -0.369028     0.638921    -0.061157      55.89
 H      -0.805886     1.553162     0.312514      21.08
 C       1.465989    -0.628475    -0.812116     -16.86
 C       3.020957    -0.674688    -1.497796     101.87
 H       2.984288    -1.629823    -2.027254      24.28
 O       3.396597     0.478104    -2.273878     265.62
 H       3.435113     1.199283    -1.705560      29.28
 C       3.954824    -0.792090    -0.270107      83.33
 H       3.700691    -1.688408     0.537971      25.67
 O       5.277288    -1.195014    -0.699907     158.51
 H       5.163194    -0.902741    -1.630982      29.32
 C       4.100038     0.386521     0.753234     106.56
 O       4.393659     1.649584     0.120489     308.27
 H       4.049332     2.331983     0.731901      26.16
 H       4.793395     0.119593     1.584440      26.43
 H       3.199261     0.376218     1.510837      25.70
55
name = lig-Water-frame_113
 C      -2.193061     1.789285     4.449959      57.53
 H      -3.021811     2.523584     4.354153      25.33
 C      -1.217714    -0.400114     3.767427      62.63
 H      -1.293753    -1.322111     3.070976      24.96
 C      -0.108750    -0.086601     4.553350      -6.42
 O       1.112072    -0.845402     4.533288     134.04
 C       1.066134    -2.393268     4.025600      93.79
 H       2.155680    -2.405775     4.249191      24.75
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 H       0.707123    -2.308727     2.933265      26.81
 H       0.536677    -2.608169     4.875180      24.40
 C       0.109422     1.230821     5.129472     -28.89
 O       1.378543     1.642606     5.364108     426.47
 H       1.446020     2.371955     4.712279      21.62
 C      -1.008092     2.122296     5.220299      50.64
 H      -0.940370     2.981366     5.725646      25.03
 C      -2.252611     0.535206     3.719022      22.59
 C      -3.422508     0.316276     2.702410      88.92
 H      -4.464322     1.080481     2.901602      21.04
 O      -3.858309    -1.086192     2.843779     287.80
 H      -4.863678    -1.211187     2.921279      26.64
 C      -2.957909     0.707148     1.261992      88.20
 H      -2.344829     1.532846     1.473983      26.23
 C      -3.980970     1.169827     0.264091     100.10
 O      -5.213812     0.438641    -0.132379     228.33
 H      -4.953772    -0.492479    -0.241019      30.03
 H      -3.402369     1.369197    -0.479985      29.53
 H      -4.547827     2.100687     0.672334      24.96
 C       0.935182     0.682594    -0.687788      72.18
 H       1.488871     1.548041    -1.156149      22.29
 C       0.885085    -1.827949    -0.611702      53.87
 H       1.350421    -2.776875    -0.908697      24.93
 C      -0.538940    -1.784408    -0.125992      -3.68
 O      -1.415533    -2.895483    -0.015356      96.57
 C      -1.223046    -3.927982    -1.231013      74.47
 H      -2.020891    -4.714409    -0.847530      21.57
 H      -1.231898    -3.298049    -2.171377      25.06
 H      -0.167847    -4.187397    -1.000856      21.70
 C      -1.085474    -0.598906     0.279033       6.39
 O      -2.381469    -0.531450     0.726526     127.24
 C      -0.336931     0.689416    -0.089352      33.62
 H      -0.820034     1.617875     0.221860      27.12
 C       1.431217    -0.622989    -0.852304      34.43
 C       2.980518    -0.650539    -1.415822      66.58
 H       2.959174    -1.658815    -1.998664      27.58
 O       3.387788     0.526975    -2.324065     165.43
 H       3.380333     1.367167    -1.637194      24.37
 C       4.020788    -0.810685    -0.206775      95.80
 H       3.717383    -1.759402     0.491144      27.48
 O       5.242888    -1.164068    -0.689734     158.51
 H       5.297559    -0.994725    -1.685687      26.83
 C       4.092929     0.357627     0.817381     114.42
 O       4.383261     1.621120     0.137276     256.16
 H       4.059038     2.359476     0.788392      25.85
 H       4.810243     0.132694     1.640285      28.27
 H       3.275285     0.670068     1.458147      28.72
55
name = lig-Water-frame_114
 C      -2.201916     1.776756     4.470876      50.06
 H      -2.918090     2.563995     4.495048      24.73
 C      -1.155863    -0.382623     3.742027      22.94
 H      -1.184410    -1.391889     3.190707      24.52
 C      -0.099621    -0.119069     4.553776      -5.80
 O       1.100856    -0.896085     4.550720     149.39
 C       1.095630    -2.308772     4.051031     108.55
 H       2.199513    -2.376469     4.031759      27.45
 H       0.915157    -2.645829     2.946674      26.47
 H       0.628498    -2.696871     5.044572      23.34
 C       0.099915     1.203400     5.128419     -44.35
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 O       1.404614     1.678674     5.348071     240.25
 H       1.553575     2.534196     4.690975      20.49
 C      -1.029217     2.123166     5.197278      40.00
 H      -1.004232     3.300311     5.546595      25.21
 C      -2.350461     0.566617     3.763653       6.92
 C      -3.471692     0.365773     2.661687     110.97
 H      -4.154480     1.065804     2.988799      28.45
 O      -3.829957    -1.099858     2.866270     278.71
 H      -4.823007    -1.106191     2.761289      27.53
 C      -2.958231     0.619088     1.298269      81.60
 H      -2.275561     1.588896     1.228043      27.54
 C      -4.047780     1.161954     0.234302      84.36
 O      -5.201661     0.467562    -0.091935     199.69
 H      -4.812180    -0.449039    -0.265425      27.16
 H      -3.134959     1.390563    -0.692644      25.63
 H      -4.429436     2.180753     0.621139      26.39
 C       0.930750     0.632933    -0.678904      87.43
 H       1.463060     1.502166    -0.956674      28.54
 C       0.880283    -1.852762    -0.619034      31.46
 H       1.418955    -2.793394    -0.834527      25.14
 C      -0.484152    -1.834529    -0.160360     -20.17
 O      -1.387650    -2.905255    -0.055478     163.44
 C      -1.260489    -3.941524    -1.156831     105.69
 H      -2.063382    -4.766312    -1.372783      24.44
 H      -1.264928    -3.559545    -2.171405      26.40
 H      -0.189068    -4.219647    -1.319721      22.95
 C      -0.996767    -0.498993     0.321582     -54.53
 O      -2.393522    -0.540219     0.671486     113.00
 C      -0.333820     0.713714    -0.090692      62.10
 H      -0.828399     1.721953     0.021754      29.06
 C       1.527500    -0.573070    -0.945942      53.00
 C       2.908141    -0.625498    -1.311936      63.33
 H       3.207844    -1.414524    -2.107347      26.65
 O       3.362902     0.556337    -2.342830     175.68
 H       3.496526     1.285511    -1.710830      29.25
 C       4.018612    -0.819271    -0.113863      87.06
 H       3.493712    -1.782605     0.336605      27.92
 O       5.267747    -1.134161    -0.701167     144.93
 H       5.396614    -1.249515    -1.680608      25.46
 C       4.088410     0.349487     0.903407     108.15
 O       4.383901     1.598890     0.148152     228.97
 H       4.118047     2.414538     0.696514      27.81
 H       5.015810     0.103712     1.493510      27.29
 H       3.017874     0.625536     1.268558      27.99
55
name = lig-Water-frame_115
 C      -2.208278     1.752839     4.502887      48.16
 H      -3.034723     2.559728     4.559234      23.45
 C      -1.184214    -0.346948     3.730890       2.01
 H      -1.149451    -1.317248     3.286686      25.27
 C      -0.022341    -0.128486     4.556359      -7.15
 O       1.070258    -0.923422     4.549035     200.57
 C       1.161221    -2.217806     4.130030     150.34
 H       2.226775    -2.633535     3.928320      28.28
 H       0.740692    -2.714368     3.156618      28.33
 H       0.760755    -3.139242     4.652441      27.42
 C       0.048552     1.212776     5.118181     -43.08
 O       1.430251     1.717896     5.328806     191.72
 H       1.599361     2.574204     4.839443      23.28
 C      -1.022880     2.099185     5.158857      75.99
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 H      -0.869992     3.174483     5.303943      25.53
 C      -2.394019     0.574760     3.772918       3.96
 C      -3.460127     0.345200     2.711313     100.66
 H      -4.330667     1.166624     3.020292      25.00
 O      -3.823339    -1.082144     2.876360     285.41
 H      -4.790197    -1.134141     2.672784      28.19
 C      -2.987874     0.582337     1.269673      97.71
 H      -2.268336     1.310433     1.202582      31.72
 C      -4.028953     1.213843     0.203018     108.20
 O      -5.182464     0.459344    -0.065853     221.01
 H      -4.933745    -0.489628    -0.279532      27.75
 H      -3.602753     1.332369    -0.675757      29.84
 H      -4.244510     2.271099     0.549829      28.72
 C       0.914362     0.605653    -0.669481      45.45
 H       1.428184     1.608188    -0.776119      27.98
 C       0.849636    -1.857153    -0.635556      53.55
 H       1.405386    -2.770131    -0.783681      26.63
 C      -0.423847    -1.836477    -0.174579     -16.38
 O      -1.359789    -2.933963    -0.111813     169.67
 C      -1.255724    -3.935825    -1.136541     120.57
 H      -2.012646    -4.723119    -1.310238      26.87
 H      -1.530221    -3.420659    -2.127007      26.88
 H      -0.330721    -4.608910    -1.265575      25.57
 C      -0.946582    -0.423398     0.310627     -53.03
 O      -2.360341    -0.553849     0.621921     116.41
 C      -0.353444     0.722833    -0.075467      82.55
 H      -0.772306     1.683789    -0.105537      29.43
 C       1.587578    -0.579040    -1.005472      47.72
 C       2.960838    -0.576156    -1.285862      88.43
 H       3.245086    -1.332629    -1.996909      28.75
 O       3.327485     0.563888    -2.323630     175.68
 H       3.680295     1.285337    -1.764135      27.55
 C       3.951419    -0.814407    -0.084659      72.55
 H       3.438818    -1.817665     0.436751      27.55
 O       5.326950    -1.109937    -0.693460      73.15
 H       5.174551    -1.457152    -1.668386      24.46
 C       4.082545     0.360879     0.950010     115.83
 O       4.395279     1.578361     0.147267     258.10
 H       4.131086     2.360258     0.668915      28.85
 H       4.920101     0.151036     1.601387      29.56
 H       3.087123     0.237027     1.346792      32.00
55
name = lig-Water-frame_116
 C      -2.262740     1.742303     4.535071      55.30
 H      -3.070290     2.374318     4.539506      26.90
 C      -1.236038    -0.291541     3.773480      42.03
 H      -1.291807    -1.353835     3.170873      25.64
 C      -0.014059    -0.093517     4.529215     -11.93
 O       1.064190    -0.928792     4.566023     169.67
 C       1.236082    -2.269080     4.151044     130.67
 H       2.246053    -2.491981     4.004547      28.16
 H       0.415008    -2.190128     3.293951      27.64
 H       0.813751    -3.167784     4.647828      27.53
 C       0.073300     1.230622     5.096331     -30.72
 O       1.425097     1.734389     5.323525     253.42
 H       1.444782     2.612808     4.773122      23.04
 C      -1.001099     2.058761     5.099757      62.62
 H      -0.698181     3.127261     5.296469      22.14
 C      -2.349899     0.551826     3.761230      -8.24
 C      -3.458384     0.305417     2.803759      98.65
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 H      -4.421165     0.884499     2.785566      23.90
 O      -3.836450    -1.051977     2.881664     279.56
 H      -4.805293    -1.243034     2.678293      27.53
 C      -3.021397     0.584607     1.182838      77.97
 H      -2.119549     1.335750     1.415528      26.66
 C      -3.982049     1.251312     0.212833      85.44
 O      -5.197477     0.436584    -0.040522     193.91
 H      -5.002232    -0.490169    -0.211464      29.07
 H      -3.639505     1.354711    -1.020882      23.93
 H      -4.256193     2.359936     0.561933      25.82
 C       0.931741     0.616123    -0.669244      56.08
 H       1.420737     1.563285    -0.739402      28.19
 C       0.875030    -1.833001    -0.687683      53.71
 H       1.336742    -2.846363    -0.845081      24.99
 C      -0.420143    -1.777152    -0.153215     -16.01
 O      -1.318212    -2.952528    -0.142703     135.52
 C      -1.245259    -3.944510    -1.200154     112.48
 H      -2.182972    -4.605083    -0.658374      22.10
 H      -1.489881    -3.274964    -1.998880      26.13
 H      -0.437249    -4.659993    -1.061474      24.43
 C      -0.992319    -0.472173     0.258637     -33.34
 O      -2.299537    -0.576392     0.584843     118.61
 C      -0.347927     0.732977    -0.073160      44.56
 H      -0.843994     1.770253    -0.043653      24.70
 C       1.529569    -0.609462    -0.987106      16.30
 C       3.112948    -0.513529    -1.339245     101.99
 H       3.182855    -1.624659    -1.893391      24.12
 O       3.289532     0.561266    -2.266646     168.80
 H       3.943872     1.288145    -1.803288      22.53
 C       3.919131    -0.801249    -0.094186      84.90
 H       3.649418    -1.691778     0.573245      27.33
 O       5.349949    -1.092501    -0.665021      69.59
 H       5.138962    -1.503756    -1.526354      27.35
 C       4.083612     0.348044     0.937934     105.07
 O       4.397483     1.547981     0.156332     255.83
 H       4.070522     2.359835     0.738256      25.66
 H       4.769013     0.205606     1.858550      27.07
 H       3.147764     0.175895     1.652455      29.27
55
name = lig-Water-frame_117
 C      -2.304999     1.714795     4.553456      42.99
 H      -3.227178     2.420892     4.556155      26.22
 C      -1.249825    -0.312860     3.820333     102.34
 H      -1.433372    -1.083794     3.226719      25.03
 C      -0.061982    -0.050777     4.481597       0.98
 O       1.088311    -0.899159     4.632005     197.01
 C       1.223439    -2.342323     4.106770      99.93
 H       2.397392    -2.239890     3.900633      23.61
 H       0.629940    -2.096565     3.218275      24.44
 H       0.806912    -2.885326     5.032945      22.72
 C       0.164321     1.209423     5.053128      12.61
 O       1.389463     1.752051     5.315410     287.06
 H       1.373565     2.554541     4.645568      22.75
 C      -0.999403     2.058408     5.037358      56.10
 H      -0.696921     3.127096     5.501407      19.07
 C      -2.295914     0.562266     3.763324     -18.12
 C      -3.494016     0.239813     2.811758      84.21
 H      -4.463911     0.876470     2.888732      25.05
 O      -3.859464    -1.065807     2.896949     239.07
 H      -4.832084    -1.160620     2.752904      25.23
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 C      -2.966538     0.627813     1.126117      83.38
 H      -2.313466     1.344206     1.490981      28.25
 C      -3.948178     1.263059     0.159005     102.93
 O      -5.229785     0.429878    -0.004242     220.23
 H      -4.877096    -0.522849    -0.099888      27.19
 H      -3.447459     1.440867    -0.682523      28.77
 H      -4.332797     2.190828     0.565987      26.52
 C       0.938498     0.646379    -0.657639      64.75
 H       1.580719     1.532260    -0.880040      26.28
 C       0.897372    -1.815759    -0.743197      62.00
 H       1.264388    -2.786068    -0.989251      27.39
 C      -0.441730    -1.729533    -0.139880       5.86
 O      -1.251701    -2.921663    -0.124644     151.57
 C      -1.290951    -3.957905    -1.196675     119.77
 H      -2.101332    -4.395554    -0.650906      25.30
 H      -1.335950    -3.511129    -2.262065      24.06
 H      -0.321031    -4.606334    -1.092120      25.52
 C      -1.050601    -0.555223     0.163687      21.54
 O      -2.284559    -0.598544     0.573398     130.45
 C      -0.333076     0.736507    -0.083896      56.64
 H      -0.832656     1.627440     0.145695      23.37
 C       1.515446    -0.618139    -0.945512     -20.84
 C       3.162577    -0.542875    -1.409753     119.83
 H       3.281311    -1.484122    -1.873277      26.01
 O       3.286371     0.570580    -2.192708     251.59
 H       3.983873     1.073288    -1.864651      28.35
 C       3.993869    -0.754925    -0.096328      89.20
 H       3.648445    -1.738831     0.533937      26.41
 O       5.335024    -1.075702    -0.602514     119.08
 H       5.399249    -1.481515    -1.553617      24.38
 C       4.073815     0.317310     0.946429     121.74
 O       4.380588     1.528605     0.196311     281.66
 H       4.059859     2.294026     0.676261      29.45
 H       4.826159     0.169691     1.695987      29.41
 H       3.169458     0.561997     1.496287      27.65
55
name = lig-Water-frame_118
 C      -2.315952     1.718121     4.565988      58.29
 H      -3.104489     2.414437     4.628079      24.11
 C      -1.249545    -0.362692     3.857623      60.76
 H      -1.436000    -1.328245     3.093527      22.87
 C      -0.040797    -0.057088     4.452376      14.06
 O       1.106444    -0.846312     4.706412     171.63
 C       1.203988    -2.325239     4.085785      97.80
 H       2.210553    -2.363042     3.882302      27.65
 H       0.845822    -2.631645     2.909494      24.17
 H       0.922051    -2.747268     4.980182      25.17
 C       0.163953     1.209658     4.981989      26.58
 O       1.367152     1.782241     5.293625     274.93
 H       1.530618     2.520594     4.670274      28.87
 C      -0.988674     2.084945     5.015931      61.25
 H      -0.933501     2.975753     5.564801      21.32
 C      -2.317769     0.593038     3.758953     -48.42
 C      -3.523387     0.216353     2.753489      82.17
 H      -4.274714     1.028527     3.191928      25.45
 O      -3.899742    -1.136689     2.922462     232.77
 H      -4.896240    -1.083415     2.836926      21.92
 C      -2.913495     0.650003     1.137070      74.14
 H      -2.200696     1.549285     1.393012      24.99
 C      -3.954287     1.229638     0.139116      77.77
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 O      -5.226358     0.423033     0.023086     196.27
 H      -4.855925    -0.497502    -0.025618      27.24
 H      -3.190515     1.569580    -0.825479      22.88
 H      -4.450383     2.215451     0.688196      23.96
 C       0.951609     0.682348    -0.641517      53.91
 H       1.605647     1.482129    -0.999294      24.04
 C       0.856145    -1.799075    -0.769249      63.30
 H       1.307996    -2.758617    -1.158843      27.52
 C      -0.418202    -1.769852    -0.195175      26.93
 O      -1.186051    -2.869764    -0.087845     191.69
 C      -1.278810    -3.935287    -1.171132     111.54
 H      -2.358663    -4.654079    -1.012818      24.51
 H      -1.291790    -3.886886    -2.250934      26.07
 H      -0.414702    -4.530278    -1.187251      28.30
 C      -1.052208    -0.541937     0.050831       8.03
 O      -2.346674    -0.603355     0.594193     122.95
 C      -0.325416     0.680833    -0.094645      64.94
 H      -0.803518     1.616852     0.324696      22.99
 C       1.596094    -0.594899    -0.926107     -25.47
 C       3.085349    -0.620143    -1.399628      81.19
 H       3.504911    -1.516132    -2.207573      21.90
 O       3.301945     0.596648    -2.144554     201.11
 H       4.137458     1.035032    -1.803702      26.10
 C       4.080866    -0.753062    -0.114711     100.82
 H       3.499551    -1.687416     0.213917      27.41
 O       5.334911    -1.060439    -0.526865     190.35
 H       5.566955    -1.307604    -1.469730      23.40
 C       4.065586     0.331092     0.951531     115.87
 O       4.377933     1.525522     0.227441     247.58
 H       3.997232     2.336160     0.707214      27.42
 H       5.009799     0.000973     1.552165      27.83
 H       3.040019     0.720077     1.261713      23.54
55
name = lig-Water-frame_119
 C      -2.265770     1.735495     4.566176      54.91
 H      -3.086232     2.497655     4.695214      26.02
 C      -1.279215    -0.442311     3.834697      56.18
 H      -1.213621    -1.313466     3.370168      25.96
 C       0.030237    -0.094873     4.446103      -9.86
 O       1.111064    -0.820940     4.735392     116.45
 C       1.193717    -2.262098     4.046883      92.53
 H       2.358635    -2.552460     4.010293      24.90
 H       0.787688    -2.846586     3.191145      26.37
 H       0.856809    -3.053204     4.875169      23.83
 C       0.074541     1.282173     4.895167      23.50
 O       1.378392     1.806782     5.273019     219.56
 H       1.617648     2.630825     4.641867      25.62
 C      -0.994448     2.085166     5.016068      61.09
 H      -1.093970     3.087963     5.745489      16.19
 C      -2.367405     0.558531     3.729371     -46.23
 C      -3.484312     0.257702     2.710350      95.45
 H      -4.226178     0.947555     3.069314      27.21
 O      -3.959539    -1.208779     2.944289     194.74
 H      -4.980431    -1.216919     2.906358      19.47
 C      -2.907701     0.665219     1.206223      86.92
 H      -2.131779     1.419269     1.168842      28.98
 C      -3.968982     1.223927     0.154442     110.50
 O      -5.175417     0.410631     0.033689     270.69
 H      -4.969008    -0.540679    -0.057677      27.76
 H      -3.591923     1.463305    -0.760719      29.93
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 H      -4.286550     2.114086     0.568293      29.01
 C       1.008785     0.671111    -0.643842      35.84
 H       1.459011     1.628315    -0.930529      24.47
 C       0.850428    -1.777613    -0.802907      83.76
 H       1.297903    -2.659766    -1.199743      28.60
 C      -0.388908    -1.801042    -0.302203      17.78
 O      -1.164778    -2.876698    -0.066278     203.08
 C      -1.282419    -3.946212    -1.138429     112.99
 H      -2.129874    -4.589085    -1.152599      28.21
 H      -1.337098    -3.587875    -2.232081      25.93
 H      -0.385088    -4.719164    -0.953064      25.61
 C      -1.054698    -0.493427    -0.029504      -8.07
 O      -2.403828    -0.588605     0.619727      99.06
 C      -0.329895     0.631269    -0.097912      71.76
 H      -0.667429     1.570766     0.302652      26.96
 C       1.669466    -0.569630    -0.922333      11.72
 C       3.025068    -0.682700    -1.390321     111.39
 H       3.242327    -1.396706    -2.074500      27.49
 O       3.324993     0.634493    -2.115578     176.29
 H       4.227897     0.996727    -1.687407      24.81
 C       4.050186    -0.790429    -0.182452      85.88
 H       3.498132    -1.805644     0.270853      26.82
 O       5.394380    -1.048453    -0.448621     179.54
 H       5.436254    -1.211375    -1.432910      26.07
 C       4.064695     0.360825     0.926157     122.10
 O       4.403311     1.562730     0.243667     280.94
 H       3.961861     2.325033     0.759432      26.86
 H       4.761585     0.003261     1.662793      31.04
 H       3.062747     0.289727     1.388111      29.16
55
name = lig-Water-frame_120
 C      -2.236148     1.730042     4.514368      44.77
 H      -3.075534     2.436963     4.683045      26.11
 C      -1.266778    -0.466297     3.833651      29.95
 H      -1.206083    -1.613539     3.406185      27.26
 C       0.010088    -0.072730     4.438825     -27.45
 O       1.123708    -0.860256     4.715395     128.40
 C       1.239445    -2.241123     4.091087     106.11
 H       2.263198    -2.453148     4.119558      28.35
 H       0.411464    -2.507417     3.180932      27.64
 H       0.770024    -2.965220     4.699202      27.55
 C       0.066051     1.338282     4.812969     -55.61
 O       1.393400     1.833182     5.236923     207.89
 H       1.452711     2.603070     4.673174      21.09
 C      -1.058305     2.138733     5.071778      42.21
 H      -0.919112     2.937040     5.606461      26.50
 C      -2.376965     0.479011     3.715689      -6.95
 C      -3.423301     0.292737     2.689883      86.80
 H      -4.529214     0.886525     2.709926      23.79
 O      -4.010239    -1.247833     2.955371     180.46
 H      -4.996383    -1.318218     2.869523      21.45
 C      -2.947489     0.642484     1.247764      88.34
 H      -2.069735     1.330234     1.263099      30.98
 C      -4.004039     1.185292     0.226032      86.92
 O      -5.126157     0.394658     0.043886     237.44
 H      -4.950040    -0.597980    -0.157884      24.69
 H      -3.696273     1.323896    -0.993241      25.15
 H      -4.279108     2.381146     0.560138      25.29
 C       1.063767     0.636584    -0.647064      60.79
 H       1.343890     1.708061    -0.707736      27.79
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 C       0.921054    -1.745314    -0.860331      62.53
 H       1.343759    -2.732458    -1.180225      27.56
 C      -0.431997    -1.760987    -0.404882     -19.74
 O      -1.184720    -2.940458    -0.059718     132.45
 C      -1.218762    -3.953564    -1.118935     106.26
 H      -2.356152    -4.582873    -0.919420      24.20
 H      -1.165945    -3.181015    -1.889041      26.07
 H      -0.518035    -4.653695    -0.868542      26.98
 C      -1.105790    -0.515332    -0.052155      -6.57
 O      -2.409125    -0.573581     0.627024      78.33
 C      -0.285805     0.634094    -0.119854      50.80
 H      -0.630796     1.624528     0.188270      30.00
 C       1.649832    -0.546150    -0.913802      45.29
 C       3.046674    -0.643609    -1.380705     116.43
 H       2.934276    -1.704290    -2.154880      22.91
 O       3.358573     0.655613    -2.092984     208.56
 H       4.088933     0.981696    -1.657275      30.01
 C       3.946318    -0.860601    -0.201581      83.51
 H       3.814706    -1.697279     0.509286      29.81
 O       5.457708    -1.050287    -0.412443     127.62
 H       5.472090    -1.276630    -1.405711      28.06
 C       4.028973     0.336673     0.872295     118.23
 O       4.429635     1.617668     0.274011     258.07
 H       3.998006     2.340960     0.772735      28.31
 H       4.658119     0.110264     1.836808      29.58
 H       3.105227     0.064156     1.500864      31.91
55
name = lig-Water-frame_121
 C      -2.265993     1.691975     4.422224      46.93
 H      -3.156965     2.275551     4.528869      25.28
 C      -1.222373    -0.496576     3.832982      64.00
 H      -1.476904    -1.455990     3.506676      29.83
 C      -0.062441    -0.014484     4.427439      16.57
 O       1.129906    -0.911982     4.671900     105.24
 C       1.216279    -2.204557     4.143574     120.65
 H       2.391677    -2.375991     3.968498      28.00
 H       0.632116    -1.958084     3.140480      28.79
 H       0.672812    -2.883145     4.909193      28.04
 C       0.125395     1.350060     4.770357     -55.05
 O       1.379850     1.847425     5.184681     176.93
 H       1.430421     2.749773     4.638033      23.03
 C      -1.089110     2.150825     5.104725      28.57
 H      -0.746655     3.231803     5.657788      20.45
 C      -2.334389     0.422230     3.744951      36.09
 C      -3.467622     0.280548     2.668265      79.69
 H      -4.318655     0.804755     2.677405      28.75
 O      -4.024504    -1.257099     2.955207     212.97
 H      -5.036599    -1.243936     2.724658      21.87
 C      -2.968369     0.601024     1.240893      84.60
 H      -2.169854     1.367075     1.549678      31.31
 C      -4.015619     1.202362     0.258648     129.80
 O      -5.127801     0.355386     0.068115     236.11
 H      -4.775120    -0.503600    -0.219134      27.76
 H      -3.437410     1.201723    -0.604407      29.68
 H      -4.337004     2.107923     0.510353      32.17
 C       1.033566     0.659362    -0.607462     120.40
 H       1.592852     1.588067    -0.572528      32.85
 C       0.947668    -1.742670    -0.908787      33.02
 H       1.426807    -2.705197    -1.085178      27.28
 C      -0.511547    -1.719909    -0.474965     -56.31
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 O      -1.198142    -2.983927    -0.036902     128.99
 C      -1.209314    -3.936531    -1.068666     110.07
 H      -2.184836    -4.321104    -0.929089      27.32
 H      -0.985981    -3.316169    -1.994762      25.55
 H      -0.332308    -4.780805    -1.004614      23.86
 C      -1.154270    -0.545541    -0.034667      -1.57
 O      -2.373558    -0.579999     0.611203      86.47
 C      -0.244802     0.649507    -0.155755      31.16
 H      -0.694606     1.666135     0.026435      31.04
 C       1.630964    -0.555297    -0.930078      38.17
 C       3.079115    -0.609250    -1.423884     132.84
 H       3.067692    -1.419823    -2.002087      28.58
 O       3.384266     0.635131    -2.079643     222.39
 H       4.122757     1.130818    -1.535730      25.62
 C       3.942230    -0.894907    -0.134627      71.57
 H       3.741459    -1.787148     0.588593      29.90
 O       5.473763    -1.071518    -0.426790      84.67
 H       5.708783    -1.381840    -1.330835      27.97
 C       3.976338     0.278904     0.850188     111.17
 O       4.441778     1.649976     0.312685     201.76
 H       3.993533     2.447336     0.865101      26.08
 H       4.784368     0.149598     1.543277      33.73
 H       2.961479     0.435613     1.300503      32.46
55
name = lig-Water-frame_122
 C      -2.290949     1.658154     4.354533      27.81
 H      -3.327035     2.176009     4.308123      19.84
 C      -1.228303    -0.488252     3.833746      73.79
 H      -1.539413    -1.546839     3.524001      27.86
 C      -0.060109    -0.011476     4.421438      11.75
 O       1.121122    -0.873749     4.657548     139.33
 C       1.168074    -2.167399     4.168900     138.19
 H       2.186139    -2.436440     3.890947      30.85
 H       1.048969    -1.927447     3.025746      31.17
 H       0.713169    -2.879992     4.805159      30.38
 C       0.137621     1.374560     4.786814     -23.31
 O       1.361096     1.869060     5.109006     193.73
 H       1.546866     2.760818     4.710608      22.73
 C      -1.050488     2.140702     5.089716      41.09
 H      -1.026480     3.077978     5.458523      26.56
 C      -2.297059     0.405731     3.762397      40.20
 C      -3.513064     0.158464     2.678783      56.65
 H      -4.369476     1.093484     3.041848      22.89
 O      -4.022018    -1.225411     2.933437     263.48
 H      -4.966438    -1.223909     2.641916      24.17
 C      -2.968842     0.568478     1.254717      86.74
 H      -2.318584     1.374292     1.533097      32.61
 C      -3.978527     1.180148     0.294869      91.95
 O      -5.152865     0.307944     0.091557     194.58
 H      -4.753626    -0.519491    -0.295954      27.55
 H      -3.118786     1.310912    -0.601144      27.14
 H      -4.539532     2.282239     0.642139      24.97
 C       1.013864     0.694064    -0.557872      57.74
 H       1.823193     1.449226    -0.550253      28.45
 C       0.873788    -1.756789    -0.925818      24.63
 H       1.451446    -2.683945    -1.048996      28.54
 C      -0.566105    -1.731954    -0.497361     -19.49
 O      -1.180105    -2.965797    -0.005604     181.21
 C      -1.146728    -3.933784    -1.052651     109.43
 H      -2.369394    -4.393417    -1.209418      25.12
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 H      -1.023467    -3.772920    -2.160214      25.28
 H      -0.463254    -4.681251    -1.057692      28.79
 C      -1.127027    -0.531504    -0.025247      14.07
 O      -2.337597    -0.596090     0.591909      99.34
 C      -0.308184     0.673150    -0.177213      78.71
 H      -0.766109     1.610517    -0.046664      32.94
 C       1.641562    -0.577602    -0.976661     -11.80
 C       3.100944    -0.557659    -1.411731      99.97
 H       3.478464    -1.463919    -2.314136      22.66
 O       3.431840     0.610772    -2.072635     222.31
 H       3.943816     1.266322    -1.433941      25.10
 C       4.018264    -0.903088    -0.070930      84.85
 H       3.420944    -1.832882     0.305073      29.41
 O       5.455616    -1.101053    -0.434178      44.56
 H       5.623027    -1.420010    -1.381418      25.73
 C       3.928745     0.281039     0.845329     108.38
 O       4.444410     1.662739     0.338470     195.82
 H       4.036789     2.339890     0.913732      28.72
 H       4.826081    -0.030484     1.483611      30.29
 H       2.963722     0.710742     1.113290      27.23
55
name = lig-Water-frame_123
 C      -2.285608     1.648541     4.335855      78.18
 H      -3.151615     2.197041     4.242797      23.87
 C      -1.248328    -0.490652     3.841797      82.37
 H      -1.248463    -1.602277     3.565016      23.79
 C       0.005718    -0.049508     4.420392     -26.10
 O       1.103389    -0.761586     4.675624     157.23
 C       1.145321    -2.135400     4.114505      98.35
 H       2.267073    -2.528257     4.197500      25.93
 H       0.874172    -2.319927     2.945874      29.23
 H       0.528893    -3.011009     4.587159      23.83
 C       0.089957     1.397323     4.830555     -35.66
 O       1.374496     1.885426     5.040201     238.53
 H       1.491880     2.791833     4.642912      24.82
 C      -1.060767     2.078971     4.985857      50.07
 H      -1.219165     3.187514     5.412677      25.59
 C      -2.317947     0.398844     3.722616      50.43
 C      -3.548874     0.058559     2.765351     110.59
 H      -4.102926     0.779869     3.102291      31.01
 O      -4.011491    -1.173047     2.893175     302.10
 H      -4.987698    -1.300708     2.630350      24.32
 C      -2.987709     0.532015     1.303686      77.75
 H      -2.213890     1.421884     1.412803      28.23
 C      -3.944312     1.176320     0.316623     109.16
 O      -5.154701     0.275216     0.099926     212.00
 H      -4.956177    -0.599592    -0.384458      25.77
 H      -3.508499     1.525279    -0.582340      29.67
 H      -4.303111     1.997606     0.679809      31.89
 C       1.045927     0.661196    -0.538231       0.51
 H       1.672128     1.578243    -0.554413      25.72
 C       0.764087    -1.762972    -0.926996      34.58
 H       1.279531    -2.736524    -1.101916      25.71
 C      -0.559102    -1.769603    -0.475648      12.47
 O      -1.143540    -2.919489    -0.011359     185.56
 C      -1.160714    -3.980632    -1.094998      89.44
 H      -2.093706    -4.452608    -1.200073      28.37
 H      -1.046997    -3.694902    -2.158782      24.92
 H      -0.415211    -4.887007    -0.701166      23.81
 C      -1.056301    -0.495821    -0.036843      -3.25
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 O      -2.322399    -0.606896     0.585851      96.82
 C      -0.404909     0.704632    -0.189911      72.81
 H      -0.925922     1.701415     0.039765      27.93
 C       1.618066    -0.585531    -1.022650      25.71
 C       3.160727    -0.582290    -1.406524     106.94
 H       3.390874    -1.226163    -2.093833      30.98
 O       3.495323     0.631653    -2.071971     254.03
 H       3.712077     1.253325    -1.414348      29.54
 C       4.058046    -0.886863    -0.114188     101.48
 H       3.452375    -1.768202     0.197169      28.62
 O       5.418687    -1.138190    -0.422629     157.17
 H       5.239820    -1.325326    -1.413373      26.72
 C       3.950951     0.330298     0.868776     114.59
 O       4.459987     1.635136     0.333404     218.75
 H       4.053108     2.361990     0.993200      25.13
 H       4.444083    -0.040733     1.814687      29.96
 H       2.879849     0.492950     1.243694      29.31
55
name = lig-Water-frame_124
 C      -2.259264     1.618485     4.326177      31.91
 H      -3.070352     2.463702     4.301704      26.61
 C      -1.198998    -0.513436     3.873109      70.30
 H      -1.134504    -1.511678     3.535518      24.32
 C       0.001599    -0.019156     4.420649      -4.67
 O       1.109073    -0.695586     4.678113     179.96
 C       1.161062    -2.149955     4.037380     102.13
 H       2.051760    -2.415617     4.609840      23.40
 H       0.724740    -2.464951     3.056512      26.08
 H       0.333480    -2.709906     4.536048      22.95
 C       0.073289     1.353351     4.858609     -30.73
 O       1.396619     1.900378     4.980039     213.65
 H       1.310319     2.845684     4.512665      18.30
 C      -1.145101     2.080519     4.868631      87.21
 H      -1.103700     3.089940     5.333010      31.69
 C      -2.361103     0.363935     3.665152     -45.31
 C      -3.488699     0.045086     2.835972     102.50
 H      -4.474310     0.893125     3.150562      25.79
 O      -4.022760    -1.199645     2.852113     266.26
 H      -5.010391    -1.253584     2.666054      24.18
 C      -2.972752     0.510800     1.329054      85.61
 H      -2.217733     1.194662     1.478172      29.16
 C      -3.956074     1.113444     0.330574      82.97
 O      -5.152760     0.269611     0.102110     246.05
 H      -5.012620    -0.543446    -0.396297      27.48
 H      -3.727105     1.566717    -0.770056      24.82
 H      -4.362500     2.140138     1.042532      24.91
 C       1.035115     0.611185    -0.544883      43.24
 H       1.377220     1.643676    -0.573005      22.48
 C       0.716150    -1.765271    -0.949980      71.17
 H       1.039134    -2.758759    -1.201214      25.73
 C      -0.512889    -1.763149    -0.419010      24.18
 O      -1.128860    -2.900883    -0.055273     177.31
 C      -1.138918    -4.061908    -1.110601      78.32
 H      -2.303733    -4.633670    -0.941263      22.25
 H      -0.845355    -3.452844    -1.984334      24.00
 H      -0.538646    -4.689002    -0.584059      25.53
 C      -1.050506    -0.478357    -0.032341       2.70
 O      -2.314083    -0.617257     0.590974     101.26
 C      -0.423850     0.758258    -0.211742      67.91
 H      -0.910663     1.624731     0.114344      25.72
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 C       1.569476    -0.574292    -1.043216      27.42
 C       3.189731    -0.582375    -1.369524      75.36
 H       3.244807    -1.606476    -2.246357      22.37
 O       3.566090     0.666431    -2.086336     159.60
 H       3.537393     1.402961    -1.283506      22.44
 C       4.038517    -0.818531    -0.170048      91.34
 H       3.661462    -1.774155     0.460678      26.45
 O       5.371511    -1.182818    -0.425904     184.79
 H       5.385635    -1.292877    -1.430175      26.37
 C       3.961282     0.365991     0.933465     123.45
 O       4.470531     1.580766     0.339403     265.21
 H       4.185780     2.388326     0.855151      25.42
 H       4.271192     0.148897     1.987239      29.27
 H       2.895992     0.222183     1.198867      29.31
55
name = lig-Water-frame_125
 C      -2.321665     1.591788     4.278307      51.97
 H      -3.033497     2.352958     4.310191      26.67
 C      -1.168332    -0.513338     3.896744      51.75
 H      -1.196481    -1.582746     3.352458      21.57
 C      -0.043484     0.057490     4.439376       6.68
 O       1.144764    -0.692493     4.638772     196.11
 C       1.135585    -2.150458     4.053031      89.00
 H       2.033952    -2.520392     4.590411      24.35
 H       1.004503    -2.243206     2.853147      24.95
 H       0.259333    -2.415742     4.726251      21.50
 C       0.072751     1.314559     4.861040      -2.19
 O       1.382980     1.920735     4.918274     220.56
 H       1.323371     2.780617     4.496196      21.02
 C      -1.122302     2.115107     4.798593     103.55
 H      -1.016795     3.124631     5.224896      25.16
 C      -2.333775     0.310500     3.682285     -52.93
 C      -3.507492     0.133375     2.836749     110.48
 H      -4.264981     0.684784     2.985483      29.64
 O      -4.040564    -1.293795     2.819183     263.18
 H      -5.004366    -1.140726     2.662033      26.64
 C      -2.941510     0.473528     1.305785      71.20
 H      -2.079569     1.236485     1.656946      25.93
 C      -4.035262     1.099310     0.372107     118.04
 O      -5.164565     0.293647     0.116580     274.67
 H      -4.845007    -0.522980    -0.396715      25.75
 H      -3.639566     1.432321    -0.587484      27.38
 H      -4.369554     1.794799     0.932313      29.85
 C       0.941926     0.610531    -0.568721      61.15
 H       1.453505     1.619643    -0.656498      21.45
 C       0.761222    -1.755342    -1.008253      57.11
 H       1.063952    -2.781144    -1.366881      23.61
 C      -0.484868    -1.709026    -0.340411       0.94
 O      -1.154155    -2.915080    -0.098922     183.64
 C      -1.165722    -4.103263    -1.057743      92.89
 H      -2.094322    -4.443029    -1.010947      26.68
 H      -0.704306    -3.603983    -1.970458      25.19
 H      -0.277426    -4.823560    -0.657494      23.66
 C      -1.112112    -0.463874     0.000708       9.82
 O      -2.311097    -0.638587     0.607497     138.40
 C      -0.379264     0.747286    -0.233493      64.38
 H      -0.807360     1.727579     0.146006      23.60
 C       1.549629    -0.568864    -1.046508      24.33
 C       3.138061    -0.603110    -1.401962      90.08
 H       3.249331    -1.377286    -1.942166      26.43
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 O       3.628882     0.690845    -2.084875     221.79
 H       3.516450     1.367667    -1.424787      26.92
 C       4.022740    -0.766971    -0.121826      86.16
 H       3.675070    -1.568949     0.547163      26.58
 O       5.351329    -1.221971    -0.452582     224.49
 H       5.710634    -1.393236    -1.398649      27.03
 C       3.936293     0.368116     0.981540     102.41
 O       4.477135     1.523027     0.349050     270.92
 H       4.234508     2.397634     0.802109      25.50
 H       4.601123     0.242186     1.918561      24.96
 H       2.786986     0.367379     0.981142      23.45
55
name = lig-Water-frame_126
 C      -2.353450     1.587399     4.247460      52.14
 H      -3.354524     2.163960     4.185695      21.34
 C      -1.204289    -0.529942     3.868372     107.59
 H      -1.194958    -1.395311     3.402000      23.34
 C      -0.026728     0.023560     4.464049     -23.59
 O       1.189287    -0.702837     4.565178     152.00
 C       1.090055    -2.106063     4.117981      96.39
 H       2.047856    -2.743910     4.293645      22.83
 H       1.434728    -1.920069     3.091137      23.66
 H       0.158485    -2.532420     4.616967      19.99
 C       0.074409     1.399829     4.845620      -0.48
 O       1.345574     1.917120     4.871125     260.81
 H       1.382751     2.874993     4.416595      23.25
 C      -1.053164     2.137568     4.757822     106.76
 H      -1.023203     3.313578     5.040223      24.92
 C      -2.294313     0.278291     3.758521     -14.15
 C      -3.503737     0.110044     2.740427      64.91
 H      -4.492842     0.992683     3.017464      19.28
 O      -4.044863    -1.369625     2.790945     232.99
 H      -5.063401    -1.256518     2.620963      24.42
 C      -2.904787     0.464361     1.294778      90.80
 H      -2.247088     1.213677     1.479646      27.31
 C      -4.077857     1.069361     0.429276      79.38
 O      -5.191598     0.305969     0.125245     265.54
 H      -4.821525    -0.522615    -0.308367      25.70
 H      -3.418652     1.445510    -0.512475      23.26
 H      -4.602358     2.109486     1.046582      21.50
 C       0.895471     0.652529    -0.635363      52.82
 H       1.592291     1.435633    -0.727949      21.24
 C       0.819664    -1.740197    -1.060427      48.16
 H       1.248795    -2.629306    -1.465868      24.89
 C      -0.457782    -1.683496    -0.298097     -13.80
 O      -1.202498    -2.931989    -0.125991     169.50
 C      -1.082039    -4.088683    -0.971609     102.71
 H      -2.338374    -4.452572    -1.249283      21.91
 H      -0.863060    -3.982405    -2.072478      25.84
 H      -0.407905    -4.900784    -0.863379      25.71
 C      -1.150436    -0.462189     0.032988      23.00
 O      -2.335039    -0.662307     0.644552     161.40
 C      -0.389063     0.711695    -0.209892      75.22
 H      -0.627305     1.741341     0.024733      24.05
 C       1.567176    -0.565607    -1.052879       8.91
 C       3.044210    -0.532211    -1.388526      51.34
 H       3.480184    -1.581630    -2.140288      18.51
 O       3.670082     0.669421    -2.097517     202.64
 H       3.614335     1.393049    -1.441427      25.56
 C       4.025891    -0.750397    -0.048621      64.79
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 H       3.408942    -1.623908     0.532447      24.03
 O       5.360897    -1.251641    -0.450234     187.97
 H       5.516324    -1.443964    -1.481473      23.49
 C       3.918564     0.371793     0.972013     104.85
 O       4.489095     1.500146     0.347557     289.85
 H       4.191033     2.324256     0.895658      26.76
 H       4.658862     0.087421     1.744190      24.21
 H       2.875204     0.649869     1.180013      22.82
55
name = lig-Water-frame_127
 C      -2.322579     1.615743     4.260194      52.90
 H      -3.351008     1.940948     4.108079      20.74
 C      -1.196826    -0.531447     3.861425      30.24
 H      -1.155791    -1.615452     3.319559      19.83
 C       0.016894    -0.057638     4.482938       0.42
 O       1.225478    -0.704144     4.508690     185.75
 C       1.098064    -2.058356     4.170638     112.84
 H       1.893255    -2.703443     4.435287      26.89
 H       1.268659    -1.922349     3.007454      27.08
 H       0.150122    -2.731846     4.249694      23.22
 C       0.087301     1.463130     4.791089     -18.62
 O       1.331598     1.929771     4.832825     276.94
 H       1.371620     2.820135     4.393657      23.77
 C      -1.087666     2.212885     4.713760      51.63
 H      -1.016644     3.206060     4.816497      29.05
 C      -2.356387     0.291562     3.803709      -1.46
 C      -3.510253     0.037122     2.665017      90.01
 H      -4.128521     0.696824     2.905411      29.55
 O      -4.040601    -1.398209     2.756625     288.70
 H      -5.009925    -1.532089     2.578113      26.86
 C      -2.959079     0.466709     1.317660      79.70
 H      -2.185658     1.401510     1.276910      23.25
 C      -4.083573     1.124562     0.497503     109.64
 O      -5.225863     0.305143     0.125466     316.58
 H      -5.039520    -0.597640    -0.210813      26.49
 H      -3.538874     1.467125    -0.385848      26.14
 H      -4.416864     1.954580     0.837742      28.04
 C       0.932127     0.652728    -0.738199      43.30
 H       1.592873     1.611222    -0.754249      22.63
 C       0.834586    -1.714062    -1.064575      59.98
 H       1.369292    -2.612286    -1.484968      25.36
 C      -0.418485    -1.725083    -0.326247      -8.90
 O      -1.240972    -2.926809    -0.142423     170.36
 C      -1.062835    -4.077693    -0.968830     123.23
 H      -1.972686    -4.443610    -1.071838      28.31
 H      -0.989183    -3.983416    -2.070950      26.48
 H      -0.474004    -5.044756    -0.567951      24.57
 C      -1.128154    -0.504242     0.051988      11.54
 O      -2.375519    -0.686506     0.688201     118.45
 C      -0.429835     0.702431    -0.162816      61.29
 H      -0.756073     1.737233    -0.020851      22.41
 C       1.581188    -0.527174    -1.069074      16.38
 C       3.045106    -0.486819    -1.387204      92.73
 H       3.254937    -1.182003    -1.978828      26.44
 O       3.674435     0.620472    -2.116186     224.90
 H       3.861402     1.416941    -1.411504      22.08
 C       3.967481    -0.806462    -0.020925      74.52
 H       3.403801    -1.643785     0.392663      26.55
 O       5.353286    -1.263772    -0.422225     223.26
 H       5.184773    -1.379618    -1.417109      23.37
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 C       3.938747     0.375992     0.937118     102.91
 O       4.508380     1.528817     0.341304     293.03
 H       4.238301     2.274638     0.903989      28.07
 H       4.527403    -0.152465     1.815892      24.64
 H       3.032733     0.667409     1.607789      23.80
55
name = lig-Water-frame_128
 C      -2.289895     1.618595     4.277328      42.72
 H      -3.214904     2.233046     4.188657      26.77
 C      -1.152746    -0.553552     3.864902      15.50
 H      -1.216466    -1.483919     3.442692      25.68
 C       0.019933    -0.057395     4.488504      24.09
 O       1.242465    -0.696589     4.491295     184.18
 C       1.135987    -2.057010     4.123420     120.77
 H       1.920765    -2.570261     4.864251      25.09
 H       1.016754    -2.268445     3.021693      28.16
 H       0.127866    -2.619081     4.101431      24.95
 C       0.059066     1.419157     4.699844     -29.64
 O       1.356418     1.954708     4.807351     211.11
 H       1.384092     2.911205     4.324911      22.48
 C      -1.152196     2.265924     4.664800      35.72
 H      -1.002817     3.508537     4.684347      17.72
 C      -2.425991     0.284270     3.797574       1.44
 C      -3.463649    -0.101670     2.662915      72.33
 H      -4.455939     0.781672     2.984364      22.51
 O      -4.006294    -1.405379     2.716361     267.43
 H      -4.999414    -1.516812     2.503647      25.95
 C      -3.024763     0.500705     1.332671      88.81
 H      -2.284095     1.200866     1.410167      27.09
 C      -4.075106     1.123380     0.499113      76.55
 O      -5.272608     0.323318     0.135628     259.08
 H      -5.099971    -0.676780    -0.085646      23.67
 H      -3.642915     1.501787    -0.556653      23.38
 H      -4.479236     2.246834     1.055542      22.33
 C       0.944552     0.692057    -0.803662      65.49
 H       1.308635     1.660079    -0.804529      29.60
 C       0.829545    -1.707432    -1.033493      70.66
 H       1.274053    -2.633980    -1.354712      28.32
 C      -0.402078    -1.806606    -0.393621       2.46
 O      -1.252890    -2.887407    -0.159186     153.48
 C      -1.038821    -4.109856    -0.989353      91.20
 H      -2.210483    -4.693563    -0.719099      21.94
 H      -0.754674    -3.745840    -1.992753      24.52
 H      -0.468080    -4.686020    -0.250085      24.10
 C      -1.084424    -0.563759     0.075722     -21.07
 O      -2.392909    -0.712499     0.710016      76.99
 C      -0.422812     0.699476    -0.146547      37.36
 H      -1.058434     1.633275     0.011029      21.77
 C       1.586363    -0.457704    -1.094969      21.81
 C       3.105615    -0.428909    -1.346997      84.87
 H       3.114811    -1.474771    -2.272298      19.48
 O       3.662081     0.590901    -2.125255     263.78
 H       4.045058     1.189389    -1.533972      28.84
 C       3.874943    -0.858665    -0.056642      65.81
 H       3.389563    -1.854399     0.463116      25.70
 O       5.301405    -1.255527    -0.372084     154.42
 H       5.226643    -1.342513    -1.465959      20.27
 C       3.980360     0.346176     0.967410     109.48
 O       4.534794     1.565777     0.335080     256.86
 H       4.297151     2.431413     0.906493      24.31
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 H       4.620338    -0.086457     1.777664      28.05
 H       3.115353     0.499129     1.555711      29.01
55
name = lig-Water-frame_129
 C      -2.338766     1.618654     4.267645      30.20
 H      -3.013421     2.528530     4.283456      18.98
 C      -1.168555    -0.522251     3.891864       1.17
 H      -1.251196    -1.594954     3.466977      27.41
 C      -0.006422     0.016710     4.466122      46.18
 O       1.239180    -0.683463     4.480835     146.66
 C       1.177936    -2.116418     4.073990     116.98
 H       1.803109    -2.478362     4.788389      32.80
 H       1.397728    -2.418979     2.999972      31.11
 H       0.076201    -2.407007     4.537614      27.11
 C       0.024733     1.384595     4.607264     -15.96
 O       1.375977     1.975686     4.782427     230.09
 H       1.404247     2.897279     4.351212      22.98
 C      -1.119458     2.298275     4.618067      31.78
 H      -1.109863     3.273027     4.679997      14.47
 C      -2.413553     0.234640     3.771549     -59.50
 C      -3.502957    -0.135531     2.754452     108.80
 H      -4.302319     0.360126     2.939973      29.40
 O      -3.956956    -1.433891     2.671630     274.94
 H      -4.918610    -1.261020     2.473209      27.39
 C      -3.066348     0.478032     1.339061      69.15
 H      -2.207279     1.221990     1.728528      28.16
 C      -4.119664     1.160660     0.449874     112.30
 O      -5.320609     0.350769     0.163632     253.47
 H      -4.952041    -0.542748     0.031097      27.34
 H      -3.735166     1.472106    -0.535061      26.83
 H      -4.408075     1.869866     1.050291      29.28
 C       0.857994     0.776665    -0.804572      81.86
 H       1.274117     1.855183    -0.956729      31.98
 C       0.842238    -1.707381    -0.991296      50.82
 H       1.284510    -2.692511    -1.253236      30.74
 C      -0.444093    -1.840221    -0.438145     -19.29
 O      -1.255908    -2.844416    -0.190152     160.31
 C      -1.076954    -4.142850    -0.931948     114.78
 H      -1.885187    -4.625806    -0.874467      29.80
 H      -0.545591    -3.844854    -1.873644      21.80
 H      -0.170882    -4.525144    -0.322621      23.78
 C      -1.040562    -0.597339     0.101381     -53.13
 O      -2.367723    -0.737613     0.697020      39.33
 C      -0.414329     0.652391    -0.162904      63.84
 H      -1.053936     1.456496     0.018501      28.72
 C       1.592191    -0.409903    -1.124610     -72.45
 C       3.137152    -0.497442    -1.372740     121.57
 H       3.168623    -1.293403    -1.947184      24.30
 O       3.647273     0.574898    -2.138943     273.63
 H       4.242529     1.148249    -1.502502      27.30
 C       3.820000    -0.897091    -0.088446      79.06
 H       3.351830    -1.699614     0.424981      30.89
 O       5.220395    -1.239384    -0.345609     194.76
 H       5.529276    -1.352100    -1.224715      26.90
 C       4.035145     0.294528     1.010753      93.05
 O       4.556724     1.595532     0.336217     221.58
 H       4.264980     2.366572     0.854926      28.17
 H       4.978302     0.093612     1.657500      28.48
 H       2.915024     0.468787     1.336072      29.12
55
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name = lig-Water-frame_130
 C      -2.377638     1.648144     4.248273      39.71
 H      -3.197294     2.332956     4.218155      26.99
 C      -1.245526    -0.498888     3.913634      93.73
 H      -1.168572    -1.555287     3.568788      28.78
 C      -0.021048     0.057864     4.401876      11.42
 O       1.224896    -0.660262     4.456400      89.42
 C       1.168574    -2.165337     4.063158     106.03
 H       2.036685    -2.678414     4.760954      27.30
 H       1.735949    -2.385711     3.129556      28.76
 H       0.351407    -2.365625     4.746898      23.25
 C       0.058863     1.462236     4.548018      12.51
 O       1.365643     1.953639     4.765667     263.65
 H       1.423133     2.980047     4.337749      21.34
 C      -1.073261     2.199051     4.555922      71.51
 H      -1.083960     3.409215     4.803258      18.78
 C      -2.363950     0.220975     3.763436     -64.35
 C      -3.521607    -0.121909     2.835573      80.63
 H      -4.651289     0.502240     3.192816      21.79
 O      -3.913721    -1.498341     2.628245     258.82
 H      -4.890628    -1.395057     2.482740      25.84
 C      -3.039308     0.425503     1.354226      71.64
 H      -2.403053     1.195339     1.706200      30.26
 C      -4.166554     1.146911     0.400415      81.20
 O      -5.352623     0.378349     0.202350     228.71
 H      -4.959687    -0.535416    -0.004591      26.28
 H      -3.686447     1.568711    -0.576743      26.39
 H      -4.568388     2.088624     1.206876      23.96
 C       0.783546     0.855916    -0.795935      72.13
 H       1.229044     1.758735    -1.058135      24.77
 C       0.877820    -1.700008    -0.954287      21.55
 H       1.440213    -2.615129    -1.201960      27.65
 C      -0.488176    -1.771661    -0.449527      11.78
 O      -1.289593    -2.853090    -0.234051     167.72
 C      -1.002909    -4.111543    -0.834717     114.57
 H      -2.054384    -4.897554    -1.122602      23.15
 H      -0.671192    -4.098437    -1.914216      24.61
 H      -0.075096    -4.678502    -0.531893      26.14
 C      -1.021851    -0.616894     0.116937       9.56
 O      -2.312764    -0.744817     0.666963      88.26
 C      -0.424762     0.582512    -0.189913      80.02
 H      -0.991757     1.559562     0.085082      28.86
 C       1.558475    -0.387857    -1.136426     -35.93
 C       3.094385    -0.556324    -1.394264      63.89
 H       3.404447    -1.715098    -2.058838      22.39
 O       3.645605     0.576648    -2.147294     212.14
 H       4.266182     1.089637    -1.480728      28.65
 C       3.854178    -0.861634    -0.096363      77.43
 H       3.121475    -1.712600     0.456088      29.46
 O       5.156702    -1.238207    -0.306520     130.25
 H       5.641614    -1.371239    -1.243917      21.80
 C       4.073548     0.270511     1.007664     119.56
 O       4.571806     1.590478     0.328349     208.42
 H       4.128129     2.343951     0.916343      25.93
 H       4.876653     0.074713     1.651866      32.93
 H       3.120574     0.501292     1.371685      30.01
55
name = lig-Water-frame_131
 C      -2.365350     1.639278     4.212312      96.48
 H      -3.456050     2.002040     4.132035      23.51
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 C      -1.252337    -0.520580     3.946209      88.08
 H      -1.204139    -1.530550     3.622651      25.13
 C      -0.015602     0.067346     4.308019     -17.06
 O       1.203735    -0.642194     4.417329     136.97
 C       1.238721    -2.179259     4.143553     108.40
 H       2.048538    -2.556077     4.625086      30.18
 H       1.484840    -2.340025     3.048274      28.36
 H       0.251728    -2.775171     4.544806      22.84
 C       0.158046     1.513384     4.509051       7.49
 O       1.350507     1.939735     4.748420     234.77
 H       1.482439     2.865254     4.395349      22.57
 C      -1.110441     2.159399     4.500197      86.98
 H      -0.935858     3.116112     4.888504      29.15
 C      -2.390780     0.299896     3.774198     -43.07
 C      -3.591343    -0.087872     2.879547      97.57
 H      -4.290406     0.455663     3.229411      31.07
 O      -3.877086    -1.564646     2.603811     252.19
 H      -4.862191    -1.772770     2.507226      24.69
 C      -3.029692     0.377175     1.357514      65.03
 H      -2.323575     1.313039     1.480464      27.89
 C      -4.201531     1.152829     0.430981     104.54
 O      -5.365435     0.387372     0.229797     231.55
 H      -5.241624    -0.552353    -0.115584      27.19
 H      -3.702375     1.601052    -0.484932      27.64
 H      -4.487044     2.014769     0.858736      29.10
 C       0.782607     0.825400    -0.814872      46.89
 H       1.162655     1.873752    -1.040200      21.47
 C       0.899026    -1.654763    -0.919401      44.91
 H       1.512712    -2.508427    -1.168036      26.46
 C      -0.475215    -1.713534    -0.457384       2.59
 O      -1.334706    -2.895184    -0.282686     148.23
 C      -0.934140    -4.138400    -0.821530     130.64
 H      -1.710475    -4.687963    -0.834973      31.21
 H      -0.882601    -4.035270    -1.935552      27.09
 H      -0.174943    -4.812885    -0.347733      27.43
 C      -1.052305    -0.614417     0.126581       8.73
 O      -2.266848    -0.730634     0.650574     127.77
 C      -0.463973     0.612659    -0.200519      64.76
 H      -0.900134     1.474323     0.157889      30.43
 C       1.496303    -0.401133    -1.132880      29.79
 C       3.045446    -0.623418    -1.444541      90.37
 H       3.301842    -1.467573    -1.975563      29.49
 O       3.644376     0.569384    -2.147477     258.32
 H       4.089702     1.031660    -1.500112      31.70
 C       3.865098    -0.799706    -0.063126      94.63
 H       3.265876    -1.567599     0.367334      30.75
 O       5.169157    -1.271211    -0.276261     180.14
 H       5.176491    -1.343633    -1.278502      27.26
 C       4.090283     0.294812     0.944214     126.38
 O       4.575415     1.562410     0.330557     227.96
 H       4.134269     2.299465     0.856086      26.26
 H       4.741730    -0.190547     1.866752      28.01
 H       3.204849     0.581432     1.681116      27.54
55
name = lig-Water-frame_132
 C      -2.376929     1.598178     4.158541      89.14
 H      -3.324012     2.073455     4.197497      30.36
 C      -1.226274    -0.529044     3.971419      47.84
 H      -1.371348    -1.666551     3.629548      23.44
 C       0.017453     0.070337     4.210884       9.24
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 O       1.178968    -0.662670     4.375884     162.21
 C       1.271431    -2.160459     4.216088     116.73
 H       2.293447    -2.426624     4.758952      23.70
 H       1.027612    -2.216507     3.094059      24.45
 H       0.517798    -2.959931     4.118622      23.28
 C       0.140649     1.446583     4.445857       4.81
 O       1.391873     1.939568     4.754330     242.40
 H       1.511708     2.945791     4.335322      19.24
 C      -1.118271     2.174006     4.476095      74.70
 H      -0.990037     3.225066     4.967310      22.98
 C      -2.431768     0.328356     3.784046     -48.59
 C      -3.581428    -0.116972     2.838860      76.80
 H      -4.595175     0.661112     3.254453      23.26
 O      -3.839674    -1.610279     2.610028     239.02
 H      -4.799919    -1.845994     2.588898      24.48
 C      -3.037956     0.392823     1.349520      76.61
 H      -2.271557     1.173346     1.309719      26.74
 C      -4.179496     1.098046     0.468281      85.19
 O      -5.398528     0.387737     0.241862     207.87
 H      -5.274335    -0.491988    -0.150564      28.38
 H      -3.706450     1.413474    -0.549023      24.81
 H      -4.539832     2.237904     0.964306      23.80
 C       0.809874     0.749402    -0.844318      57.94
 H       1.097812     1.793517    -0.882502      23.09
 C       0.870175    -1.613470    -0.884681      64.27
 H       1.439180    -2.544861    -1.136501      25.45
 C      -0.444302    -1.749893    -0.456116     -14.36
 O      -1.350242    -2.906031    -0.324306     110.97
 C      -0.856132    -4.172484    -0.856032      90.40
 H      -1.979428    -4.847937    -0.384437      20.89
 H      -0.744211    -3.979407    -1.923144      25.47
 H      -0.127605    -4.665573    -0.104342      24.02
 C      -1.082385    -0.557032     0.105920     -18.78
 O      -2.284419    -0.712966     0.671297     123.76
 C      -0.486308     0.692439    -0.203823      58.61
 H      -0.993279     1.613970     0.268172      26.50
 C       1.477192    -0.415498    -1.132241      65.71
 C       2.998892    -0.571153    -1.438898      73.62
 H       3.132337    -1.621959    -2.281819      22.81
 O       3.626881     0.535874    -2.161253     179.42
 H       3.935447     1.187636    -1.320263      21.92
 C       3.836048    -0.734962    -0.034221      71.58
 H       3.300905    -1.670613     0.587419      26.52
 O       5.208598    -1.324222    -0.288772     156.82
 H       5.074678    -1.417953    -1.226647      28.65
 C       4.069347     0.353999     0.954224     130.34
 O       4.581809     1.513317     0.337757     297.15
 H       4.262110     2.332138     0.815507      26.92
 H       4.700267    -0.205459     1.591707      28.84
 H       3.281645     0.592295     1.599558      28.55
55
name = lig-Water-frame_133
 C      -2.376293     1.623926     4.130777      38.53
 H      -3.172336     2.439412     4.265141      18.68
 C      -1.251015    -0.536601     3.952458      83.52
 H      -1.386347    -1.510776     3.778505      25.85
 C       0.042689     0.019674     4.125949      14.41
 O       1.160384    -0.703843     4.356239     191.31
 C       1.299103    -2.122608     4.212032     117.94
 H       2.261840    -2.321961     4.588845      27.13
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 H       1.315785    -2.106997     3.116703      26.60
 H       0.509463    -2.950785     4.546508      24.71
 C       0.061002     1.397522     4.383697     -18.22
 O       1.445532     1.954155     4.760210     250.10
 H       1.448994     2.825107     4.280739      25.65
 C      -1.078326     2.211360     4.480475      61.66
 H      -1.215100     3.273709     4.882213      16.78
 C      -2.437401     0.214590     3.770429     -67.01
 C      -3.576914    -0.134576     2.770447     104.76
 H      -4.448893     0.247290     2.872266      26.62
 O      -3.800570    -1.618341     2.645434     272.18
 H      -4.795377    -1.607487     2.650587      25.65
 C      -3.064907     0.422320     1.332403      78.85
 H      -2.268123     1.202487     1.523678      24.47
 C      -4.143800     1.061481     0.500288     104.36
 O      -5.439514     0.391232     0.251858     223.94
 H      -5.105539    -0.510067    -0.093428      25.52
 H      -3.735686     1.110278    -0.553325      22.61
 H      -4.387880     1.917877     1.005765      26.22
 C       0.792322     0.715530    -0.836079      67.89
 H       1.324925     1.681677    -0.863305      25.30
 C       0.815889    -1.658862    -0.864647      76.23
 H       1.302556    -2.572200    -1.112103      25.62
 C      -0.477073    -1.791056    -0.412390     -10.29
 O      -1.321921    -2.878372    -0.367345     174.80
 C      -0.866786    -4.227454    -0.816947     120.71
 H      -1.551632    -4.776780    -0.550629      29.78
 H      -0.476931    -4.283885    -1.889055      26.83
 H       0.060355    -4.407265    -0.255253      26.90
 C      -1.095574    -0.482567     0.042077     -47.38
 O      -2.352751    -0.707046     0.711515     112.20
 C      -0.500840     0.766557    -0.198106      80.95
 H      -0.904213     1.694334     0.151708      24.44
 C       1.519949    -0.416311    -1.136615      27.70
 C       2.970958    -0.515266    -1.437254     113.65
 H       2.994965    -1.340910    -2.080349      24.99
 O       3.609296     0.516387    -2.148063     282.79
 H       3.692522     1.232556    -1.529225      28.26
 C       3.782783    -0.765392    -0.017882      72.83
 H       3.331075    -1.440819     0.627725      28.65
 O       5.225369    -1.367935    -0.315782     108.39
 H       5.407821    -1.614148    -1.383731      23.68
 C       4.029007     0.407161     0.983877      93.66
 O       4.600214     1.487767     0.329378     267.36
 H       4.462199     2.379996     0.859803      25.74
 H       5.015263    -0.089019     1.502608      23.65
 H       3.022097     0.651411     1.534403      23.59
55
name = lig-Water-frame_134
 C      -2.333448     1.668140     4.125548      13.18
 H      -3.087471     2.455998     4.161849      21.34
 C      -1.286459    -0.547950     3.903037      57.86
 H      -1.330168    -1.768434     3.850420      22.75
 C       0.012330    -0.042308     4.069749      -5.53
 O       1.158708    -0.725916     4.365581     203.26
 C       1.293839    -2.108048     4.149889     120.23
 H       2.376287    -2.340534     4.546378      24.40
 H       1.702358    -2.408722     3.094767      23.67
 H       0.726060    -2.446134     5.068261      22.59
 C       0.066135     1.408746     4.358634     -53.66
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 O       1.449883     1.933935     4.755363     236.06
 H       1.496231     2.861253     4.221877      21.66
 C      -1.088664     2.218348     4.475160      31.08
 H      -1.099559     3.248204     4.764881      24.56
 C      -2.461176     0.160817     3.753729     -36.00
 C      -3.505621    -0.202028     2.680954      93.57
 H      -4.769701     0.183618     2.762014      20.56
 O      -3.782123    -1.592576     2.694606     256.97
 H      -4.776987    -1.550421     2.609859      24.68
 C      -3.061398     0.422887     1.342177      85.99
 H      -2.445561     1.263800     1.810945      24.64
 C      -4.118873     0.993609     0.484754      92.73
 O      -5.449695     0.377374     0.265268     212.58
 H      -5.200948    -0.576185     0.064315      26.47
 H      -3.672147     1.135269    -0.530830      23.97
 H      -4.342925     2.102952     1.099480      23.10
 C       0.786515     0.742667    -0.805127      78.57
 H       1.528303     1.570184    -0.926270      26.80
 C       0.785152    -1.732508    -0.871759      51.30
 H       1.286652    -2.703154    -1.159585      22.63
 C      -0.543726    -1.754302    -0.354713       7.01
 O      -1.294415    -2.858398    -0.418963     161.74
 C      -0.798201    -4.216195    -0.777656      93.26
 H      -1.709415    -5.240518    -0.592668      21.26
 H      -0.483106    -4.547994    -1.798182      25.23
 H       0.276382    -4.276719    -0.342452      23.40
 C      -1.153200    -0.447194    -0.012109     -27.20
 O      -2.407359    -0.695352     0.731718      90.60
 C      -0.494516     0.798068    -0.209085      57.71
 H      -0.855259     1.819320     0.039563      22.26
 C       1.505618    -0.440027    -1.105799     -16.67
 C       2.970493    -0.460868    -1.376382      89.86
 H       3.108089    -1.590850    -2.100716      19.02
 O       3.590203     0.520975    -2.146522     254.36
 H       3.609501     1.377604    -1.648333      28.56
 C       3.777390    -0.807989    -0.052551      55.50
 H       3.120918    -1.581026     0.701720      24.45
 O       5.219140    -1.411320    -0.355115     153.01
 H       5.503418    -1.543931    -1.221728      29.61
 C       4.017379     0.413388     1.007806     108.17
 O       4.624144     1.519462     0.299854     295.85
 H       4.570958     2.279889     0.885414      28.87
 H       4.748638     0.145249     1.695191      27.99
 H       3.074073     0.626254     1.482191      27.55
55
name = lig-Water-frame_135
 C      -2.293818     1.647711     4.106246      43.85
 H      -3.234347     2.214604     4.010588      27.50
 C      -1.303817    -0.647089     3.840865      40.31
 H      -1.322680    -1.649679     3.790173      24.63
 C      -0.041106    -0.030425     4.062934     -19.12
 O       1.174375    -0.705071     4.356814     184.13
 C       1.363297    -2.122055     4.129859     123.71
 H       2.330685    -2.230191     4.609276      26.12
 H       1.369414    -2.790696     3.237040      27.24
 H       0.811468    -2.441337     5.014656      24.64
 C       0.145180     1.410612     4.359557     -66.30
 O       1.406158     1.904701     4.722420     260.64
 H       1.559757     2.795967     4.330245      26.02
 C      -1.092353     2.192271     4.459481      55.74
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 H      -0.770553     3.341289     4.680321      23.25
 C      -2.495349     0.236172     3.742427     -26.78
 C      -3.523057    -0.241178     2.644944     110.53
 H      -4.287512     0.316552     2.905836      30.42
 O      -3.784683    -1.581579     2.738737     298.39
 H      -4.726100    -1.791653     2.522010      24.75
 C      -3.049664     0.392255     1.387426      91.51
 H      -2.468289     1.268483     1.676551      29.07
 C      -4.135407     0.993155     0.460811     106.19
 O      -5.425605     0.348029     0.287060     224.23
 H      -5.430660    -0.630852     0.174044      26.58
 H      -3.610223     1.331308    -0.521776      24.87
 H      -4.337695     1.975251     0.794053      27.91
 C       0.837789     0.763323    -0.778470     105.86
 H       1.389364     1.673580    -0.913233      31.11
 C       0.773039    -1.766762    -0.890324      67.14
 H       1.225761    -2.687178    -1.190364      25.22
 C      -0.556679    -1.668561    -0.343811     -25.60
 O      -1.311282    -2.880877    -0.472511     141.31
 C      -0.714537    -4.240720    -0.732712     119.64
 H      -1.319294    -4.887564    -0.432580      30.52
 H      -0.685631    -4.357196    -1.860460      26.26
 H       0.166876    -4.390825    -0.181852      27.30
 C      -1.249191    -0.446839    -0.027032     -15.51
 O      -2.410261    -0.671196     0.710143      97.91
 C      -0.486624     0.805935    -0.231842      10.56
 H      -0.941491     1.813271     0.001773      24.81
 C       1.419976    -0.502074    -1.038005      -4.79
 C       2.999530    -0.506458    -1.313901     101.10
 H       3.239590    -1.394038    -1.900607      25.52
 O       3.574640     0.549141    -2.153787     217.29
 H       3.628467     1.502215    -1.654009      26.05
 C       3.814168    -0.853966    -0.057776      88.58
 H       3.242944    -1.602709     0.342729      29.69
 O       5.176236    -1.444885    -0.350687     143.42
 H       5.336540    -1.366952    -1.436482      23.39
 C       4.023463     0.390306     0.975466      98.36
 O       4.644758     1.557976     0.259304     212.56
 H       4.557409     2.367540     0.934070      24.00
 H       4.473321     0.130864     2.120851      26.42
 H       3.009600     0.695160     1.452399      27.59
55
name = lig-Water-frame_136
 C      -2.312789     1.580830     4.064953      67.73
 H      -3.335988     2.061930     3.919732      25.06
 C      -1.316528    -0.673511     3.788285      14.78
 H      -1.412138    -1.856859     3.591309      21.52
 C      -0.064086     0.003071     4.101407     -17.06
 O       1.189000    -0.661722     4.303170     154.69
 C       1.439087    -2.161274     4.185119     108.46
 H       2.490811    -2.215625     4.537017      25.28
 H       0.842115    -2.748689     3.341580      25.43
 H       0.694976    -2.874140     4.793147      23.66
 C       0.165176     1.388499     4.363128       4.44
 O       1.361379     1.865061     4.684766     241.13
 H       1.457095     2.841814     4.341573      25.35
 C      -0.996583     2.183633     4.440805      58.20
 H      -0.844985     3.154179     4.598641      24.09
 C      -2.449225     0.286662     3.724670     -56.69
 C      -3.546233    -0.205431     2.708379      85.84
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 H      -4.386970     0.662996     3.158994      23.44
 O      -3.802754    -1.610464     2.776835     271.90
 H      -4.702799    -1.860308     2.433980      24.26
 C      -3.063114     0.368434     1.383137      86.74
 H      -2.275795     1.229679     1.403946      29.01
 C      -4.151539     0.997771     0.411029      89.42
 O      -5.399927     0.324681     0.313201     199.98
 H      -5.351813    -0.700837     0.149405      24.81
 H      -3.664753     1.220592    -0.545738      25.20
 H      -4.536279     2.161558     0.812970      23.42
 C       0.860717     0.752880    -0.736698      60.86
 H       1.245764     1.802652    -0.874274      27.52
 C       0.734766    -1.729698    -0.890958     100.23
 H       1.183145    -2.690475    -1.203781      26.62
 C      -0.553975    -1.650138    -0.396769     -33.77
 O      -1.347560    -2.900605    -0.502047     113.33
 C      -0.615530    -4.194697    -0.717007      87.54
 H      -1.542986    -4.959983    -0.001042      21.59
 H      -0.695377    -4.147004    -1.805015      24.47
 H       0.303145    -4.508712    -0.037753      23.92
 C      -1.290742    -0.437426    -0.028180     -13.52
 O      -2.385989    -0.654705     0.658705     106.45
 C      -0.506496     0.784163    -0.257120      44.11
 H      -1.002641     1.685521    -0.010727      29.51
 C       1.403843    -0.549131    -0.974937      -5.19
 C       3.015726    -0.545015    -1.256081      80.23
 H       3.363768    -1.519208    -2.073840      22.47
 O       3.556955     0.590878    -2.145051     239.83
 H       3.683257     1.307514    -1.587851      30.54
 C       3.902409    -0.846944    -0.030454      86.70
 H       3.240588    -1.871581     0.304304      26.72
 O       5.120283    -1.470289    -0.371331     186.10
 H       5.126177    -1.192138    -1.336514      25.56
 C       4.005200     0.363142     0.970977     117.71
 O       4.664054     1.577359     0.244134     223.28
 H       4.436687     2.379866     0.786860      26.98
 H       4.369893     0.090945     1.860515      32.32
 H       2.982200     0.760443     1.072165      29.35
55
name = lig-Water-frame_137
 C      -2.313698     1.566854     4.041871      66.69
 H      -3.164006     2.184762     3.962506      27.06
 C      -1.295186    -0.642687     3.758282     116.91
 H      -1.456663    -1.634028     3.404673      29.61
 C      -0.059237    -0.043372     4.150063       3.90
 O       1.202019    -0.648624     4.238985     114.88
 C       1.420384    -2.218128     4.255527     110.05
 H       2.552829    -2.414775     4.170866      27.33
 H       0.996313    -2.246260     3.246847      29.00
 H       0.918153    -2.849737     4.927419      28.47
 C       0.098123     1.353414     4.366076      26.51
 O       1.363053     1.848881     4.645622     242.42
 H       1.284858     2.803915     4.345385      32.21
 C      -0.957590     2.142040     4.392628      77.49
 H      -1.027065     3.344309     4.632214      13.84
 C      -2.357226     0.206063     3.673284      -0.19
 C      -3.589830    -0.080358     2.850045      80.22
 H      -4.476933     0.345003     3.018568      26.11
 O      -3.829980    -1.628825     2.814176     294.28
 H      -4.749070    -1.662117     2.403335      25.25
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 C      -3.084558     0.396335     1.313053      84.62
 H      -2.314484     1.083933     1.453316      30.22
 C      -4.177013     1.041879     0.392450     101.63
 O      -5.389922     0.281914     0.336628     216.75
 H      -5.079709    -0.588042     0.019202      26.18
 H      -3.738615     0.980927    -0.698093      25.04
 H      -4.510873     1.955962     0.821128      26.89
 C       0.822695     0.721795    -0.678415      41.95
 H       1.314564     1.657981    -0.836868      29.13
 C       0.689681    -1.689159    -0.885395      70.79
 H       1.154538    -2.638545    -1.169924      29.75
 C      -0.615647    -1.699609    -0.477651      -0.64
 O      -1.364659    -2.883688    -0.496254     154.18
 C      -0.603424    -4.166340    -0.632913     121.34
 H      -1.243826    -4.732938    -0.289915      32.13
 H      -0.462552    -4.405142    -1.728826      27.51
 H       0.374009    -4.287141    -0.259400      29.39
 C      -1.213564    -0.436840    -0.057649     -30.91
 O      -2.396583    -0.670826     0.609737     129.25
 C      -0.545597     0.728421    -0.279177      99.35
 H      -1.036531     1.752770    -0.025971      28.94
 C       1.509593    -0.505674    -0.934186     -45.08
 C       3.029798    -0.595323    -1.271115      97.28
 H       3.185402    -1.450293    -1.976102      23.30
 O       3.530815     0.600676    -2.103736     213.36
 H       3.828834     1.292971    -1.353862      25.64
 C       3.929713    -0.866185     0.022146     109.06
 H       3.400133    -1.557082     0.579601      31.28
 O       5.085838    -1.480681    -0.409217     224.21
 H       5.304433    -1.239882    -1.317662      25.95
 C       3.951819     0.366550     0.899741     102.50
 O       4.687351     1.560106     0.238431     198.09
 H       4.324381     2.392071     0.740826      26.17
 H       4.601692     0.038100     1.916120      27.07
 H       2.908069     0.690952     0.890274      27.48
55
name = lig-Water-frame_138
 C      -2.236977     1.571691     4.041545      43.46
 H      -3.071366     2.381950     4.045482      24.82
 C      -1.218496    -0.610547     3.735736      76.36
 H      -1.349284    -1.621747     3.287461      29.62
 C      -0.022860    -0.131331     4.193549      15.13
 O       1.231819    -0.668398     4.202942     151.11
 C       1.384110    -2.222417     4.247516     116.52
 H       2.378375    -2.438373     4.023932      29.78
 H       1.218884    -2.223775     3.132938      27.70
 H       1.066179    -2.678805     5.311939      24.82
 C       0.072460     1.292360     4.384801     -30.60
 O       1.373268     1.844596     4.601514     178.92
 H       1.335527     2.808150     4.367519      22.85
 C      -1.076505     2.158160     4.333326      59.77
 H      -0.981289     3.129066     4.613650      22.49
 C      -2.341879     0.176251     3.630456     -40.33
 C      -3.591893    -0.040779     2.921651      63.12
 H      -4.774434     0.264593     3.066014      20.98
 O      -3.867437    -1.602194     2.847167     252.91
 H      -4.793144    -1.545463     2.506921      26.15
 C      -3.115025     0.436316     1.243526      63.15
 H      -2.336734     1.228909     1.651039      28.49
 C      -4.181282     1.040955     0.366273     102.21
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 O      -5.388500     0.228807     0.358738     197.73
 H      -5.081636    -0.624008    -0.121811      24.63
 H      -3.836997     1.063991    -0.639562      27.53
 H      -4.446916     2.199261     0.838463      24.82
 C       0.800072     0.675916    -0.630154      47.33
 H       1.420352     1.588596    -0.774146      26.95
 C       0.701580    -1.647922    -0.892784      19.99
 H       1.169323    -2.580283    -1.162020      27.54
 C      -0.687367    -1.744939    -0.563414      46.20
 O      -1.367091    -2.861031    -0.477087     159.42
 C      -0.586567    -4.102174    -0.611126      88.03
 H      -1.422237    -5.142254    -0.218407      22.95
 H      -0.309527    -4.633703    -1.565854      25.73
 H       0.500463    -3.897277    -0.196383      25.96
 C      -1.152921    -0.507397    -0.082264       0.24
 O      -2.436444    -0.701106     0.564073      96.04
 C      -0.570179     0.724792    -0.293928      99.47
 H      -0.971617     1.637766    -0.097993      28.59
 C       1.597344    -0.440074    -0.897921       7.40
 C       3.026856    -0.602286    -1.287288      81.03
 H       2.972668    -1.660499    -2.032366      22.35
 O       3.503800     0.589720    -2.010137     175.37
 H       4.046759     1.149039    -1.322681      24.08
 C       3.902936    -0.866052     0.017278      81.23
 H       3.410720    -1.428912     1.047151      26.82
 O       5.095587    -1.506087    -0.439237     167.79
 H       5.561113    -1.287872    -1.394596      22.06
 C       3.956550     0.398735     0.832422     117.59
 O       4.699397     1.521167     0.237074     241.67
 H       4.377129     2.342663     0.766223      24.66
 H       4.414687     0.248020     1.699114      31.77
 H       2.847569     0.570360     1.125392      29.42
55
name = lig-Water-frame_139
 C      -2.243674     1.564893     4.025889      87.45
 H      -3.075840     2.166762     4.063577      29.86
 C      -1.166528    -0.638225     3.691117      20.93
 H      -1.112625    -1.720490     3.261714      25.53
 C       0.051392    -0.149549     4.237769       5.20
 O       1.289751    -0.728481     4.192174     174.89
 C       1.353179    -2.170366     4.197922     120.19
 H       2.545528    -2.294419     4.253823      25.73
 H       0.868823    -2.845678     3.332815      26.84
 H       1.038999    -2.454351     5.130962      28.59
 C       0.078390     1.263336     4.415909     -24.06
 O       1.365799     1.834725     4.555860     150.55
 H       1.439782     2.837930     4.352123      19.45
 C      -1.096340     2.152100     4.302067      62.45
 H      -0.901690     3.254698     4.624297      21.60
 C      -2.370204     0.245139     3.641409     -10.09
 C      -3.632589    -0.116923     2.881848      79.98
 H      -4.405114     0.499909     3.310351      28.24
 O      -3.901489    -1.534379     2.880132     258.07
 H      -4.893523    -1.660284     2.653697      24.52
 C      -3.114462     0.480403     1.228035      64.10
 H      -2.490088     1.253733     1.476329      30.90
 C      -4.201333     1.051553     0.365247     108.78
 O      -5.389517     0.188256     0.373731     208.49
 H      -5.330914    -0.712647    -0.068007      23.63
 H      -3.827164     1.334454    -0.735543      26.44
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 H      -4.371441     2.094454     0.649322      28.24
 C       0.839910     0.684746    -0.601449      58.49
 H       1.304702     1.674742    -0.645159      25.05
 C       0.756765    -1.612751    -0.916398      36.72
 H       1.271488    -2.552941    -1.247735      25.26
 C      -0.650248    -1.728308    -0.650686      25.95
 O      -1.390763    -2.890708    -0.470380     190.25
 C      -0.584448    -4.104776    -0.569258     124.92
 H      -0.985187    -4.799268    -0.088738      31.45
 H      -0.359450    -4.407094    -1.602022      26.81
 H       0.180657    -3.797341     0.079776      28.71
 C      -1.206335    -0.586314    -0.076007     -12.91
 O      -2.481889    -0.713913     0.523703      88.34
 C      -0.548698     0.706339    -0.306487      57.44
 H      -1.089288     1.723191    -0.083034      24.62
 C       1.559312    -0.447289    -0.862311      60.66
 C       2.998537    -0.615098    -1.286761      96.29
 H       3.034350    -1.531796    -1.968366      25.50
 O       3.490982     0.558114    -1.903773     233.06
 H       4.134220     1.021549    -1.372607      26.77
 C       3.859576    -0.868306    -0.008493      96.69
 H       3.539413    -1.499152     0.708083      29.72
 O       5.141829    -1.548498    -0.448633     209.01
 H       5.328008    -1.239850    -1.322007      29.01
 C       3.964946     0.453471     0.778797     115.06
 O       4.702462     1.488282     0.226849     250.64
 H       4.517908     2.325925     0.759116      24.05
 H       4.453372     0.270194     1.931721      26.02
 H       2.999547     0.641675     1.205351      28.33
55
name = lig-Water-frame_140
 C      -2.332284     1.556347     4.005761      40.35
 H      -3.384914     2.066157     4.010836      18.69
 C      -1.141892    -0.660440     3.654192      25.89
 H      -1.076285    -1.638946     3.307778      24.52
 C       0.092587    -0.117658     4.249482     -32.92
 O       1.343955    -0.791860     4.172596     147.28
 C       1.370449    -2.151068     4.136789     139.67
 H       2.352338    -2.299285     4.356901      28.67
 H       0.706394    -3.010986     3.815585      24.46
 H       0.800919    -2.462062     5.187065      24.04
 C       0.100430     1.302273     4.442878      10.69
 O       1.360971     1.824390     4.517464     270.22
 H       1.360307     2.763785     4.266780      27.43
 C      -0.967010     2.144893     4.324025      64.30
 H      -0.948043     3.252968     4.514296      25.15
 C      -2.357025     0.231654     3.651450     -15.90
 C      -3.622862    -0.189895     2.794385      77.97
 H      -4.257029     0.695504     3.355111      22.02
 O      -3.943372    -1.463855     2.913803     263.19
 H      -4.907586    -1.682713     2.804100      24.29
 C      -3.128807     0.476939     1.232548      52.55
 H      -2.322919     1.348447     1.294711      26.32
 C      -4.223307     1.028442     0.319014      96.26
 O      -5.412348     0.185688     0.385542     214.47
 H      -5.260980    -0.764929     0.068803      24.51
 H      -3.860024     1.281655    -0.624754      27.83
 H      -4.619215     2.175689     0.777275      23.75
 C       0.865105     0.766170    -0.569047      48.58
 H       1.245558     1.778782    -0.550918      23.48
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 C       0.805276    -1.637612    -0.960941      70.59
 H       1.339075    -2.472823    -1.314959      25.92
 C      -0.577247    -1.706768    -0.699973     -10.60
 O      -1.423336    -2.927062    -0.484316     147.53
 C      -0.561066    -4.061106    -0.527634      89.77
 H      -1.108506    -5.021053     0.287154      22.29
 H      -0.319868    -4.118190    -1.627896      23.34
 H       0.291346    -3.913764     0.265473      25.44
 C      -1.301269    -0.584550    -0.074473     -16.01
 O      -2.525652    -0.707088     0.492845      93.29
 C      -0.536693     0.660103    -0.292020      60.60
 H      -1.059106     1.547077    -0.107274      27.30
 C       1.480899    -0.499233    -0.850298      55.84
 C       2.961228    -0.612563    -1.229348      74.00
 H       3.240368    -1.508887    -2.093653      23.77
 O       3.473061     0.532593    -1.836175     175.86
 H       4.313992     0.993287    -1.300871      20.57
 C       3.858674    -0.866265    -0.061252      81.49
 H       3.357562    -1.903210     0.463033      25.13
 O       5.176186    -1.575665    -0.438606     160.89
 H       5.196686    -1.229749    -1.391051      26.05
 C       3.999537     0.456853     0.840696     116.98
 O       4.725692     1.482673     0.191603     241.28
 H       4.572691     2.366478     0.727460      23.69
 H       4.448875     0.134372     1.674911      29.73
 H       2.931681     0.935651     1.045046      25.65
55
name = lig-Water-frame_141
 C      -2.363495     1.574733     4.018012      17.60
 H      -3.288852     2.087226     3.942957      20.87
 C      -1.107227    -0.611859     3.671372      72.10
 H      -1.207245    -1.747842     3.249993      26.15
 C       0.079282    -0.104034     4.201871     -26.47
 O       1.358106    -0.783706     4.130489     145.75
 C       1.352636    -2.220083     4.211773     120.72
 H       2.444467    -2.683595     4.277141      27.54
 H       0.617390    -2.857331     3.512841      28.38
 H       0.948538    -2.369507     5.165137      30.55
 C       0.158322     1.333019     4.455570       9.55
 O       1.388695     1.827294     4.490915     255.81
 H       1.317495     2.775977     4.155998      26.57
 C      -0.955990     2.131620     4.345729      56.80
 H      -0.854824     3.198606     4.443371      26.43
 C      -2.312035     0.133161     3.624335     -61.12
 C      -3.541318    -0.123372     2.719131      88.22
 H      -4.436267     0.506291     2.962564      23.89
 O      -3.987531    -1.453759     2.948351     257.90
 H      -5.020588    -1.477997     2.822208      25.26
 C      -3.139026     0.456545     1.236287      78.78
 H      -2.335777     1.115336     1.298190      28.69
 C      -4.279353     1.027178     0.327150      98.28
 O      -5.446786     0.193149     0.383015     208.96
 H      -5.049180    -0.719762     0.186113      25.34
 H      -3.843286     1.133994    -0.786949      25.45
 H      -4.766959     1.825706     0.846311      25.52
 C       0.839863     0.808567    -0.535385      55.90
 H       1.365795     1.803824    -0.525954      24.33
 C       0.786939    -1.724485    -1.013029      55.19
 H       1.405430    -2.583903    -1.391072      26.12
 C      -0.597290    -1.709460    -0.670285     -29.01
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 O      -1.426259    -2.925861    -0.507320     154.73
 C      -0.546746    -4.058454    -0.411810     129.87
 H      -1.137547    -4.813628    -0.257630      30.74
 H      -0.175599    -4.279264    -1.412452      27.27
 H       0.434570    -4.001841     0.025015      28.97
 C      -1.316283    -0.551077    -0.129251       2.82
 O      -2.572443    -0.695968     0.467274      99.17
 C      -0.544232     0.604792    -0.251921      67.28
 H      -1.077952     1.593630    -0.067824      27.96
 C       1.469542    -0.468329    -0.863050     -20.30
 C       2.956455    -0.605633    -1.190636      78.75
 H       3.140489    -1.524413    -2.013809      23.75
 O       3.466969     0.552723    -1.809174     215.32
 H       4.140298     0.898343    -1.295511      26.79
 C       3.856090    -0.944254    -0.060067      99.87
 H       3.297238    -1.628454     0.372311      30.50
 O       5.184388    -1.562054    -0.434694     131.43
 H       5.412063    -1.428266    -1.490718      22.45
 C       3.987037     0.422943     0.896439      99.59
 O       4.785954     1.497254     0.149092     217.68
 H       4.506589     2.318322     0.608885      27.47
 H       4.605844    -0.030863     1.860535      24.93
 H       3.078809     0.890814     0.952448      26.57
55
name = lig-Water-frame_142
 C      -2.270011     1.537194     4.043015      45.58
 H      -3.131221     2.262658     3.900451      26.50
 C      -1.104043    -0.604101     3.687406      84.12
 H      -1.198097    -1.513261     3.334662      30.61
 C       0.090022    -0.089058     4.136684       1.61
 O       1.352480    -0.750735     4.076208     121.60
 C       1.328680    -2.322067     4.308771     113.86
 H       2.227792    -2.779385     4.010111      30.00
 H       0.773378    -2.540768     3.228068      27.42
 H       1.023847    -2.481184     5.431160      25.75
 C       0.190310     1.300247     4.439483     -14.71
 O       1.457508     1.866239     4.469899     161.34
 H       1.483058     2.815970     4.115710      26.00
 C      -1.065246     2.111639     4.362071      42.45
 H      -0.727199     3.263184     4.433002      23.36
 C      -2.293111     0.130393     3.595143     -29.51
 C      -3.453070    -0.046208     2.645403      86.32
 H      -4.522472     0.544667     2.770046      22.75
 O      -4.027358    -1.467558     2.967153     246.79
 H      -4.999245    -1.353056     2.772716      26.58
 C      -3.153495     0.391769     1.216132      89.06
 H      -2.308914     1.149293     1.453435      29.43
 C      -4.326086     1.005231     0.354871      96.69
 O      -5.476752     0.176707     0.366784     215.29
 H      -5.184806    -0.757413     0.165744      25.72
 H      -3.992463     1.115553    -0.617048      28.92
 H      -4.743862     2.096553     0.879196      24.92
 C       0.806748     0.759110    -0.516041     134.75
 H       1.373699     1.656353    -0.516048      31.44
 C       0.730522    -1.765199    -1.049477      13.32
 H       1.250025    -2.643890    -1.376330      31.01
 C      -0.677563    -1.759202    -0.599030      -0.34
 O      -1.385616    -2.888768    -0.528131     127.33
 C      -0.520491    -4.065839    -0.367045     103.04
 H      -1.403738    -5.055288    -0.443707      23.17
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 H      -0.072618    -4.498047    -1.349890      26.06
 H       0.475859    -3.953185     0.200064      26.23
 C      -1.285952    -0.543075    -0.206956      28.44
 O      -2.603689    -0.693151     0.428986     112.18
 C      -0.571135     0.640466    -0.193473      75.29
 H      -1.084794     1.584204     0.040038      30.26
 C       1.483104    -0.423217    -0.891464    -102.39
 C       2.973060    -0.584380    -1.202833      97.87
 H       2.838307    -1.547809    -1.856658      23.22
 O       3.443266     0.588478    -1.831931     166.22
 H       4.171370     1.052151    -1.145831      16.78
 C       3.883680    -0.984675    -0.032996      81.94
 H       3.208215    -1.705006     0.802520      27.70
 O       5.180832    -1.537948    -0.438818     186.90
 H       5.486328    -1.532387    -1.298975      26.26
 C       4.039844     0.331523     0.921503      81.09
 O       4.856218     1.487245     0.125675     203.14
 H       4.414940     2.369840     0.527924      24.45
 H       4.475189     0.199271     1.864443      29.72
 H       2.940902     0.739934     1.183464      28.09
55
name = lig-Water-frame_143
 C      -2.184378     1.484674     4.052604      98.37
 H      -2.959851     2.250862     3.869698      27.29
 C      -1.144074    -0.603604     3.697429      28.15
 H      -1.100429    -1.758318     3.267287      29.34
 C       0.154333    -0.060956     4.087128     -22.77
 O       1.351220    -0.742908     4.036331     110.86
 C       1.275511    -2.373867     4.367050     115.35
 H       2.309051    -2.663986     3.975993      28.20
 H       0.692315    -2.431483     3.426421      26.74
 H       0.961314    -2.729729     5.290539      27.69
 C       0.175004     1.293793     4.391897     -23.01
 O       1.528040     1.916031     4.451792     173.29
 H       1.585498     2.847349     4.151507      24.76
 C      -1.058597     2.098252     4.399094      61.58
 H      -0.988871     3.092804     4.496426      29.40
 C      -2.295676     0.227146     3.576748     -18.51
 C      -3.443886    -0.044873     2.606094      85.47
 H      -4.185647     0.772455     2.937817      23.84
 O      -4.023128    -1.459527     2.964060     230.08
 H      -5.062906    -1.499152     2.765375      22.96
 C      -3.136967     0.341245     1.170065      94.01
 H      -2.516965     1.216414     1.393469      30.58
 C      -4.376933     1.005298     0.444618     103.64
 O      -5.523823     0.149387     0.352569     224.49
 H      -5.409001    -0.795386     0.006422      23.02
 H      -4.005979     1.241503    -0.680285      26.07
 H      -4.427915     2.076952     0.631647      26.30
 C       0.778778     0.662334    -0.508656     117.15
 H       1.329682     1.647330    -0.464190      32.45
 C       0.644653    -1.696471    -1.043561      49.54
 H       1.066762    -2.667477    -1.352042      34.31
 C      -0.680572    -1.787944    -0.555334      -5.83
 O      -1.341913    -2.892997    -0.539694     155.88
 C      -0.525949    -4.149175    -0.391932     117.87
 H      -1.190775    -4.824878    -0.046613      30.75
 H      -0.030417    -4.344371    -1.308135      27.60
 H       0.009350    -3.964229     0.568098      28.50
 C      -1.297932    -0.541453    -0.243771      -0.98
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 O      -2.601105    -0.702058     0.366190     109.64
 C      -0.594467     0.719947    -0.140195      53.95
 H      -1.119903     1.596420     0.194686      30.35
 C       1.461864    -0.464669    -0.924092     -23.06
 C       2.960415    -0.558736    -1.213682      95.50
 H       2.908066    -1.587830    -2.003231      24.99
 O       3.442517     0.632045    -1.866304     179.18
 H       3.965613     1.173819    -1.240025      23.09
 C       3.899504    -0.991244     0.050914      98.85
 H       3.594395    -1.635991     0.729865      32.07
 O       5.166246    -1.526990    -0.397646     155.57
 H       5.394303    -1.402992    -1.478270      19.47
 C       4.084434     0.265577     0.903811      94.34
 O       4.896038     1.455145     0.131200     230.02
 H       4.533635     2.275100     0.487852      29.28
 H       4.614388     0.283000     1.987653      28.18
 H       3.137167     0.484724     1.254075      32.89
55
name = lig-Water-frame_144
 C      -2.171396     1.495858     4.051021      76.20
 H      -3.033383     2.118689     3.883298      26.58
 C      -1.156012    -0.632486     3.690336      73.95
 H      -1.140384    -1.583266     3.353261      31.20
 C       0.173396    -0.055848     4.039829     -30.60
 O       1.359750    -0.769002     4.027413      99.38
 C       1.243360    -2.361896     4.344289      86.06
 H       2.353439    -2.499042     4.270393      25.49
 H       0.373217    -2.806887     3.608631      22.90
 H       0.782582    -2.851537     5.319729      24.47
 C       0.205628     1.374250     4.335010       9.37
 O       1.560696     1.946374     4.436738     230.14
 H       1.497023     2.958421     4.181833      25.43
 C      -0.920209     2.065572     4.458810      58.23
 H      -1.223497     3.236855     4.704638      18.36
 C      -2.279838     0.245122     3.528852     -11.64
 C      -3.471592    -0.098825     2.637911      81.54
 H      -4.114908     0.885626     3.078241      22.73
 O      -3.991370    -1.424972     2.941674     252.38
 H      -4.971185    -1.547360     2.802470      24.34
 C      -3.152581     0.324880     1.113413      88.36
 H      -2.518638     1.244128     1.155095      27.90
 C      -4.368725     0.961949     0.450940      98.06
 O      -5.600181     0.143342     0.352974     222.24
 H      -5.345438    -0.693766    -0.174463      24.74
 H      -4.029406     1.144769    -0.504456      26.58
 H      -4.564897     2.135356     0.830444      23.86
 C       0.756821     0.626051    -0.492440      69.75
 H       1.284082     1.545348    -0.400189      30.55
 C       0.594443    -1.607803    -1.025031     105.73
 H       1.028300    -2.562126    -1.346510      32.83
 C      -0.629686    -1.726976    -0.545430     -26.13
 O      -1.338228    -2.963053    -0.546416     155.56
 C      -0.544484    -4.181776    -0.376387     108.47
 H      -1.365406    -5.027609     0.173009      23.24
 H       0.151494    -4.312632    -1.269865      24.61
 H      -0.186098    -4.018531     0.646907      27.46
 C      -1.348246    -0.508293    -0.213279       2.68
 O      -2.577248    -0.718125     0.289244     125.88
 C      -0.614103     0.732719    -0.117960      50.64
 H      -1.076473     1.685997     0.347154      27.22
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 C       1.408615    -0.564617    -0.956112      12.69
 C       2.926914    -0.571270    -1.227645      78.35
 H       3.338678    -1.234150    -2.009841      26.59
 O       3.434722     0.657804    -1.913609     179.10
 H       3.905052     1.258292    -1.231089      23.39
 C       3.945609    -0.934498     0.089327      73.53
 H       3.564197    -1.910456     0.825863      27.04
 O       5.169417    -1.529147    -0.382585     190.25
 H       5.185406    -1.160855    -1.272973      26.59
 C       4.176693     0.254012     0.911928      96.40
 O       4.903645     1.385518     0.147567     223.36
 H       4.649913     2.269633     0.684600      26.34
 H       4.874974     0.062297     1.741148      28.84
 H       3.065840     0.563998     1.214298      28.87
55
name = lig-Water-frame_145
 C      -2.157522     1.544988     4.046818      22.51
 H      -3.170517     2.120337     4.051486      23.69
 C      -1.107245    -0.610883     3.688872      91.84
 H      -1.247968    -1.752640     3.330484      28.14
 C       0.128425    -0.051665     3.991510     -26.63
 O       1.349503    -0.835020     4.042551     148.16
 C       1.184566    -2.323290     4.302962     116.37
 H       2.201447    -2.627555     4.395504      28.08
 H       0.660625    -3.191795     3.799435      26.18
 H       0.825951    -2.378178     5.348450      27.54
 C       0.350349     1.430196     4.274852      -8.25
 O       1.549036     1.980559     4.416370     227.37
 H       1.455908     2.933950     4.228078      28.33
 C      -0.882759     2.102644     4.519903      55.03
 H      -0.895581     3.031261     4.931337      26.32
 C      -2.235462     0.188751     3.473301      -0.91
 C      -3.499822    -0.129075     2.699714      87.11
 H      -4.322522     0.622838     2.940059      24.52
 O      -3.936974    -1.389143     2.912962     276.50
 H      -4.962027    -1.377468     2.771149      23.75
 C      -3.201370     0.324872     1.094471      77.60
 H      -2.398375     1.122065     1.019033      27.46
 C      -4.377802     0.930947     0.429401      91.29
 O      -5.662869     0.153884     0.353160     169.57
 H      -5.356571    -0.599019    -0.167739      27.66
 H      -4.022370     1.129198    -0.689808      24.50
 H      -4.836042     1.634800     1.149873      24.65
 C       0.744055     0.626876    -0.471651      53.52
 H       1.391558     1.528259    -0.354588      28.05
 C       0.607492    -1.639896    -1.043233     104.15
 H       1.106141    -2.518085    -1.389951      34.58
 C      -0.681610    -1.661960    -0.533727     -43.33
 O      -1.352940    -3.014400    -0.559129     141.54
 C      -0.603482    -4.209174    -0.289339     123.66
 H      -1.265314    -5.030709    -0.458859      26.46
 H       0.156052    -4.541866    -0.979719      27.58
 H       0.161611    -4.067364     0.558805      27.57
 C      -1.362378    -0.478724    -0.152795      20.44
 O      -2.592302    -0.734677     0.228086     118.14
 C      -0.619948     0.699121    -0.111922      84.84
 H      -0.875445     1.604474     0.295898      29.71
 C       1.399701    -0.548665    -0.970606     -37.19
 C       2.937578    -0.567458    -1.226465      58.35
 H       3.441417    -1.356316    -2.073177      24.93
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 O       3.418532     0.676053    -1.948375     168.67
 H       3.826675     1.287637    -1.189754      22.92
 C       3.956449    -0.930528     0.109465      98.12
 H       3.361028    -1.531841     0.646328      30.89
 O       5.175928    -1.523645    -0.382046     189.48
 H       5.348760    -1.041239    -1.222654      24.02
 C       4.261624     0.293136     0.934767     106.48
 O       4.887138     1.318909     0.178151     260.93
 H       4.809188     2.074297     0.810168      29.49
 H       5.035133    -0.165515     1.706576      25.07
 H       3.367390     0.740652     1.271399      28.38
55
name = lig-Water-frame_146
 C      -2.130961     1.572332     4.035924      35.67
 H      -2.982804     2.123857     4.260215      23.30
 C      -1.066033    -0.618876     3.649378      87.91
 H      -1.175424    -1.680677     3.465330      27.09
 C       0.149514    -0.021030     3.958757      14.84
 O       1.307606    -0.910883     4.039372     169.53
 C       1.153307    -2.275060     4.327449     113.62
 H       2.192426    -2.838883     4.437485      25.52
 H       0.788020    -3.138681     3.578820      25.14
 H       0.808569    -1.984128     5.383866      23.73
 C       0.406216     1.397851     4.212478     -14.88
 O       1.557449     2.022574     4.399343     205.71
 H       1.561777     3.026684     4.193584      23.55
 C      -0.887568     2.113219     4.545428      36.90
 H      -0.553728     3.110720     5.212367      21.43
 C      -2.195867     0.209864     3.466802      29.87
 C      -3.486748    -0.113438     2.715181      77.06
 H      -4.555684     0.576807     2.969176      22.32
 O      -3.908716    -1.402570     2.883602     270.50
 H      -4.878901    -1.359864     2.746631      26.42
 C      -3.231992     0.304215     1.099302      81.66
 H      -2.493975     1.047932     1.174171      29.22
 C      -4.438705     0.889415     0.388189      98.74
 O      -5.697072     0.159238     0.340956     176.65
 H      -5.612245    -0.786574    -0.095152      24.82
 H      -4.224442     1.352905    -0.541748      27.61
 H      -4.803890     1.623667     1.232453      25.17
 C       0.773514     0.644771    -0.459594      82.50
 H       1.385268     1.532424    -0.320159      26.93
 C       0.631728    -1.732076    -1.068902       4.63
 H       1.112975    -2.681026    -1.457202      25.59
 C      -0.741840    -1.687568    -0.553443     -16.55
 O      -1.376834    -3.012001    -0.570613     147.51
 C      -0.607791    -4.226541    -0.214966     107.45
 H      -1.359405    -5.122629    -0.660530      23.24
 H       0.146570    -4.567909    -1.037393      25.38
 H       0.111947    -4.242939     0.588929      27.65
 C      -1.340170    -0.500255    -0.099568      19.21
 O      -2.675000    -0.743205     0.202538     133.41
 C      -0.578725     0.663515    -0.115096      74.63
 H      -0.883170     1.719964     0.285637      26.52
 C       1.436116    -0.454829    -0.968659     -59.53
 C       3.003955    -0.556717    -1.246611      89.92
 H       2.991645    -1.524477    -1.827018      25.40
 O       3.397873     0.684461    -1.954319     226.64
 H       3.712360     1.242955    -1.310276      29.96
 C       3.924248    -0.880535     0.055799      83.29
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 H       3.107673    -1.537925     0.729511      26.47
 O       5.174714    -1.520841    -0.385636     135.02
 H       5.720389    -1.041557    -1.199286      22.49
 C       4.353655     0.305112     0.980554     111.56
 O       4.893496     1.273227     0.199592     257.82
 H       4.928208     2.084701     0.751586      29.51
 H       4.986516    -0.199072     1.779275      26.29
 H       3.516627     0.801570     1.643750      26.50
55
name = lig-Water-frame_147
 C      -2.056892     1.590358     4.046050      49.83
 H      -3.006915     2.191556     4.387188      19.66
 C      -1.057505    -0.599036     3.595192      34.74
 H      -1.044956    -1.723520     3.492614      25.27
 C       0.247660    -0.014389     3.938848      -1.00
 O       1.284795    -0.928352     3.989319     219.15
 C       1.151479    -2.275035     4.406487     126.58
 H       2.107468    -2.639919     4.512714      28.84
 H       0.592174    -2.596058     3.478034      27.20
 H       0.508313    -2.380456     5.359485      26.30
 C       0.326466     1.354891     4.168362      -7.18
 O       1.601561     2.063484     4.389181     214.95
 H       1.625288     3.025966     4.020046      21.46
 C      -0.841128     2.096040     4.536535      51.28
 H      -0.632382     2.889174     5.206404      24.56
 C      -2.179624     0.295044     3.497663      13.59
 C      -3.480020    -0.056354     2.683920      93.83
 H      -4.269444     0.573705     3.109865      26.86
 O      -3.891095    -1.464806     2.859422     268.47
 H      -4.887579    -1.539911     2.732669      26.67
 C      -3.273540     0.264185     1.107661      78.75
 H      -2.587185     1.207514     1.324805      26.09
 C      -4.540133     0.873857     0.406461     109.90
 O      -5.731331     0.135953     0.313711     221.87
 H      -5.746454    -0.812835     0.098116      25.20
 H      -4.353966     1.577061    -0.520087      25.11
 H      -4.580962     1.858854     1.020507      25.39
 C       0.831133     0.680293    -0.452530      71.14
 H       1.320629     1.645482    -0.292959      26.39
 C       0.654910    -1.753365    -1.071277      35.68
 H       1.001915    -2.689830    -1.427593      23.41
 C      -0.707350    -1.804896    -0.615960     -15.17
 O      -1.407389    -2.981030    -0.564543     161.86
 C      -0.595341    -4.268738    -0.240500      99.28
 H      -1.439521    -5.019405    -0.185318      26.18
 H       0.053217    -4.256127    -1.087093      24.81
 H      -0.266079    -4.349003     0.844916      26.42
 C      -1.334266    -0.571973    -0.065513     -60.20
 O      -2.761627    -0.732647     0.207882      99.73
 C      -0.539493     0.672575    -0.096231      71.68
 H      -1.025054     1.546855     0.188337      29.03
 C       1.471830    -0.452819    -0.961945     -10.23
 C       3.020641    -0.520080    -1.234601     104.28
 H       2.906059    -1.588176    -1.858779      24.02
 O       3.377227     0.657791    -1.971038     198.74
 H       3.749825     1.347466    -1.236319      22.59
 C       3.849307    -0.804665    -0.004005      97.20
 H       3.470390    -1.601266     0.561669      30.33
 O       5.181314    -1.527878    -0.387899     150.59
 H       5.624325    -1.141023    -1.089941      30.23
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 C       4.371348     0.267297     1.070154     106.64
 O       4.944402     1.271987     0.195546     229.44
 H       4.946440     2.234879     0.611835      25.92
 H       5.155650    -0.168477     1.835120      26.31
 H       3.683492     0.594169     1.821551      28.18
55
name = lig-Water-frame_148
 C      -2.017280     1.632996     4.094617      73.57
 H      -2.905016     2.121298     4.262298      22.91
 C      -1.037703    -0.527289     3.552506      47.03
 H      -1.107921    -1.684904     3.364945      25.61
 C       0.284807    -0.064465     3.907576      -7.18
 O       1.318611    -0.881632     3.945158     197.50
 C       1.086339    -2.278980     4.464655     102.03
 H       2.237181    -2.585791     4.605450      24.93
 H       0.480707    -2.617131     3.583308      26.97
 H       0.368121    -2.759456     5.249648      25.52
 C       0.308437     1.370063     4.159156      -2.23
 O       1.622635     2.070393     4.375665     196.37
 H       1.611892     2.922882     3.859164      24.40
 C      -0.787073     2.040043     4.491031      59.74
 H      -0.781799     2.967984     5.203002      26.77
 C      -2.169977     0.341109     3.512202       3.21
 C      -3.451599    -0.051535     2.648643      77.55
 H      -4.269375     0.811113     3.193440      22.66
 O      -3.868514    -1.530312     2.839396     241.83
 H      -4.874401    -1.590037     2.756750      25.78
 C      -3.336914     0.285621     1.121620      92.68
 H      -2.746801     1.132071     1.110667      27.89
 C      -4.601599     0.920769     0.435531      97.39
 O      -5.794160     0.117838     0.298106     216.85
 H      -5.499965    -0.842640     0.163037      24.69
 H      -4.334602     1.248245    -0.565295      26.10
 H      -4.805858     1.886102     1.045171      25.31
 C       0.872784     0.716182    -0.442978      45.62
 H       1.343923     1.723339    -0.343697      26.55
 C       0.677752    -1.697620    -1.052497      89.60
 H       1.142047    -2.648354    -1.444451      26.73
 C      -0.643598    -1.882592    -0.656979      -6.84
 O      -1.443588    -2.967571    -0.543182     150.69
 C      -0.631315    -4.271622    -0.262893      99.72
 H      -1.522173    -5.088362    -0.031318      23.91
 H       0.156797    -4.278311    -1.042247      24.16
 H      -0.413278    -4.085442     0.775235      27.10
 C      -1.314233    -0.657325    -0.070520    -109.96
 O      -2.795170    -0.714723     0.229535      48.17
 C      -0.543913     0.624015    -0.074107      47.25
 H      -1.177341     1.546437     0.167699      27.28
 C       1.481284    -0.524016    -0.937820      15.39
 C       2.960513    -0.498087    -1.227412     104.66
 H       3.331260    -1.288749    -1.974320      26.45
 O       3.373857     0.637610    -1.981505     245.66
 H       3.802745     1.241489    -1.324023      26.33
 C       3.857884    -0.757401    -0.015221      86.77
 H       3.516962    -1.758900     0.503328      28.25
 O       5.173065    -1.533679    -0.382315     102.44
 H       5.491196    -1.120201    -1.294708      24.29
 C       4.376543     0.208543     1.143097      88.99
 O       5.010644     1.304259     0.189735     238.37
 H       4.766466     2.159024     0.584973      28.24
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 H       5.362018    -0.207781     1.541150      25.38
 H       3.563642     0.580092     1.855799      26.13
55
name = lig-Water-frame_149
 C      -2.041320     1.620476     4.117453      37.19
 H      -2.977843     2.315946     4.188411      22.53
 C      -1.013619    -0.462563     3.510935      88.47
 H      -1.263126    -1.433949     3.180625      29.70
 C       0.228548    -0.059494     3.867090       9.24
 O       1.389342    -0.843032     3.938628     188.02
 C       1.036792    -2.300533     4.465791      97.82
 H       1.961177    -2.677209     4.625750      29.55
 H       0.740450    -3.073405     3.604845      27.12
 H       0.383154    -2.547555     5.392793      27.12
 C       0.435504     1.366627     4.166679      -8.22
 O       1.607070     2.033578     4.358410     281.08
 H       1.658788     2.917220     3.810038      25.85
 C      -0.767281     2.053969     4.481716      59.13
 H      -0.762706     3.108427     4.971955      24.28
 C      -2.158490     0.344975     3.494255      19.02
 C      -3.440135    -0.061993     2.661040      84.43
 H      -4.214202     0.634762     2.956447      27.00
 O      -3.841198    -1.561821     2.820460     254.87
 H      -4.815339    -1.467980     2.803907      27.08
 C      -3.412926     0.340794     1.131971      78.02
 H      -2.670142     1.246003     0.893774      25.83
 C      -4.645329     0.967090     0.464141      90.39
 O      -5.855114     0.084011     0.291217     168.59
 H      -5.334546    -0.758965     0.129540      26.83
 H      -4.233839     0.965399    -0.618684      24.23
 H      -5.214965     1.778012     1.072496      23.62
 C       0.858909     0.702949    -0.433259      50.92
 H       1.411406     1.625006    -0.453009      28.30
 C       0.726760    -1.678147    -1.044874      79.40
 H       1.376459    -2.441888    -1.434641      31.37
 C      -0.638416    -1.860912    -0.634288      12.82
 O      -1.468321    -2.994415    -0.536897     122.57
 C      -0.720978    -4.224402    -0.265336     108.97
 H      -1.376839    -5.191081    -0.294596      25.72
 H       0.160203    -4.619788    -0.839738      26.56
 H      -0.155853    -3.859503     0.661540      27.50
 C      -1.278844    -0.706491    -0.103474     -34.02
 O      -2.774244    -0.712119     0.247104     -12.10
 C      -0.570620     0.536891    -0.060666      37.41
 H      -1.084398     1.468632     0.165171      27.72
 C       1.458980    -0.544347    -0.888090       3.53
 C       2.934233    -0.484474    -1.237817      77.90
 H       3.457305    -1.306960    -2.018967      24.98
 O       3.376439     0.647891    -1.992298     225.34
 H       3.908131     1.198445    -1.390707      27.46
 C       3.921058    -0.807647     0.051143      86.83
 H       3.196769    -1.565344     0.491625      30.48
 O       5.166104    -1.501586    -0.407401     107.30
 H       5.335120    -1.279889    -1.429646      22.80
 C       4.392691     0.169428     1.120056     108.48
 O       5.059463     1.336931     0.204177     195.32
 H       4.602340     2.182763     0.651220      25.80
 H       5.248596    -0.330582     1.515819      29.84
 H       3.613073     0.613594     1.771428      27.26
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name = lig-Water-frame_150
 C      -2.106531     1.596988     4.116830      54.49
 H      -2.819535     2.381736     4.149685      26.31
 C      -1.033775    -0.429906     3.452102      54.32
 H      -1.269673    -1.484702     2.882587      26.66
 C       0.240032     0.010240     3.845231      18.84
 O       1.430602    -0.854763     3.952325     143.19
 C       1.011642    -2.332636     4.425206      85.65
 H       2.068921    -2.803835     4.825669      25.69
 H       0.864357    -3.092530     3.671378      26.58
 H       0.413126    -2.024107     5.407580      25.03
 C       0.499365     1.350681     4.188632      12.74
 O       1.620547     1.988133     4.335826     298.38
 H       1.709979     2.889196     3.996712      26.07
 C      -0.752371     2.104393     4.465989      65.02
 H      -0.583483     3.157482     4.751377      20.50
 C      -2.175634     0.358618     3.463550      33.57
 C      -3.407418    -0.103319     2.666380      82.60
 H      -4.493372     0.567080     3.058150      22.82
 O      -3.811907    -1.545614     2.799922     229.27
 H      -4.820708    -1.422758     2.868041      24.80
 C      -3.412923     0.419205     1.137032      66.36
 H      -2.784043     1.230484     1.072188      27.92
 C      -4.724133     0.959992     0.465893     100.92
 O      -5.881641     0.038833     0.290090     183.93
 H      -5.605147    -0.864420    -0.006765      26.19
 H      -4.285032     1.177271    -0.543776      25.64
 H      -5.136406     1.841127     0.920975      26.99
 C       0.783347     0.622507    -0.421363     101.48
 H       1.387400     1.567254    -0.506137      27.18
 C       0.759197    -1.720994    -1.033987      39.03
 H       1.419482    -2.508432    -1.441366      27.88
 C      -0.660975    -1.828202    -0.586627      -9.44
 O      -1.471644    -3.028443    -0.567011     167.00
 C      -0.757533    -4.177402    -0.243471     119.50
 H      -1.471783    -5.121054    -0.270887      25.34
 H      -0.024317    -4.624477    -0.954233      26.76
 H      -0.063297    -4.068714     0.621483      28.26
 C      -1.286835    -0.690721    -0.125605      32.71
 O      -2.725347    -0.726487     0.253668      14.19
 C      -0.552602     0.470905    -0.065359      67.04
 H      -1.033284     1.395050     0.245784      27.20
 C       1.452885    -0.474658    -0.836556     -21.81
 C       2.988199    -0.491258    -1.251017      78.98
 H       3.019455    -1.506285    -1.806084      26.36
 O       3.372590     0.687198    -2.001591     177.91
 H       4.106613     1.202105    -1.399996      23.46
 C       3.947713    -0.892466     0.092648      90.62
 H       3.138027    -1.507752     0.660512      29.48
 O       5.151217    -1.458171    -0.448232     206.27
 H       5.251139    -1.424711    -1.343810      27.59
 C       4.427705     0.173775     1.014075     112.13
 O       5.079350     1.357755     0.250769     179.57
 H       4.723405     2.222468     0.635622      24.93
 H       5.112165    -0.426397     1.874669      26.86
 H       3.717486     0.609909     1.704359      27.52
55
name = lig-Water-frame_151
 C      -2.095502     1.620112     4.118286      60.58
 H      -2.926876     2.378587     4.133955      26.56
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 C      -1.053055    -0.448431     3.360384      34.88
 H      -0.986085    -1.328148     2.889182      27.18
 C       0.317519     0.035431     3.831356      -7.43
 O       1.435898    -0.893017     3.952474     128.18
 C       1.072002    -2.326179     4.434816      85.63
 H       1.885082    -2.614097     5.002088      27.71
 H       0.557338    -2.984683     3.559710      24.11
 H       0.322703    -1.758405     5.059187      25.62
 C       0.400546     1.368023     4.220831      19.71
 O       1.706626     1.943056     4.325110     186.77
 H       1.676350     2.970829     4.159497      24.81
 C      -0.750851     2.112983     4.417246      63.48
 H      -0.458500     3.288786     4.570225      20.61
 C      -2.220088     0.368491     3.431439       7.76
 C      -3.447996    -0.107463     2.666261     109.74
 H      -4.262467     0.267324     3.198233      27.32
 O      -3.784633    -1.504687     2.779017     249.58
 H      -4.762440    -1.532657     2.892119      25.53
 C      -3.385256     0.452168     1.155821      40.72
 H      -2.737918     1.440056     1.306351      23.45
 C      -4.787768     0.894077     0.433861     102.81
 O      -5.892745     0.001037     0.295831     222.24
 H      -5.840980    -0.903762    -0.128020      24.45
 H      -4.490987     1.463217    -0.556842      25.12
 H      -4.955890     2.011401     0.895929      24.07
 C       0.722889     0.574198    -0.409564     119.26
 H       1.134696     1.555777    -0.391257      28.77
 C       0.756190    -1.757334    -0.991754      36.76
 H       1.176531    -2.708396    -1.390192      24.68
 C      -0.650448    -1.854401    -0.562801     -25.98
 O      -1.460650    -3.019083    -0.611152     189.00
 C      -0.739791    -4.206597    -0.239448      99.73
 H      -1.730637    -4.849149     0.091225      22.66
 H      -0.282147    -4.356603    -1.274830      22.66
 H      -0.205198    -4.275178     0.723495      27.18
 C      -1.360793    -0.647236    -0.122326      21.25
 O      -2.668987    -0.732356     0.258279      34.27
 C      -0.552596     0.475864    -0.061006      76.27
 H      -1.070954     1.376149     0.399795      26.63
 C       1.492320    -0.472528    -0.831075       8.55
 C       3.010619    -0.501500    -1.203020      76.84
 H       2.872266    -1.612163    -1.856793      23.64
 O       3.385619     0.721888    -1.992584     205.12
 H       4.097813     1.083295    -1.532049      28.75
 C       3.926031    -0.938334     0.058432      84.85
 H       3.461127    -1.669298     0.851417      28.22
 O       5.147022    -1.438193    -0.463925     150.69
 H       5.159958    -1.502115    -1.543353      21.79
 C       4.477229     0.217909     0.949630     125.35
 O       5.098705     1.338418     0.301910     235.22
 H       4.841990     2.269045     0.733963      22.80
 H       5.028772    -0.190998     1.765151      30.16
 H       3.584311     0.635639     1.562168      27.19
55
name = lig-Water-frame_152
 C      -2.054700     1.668891     4.097458      44.27
 H      -3.019134     2.219185     4.170141      22.56
 C      -0.996916    -0.422819     3.303251      17.70
 H      -0.818005    -1.515941     2.759457      24.01
 C       0.341735    -0.020928     3.807705     -17.13
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 O       1.437715    -0.908680     3.922537     161.48
 C       1.071100    -2.241751     4.425349     105.21
 H       1.939453    -2.626643     5.144252      24.19
 H       0.577137    -2.784765     3.708972      25.52
 H       0.053221    -2.117667     5.059673      25.29
 C       0.344723     1.392655     4.249896      -2.24
 O       1.777900     1.905488     4.321548      87.70
 H       1.692655     2.887838     4.253150      26.13
 C      -0.783926     2.153437     4.350046      45.64
 H      -0.648929     3.137202     4.518080      31.16
 C      -2.223059     0.354768     3.411768     -17.55
 C      -3.495526    -0.101052     2.654467      86.94
 H      -4.456260     0.510006     3.364983      22.98
 O      -3.751140    -1.487161     2.756899     255.52
 H      -4.718979    -1.594650     2.835788      24.95
 C      -3.367090     0.464965     1.166067      51.51
 H      -2.838854     1.372613     1.273917      26.21
 C      -4.774346     0.856386     0.383758      97.11
 O      -5.914535    -0.015739     0.317532     229.35
 H      -5.659942    -0.846353    -0.213060      25.45
 H      -4.694194     1.349395    -0.598822      26.66
 H      -5.100171     1.632501     1.081652      27.91
 C       0.739192     0.578305    -0.408119      45.39
 H       1.042638     1.646753    -0.216717      26.38
 C       0.713390    -1.775083    -0.921185      63.23
 H       1.021934    -2.742166    -1.275958      26.87
 C      -0.637959    -1.861447    -0.552077      -9.03
 O      -1.438135    -2.961687    -0.635881     206.14
 C      -0.769759    -4.263145    -0.264590     102.99
 H      -1.682372    -4.853259     0.053109      24.25
 H      -0.366120    -4.555570    -1.201151      25.02
 H      -0.131583    -4.206298     0.673473      27.08
 C      -1.397789    -0.639774    -0.124605      18.57
 O      -2.648437    -0.712386     0.284809      51.38
 C      -0.654387     0.523645    -0.019679      70.05
 H      -1.022485     1.381712     0.437771      28.45
 C       1.525965    -0.561911    -0.855158      18.12
 C       2.974413    -0.544071    -1.138401      93.87
 H       3.191064    -1.228226    -1.989944      25.60
 O       3.391905     0.715332    -1.967142     194.52
 H       4.240686     1.105377    -1.551918      25.08
 C       3.927579    -0.917623     0.007949      86.38
 H       3.635356    -1.762836     0.728648      27.66
 O       5.170323    -1.451574    -0.505595     133.48
 H       5.107464    -1.532869    -1.507104      26.48
 C       4.437553     0.295205     0.925294     108.89
 O       5.136866     1.313042     0.329237     221.22
 H       4.852293     2.171004     0.826406      24.92
 H       5.294042    -0.111695     1.734224      24.72
 H       3.503540     0.614084     1.324277      26.28
55
name = lig-Water-frame_153
 C      -2.068031     1.644365     4.020565      50.98
 H      -2.954794     2.205371     4.258336      25.51
 C      -0.894858    -0.425087     3.251799      65.06
 H      -1.032046    -1.301929     2.790208      29.63
 C       0.292445    -0.047155     3.796094       3.59
 O       1.427976    -0.900435     3.888823     199.33
 C       1.014225    -2.125221     4.472586     124.81
 H       1.860360    -2.666725     4.933331      28.63
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 H       0.919955    -2.965857     3.504798      26.47
 H       0.217245    -2.526771     5.113633      27.33
 C       0.415386     1.355542     4.247455     -20.07
 O       1.782668     1.868120     4.328769     134.19
 H       1.844146     2.853327     4.210533      26.80
 C      -0.818180     2.205198     4.286265      71.35
 H      -0.847988     3.411044     4.687562      22.89
 C      -2.159450     0.341177     3.411755     -21.57
 C      -3.562160    -0.044265     2.680227      94.14
 H      -4.279991     0.619257     2.985266      28.82
 O      -3.723225    -1.487642     2.738081     262.88
 H      -4.740123    -1.590618     2.704832      26.08
 C      -3.396393     0.422747     1.134524      68.93
 H      -2.783155     1.402883     1.076949      27.79
 C      -4.738118     0.834937     0.375397      93.00
 O      -5.920449    -0.051420     0.331289     177.78
 H      -5.540861    -0.808818    -0.140191      28.39
 H      -4.599686     1.208777    -0.688844      26.58
 H      -5.282423     1.340016     1.291667      24.48
 C       0.760010     0.591750    -0.398803     -13.35
 H       1.279997     1.524235    -0.176080      27.89
 C       0.676123    -1.789890    -0.851902      82.21
 H       1.163943    -2.748996    -1.189639      27.08
 C      -0.662382    -1.800648    -0.534631      39.42
 O      -1.413001    -2.925427    -0.643816     171.58
 C      -0.820555    -4.288779    -0.299568      95.02
 H      -1.725138    -5.162064    -0.112009      23.77
 H      -0.222454    -5.003338    -1.053796      25.17
 H      -0.024432    -4.060695     0.388136      28.25
 C      -1.364571    -0.643893    -0.128412      26.17
 O      -2.693653    -0.682182     0.339771      68.03
 C      -0.707455     0.567398     0.000127       6.82
 H      -1.072952     1.553957     0.480757      25.59
 C       1.473244    -0.629345    -0.852060     -28.18
 C       2.968098    -0.554018    -1.119782      74.63
 H       3.401649    -1.299594    -2.122654      24.38
 O       3.390287     0.693872    -1.914594     173.82
 H       4.276291     1.115951    -1.553718      22.54
 C       3.984035    -0.855811    -0.023696      88.43
 H       3.439628    -1.732758     0.579882      27.72
 O       5.209420    -1.480533    -0.562338     116.56
 H       5.216926    -1.530757    -1.483214      28.74
 C       4.380334     0.308692     0.942636     116.25
 O       5.191393     1.315486     0.320846     261.32
 H       4.862421     2.176916     0.706607      26.68
 H       5.021112    -0.135366     1.643148      28.53
 H       3.371842     0.716862     1.398055      25.39
55
name = lig-Water-frame_154
 C      -2.085983     1.586985     3.927178      47.76
 H      -2.941806     2.253584     4.286339      23.72
 C      -0.893949    -0.414466     3.206814      66.20
 H      -1.179783    -1.446527     2.702477      28.26
 C       0.276722     0.000937     3.812326      15.80
 O       1.390641    -0.865736     3.874150     182.62
 C       0.995918    -2.150762     4.451983     130.46
 H       2.018406    -2.536738     4.873794      27.84
 H       1.162444    -2.785988     3.656180      29.70
 H       0.175755    -2.279234     5.214602      27.30
 C       0.483929     1.348300     4.212767       1.19
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 O       1.747478     1.827705     4.345973     181.06
 H       1.903122     2.819378     4.053879      24.56
 C      -0.794595     2.263985     4.255041      42.96
 H      -0.823280     3.133902     4.675286      22.61
 C      -2.087433     0.333947     3.400488      12.41
 C      -3.513758     0.000913     2.662548      64.96
 H      -4.532399     0.785961     3.013408      22.73
 O      -3.729011    -1.476632     2.729680     243.63
 H      -4.678838    -1.619587     2.579978      28.13
 C      -3.419162     0.363889     1.069626      96.59
 H      -2.823385     1.282443     0.924406      29.22
 C      -4.735183     0.807662     0.438489     100.92
 O      -5.898132    -0.109192     0.327779     198.71
 H      -5.674548    -1.068203    -0.057621      23.02
 H      -4.389002     1.246704    -0.562025      25.79
 H      -5.045778     1.624924     1.060124      27.71
 C       0.750829     0.579910    -0.376786      63.48
 H       1.531498     1.361240    -0.265050      28.53
 C       0.689076    -1.817352    -0.807345      23.26
 H       1.225173    -2.693822    -1.068682      28.64
 C      -0.704224    -1.754418    -0.518363      25.94
 O      -1.410547    -2.948052    -0.657328     140.03
 C      -0.856147    -4.333427    -0.364854     107.81
 H      -1.656041    -4.997315    -0.044459      27.89
 H      -0.271907    -4.907816    -1.022868      29.21
 H      -0.034639    -4.047406     0.413607      27.86
 C      -1.363736    -0.592490    -0.089313      -9.35
 O      -2.758041    -0.669259     0.391689      60.41
 C      -0.636605     0.629387    -0.011635      86.31
 H      -1.124418     1.469238     0.374176      32.52
 C       1.385370    -0.615430    -0.812810     -72.52
 C       3.019861    -0.553783    -1.199695      90.54
 H       3.130820    -1.482033    -1.736265      31.45
 O       3.371931     0.676298    -1.851831     238.63
 H       4.124778     1.012015    -1.462688      30.80
 C       4.026282    -0.809367    -0.049778      92.40
 H       3.371345    -1.532167     0.557696      29.97
 O       5.245459    -1.508523    -0.590688      82.12
 H       5.415837    -1.415798    -1.681683      19.24
 C       4.298860     0.305306     0.952443     116.01
 O       5.243531     1.321346     0.300269     183.22
 H       4.877236     2.315475     0.498259      24.57
 H       4.747340    -0.313570     1.955184      25.26
 H       3.512028     0.768559     1.440690      26.71
55
name = lig-Water-frame_155
 C      -2.028678     1.622098     3.890690      63.16
 H      -2.953133     2.098379     4.069971      26.56
 C      -0.970565    -0.429344     3.167931      46.33
 H      -0.934690    -1.432670     2.786500      29.38
 C       0.296346     0.053873     3.818422      -8.90
 O       1.339767    -0.812935     3.874373     130.99
 C       1.058475    -2.214449     4.447568      92.30
 H       1.978387    -2.201729     5.096747      26.45
 H       0.927326    -3.007905     3.449119      25.13
 H       0.198937    -1.849639     5.064096      25.19
 C       0.448012     1.411701     4.152176      27.80
 O       1.732157     1.808512     4.366117     307.02
 H       1.779778     2.694240     3.988709      26.91
 C      -0.744284     2.190341     4.208555      79.00
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 H      -0.657999     3.302535     4.823627      20.42
 C      -2.093527     0.315390     3.336929      34.42
 C      -3.442479     0.041143     2.621766      94.81
 H      -4.237910     0.399305     3.156107      30.11
 O      -3.743784    -1.445956     2.732681     269.26
 H      -4.690677    -1.595309     2.513431      28.09
 C      -3.427366     0.326009     1.048148     103.44
 H      -2.857575     1.286283     0.948465      30.99
 C      -4.740566     0.771816     0.486932     121.34
 O      -5.863278    -0.161813     0.327604     220.73
 H      -5.661026    -1.081606     0.062537      24.59
 H      -4.395425     1.188663    -0.493908      26.16
 H      -4.887212     1.928112     0.782263      24.48
 C       0.760010     0.573499    -0.354819     121.31
 H       1.486280     1.403946    -0.375478      31.61
 C       0.696492    -1.816153    -0.771411      10.47
 H       1.190778    -2.810099    -0.991173      26.37
 C      -0.729150    -1.781770    -0.507892     -28.96
 O      -1.440515    -2.993231    -0.679826     118.11
 C      -0.837317    -4.320066    -0.400238     103.30
 H      -1.848195    -4.795066     0.241056      22.44
 H      -0.365818    -4.681621    -1.416348      24.26
 H      -0.267040    -4.289457     0.500877      27.14
 C      -1.406592    -0.505342    -0.020757     -64.77
 O      -2.784997    -0.698537     0.402215      73.23
 C      -0.540760     0.661927    -0.037468     118.99
 H      -1.106472     1.576578     0.306360      34.00
 C       1.356324    -0.570134    -0.764731      19.76
 C       3.029437    -0.541420    -1.239526      67.27
 H       2.974025    -1.782920    -1.846048      26.11
 O       3.329287     0.654033    -1.816196     160.33
 H       4.166451     1.018859    -1.253109      28.11
 C       4.025701    -0.785752    -0.085363      89.73
 H       3.490347    -1.556861     0.657141      31.26
 O       5.270235    -1.528293    -0.610406      84.10
 H       5.568238    -1.200593    -1.464306      24.64
 C       4.287314     0.294684     0.976862     108.08
 O       5.275067     1.316910     0.286813     191.35
 H       4.918795     2.166728     0.507378      30.66
 H       4.634318    -0.116988     1.858274      31.47
 H       3.346550     0.924767     1.350314      29.14
55
name = lig-Water-frame_156
 C      -1.936325     1.667712     3.865339      41.49
 H      -2.966342     2.148325     3.865018      22.23
 C      -0.967087    -0.444951     3.188866      37.42
 H      -0.781305    -1.469895     2.796477      27.76
 C       0.247586     0.069483     3.771628      -9.13
 O       1.320224    -0.767174     3.867530     177.31
 C       1.118302    -2.217455     4.422467     105.17
 H       1.866148    -2.327060     5.225381      26.29
 H       0.776241    -2.966096     3.816730      26.90
 H       0.179829    -1.990850     4.914675      24.95
 C       0.384366     1.440593     4.075278      18.99
 O       1.726864     1.818734     4.386742     272.84
 H       1.822008     2.786211     4.044369      25.17
 C      -0.715232     2.153618     4.203867      56.09
 H      -0.545261     3.036286     4.603837      30.13
 C      -2.153333     0.332228     3.245333      -7.63
 C      -3.355135    -0.008531     2.572185      92.02
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 H      -4.255788     0.490739     3.377318      24.58
 O      -3.747356    -1.418329     2.738696     251.07
 H      -4.742326    -1.443279     2.553160      25.11
 C      -3.427815     0.355157     1.106872      83.75
 H      -2.837942     1.328381     1.005527      26.98
 C      -4.737389     0.763275     0.460931     107.21
 O      -5.839976    -0.171412     0.361010     173.56
 H      -5.359158    -1.056110     0.013202      22.85
 H      -4.512366     0.827457    -0.685064      24.06
 H      -5.102504     1.675185     0.848762      27.55
 C       0.827575     0.615419    -0.350914      50.52
 H       1.251307     1.619647    -0.428499      28.55
 C       0.662027    -1.797300    -0.734489      66.00
 H       1.101652    -2.755236    -0.940668      29.91
 C      -0.741508    -1.816159    -0.484573     -39.64
 O      -1.485513    -3.008698    -0.691276     127.51
 C      -0.859111    -4.282629    -0.413688     119.22
 H      -1.727624    -4.814347    -0.107619      28.00
 H      -0.644443    -4.600384    -1.399064      27.21
 H      -0.139865    -4.485249     0.467908      26.08
 C      -1.422360    -0.485116     0.019901     -77.04
 O      -2.760744    -0.749465     0.369929      48.68
 C      -0.572308     0.681054    -0.028126      95.48
 H      -0.839680     1.730176     0.205955      33.35
 C       1.427798    -0.583814    -0.736006      53.56
 C       2.965499    -0.609888    -1.224906     107.77
 H       3.066839    -1.258210    -1.978654      34.24
 O       3.304504     0.655803    -1.807123     216.79
 H       4.024099     1.089634    -1.282545      31.86
 C       4.006204    -0.826302    -0.091213      93.42
 H       3.663688    -1.687744     0.550989      31.18
 O       5.271627    -1.527647    -0.594992      95.29
 H       5.686354    -1.055953    -1.394408      23.92
 C       4.284826     0.346267     0.944672     107.99
 O       5.287225     1.278702     0.281947     208.02
 H       4.930643     2.219438     0.704779      26.38
 H       4.889336     0.014957     1.997707      27.19
 H       3.366213     0.825023     1.005878      30.05
55
name = lig-Water-frame_157
 C      -1.950665     1.652819     3.789991      64.21
 H      -2.700343     2.448637     3.823092      26.77
 C      -0.941253    -0.456549     3.238311      55.92
 H      -0.893769    -1.494777     2.752623      28.69
 C       0.174966     0.050448     3.696152      28.06
 O       1.343848    -0.755389     3.858279     176.07
 C       1.127567    -2.124507     4.436809     101.02
 H       1.870806    -2.658702     5.193018      26.26
 H       0.890827    -3.192776     3.747262      25.72
 H       0.128410    -2.298593     5.023292      25.97
 C       0.431666     1.386150     4.003180       3.29
 O       1.700810     1.855560     4.393833     238.49
 H       1.961239     2.812356     4.236999      24.87
 C      -0.721538     2.173883     4.208458      72.30
 H      -0.543428     3.322073     4.596693      17.86
 C      -2.102953     0.386607     3.193406      32.60
 C      -3.390966    -0.075901     2.584013     115.80
 H      -3.977106     0.695220     2.979417      28.99
 O      -3.749070    -1.405057     2.741449     300.69
 H      -4.719639    -1.346058     2.742517      27.69
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 C      -3.413660     0.418846     1.161480      62.18
 H      -2.799723     1.280054     1.024665      26.36
 C      -4.736914     0.737642     0.365660     102.17
 O      -5.814228    -0.196584     0.422689     177.18
 H      -5.408062    -0.960690    -0.073529      26.60
 H      -4.497351     0.768515    -0.671488      25.87
 H      -5.323320     1.549263     1.002251      23.89
 C       0.869148     0.662122    -0.361104     -55.52
 H       1.178826     1.731478    -0.493745      22.42
 C       0.608183    -1.765325    -0.696629      59.15
 H       1.117066    -2.712621    -0.974195      28.37
 C      -0.750460    -1.803888    -0.444579      29.15
 O      -1.529982    -2.969287    -0.672656     157.28
 C      -0.903463    -4.258697    -0.420185     120.66
 H      -1.791965    -5.181408    -0.483469      24.38
 H      -0.546174    -4.756410    -1.433113      26.32
 H      -0.000363    -4.372676     0.137102      28.32
 C      -1.394623    -0.548449     0.014602     -33.29
 O      -2.718982    -0.771143     0.329235      41.42
 C      -0.626196     0.686932    -0.010188      37.11
 H      -0.819748     1.730798     0.190686      29.15
 C       1.529496    -0.613099    -0.709412      -0.93
 C       2.895459    -0.626248    -1.157417      76.95
 H       3.189032    -1.300266    -2.345547      23.56
 O       3.274225     0.679850    -1.822674     203.36
 H       3.893540     1.183044    -1.319383      30.76
 C       4.011197    -0.917898    -0.065820      84.32
 H       3.676994    -1.913204     0.541257      28.99
 O       5.252864    -1.507081    -0.574254     100.74
 H       5.752966    -1.042798    -1.416462      20.94
 C       4.336820     0.378247     0.880045     119.42
 O       5.270001     1.256319     0.290672     255.22
 H       5.143251     2.119916     0.700396      29.28
 H       4.719621     0.136844     1.756127      32.68
 H       3.256752     0.848748     0.931052      28.01
55
name = lig-Water-frame_158
 C      -1.992133     1.678192     3.709111      76.29
 H      -2.647778     2.546032     3.752295      23.29
 C      -1.004688    -0.494397     3.248480      79.90
 H      -1.103458    -1.435331     2.857901      29.80
 C       0.236613     0.016814     3.652110      14.60
 O       1.378751    -0.790760     3.862443     201.96
 C       1.088627    -2.109413     4.456979     121.58
 H       1.975038    -2.435398     4.956667      29.27
 H       1.226631    -2.764703     3.584774      27.83
 H       0.264438    -2.197746     5.094340      29.66
 C       0.486111     1.390598     3.972887      -4.95
 O       1.682146     1.871977     4.398378     227.69
 H       1.826225     2.824226     4.247600      27.89
 C      -0.698072     2.217692     4.200639      46.99
 H      -0.720657     3.261987     4.508196      18.65
 C      -2.009284     0.411395     3.172275      48.90
 C      -3.420003    -0.070611     2.583881      82.90
 H      -4.247672     0.898929     2.926304      23.81
 O      -3.767659    -1.409523     2.755803     271.24
 H      -4.751379    -1.490237     3.009130      24.42
 C      -3.400050     0.436854     1.135522      51.74
 H      -2.683819     1.372906     1.050403      23.02
 C      -4.746161     0.724306     0.323556     100.63
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 O      -5.793610    -0.247145     0.487536     183.49
 H      -5.693962    -1.118455    -0.069657      22.87
 H      -4.388229     1.118226    -0.752470      25.01
 H      -5.119352     1.631795     0.790383      27.26
 C       0.837080     0.669420    -0.378412      -0.29
 H       1.365302     1.595228    -0.538980      25.48
 C       0.620987    -1.738262    -0.674338      49.95
 H       1.081017    -2.664748    -1.050680      30.05
 C      -0.753471    -1.769014    -0.401450      38.68
 O      -1.570218    -2.914357    -0.629480     156.07
 C      -0.966333    -4.308142    -0.524405     118.63
 H      -1.640077    -5.025520    -0.318516      29.30
 H      -0.330425    -4.540896    -1.380548      27.60
 H      -0.022173    -4.153566     0.145393      26.86
 C      -1.356373    -0.617464    -0.010586      -7.92
 O      -2.684463    -0.751250     0.299169      25.46
 C      -0.602905     0.650430    -0.014996      23.03
 H      -1.179589     1.626242     0.280700      25.10
 C       1.513906    -0.596118    -0.654452     -60.65
 C       2.933460    -0.633780    -1.171740     108.80
 H       3.005069    -1.340980    -1.826401      26.98
 O       3.227746     0.701075    -1.848447     169.71
 H       3.818916     1.321998    -1.203026      24.61
 C       4.033196    -1.021005    -0.031341      96.93
 H       3.590694    -1.769866     0.622553      29.57
 O       5.243613    -1.483603    -0.571461     218.07
 H       5.533881    -1.155782    -1.368175      27.96
 C       4.316070     0.374274     0.778816     106.79
 O       5.274133     1.240821     0.269361     241.95
 H       5.186188     2.165200     0.693558      27.19
 H       4.566315    -0.013536     1.985614      26.58
 H       3.419570     0.884107     1.051734      28.20
55
name = lig-Water-frame_159
 C      -1.949389     1.777244     3.663460      56.36
 H      -2.955098     2.362525     3.564731      22.11
 C      -1.026279    -0.523493     3.256579      37.10
 H      -1.317543    -1.660013     2.985416      28.03
 C       0.359390    -0.014798     3.632167     -17.39
 O       1.405600    -0.816247     3.877531     190.50
 C       1.098213    -2.120869     4.447616     102.80
 H       2.185016    -2.071689     4.941553      23.86
 H       1.234928    -2.544189     3.332254      22.87
 H       0.197709    -2.048202     5.153066      25.62
 C       0.461627     1.437526     3.977483       0.71
 O       1.695441     1.871960     4.405172     209.45
 H       1.637844     2.854466     4.109555      27.90
 C      -0.696258     2.197221     4.132219      49.83
 H      -0.705604     3.278539     4.531688      25.12
 C      -2.040275     0.418650     3.157567       7.65
 C      -3.453972     0.047908     2.577171      94.97
 H      -4.279621     0.427135     3.040091      26.95
 O      -3.798306    -1.426043     2.782589     266.72
 H      -4.688257    -1.599378     3.195640      23.14
 C      -3.375618     0.414109     1.038080      84.13
 H      -2.855993     1.296774     1.078976      25.45
 C      -4.707292     0.732734     0.295830     106.92
 O      -5.785488    -0.289516     0.541423     171.74
 H      -5.704904    -1.186068     0.030703      22.37
 H      -4.516495     1.112168    -0.653324      28.06
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 H      -5.023899     1.804572     0.666593      25.50
 C       0.763431     0.643927    -0.387894     114.33
 H       1.501793     1.479392    -0.496435      31.68
 C       0.683803    -1.729246    -0.670731      52.75
 H       1.062478    -2.645866    -1.093490      30.11
 C      -0.717122    -1.797294    -0.386822     -25.90
 O      -1.610329    -2.873279    -0.580013     115.87
 C      -0.941564    -4.282247    -0.632983      95.95
 H      -1.778841    -5.004613     0.038530      21.94
 H      -0.371749    -4.371584    -1.575770      24.22
 H      -0.427488    -4.142751     0.316483      26.60
 C      -1.334340    -0.597866    -0.019057      -3.00
 O      -2.670350    -0.698344     0.284696      70.41
 C      -0.560688     0.595803    -0.030754      92.66
 H      -1.234083     1.309132     0.238761      29.25
 C       1.419278    -0.550917    -0.593819     -23.76
 C       2.989892    -0.597100    -1.137617      65.56
 H       2.924491    -1.801050    -1.924919      23.97
 O       3.189890     0.705055    -1.866402     178.18
 H       3.628885     1.251428    -1.213149      28.15
 C       4.039417    -1.017914    -0.028861      99.50
 H       3.460111    -1.666775     0.846300      27.16
 O       5.241553    -1.494924    -0.559499     161.96
 H       5.313681    -1.136522    -1.579766      22.35
 C       4.269022     0.303008     0.784087     104.61
 O       5.304730     1.233828     0.222093     275.30
 H       5.011666     2.140392     0.669783      28.19
 H       4.529760    -0.024222     1.677868      30.56
 H       3.348881     0.958744     1.015260      27.06
55
name = lig-Water-frame_160
 C      -1.930320     1.828369     3.590823      57.64
 H      -2.868345     2.232680     3.535752      23.36
 C      -0.983955    -0.544692     3.272049       6.58
 H      -1.254991    -1.514582     3.222998      28.16
 C       0.377107    -0.006037     3.612935      -1.61
 O       1.439140    -0.790683     3.891944     210.22
 C       1.179836    -2.116373     4.403888     132.01
 H       1.965779    -2.319321     5.064336      28.78
 H       0.928554    -2.903395     3.649392      27.34
 H       0.277926    -2.119433     4.990948      28.40
 C       0.425116     1.403153     3.987354       1.81
 O       1.706775     1.887362     4.404805     213.52
 H       1.852196     2.814887     4.067871      25.56
 C      -0.718891     2.213519     4.047036      47.34
 H      -0.464012     3.206738     4.621125      25.42
 C      -2.130372     0.444182     3.169055     -46.05
 C      -3.475390     0.097388     2.559996      81.56
 H      -4.433221     0.470494     3.252258      22.39
 O      -3.794742    -1.442298     2.804908     230.38
 H      -4.697053    -1.447250     3.187700      22.00
 C      -3.376696     0.364246     0.934896      93.56
 H      -2.846809     1.449717     0.951094      25.63
 C      -4.672775     0.742368     0.306410      91.82
 O      -5.779128    -0.296467     0.583988     149.16
 H      -5.388651    -1.085873     0.121977      26.93
 H      -4.647691     0.758527    -0.926854      26.17
 H      -5.098981     1.655633     0.767727      26.37
 C       0.738305     0.637737    -0.388569     129.15
 H       1.281353     1.559993    -0.363409      32.80
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 C       0.713383    -1.768271    -0.671719      63.85
 H       1.246717    -2.668297    -1.096149      28.23
 C      -0.674003    -1.844470    -0.392293     -29.27
 O      -1.633779    -2.850539    -0.539306     142.28
 C      -0.956025    -4.207063    -0.642237     111.20
 H      -1.697928    -4.835633    -0.453315      29.19
 H      -0.589639    -4.474966    -1.670578      26.19
 H      -0.350736    -4.294128     0.299181      27.15
 C      -1.305978    -0.569513    -0.021630       4.26
 O      -2.674950    -0.627152     0.282919     108.28
 C      -0.577664     0.538849    -0.040500      72.48
 H      -1.164726     1.546738     0.222821      26.86
 C       1.388304    -0.541486    -0.576453      -8.06
 C       2.969551    -0.627876    -1.125877     102.15
 H       2.982959    -1.279600    -1.763339      30.39
 O       3.160766     0.667456    -1.877819     235.50
 H       3.605006     1.258721    -1.244110      29.55
 C       3.988206    -0.926640    -0.024075     111.57
 H       3.584819    -1.649849     0.630509      29.90
 O       5.239475    -1.523660    -0.565250     159.52
 H       5.243742    -1.233140    -1.526553      27.41
 C       4.230764     0.261161     0.799951      92.79
 O       5.310376     1.224389     0.179503     240.71
 H       4.997318     2.063902     0.531812      30.55
 H       4.799658    -0.083203     1.876971      25.73
 H       3.279886     0.799323     0.839319      27.74
55
name = lig-Water-frame_161
 C      -1.959652     1.790155     3.488602      44.59
 H      -2.857019     2.612934     3.644463      23.22
 C      -0.950232    -0.467477     3.299664      29.58
 H      -1.106049    -1.645245     3.356793      28.13
 C       0.287496     0.017728     3.604071      23.53
 O       1.489076    -0.770033     3.898430     113.87
 C       1.238110    -2.135316     4.356790     131.86
 H       1.895526    -2.725211     5.166708      26.19
 H       0.840313    -3.170173     3.994885      26.47
 H       0.273113    -2.080973     4.989390      27.59
 C       0.428353     1.345480     3.989933      -4.74
 O       1.701994     1.892323     4.401632     239.66
 H       2.102277     2.777949     4.027498      24.64
 C      -0.680997     2.267061     3.990216      46.70
 H      -0.436070     3.137539     4.522056      19.20
 C      -2.155108     0.449900     3.200246      -7.79
 C      -3.517370     0.064799     2.561272      89.54
 H      -4.204017     0.817466     2.985281      26.93
 O      -3.763643    -1.429011     2.821032     247.16
 H      -4.785033    -1.336631     2.996677      22.46
 C      -3.373464     0.401643     0.899567     106.04
 H      -2.843772     1.262656     0.746000      32.66
 C      -4.706358     0.708685     0.280909     108.96
 O      -5.753628    -0.286343     0.612612     171.68
 H      -5.238757    -1.122418     0.250272      27.52
 H      -4.659370     0.557468    -0.710025      31.31
 H      -5.116708     1.598257     0.790234      27.99
 C       0.752090     0.651061    -0.373808      19.50
 H       1.044693     1.730836    -0.280028      30.49
 C       0.719455    -1.847009    -0.676783      47.58
 H       1.363958    -2.630468    -0.974501      29.12
 C      -0.669891    -1.845892    -0.397674      30.93
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 O      -1.615749    -2.849679    -0.506056     187.15
 C      -0.993795    -4.119382    -0.622983     118.21
 H      -1.970534    -4.939452    -0.950237      23.83
 H      -0.615280    -4.393743    -1.615523      28.86
 H      -0.083819    -4.454721    -0.042287      27.89
 C      -1.301742    -0.616765    -0.024245      41.08
 O      -2.675874    -0.589208     0.265820      88.79
 C      -0.641928     0.601142    -0.031677      54.21
 H      -0.898760     1.562947     0.144077      30.42
 C       1.447905    -0.581137    -0.607994     -81.57
 C       2.878511    -0.575465    -1.082986      89.86
 H       3.040419    -1.427175    -2.232090      21.19
 O       3.140238     0.609515    -1.878821     195.98
 H       3.709662     1.346160    -1.337057      23.81
 C       3.947981    -0.847702    -0.050416      88.27
 H       3.588923    -1.901483     0.482017      28.31
 O       5.216666    -1.554524    -0.572207     103.08
 H       5.439091    -1.304059    -1.468267      26.25
 C       4.277582     0.264965     0.860888     125.49
 O       5.277553     1.190324     0.139971     209.46
 H       5.061312     2.195833     0.482650      24.67
 H       4.669809     0.067517     1.731661      33.28
 H       3.248846     0.703710     0.974347      28.87
55
name = lig-Water-frame_162
 C      -1.982880     1.811553     3.438603      30.89
 H      -2.580027     2.592763     3.560653      24.42
 C      -1.002849    -0.406769     3.326352      75.61
 H      -0.960393    -1.457370     3.280164      33.74
 C       0.247482     0.023843     3.636009     -15.80
 O       1.523416    -0.779930     3.882339      73.29
 C       1.219692    -2.218004     4.402381     104.01
 H       2.060998    -2.510349     4.990636      28.77
 H       1.021293    -2.972129     3.590338      26.50
 H       0.438705    -1.893369     5.066030      25.60
 C       0.456368     1.393226     3.985019       3.86
 O       1.696764     1.864797     4.405837     266.78
 H       1.966247     2.720372     3.904590      27.56
 C      -0.631464     2.253839     3.918042      61.85
 H      -0.556573     3.419439     4.381645      20.20
 C      -2.141353     0.415523     3.214717      33.57
 C      -3.486178     0.013158     2.535026      87.83
 H      -4.243960     0.946115     2.794775      24.35
 O      -3.753441    -1.358988     2.834026     277.32
 H      -4.732431    -1.541658     2.792746      23.01
 C      -3.370997     0.462676     0.936351      70.92
 H      -2.714293     1.431920     0.730191      29.56
 C      -4.776266     0.646121     0.290020     105.48
 O      -5.712144    -0.298890     0.638418     194.27
 H      -5.545201    -1.205770     0.351749      26.00
 H      -4.581452     0.716974    -0.929116      26.64
 H      -5.082524     1.767252     0.561353      25.67
 C       0.749488     0.645774    -0.342019      12.55
 H       1.158864     1.664357    -0.355335      29.73
 C       0.729660    -1.877839    -0.670417      42.26
 H       1.330894    -2.829286    -0.875253      28.10
 C      -0.682610    -1.820395    -0.400582      23.26
 O      -1.570761    -2.857494    -0.463690     198.26
 C      -1.067635    -4.131028    -0.682276     133.48
 H      -1.799072    -4.733078    -0.787637      31.77
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 H      -0.477155    -3.924999    -1.707414      27.38
 H      -0.216583    -4.507367    -0.130341      30.48
 C      -1.329643    -0.625025    -0.014284     -11.12
 O      -2.676755    -0.626434     0.217535      23.34
 C      -0.636872     0.662734    -0.042250      40.08
 H      -1.081356     1.736056     0.208076      33.58
 C       1.477876    -0.617303    -0.650587     -53.73
 C       2.818595    -0.549339    -1.153653     133.22
 H       2.928537    -1.261105    -1.723960      33.23
 O       3.129960     0.586296    -1.879778     293.62
 H       3.703147     1.171879    -1.474207      33.82
 C       3.939136    -0.891727    -0.087196      95.41
 H       3.516537    -1.621851     0.457669      34.07
 O       5.177264    -1.579180    -0.578018      84.04
 H       5.722111    -1.230969    -1.478118      21.72
 C       4.320129     0.326362     0.880615     116.55
 O       5.214283     1.166708     0.111491     193.53
 H       5.119048     2.034652     0.485329      29.05
 H       4.752081     0.000751     2.040901      29.19
 H       3.372864     0.819291     1.297005      30.80
55
name = lig-Water-frame_163
 C      -1.898123     1.828218     3.439958      35.33
 H      -2.810083     2.659470     3.356125      20.76
 C      -1.059134    -0.396002     3.351539      15.26
 H      -1.131815    -1.498271     3.046183      32.25
 C       0.306923     0.051055     3.716530     -79.26
 O       1.506439    -0.804036     3.847175     109.19
 C       1.200839    -2.261002     4.433130      99.49
 H       2.309021    -2.309308     4.826457      24.55
 H       1.157764    -2.543938     3.339275      25.05
 H       0.419854    -2.080966     5.224090      20.66
 C       0.489539     1.460698     3.969237      -0.25
 O       1.700264     1.827410     4.407483     246.84
 H       1.796854     2.707183     3.982942      24.38
 C      -0.642064     2.265778     3.839890      32.30
 H      -0.619742     3.210065     4.035389      32.74
 C      -2.157567     0.418851     3.204060      50.28
 C      -3.417242     0.023892     2.491182     106.72
 H      -4.340786     0.565918     2.833155      26.59
 O      -3.747419    -1.282987     2.840014     306.99
 H      -4.665509    -1.608039     2.732547      23.72
 C      -3.354861     0.496292     0.976143      66.46
 H      -2.882374     1.433107     0.978072      28.11
 C      -4.781521     0.634190     0.245594     117.33
 O      -5.709699    -0.331353     0.677663     192.31
 H      -5.687782    -1.215235     0.156690      24.35
 H      -4.610086     0.810402    -0.730319      30.36
 H      -5.184656     1.612867     0.405632      28.57
 C       0.751299     0.607822    -0.318006      90.66
 H       1.464807     1.441806    -0.484465      28.89
 C       0.742771    -1.867466    -0.653729      60.30
 H       1.077207    -2.864408    -0.790646      29.56
 C      -0.677833    -1.791413    -0.395550     -20.79
 O      -1.544866    -2.851714    -0.391287     143.69
 C      -1.052689    -4.133314    -0.820281     101.81
 H      -2.071618    -4.981773    -0.680714      22.86
 H      -0.570288    -3.837775    -1.689891      27.15
 H      -0.457098    -4.520767     0.118263      25.73
 C      -1.345003    -0.541809    -0.008209     -20.16
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 O      -2.701174    -0.688336     0.164668      57.64
 C      -0.610560     0.697101    -0.053616     124.12
 H      -1.237079     1.490270     0.207143      36.16
 C       1.397815    -0.618280    -0.666754      23.34
 C       2.841338    -0.528222    -1.185552      75.14
 H       2.910318    -1.825312    -1.823445      25.19
 O       3.112341     0.599077    -1.925728     214.27
 H       3.840574     1.090834    -1.409622      28.45
 C       3.956366    -0.917951    -0.106955      83.10
 H       3.318534    -1.585712     0.740137      30.00
 O       5.144430    -1.598139    -0.593919     158.58
 H       5.512464    -1.152237    -1.319233      28.67
 C       4.352529     0.351681     0.937864     113.07
 O       5.152807     1.145993     0.085259     167.65
 H       5.098895     2.078063     0.562908      26.11
 H       4.876524    -0.069918     1.685824      32.24
 H       3.557563     0.984715     1.328069      29.98
55
name = lig-Water-frame_164
 C      -1.866418     1.835002     3.439028      69.44
 H      -2.684126     2.358337     3.177498      26.21
 C      -1.039935    -0.442059     3.382541     -30.23
 H      -1.350751    -1.381976     2.852055      33.25
 C       0.351579     0.068074     3.799622      -3.92
 O       1.435301    -0.801912     3.819774     113.67
 C       1.233963    -2.219279     4.426789     116.67
 H       2.261919    -2.489851     4.727860      28.53
 H       0.994701    -2.694665     3.460535      27.21
 H       0.475844    -2.579187     5.162319      28.32
 C       0.487947     1.438479     3.944578      33.65
 O       1.724633     1.814888     4.408843     168.49
 H       1.968584     2.858740     4.258173      19.32
 C      -0.659963     2.282956     3.759658      59.53
 H      -0.515125     3.509816     3.848792      23.30
 C      -2.158699     0.488943     3.193535     -48.64
 C      -3.388298     0.060700     2.450936     105.58
 H      -4.376379     0.578520     2.992399      23.55
 O      -3.708542    -1.260894     2.842541     239.68
 H      -4.734038    -1.338544     2.739537      19.74
 C      -3.388023     0.455596     0.990332      75.38
 H      -2.888864     1.511533     1.074192      24.77
 C      -4.732812     0.653479     0.239872      81.20
 O      -5.737755    -0.391048     0.702434     152.72
 H      -5.584870    -1.008949    -0.072608      27.19
 H      -4.591782     0.590101    -0.987070      24.69
 H      -5.426851     1.578989     0.586551      23.89
 C       0.789842     0.570118    -0.319747      85.56
 H       1.560872     1.339500    -0.520528      25.08
 C       0.683112    -1.838710    -0.620973      71.44
 H       1.096439    -2.860288    -0.828417      27.94
 C      -0.666433    -1.742370    -0.369694     -10.26
 O      -1.546757    -2.840945    -0.310921     144.26
 C      -1.068860    -4.167714    -0.882314     115.02
 H      -1.868163    -4.735801    -0.977880      30.38
 H      -0.533498    -4.218537    -1.958291      26.60
 H      -0.557404    -4.523843    -0.045882      28.85
 C      -1.325411    -0.476827    -0.037277     -11.34
 O      -2.733088    -0.706614     0.132692      56.62
 C      -0.612827     0.677937    -0.053149     105.19
 H      -1.212984     1.599793     0.199453      32.15
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 C       1.329958    -0.608582    -0.682477      24.92
 C       2.883956    -0.647062    -1.205801      85.25
 H       2.935878    -1.427114    -1.828363      31.57
 O       3.107285     0.633903    -1.986110     208.49
 H       3.952901     0.987307    -1.471267      26.04
 C       3.919602    -0.911570    -0.043757      94.92
 H       3.500481    -1.569151     0.566559      31.66
 O       5.091450    -1.613217    -0.583849     168.93
 H       5.293023    -1.095476    -1.459796      25.63
 C       4.363686     0.311308     0.931314      97.34
 O       5.122280     1.169396     0.052515     175.78
 H       5.060985     2.106324     0.448091      26.01
 H       5.208091    -0.252659     1.658327      24.78
 H       3.529608     1.003922     1.356210      24.57
55
name = lig-Water-frame_165
 C      -1.901484     1.818512     3.411606      71.96
 H      -2.765697     2.582063     3.063376      22.10
 C      -1.014616    -0.445017     3.400845      37.27
 H      -1.188479    -1.395947     2.937538      34.10
 C       0.286947     0.018112     3.840423      14.61
 O       1.355711    -0.806229     3.826224     181.45
 C       1.272118    -2.189137     4.362813     124.82
 H       2.238512    -2.656235     4.731617      28.83
 H       0.863732    -3.060635     3.651034      27.39
 H       0.577715    -2.622981     5.109794      27.81
 C       0.472778     1.418529     3.934805      15.21
 O       1.765618     1.832179     4.419301     211.21
 H       2.063427     2.713673     4.344229      18.29
 C      -0.597542     2.348750     3.703972      65.48
 H      -0.383603     3.367152     3.855588      24.67
 C      -2.072050     0.509943     3.194701     -18.23
 C      -3.418887     0.112604     2.471195     102.50
 H      -4.067201     0.900359     2.934079      27.38
 O      -3.676139    -1.272949     2.835191     261.97
 H      -4.644058    -1.208388     2.860814      22.76
 C      -3.435335     0.405981     0.959530      88.25
 H      -2.837530     1.315309     0.843462      26.31
 C      -4.729256     0.684362     0.258326     105.05
 O      -5.754365    -0.447559     0.686570     166.69
 H      -5.600418    -1.095622    -0.011340      29.01
 H      -4.629155     0.422729    -0.716335      28.31
 H      -5.167570     1.530522     0.579951      28.65
 C       0.820945     0.581862    -0.335747      32.18
 H       1.374418     1.507265    -0.427123      22.63
 C       0.608134    -1.829868    -0.597602      67.80
 H       1.208592    -2.676990    -0.899808      27.22
 C      -0.704147    -1.712774    -0.323114      37.97
 O      -1.546924    -2.840545    -0.261498     123.29
 C      -1.062294    -4.161707    -0.938077      94.87
 H      -2.205271    -4.762163    -1.290016      24.26
 H      -0.564361    -4.383950    -1.824342      28.58
 H      -0.319375    -4.752518    -0.225480      27.06
 C      -1.335754    -0.495490    -0.087067      18.96
 O      -2.747361    -0.662882     0.127803      81.67
 C      -0.609461     0.691881    -0.039934      49.79
 H      -0.885749     1.762711     0.127345      28.09
 C       1.369138    -0.640942    -0.717907       1.74
 C       2.877299    -0.707471    -1.172602      50.22
 H       3.059108    -1.451969    -2.320840      22.77
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 O       3.123672     0.646638    -2.023223     185.11
 H       3.890215     1.027644    -1.703880      29.03
 C       3.875275    -0.880976     0.018690      84.92
 H       3.448984    -1.869718     0.670860      26.16
 O       5.037359    -1.601897    -0.573155     129.05
 H       5.155238    -1.364107    -1.614270      24.92
 C       4.394125     0.226208     0.897708     125.65
 O       5.114067     1.212432     0.002006     243.36
 H       4.929415     2.112491     0.362000      26.35
 H       5.070698    -0.130696     1.585291      29.96
 H       3.597979     0.629554     1.463062      29.14
55
name = lig-Water-frame_166
 C      -1.915028     1.894903     3.372168      66.17
 H      -2.600691     2.684380     3.171870      22.58
 C      -0.996382    -0.420019     3.409598      93.47
 H      -0.906277    -1.568762     3.192462      28.51
 C       0.159794    -0.034495     3.847623      12.76
 O       1.306330    -0.854672     3.857577     172.22
 C       1.282394    -2.227674     4.280562     117.31
 H       2.360167    -2.490877     4.664163      27.06
 H       0.947385    -3.017375     3.637661      28.37
 H       0.626386    -2.039574     5.255722      25.29
 C       0.479242     1.437701     3.953283       4.18
 O       1.785973     1.808014     4.438268     166.86
 H       2.017449     2.816597     4.066630      21.45
 C      -0.529108     2.357201     3.666922      75.08
 H      -0.265138     3.380185     3.953644      25.17
 C      -2.000275     0.460044     3.166707      20.82
 C      -3.394517     0.159127     2.520645      86.14
 H      -4.103561     1.083045     2.918183      25.82
 O      -3.664553    -1.261266     2.826366     217.00
 H      -4.671321    -1.480270     3.010930      21.39
 C      -3.433970     0.356728     0.901375      99.75
 H      -2.794250     1.243139     0.621339      26.45
 C      -4.768278     0.632506     0.322125      92.62
 O      -5.765050    -0.471779     0.659237     124.43
 H      -5.602709    -1.378447     0.182932      24.06
 H      -4.626798     0.527446    -0.854042      25.88
 H      -5.024889     1.851526     0.525730      24.31
 C       0.815316     0.613821    -0.361431      30.03
 H       1.221915     1.669328    -0.311072      24.64
 C       0.609383    -1.800782    -0.606907      68.91
 H       1.117756    -2.724080    -0.925289      29.15
 C      -0.777388    -1.746489    -0.278959      34.20
 O      -1.536256    -2.876655    -0.246760     143.56
 C      -1.102588    -4.187249    -0.953944     114.11
 H      -2.008377    -4.527049    -1.180615      29.48
 H      -0.456363    -3.971536    -1.984557      26.02
 H      -0.509618    -4.862003    -0.424827      29.15
 C      -1.404732    -0.498850    -0.111712      36.72
 O      -2.751637    -0.599480     0.134534      87.80
 C      -0.544706     0.717276    -0.039428      31.80
 H      -0.796304     1.740831     0.115568      23.63
 C       1.450475    -0.669055    -0.751252      -4.54
 C       2.850853    -0.704190    -1.205118      91.64
 H       3.055463    -1.415234    -1.904313      28.52
 O       3.124227     0.625002    -2.041319     159.74
 H       3.988595     1.141096    -1.779146      23.23
 C       3.837082    -0.951252     0.040924      94.31
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 H       3.392578    -1.580364     0.703058      30.42
 O       4.998522    -1.590055    -0.575141     220.63
 H       5.077648    -1.620536    -1.467809      30.06
 C       4.417156     0.170278     0.830018      92.78
 O       5.101873     1.241497    -0.045908     248.37
 H       4.710832     2.134701     0.432479      23.44
 H       5.197235    -0.218097     1.683921      25.57
 H       3.540827     0.461306     1.592727      26.68
55
name = lig-Water-frame_167
 C      -1.811813     1.950557     3.340830      60.78
 H      -2.652245     2.724704     3.235127      23.93
 C      -1.024059    -0.485571     3.395314      78.31
 H      -1.044464    -1.503807     3.374931      30.44
 C       0.178251     0.005506     3.873878      11.39
 O       1.279893    -0.888213     3.868136     171.41
 C       1.276251    -2.237260     4.284978     126.97
 H       2.350624    -2.309442     4.493852      28.63
 H       0.904727    -2.952470     3.418708      27.69
 H       0.815067    -1.952151     5.182060      27.94
 C       0.501534     1.411184     3.989729      22.64
 O       1.777993     1.797629     4.440315     238.43
 H       1.976740     2.516853     3.815518      27.84
 C      -0.497220     2.337790     3.650963      70.46
 H      -0.231485     3.454319     4.076122      24.63
 C      -2.038276     0.493868     3.110341       6.87
 C      -3.344175     0.184040     2.553118      92.86
 H      -4.227825     0.804184     2.882651      27.53
 O      -3.678304    -1.235978     2.827916     257.89
 H      -4.570147    -1.576688     3.024356      20.92
 C      -3.387096     0.367889     0.877999      89.26
 H      -2.959818     1.409576     0.661940      29.12
 C      -4.827071     0.562060     0.329837     117.57
 O      -5.787710    -0.470781     0.637594     175.49
 H      -5.368058    -1.338408     0.372918      24.19
 H      -4.701559     0.791696    -0.717774      28.44
 H      -5.107371     1.482650     0.578243      30.22
 C       0.818078     0.634331    -0.397553      81.28
 H       1.361619     1.541877    -0.322886      30.85
 C       0.642886    -1.771584    -0.640045      42.77
 H       0.881241    -2.833996    -0.860658      29.65
 C      -0.799557    -1.781876    -0.262245     -12.75
 O      -1.534324    -2.954677    -0.237137     111.73
 C      -1.101883    -4.138788    -1.000822     116.83
 H      -2.297813    -4.644375    -1.253107      23.64
 H      -0.680631    -3.566611    -1.742032      25.53
 H      -0.617448    -4.977008    -0.325261      25.46
 C      -1.442428    -0.466465    -0.104321      25.18
 O      -2.764161    -0.576978     0.129085     107.35
 C      -0.499566     0.690662    -0.055777      34.46
 H      -1.021955     1.698927     0.212604      25.17
 C       1.460311    -0.632753    -0.756504      36.20
 C       2.851920    -0.607748    -1.219912      70.26
 H       3.081974    -1.876592    -1.705326      25.17
 O       3.116405     0.574106    -2.047272     168.86
 H       3.973142     0.998522    -1.657339      23.56
 C       3.835473    -1.008410    -0.019907      76.46
 H       3.177546    -1.604259     0.902736      27.90
 O       4.981499    -1.606856    -0.546509     117.96
 H       4.963398    -1.751352    -1.622624      23.01
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 C       4.441133     0.148418     0.810797     109.16
 O       5.053749     1.256621    -0.062273     268.87
 H       4.809436     2.048113     0.405430      30.39
 H       5.248337    -0.299145     1.365552      28.34
 H       3.691159     0.602819     1.367130      30.64
55
name = lig-Water-frame_168
 C      -1.693279     1.951277     3.291695      64.04
 H      -2.620021     2.608472     3.297938      22.56
 C      -1.087876    -0.499929     3.387452     -14.21
 H      -1.442002    -1.636547     3.391587      26.25
 C       0.264020     0.038321     3.885216      10.93
 O       1.276856    -0.855966     3.848125     169.07
 C       1.266548    -2.225518     4.302823     120.57
 H       2.450448    -2.463163     4.287960      27.55
 H       0.804525    -2.838177     3.518515      31.45
 H       0.748504    -2.591845     5.376378      27.27
 C       0.514390     1.349947     4.025037      45.95
 O       1.752110     1.779271     4.428804     184.86
 H       2.175937     2.427591     3.777711      24.50
 C      -0.462535     2.349119     3.689446      23.58
 H      -0.314222     3.286064     3.940972      26.21
 C      -2.063997     0.580066     3.083752     -14.95
 C      -3.351192     0.147506     2.520855      99.64
 H      -4.292789     0.725371     2.954811      27.59
 O      -3.670419    -1.220250     2.832323     260.74
 H      -4.671828    -1.288299     2.970327      20.49
 C      -3.390387     0.461394     0.909835      72.91
 H      -3.079464     1.499887     0.800173      27.88
 C      -4.859062     0.495048     0.326221      80.88
 O      -5.809646    -0.475306     0.619950     172.11
 H      -5.264266    -1.255142     0.415171      26.59
 H      -4.808350     0.763135    -0.796100      26.68
 H      -5.482059     1.403137     1.016393      23.51
 C       0.848164     0.627332    -0.439361     106.36
 H       1.617723     1.461782    -0.413664      30.37
 C       0.618810    -1.774806    -0.666452      34.72
 H       0.995442    -2.777003    -0.827064      29.31
 C      -0.758309    -1.767734    -0.278830     -42.01
 O      -1.552025    -3.020458    -0.195774     120.81
 C      -1.178827    -4.091265    -1.021708     132.07
 H      -1.967805    -4.613539    -1.441445      29.55
 H      -0.628967    -3.594790    -1.937114      25.35
 H      -0.579940    -4.781709    -0.455580      28.31
 C      -1.378373    -0.482626    -0.089135       7.86
 O      -2.778311    -0.582134     0.110100      75.22
 C      -0.561408     0.655232    -0.064979      62.73
 H      -1.041026     1.496046     0.257529      30.68
 C       1.402006    -0.564476    -0.750734      -4.16
 C       2.879101    -0.583426    -1.219870     110.94
 H       2.918654    -1.646888    -1.770143      26.70
 O       3.120374     0.496008    -2.035958     259.50
 H       3.866290     0.843172    -1.551298      26.17
 C       3.820689    -1.001642    -0.059804     104.72
 H       3.278591    -1.612656     0.533004      31.96
 O       4.991251    -1.665822    -0.535763     172.45
 H       4.858996    -1.762630    -1.528751      27.08
 C       4.466447     0.152951     0.759906     105.93
 O       4.997460     1.233086    -0.085469     167.10
 H       4.961070     2.192258     0.464091      24.18
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 H       5.370447    -0.358589     1.288420      28.13
 H       3.710834     0.837653     1.376209      25.86
55
name = lig-Water-frame_169
 C      -1.649142     1.922192     3.228692      92.56
 H      -2.424322     2.660409     3.228805      31.87
 C      -1.147067    -0.421635     3.405885      44.63
 H      -1.555691    -1.371036     3.377265      30.60
 C       0.241439    -0.038823     3.845625      13.77
 O       1.316111    -0.821979     3.848515     227.67
 C       1.268226    -2.247612     4.339304     128.52
 H       2.225018    -2.641164     4.226010      32.06
 H       0.660467    -2.852152     3.550222      32.74
 H       0.900596    -2.816156     5.125257      29.76
 C       0.518207     1.356992     4.038698      36.00
 O       1.755422     1.756320     4.426896     253.12
 H       2.295790     2.464789     3.896433      26.65
 C      -0.413685     2.323900     3.755209      43.50
 H      -0.237487     3.568321     3.875933      17.15
 C      -2.014697     0.601703     3.093206      44.13
 C      -3.409529     0.128319     2.452333     111.41
 H      -4.149156     0.835434     3.018325      29.14
 O      -3.669889    -1.214065     2.834711     280.82
 H      -4.652701    -1.069279     2.931014      21.84
 C      -3.464860     0.532672     0.962931      62.61
 H      -2.996406     1.612175     0.818799      26.47
 C      -4.906703     0.556976     0.368410     101.42
 O      -5.822744    -0.535936     0.606663      93.51
 H      -5.473114    -1.477160     0.308936      21.77
 H      -4.940598     0.674070    -0.733978      28.73
 H      -5.325550     1.211594     0.940818      32.33
 C       0.835978     0.653772    -0.453697      84.48
 H       1.510012     1.480434    -0.499352      32.83
 C       0.580728    -1.788126    -0.682906      35.08
 H       1.288186    -2.640635    -0.854805      30.15
 C      -0.706163    -1.776961    -0.319281      32.10
 O      -1.577878    -3.020723    -0.134965     112.55
 C      -1.193842    -4.023595    -1.083208     121.37
 H      -2.156736    -4.711557    -1.666618      25.17
 H      -0.593774    -3.963332    -1.974758      26.65
 H      -0.385041    -4.705494    -0.589667      27.00
 C      -1.310114    -0.553099    -0.066131      -2.38
 O      -2.768187    -0.568976     0.096065     -28.33
 C      -0.610941     0.630371    -0.082882      -0.91
 H      -1.063217     1.629920     0.320794      29.86
 C       1.350515    -0.561345    -0.755865     -52.25
 C       2.852830    -0.648140    -1.192579     109.14
 H       2.718931    -1.371769    -2.169747      24.60
 O       3.150893     0.434625    -2.029208     202.85
 H       3.884833     1.056831    -1.544029      22.60
 C       3.833448    -0.928536    -0.106674      93.16
 H       3.198681    -1.837852     0.494870      27.92
 O       5.011238    -1.748946    -0.542138     177.01
 H       5.004675    -1.786711    -1.474332      29.85
 C       4.471257     0.195641     0.732803     132.95
 O       4.956094     1.221192    -0.127482     223.12
 H       4.984007     2.013390     0.398989      28.22
 H       5.283565    -0.264293     1.370084      30.93
 H       3.849352     0.556131     1.493500      31.35
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name = lig-Water-frame_170
 C      -1.633533     1.930300     3.185199      79.69
 H      -2.296848     2.899912     2.948371      27.52
 C      -1.125422    -0.326398     3.456529      86.55
 H      -1.476438    -1.386736     3.374243      30.56
 C       0.140255    -0.098452     3.787924      21.53
 O       1.384370    -0.836842     3.888804     184.14
 C       1.254676    -2.300213     4.291774      92.23
 H       2.364680    -2.811604     4.090430      26.62
 H       0.560909    -2.716378     3.508482      29.87
 H       0.838854    -2.524962     5.473259      23.70
 C       0.524553     1.363500     4.028039       9.07
 O       1.811246     1.726013     4.449844     253.23
 H       2.066403     2.513314     3.975697      28.77
 C      -0.398644     2.342211     3.808111      43.03
 H      -0.112497     3.274081     3.885076      25.75
 C      -2.004851     0.591266     3.076706      64.13
 C      -3.410310     0.181366     2.426019      97.70
 H      -4.129133     0.927663     2.977710      25.38
 O      -3.690405    -1.192512     2.825354     278.29
 H      -4.642671    -1.368498     3.027930      21.87
 C      -3.536602     0.553776     0.976212      74.48
 H      -3.035899     1.449992     0.825755      27.95
 C      -4.934024     0.601251     0.398247      88.85
 O      -5.837616    -0.641031     0.610935      72.71
 H      -5.644768    -1.424654     0.061948      22.45
 H      -4.939086     0.810980    -0.672219      26.21
 H      -5.428753     1.684003     0.974646      24.16
 C       0.743351     0.688890    -0.444632      43.46
 H       1.251812     1.686044    -0.539834      28.98
 C       0.635888    -1.797179    -0.712012      81.90
 H       1.299669    -2.630925    -0.897563      34.02
 C      -0.722831    -1.852992    -0.344761     -16.90
 O      -1.576415    -2.972608    -0.109081     117.83
 C      -1.193977    -4.043423    -1.164089      99.36
 H      -2.118112    -4.501751    -1.326156      29.11
 H      -0.592235    -3.732137    -2.107851      25.40
 H      -0.541533    -4.745882    -0.643864      26.20
 C      -1.323117    -0.597987    -0.028060     -89.68
 O      -2.737401    -0.536274     0.095982     -27.08
 C      -0.599548     0.662959    -0.097777      80.86
 H      -1.046630     1.561171     0.206750      38.38
 C       1.327925    -0.601958    -0.762258      10.65
 C       2.772080    -0.719898    -1.226122      98.96
 H       2.750235    -1.541313    -2.115978      26.41
 O       3.212042     0.431191    -2.034054     240.98
 H       3.645222     1.156552    -1.631989      30.82
 C       3.855807    -0.946351    -0.123358      97.82
 H       3.397572    -1.557178     0.588754      33.84
 O       5.027643    -1.831307    -0.552050     102.50
 H       5.360426    -1.713655    -1.627635      22.16
 C       4.457787     0.209466     0.728826     120.02
 O       4.929024     1.212858    -0.185084     199.85
 H       4.906881     2.106359     0.397931      25.31
 H       5.309281    -0.237411     1.343663      31.48
 H       3.697315     0.427340     1.623332      30.45
55
name = lig-Water-frame_171
 C      -1.635121     2.010959     3.154236      45.09
 H      -2.159711     2.743412     2.684545      26.80
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 C      -1.105083    -0.361344     3.506723      52.53
 H      -1.279995    -1.469203     3.360174      32.22
 C       0.190284    -0.052380     3.778770      22.44
 O       1.421527    -0.881841     3.946803     181.03
 C       1.245557    -2.347344     4.248481     122.53
 H       2.146183    -2.732673     4.113438      31.24
 H       0.462713    -2.741887     3.546989      28.48
 H       0.984379    -2.076209     5.235105      26.25
 C       0.536198     1.308397     4.014887      14.06
 O       1.867473     1.684513     4.476470     162.30
 H       1.900261     2.618560     4.039967      27.14
 C      -0.423250     2.318986     3.822532      23.75
 H       0.018529     3.479224     3.974437      22.34
 C      -2.070262     0.649999     3.020958      61.16
 C      -3.391163     0.252130     2.470122     103.22
 H      -4.233048     0.955074     2.924258      24.30
 O      -3.715670    -1.162272     2.808739     310.65
 H      -4.581215    -1.579622     3.077792      22.30
 C      -3.572498     0.501750     0.953698      62.69
 H      -3.041568     1.581877     0.758257      24.20
 C      -4.998433     0.654278     0.437037      99.84
 O      -5.851708    -0.709515     0.626694      69.32
 H      -5.495767    -1.231040    -0.189596      22.87
 H      -4.871153     0.955304    -0.676027      25.62
 H      -5.450839     1.441819     0.755158      31.10
 C       0.668052     0.695832    -0.450104      86.27
 H       1.031845     1.716350    -0.570449      28.19
 C       0.691516    -1.827692    -0.732551      44.41
 H       1.144905    -2.813718    -0.978143      27.86
 C      -0.772437    -1.900703    -0.332476     -38.37
 O      -1.539969    -2.929398    -0.136882     118.04
 C      -1.173967    -4.055650    -1.206127      79.53
 H      -2.381635    -4.530980    -1.258364      22.25
 H      -0.886347    -3.352894    -2.001194      23.62
 H      -0.640193    -4.871158    -0.661872      22.17
 C      -1.365423    -0.587031     0.005155     -46.97
 O      -2.721179    -0.502100     0.106138      42.62
 C      -0.606665     0.661284    -0.102000      77.16
 H      -1.172430     1.622864     0.096760      30.59
 C       1.331598    -0.590016    -0.769744      47.63
 C       2.725218    -0.740549    -1.295600      89.59
 H       2.970333    -1.838207    -1.700393      25.08
 O       3.250641     0.425371    -2.076881     209.77
 H       3.471205     1.154466    -1.408925      27.86
 C       3.912479    -1.006798    -0.132261      62.64
 H       3.444050    -1.588123     0.905124      29.46
 O       5.049951    -1.897788    -0.596312     146.81
 H       5.475753    -1.550863    -1.341562      28.18
 C       4.421758     0.183032     0.733968     100.50
 O       4.904480     1.243041    -0.215837     205.28
 H       4.816109     2.157680     0.245340      28.55
 H       5.394797    -0.223294     1.193336      28.59
 H       3.625718     0.572434     1.314072      28.45
55
name = lig-Water-frame_172
 C      -1.642776     2.064805     3.132809      41.63
 H      -2.243229     2.843164     2.421673      21.26
 C      -1.128419    -0.423081     3.511127      22.95
 H      -1.244069    -1.455013     3.379334      30.16
 C       0.350844    -0.006479     3.808729      12.38
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 O       1.424123    -0.905462     3.973386     177.22
 C       1.201605    -2.328107     4.196615      98.61
 H       2.302917    -2.890018     4.121792      25.24
 H       0.316563    -2.950684     3.710692      25.77
 H       0.975255    -2.142934     5.399899      23.72
 C       0.567473     1.282537     4.026489      28.14
 O       1.879698     1.648274     4.485195     140.27
 H       2.061637     2.606245     4.222316      27.85
 C      -0.419637     2.315704     3.811242      32.00
 H      -0.163511     3.319641     4.016161      28.27
 C      -2.068839     0.700077     3.008231      35.39
 C      -3.438230     0.295374     2.518644     108.74
 H      -4.262801     0.953775     2.949243      26.26
 O      -3.708179    -1.133649     2.791597     278.26
 H      -4.698613    -1.284537     3.032711      21.90
 C      -3.543116     0.473797     0.925235      88.56
 H      -3.259311     1.435943     0.728479      27.33
 C      -5.041165     0.620397     0.424537      78.57
 O      -5.846976    -0.717662     0.619149     119.18
 H      -5.356564    -1.155289    -0.150769      26.22
 H      -4.938055     0.820020    -0.614604      26.88
 H      -5.775409     1.524859     1.014929      24.09
 C       0.670084     0.664973    -0.487635      80.65
 H       1.121734     1.647491    -0.641081      27.53
 C       0.649410    -1.870418    -0.720496      40.38
 H       1.045734    -2.839873    -1.091354      24.17
 C      -0.749246    -1.814192    -0.297773     -34.55
 O      -1.514331    -2.954285    -0.184768     152.69
 C      -1.246207    -4.044530    -1.188111     111.44
 H      -2.212632    -4.459144    -1.462002      26.96
 H      -1.049506    -3.410026    -2.035348      26.39
 H      -0.478337    -4.870356    -0.903150      24.62
 C      -1.377486    -0.553009     0.018748       7.88
 O      -2.766094    -0.475861     0.124772     105.48
 C      -0.707038     0.627236    -0.077310      62.68
 H      -1.250195     1.598036    -0.054001      24.97
 C       1.347505    -0.559416    -0.792909     -25.64
 C       2.779511    -0.747964    -1.313975      90.18
 H       2.947817    -1.800316    -1.746481      23.11
 O       3.267979     0.404348    -2.130285     227.05
 H       3.334619     0.918781    -1.223398      25.87
 C       3.955792    -1.087724    -0.085760      79.57
 H       3.543864    -1.704564     0.661322      29.46
 O       5.051671    -1.939461    -0.618455     162.36
 H       5.504172    -1.362616    -1.371988      24.68
 C       4.419229     0.159197     0.669446     101.44
 O       4.877319     1.291594    -0.239982     263.99
 H       4.788292     2.125918     0.262257      30.40
 H       5.277950    -0.143253     1.283778      27.56
 H       3.547543     0.722001     1.199357      25.00
55
name = lig-Water-frame_173
 C      -1.657226     2.087978     3.092383      38.03
 H      -2.157017     2.866544     2.680676      24.59
 C      -1.098375    -0.385165     3.488126      35.36
 H      -1.407784    -1.531265     3.395317      27.10
 C       0.405671    -0.072333     3.822677       4.82
 O       1.420735    -0.913838     3.963665     213.26
 C       1.170501    -2.319390     4.230106     135.44
 H       2.016810    -2.811635     4.057910      30.96
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 H       0.371648    -2.881313     3.768032      28.31
 H       0.938861    -2.651788     5.279663      28.31
 C       0.619471     1.362198     4.061610      23.06
 O       1.876808     1.623966     4.496447     202.51
 H       2.246485     2.470397     4.294090      27.48
 C      -0.416668     2.293507     3.770512      38.70
 H      -0.197297     3.426716     4.054977      26.47
 C      -1.999006     0.681053     3.052024      41.95
 C      -3.483627     0.301287     2.520543     104.40
 H      -4.319618     1.017226     3.060446      24.32
 O      -3.711102    -1.092114     2.787150     293.21
 H      -4.645583    -0.975013     2.904855      24.82
 C      -3.532533     0.471122     0.929660      81.66
 H      -3.234076     1.625714     0.638716      23.08
 C      -5.103007     0.555096     0.443711      96.62
 O      -5.823103    -0.678114     0.591291     159.55
 H      -5.435868    -1.438618     0.092601      25.10
 H      -5.168779     0.726870    -0.711237      26.14
 H      -5.538976     1.182640     1.064132      29.77
 C       0.677105     0.610469    -0.528899      50.82
 H       1.295328     1.532634    -0.699617      27.12
 C       0.562379    -1.845423    -0.693166      57.92
 H       1.018927    -2.716625    -1.117745      25.51
 C      -0.688529    -1.722585    -0.263247      22.61
 O      -1.505672    -3.005389    -0.227134     165.20
 C      -1.303208    -3.993956    -1.179744     123.31
 H      -2.402503    -4.608432    -1.550248      23.80
 H      -0.954741    -3.688299    -2.260168      26.15
 H      -0.431581    -4.644874    -1.084977      27.08
 C      -1.412244    -0.533294     0.028953      32.12
 O      -2.852200    -0.478504     0.145021      95.79
 C      -0.753320     0.634421    -0.078229      29.17
 H      -1.302147     1.542029    -0.080513      21.18
 C       1.358958    -0.584383    -0.825125     -58.56
 C       2.884780    -0.768960    -1.293465      79.27
 H       2.708525    -1.592836    -2.215594      20.88
 O       3.265410     0.360118    -2.148069     263.25
 H       3.509365     1.039897    -1.522937      26.50
 C       3.984618    -1.147793    -0.081949      68.89
 H       3.403953    -2.001598     0.638837      23.51
 O       5.050711    -1.940646    -0.632588     182.32
 H       5.397052    -1.480992    -1.523753      24.60
 C       4.425324     0.179429     0.588516     106.37
 O       4.850550     1.323716    -0.266545     286.73
 H       4.810257     2.128196     0.488994      24.84
 H       5.099948     0.014299     1.550716      25.74
 H       3.569214     0.511144     1.191554      27.01
55
name = lig-Water-frame_174
 C      -1.621952     2.033254     3.093461      62.97
 H      -2.291940     3.020473     2.942638      25.16
 C      -1.009894    -0.328172     3.457405      80.53
 H      -1.471213    -1.223905     3.452031      27.28
 C       0.311990    -0.085603     3.822849      10.91
 O       1.427056    -0.948863     3.961489     185.27
 C       1.127341    -2.327293     4.294476     112.21
 H       2.131484    -2.861967     3.815718      25.72
 H       0.289108    -2.614253     3.408841      25.88
 H       0.915200    -2.901916     5.299826      25.79
 C       0.628890     1.394243     4.066251       0.96
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 O       1.900975     1.612640     4.532498     246.26
 H       2.330125     2.498348     4.138772      22.21
 C      -0.392808     2.319248     3.724141      69.13
 H      -0.163061     3.401637     4.005286      25.82
 C      -1.951028     0.647141     3.095643      50.00
 C      -3.445975     0.314445     2.499460      91.58
 H      -4.163403     0.959293     2.984102      25.47
 O      -3.733222    -1.037066     2.796201     262.10
 H      -4.773815    -1.168258     2.839668      21.95
 C      -3.573972     0.550990     0.935158      88.10
 H      -3.180209     1.444944     0.692853      25.97
 C      -5.092677     0.440499     0.417824     103.64
 O      -5.821727    -0.664259     0.575409     199.11
 H      -5.477317    -1.604728     0.389352      21.46
 H      -5.283069     0.882460    -0.537689      28.38
 H      -5.554943     1.301734     1.272383      23.88
 C       0.675859     0.563272    -0.562258      62.36
 H       1.255193     1.447704    -0.673485      28.80
 C       0.562056    -1.751591    -0.691375      72.24
 H       0.974454    -2.753673    -1.051206      26.66
 C      -0.731802    -1.724320    -0.224810      11.52
 O      -1.506314    -3.013332    -0.250871     174.62
 C      -1.354905    -3.964747    -1.269517     137.88
 H      -2.198924    -4.656536    -1.216223      27.64
 H      -1.065177    -3.701709    -2.256402      26.73
 H      -0.447919    -4.634135    -0.900344      25.12
 C      -1.492177    -0.524112     0.044036     -25.90
 O      -2.921861    -0.519846     0.160989      79.75
 C      -0.700476     0.678168    -0.121205      18.50
 H      -1.315030     1.672903    -0.001050      20.29
 C       1.363888    -0.652273    -0.839126      -0.08
 C       2.938263    -0.787178    -1.304197      84.55
 H       2.765259    -1.470047    -2.202525      21.32
 O       3.266867     0.320545    -2.150528     254.32
 H       3.775281     1.180404    -1.890258      22.43
 C       3.982380    -1.205617    -0.131041      87.17
 H       3.398671    -1.821232     0.558392      26.52
 O       5.062034    -1.928707    -0.652979     254.46
 H       5.285118    -1.791597    -1.598882      28.07
 C       4.416770     0.197628     0.570039      93.45
 O       4.821718     1.349257    -0.258533     325.78
 H       4.875744     2.060262     0.342846      30.30
 H       5.086516     0.091766     1.372066      26.94
 H       3.385621     0.380652     1.096369      26.69
55
name = lig-Water-frame_175
 C      -1.579860     1.982113     3.134456      81.61
 H      -2.363400     2.698723     3.166247      27.31
 C      -0.953796    -0.291803     3.418152      54.81
 H      -1.449996    -1.355907     3.494633      21.81
 C       0.254214    -0.005540     3.846867      18.21
 O       1.411516    -0.972998     3.991631     164.51
 C       1.099785    -2.389375     4.254586     136.22
 H       1.935521    -2.817794     3.836380      30.31
 H       0.376122    -2.494716     3.516056      30.36
 H       0.868878    -2.602103     5.298833      28.36
 C       0.598913     1.341340     4.032078       7.28
 O       1.946123     1.636027     4.570518     247.12
 H       2.180717     2.377661     3.982757      27.22
 C      -0.324338     2.369833     3.688872      67.31
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 H      -0.105292     3.426388     3.886310      18.56
 C      -1.956880     0.659083     3.095528      31.13
 C      -3.342265     0.322088     2.465411      86.15
 H      -4.128323     1.157493     3.017297      22.80
 O      -3.783291    -1.006652     2.821008     251.38
 H      -4.670766    -1.399857     2.831850      22.90
 C      -3.641998     0.582589     0.935303      64.22
 H      -3.090825     1.627261     0.638709      20.02
 C      -5.042813     0.452571     0.448966     114.79
 O      -5.870285    -0.721896     0.588649     242.03
 H      -5.263464    -1.500030     0.398869      25.06
 H      -5.198020     1.075489    -0.511335      26.09
 H      -5.537860     1.109826     1.030208      27.98
 C       0.672995     0.544111    -0.583195      68.83
 H       1.202273     1.546924    -0.648706      25.98
 C       0.584144    -1.729440    -0.702403      33.60
 H       0.892807    -2.715902    -0.871434      28.21
 C      -0.860043    -1.769976    -0.202796      -4.40
 O      -1.523438    -2.963967    -0.254177     128.24
 C      -1.327434    -3.979080    -1.322896     121.57
 H      -2.344426    -4.790958    -1.060935      22.20
 H      -1.304161    -3.448949    -2.388163      23.78
 H      -0.602453    -4.628250    -0.911090      25.68
 C      -1.552404    -0.506290     0.040915     -33.46
 O      -2.950625    -0.574192     0.178241      44.61
 C      -0.653375     0.701773    -0.171987      54.45
 H      -0.976643     1.656592     0.031393      25.31
 C       1.398209    -0.673128    -0.837702      25.20
 C       2.929270    -0.779392    -1.316089      78.67
 H       3.022615    -1.832094    -2.012664      20.97
 O       3.269367     0.305148    -2.178216     228.30
 H       4.022362     0.978796    -1.877546      21.25
 C       3.978107    -1.168570    -0.239756      73.99
 H       3.370166    -1.765694     0.700103      24.70
 O       5.092377    -1.937952    -0.662528     202.95
 H       5.179369    -2.038312    -1.749760      24.46
 C       4.351584     0.198031     0.570892      76.37
 O       4.790970     1.342475    -0.259656     259.52
 H       4.898214     2.265189     0.342582      23.59
 H       5.323571     0.002119     1.249784      22.93
 H       3.345846     0.440116     0.937353      27.07
55
name = lig-Water-frame_176
 C      -1.537038     1.967306     3.219257      73.96
 H      -2.461495     2.635420     3.164690      24.67
 C      -1.025952    -0.336341     3.366080      23.49
 H      -1.106978    -1.391642     3.397057      23.38
 C       0.318586     0.040475     3.896454      13.47
 O       1.369647    -0.952638     4.036138     129.45
 C       1.071117    -2.409083     4.188021      93.39
 H       2.030026    -3.050408     3.931021      25.86
 H      -0.001810    -2.814250     3.584406      24.10
 H       0.794973    -2.283373     5.331595      22.63
 C       0.615900     1.330100     4.010136      38.99
 O       1.956823     1.666199     4.582994     227.62
 H       2.198542     2.372629     3.935699      30.22
 C      -0.248490     2.387222     3.657107      40.01
 H       0.006917     3.579865     3.738425      17.52
 C      -1.962405     0.649892     3.055031      40.04
 C      -3.305105     0.357249     2.455436     117.38
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 H      -3.900033     1.119212     2.903846      29.47
 O      -3.800492    -1.004327     2.865228     193.81
 H      -4.798786    -1.193923     2.785005      19.67
 C      -3.627381     0.578175     0.934132      79.08
 H      -3.330863     1.506215     0.608174      24.27
 C      -5.039115     0.534807     0.473374      85.17
 O      -5.894675    -0.798091     0.601125     227.23
 H      -5.247042    -1.424535     0.237571      26.04
 H      -4.985231     0.848336    -0.565995      26.03
 H      -5.760000     1.289031     1.169466      23.01
 C       0.707451     0.571228    -0.601531      81.76
 H       1.180071     1.513609    -0.673551      27.45
 C       0.520826    -1.788731    -0.676891     -22.49
 H       0.988394    -2.849874    -0.762356      25.84
 C      -0.925454    -1.759030    -0.233412      14.26
 O      -1.571167    -2.923361    -0.249710     137.21
 C      -1.347826    -3.991887    -1.337419     121.34
 H      -2.264602    -4.515811    -1.222839      27.86
 H      -1.487454    -3.488580    -2.214260      28.11
 H      -0.347835    -4.691707    -1.212892      24.14
 C      -1.562654    -0.499916     0.005995      -3.78
 O      -2.950719    -0.606632     0.198828      34.83
 C      -0.645625     0.655723    -0.209199      32.10
 H      -0.756743     1.799541     0.091775      23.84
 C       1.447565    -0.639051    -0.839058     -14.78
 C       2.902307    -0.807050    -1.341013      91.68
 H       3.041605    -1.962280    -1.850414      19.50
 O       3.276927     0.293400    -2.219187     252.82
 H       3.986746     0.608311    -1.654256      22.92
 C       3.958488    -1.072187    -0.301489      86.76
 H       3.561062    -1.640898     0.526501      26.16
 O       5.117709    -1.964662    -0.676633     227.64
 H       5.204964    -1.955481    -1.600245      28.64
 C       4.322163     0.184706     0.555997      92.04
 O       4.767168     1.344227    -0.267647     295.41
 H       4.744890     2.128253     0.289544      28.32
 H       5.071791    -0.121860     1.180421      26.42
 H       3.389134     0.553533     1.113715      28.00
55
name = lig-Water-frame_177
 C      -1.522016     2.000883     3.313903      66.29
 H      -2.270880     2.816028     3.030524      18.07
 C      -1.033531    -0.394944     3.349766      46.14
 H      -1.048375    -1.489952     3.126308      26.79
 C       0.338266    -0.029789     3.906512       9.63
 O       1.323306    -0.915855     4.061772     177.00
 C       0.991429    -2.402435     4.151876     121.39
 H       1.870327    -3.062372     4.139335      27.78
 H       0.213405    -2.933561     3.776157      30.38
 H       0.797940    -2.475769     5.168607      28.10
 C       0.715638     1.406819     4.026105      24.64
 O       1.941048     1.700124     4.565949     199.71
 H       2.401649     2.464871     4.019425      25.76
 C      -0.207566     2.400141     3.619529      49.38
 H       0.070484     3.359287     3.655366      31.99
 C      -1.928986     0.603875     3.002365      25.95
 C      -3.322565     0.364606     2.447531      84.02
 H      -4.019425     1.293183     2.987529      23.44
 O      -3.808073    -0.994707     2.916679     193.38
 H      -4.774807    -0.773983     2.741731      21.52
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 C      -3.574274     0.509229     0.955731      74.49
 H      -3.288954     1.601073     0.498206      20.32
 C      -5.120184     0.598900     0.514801      79.51
 O      -5.877059    -0.833828     0.609722     195.23
 H      -5.392484    -1.573581     0.050847      23.35
 H      -4.982796     0.600522    -0.595874      23.63
 H      -5.701578     1.350721     1.019295      25.40
 C       0.765884     0.586072    -0.622524      57.63
 H       1.296527     1.578427    -0.746210      23.56
 C       0.467555    -1.844860    -0.630227      28.89
 H       0.947915    -2.764930    -0.708453      28.35
 C      -0.875373    -1.712706    -0.318542       7.72
 O      -1.648174    -2.929334    -0.244798     144.82
 C      -1.347217    -3.974035    -1.314844      96.54
 H      -2.453358    -4.664793    -1.262996      22.73
 H      -1.475601    -3.419471    -2.384564      26.73
 H      -0.435157    -4.433467    -1.490377      24.74
 C      -1.533272    -0.490663    -0.053372      14.92
 O      -2.934869    -0.600253     0.218993      43.07
 C      -0.659377     0.619229    -0.217266      52.39
 H      -0.933137     1.569111     0.087883      28.22
 C       1.417466    -0.645522    -0.833108     -67.28
 C       2.857126    -0.864273    -1.388382      94.27
 H       2.768298    -1.878478    -1.909978      21.30
 O       3.282163     0.256103    -2.255150     224.35
 H       4.003627     0.637962    -1.576638      18.26
 C       3.964572    -0.968441    -0.313584      74.06
 H       3.444225    -1.736465     0.536614      22.98
 O       5.114028    -1.971433    -0.664779     143.74
 H       5.473265    -1.737280    -1.715823      20.26
 C       4.292236     0.191355     0.517049      96.47
 O       4.748493     1.323875    -0.283219     271.85
 H       4.662505     2.166669     0.333274      24.44
 H       5.043479    -0.251569     1.368099      23.82
 H       3.551840     0.517112     1.309586      26.19
55
name = lig-Water-frame_178
 C      -1.532279     2.020410     3.355654      53.84
 H      -2.038469     2.906090     2.998590      20.81
 C      -0.948247    -0.456334     3.360398      52.37
 H      -1.244911    -1.405934     2.809002      28.05
 C       0.286016    -0.050585     3.873312       8.42
 O       1.296511    -0.928377     4.076624     164.51
 C       0.943929    -2.366312     4.195303      95.77
 H       1.916277    -2.895834     4.060805      26.79
 H       0.094524    -3.010326     3.403484      24.59
 H       0.679761    -2.747866     5.317790      24.36
 C       0.774976     1.431058     4.028920      19.48
 O       1.965349     1.746656     4.545630     210.83
 H       2.412428     2.469898     4.144282      30.14
 C      -0.186134     2.358502     3.600329      44.01
 H       0.194736     3.571500     3.618206      26.05
 C      -1.876385     0.610517     2.977301       3.00
 C      -3.353863     0.381792     2.484642     105.96
 H      -3.974780     1.105662     2.896356      27.70
 O      -3.817588    -0.936491     2.954905     232.36
 H      -4.789215    -0.860855     2.837144      24.28
 C      -3.546612     0.473934     0.956551      93.17
 H      -3.093987     1.364613     0.636608      22.69
 C      -5.161910     0.537369     0.512597      76.04
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 O      -5.848544    -0.829584     0.625721     251.55
 H      -5.501168    -1.534971     0.071925      26.25
 H      -5.192670     0.696291    -0.602063      24.61
 H      -5.787846     1.466625     0.968636      23.23
 C       0.796344     0.589459    -0.633828      72.00
 H       1.339555     1.501850    -0.807079      24.14
 C       0.494407    -1.828897    -0.596159      73.95
 H       0.887325    -2.897054    -0.706183      26.26
 C      -0.833508    -1.726461    -0.410309     -37.33
 O      -1.710425    -2.946054    -0.255269     133.57
 C      -1.440537    -3.899266    -1.329703     117.20
 H      -2.030470    -4.844909    -1.240802      26.13
 H      -1.489854    -3.435690    -2.249318      30.66
 H      -0.307487    -4.339244    -1.387583      23.97
 C      -1.492307    -0.484106    -0.122994     -32.78
 O      -2.895186    -0.573519     0.230852      82.00
 C      -0.652814     0.602640    -0.215179      60.28
 H      -1.281180     1.550449     0.088897      25.00
 C       1.322598    -0.693983    -0.822084      -4.77
 C       2.803055    -0.884787    -1.427602      74.43
 H       2.646433    -1.932584    -2.183800      22.81
 O       3.290123     0.197620    -2.278267     257.61
 H       3.812913     0.939815    -1.952833      24.46
 C       3.939602    -0.992355    -0.285454      87.14
 H       3.372749    -1.630316     0.390200      27.91
 O       5.092861    -1.935619    -0.680946     202.42
 H       5.664804    -1.616058    -1.372020      28.01
 C       4.313829     0.206172     0.547198     105.71
 O       4.734577     1.304938    -0.285531     280.11
 H       4.769150     2.207300     0.243643      25.21
 H       5.092748    -0.119413     1.130617      27.86
 H       3.460415     0.467447     1.203908      28.49
55
name = lig-Water-frame_179
 C      -1.530035     1.991443     3.334855      49.05
 H      -2.124871     2.957410     2.968541      20.29
 C      -0.914184    -0.454728     3.322449      50.42
 H      -1.203716    -1.325225     2.846962      30.61
 C       0.274129    -0.008842     3.838376      10.49
 O       1.275626    -0.983346     4.100627     178.99
 C       0.904448    -2.385896     4.251694     119.12
 H       1.944282    -2.678983     3.855215      26.01
 H       0.354918    -2.541483     3.384765      29.53
 H       0.531512    -2.663365     5.151269      29.39
 C       0.734537     1.380284     3.995627      19.46
 O       2.031861     1.775743     4.546529     164.72
 H       2.318758     2.622148     4.028137      27.74
 C      -0.140749     2.354707     3.612905      55.03
 H       0.067216     3.295105     3.601684      29.24
 C      -1.833342     0.672812     3.006035      -0.52
 C      -3.339093     0.358461     2.518527      99.48
 H      -4.122803     1.280481     2.983384      22.53
 O      -3.828806    -0.869459     2.986945     245.52
 H      -4.794335    -1.219793     2.988900      20.80
 C      -3.559749     0.462164     0.956340      81.16
 H      -2.983322     1.469732     0.717954      21.03
 C      -5.163790     0.424255     0.467353      96.58
 O      -5.831624    -0.785056     0.663529     246.62
 H      -5.350674    -1.458361     0.112552      25.27
 H      -5.297247     0.902095    -0.543112      25.57
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 H      -5.761170     1.216823     1.041767      24.72
 C       0.746281     0.571395    -0.623776      69.49
 H       1.371397     1.452918    -0.852493      24.07
 C       0.565504    -1.842924    -0.588384      48.71
 H       0.895721    -2.847342    -0.723121      26.05
 C      -0.884251    -1.786582    -0.461782     -40.78
 O      -1.742012    -2.940971    -0.280468     100.15
 C      -1.463707    -3.842797    -1.336678     112.44
 H      -1.990158    -5.011147    -1.164659      23.68
 H      -1.718545    -3.324800    -2.397581      26.75
 H      -0.503996    -4.125339    -1.093691      25.23
 C      -1.459824    -0.518496    -0.187887     -39.45
 O      -2.825855    -0.561678     0.223128      64.57
 C      -0.634132     0.655689    -0.205537      66.28
 H      -1.235118     1.534187    -0.052226      23.39
 C       1.271755    -0.723237    -0.831526      31.55
 C       2.774293    -0.875739    -1.445697      80.47
 H       2.790932    -1.671152    -2.219540      24.46
 O       3.270988     0.130417    -2.338439     294.15
 H       3.529934     1.026854    -2.036090      25.89
 C       3.896543    -1.098567    -0.292580      71.04
 H       3.316494    -1.784450     0.586478      24.94
 O       5.044919    -1.881997    -0.660753     232.98
 H       5.652658    -1.443024    -1.334007      28.32
 C       4.336413     0.226871     0.571885      74.32
 O       4.728963     1.309311    -0.298602     289.91
 H       4.893043     2.107641     0.225664      28.79
 H       5.355314    -0.037807     1.128505      23.43
 H       3.312088     0.473390     1.048033      25.45
55
name = lig-Water-frame_180
 C      -1.491063     2.000744     3.268027      55.91
 H      -2.251619     2.660622     3.077093      23.36
 C      -0.946906    -0.346213     3.252090      18.86
 H      -1.061781    -1.517623     3.045319      23.30
 C       0.345472    -0.007274     3.824069      13.26
 O       1.260512    -0.994960     4.149566     174.65
 C       0.925413    -2.384496     4.242588     107.64
 H       1.830629    -2.906135     4.025848      28.19
 H       0.235958    -2.343655     3.170380      27.35
 H       0.315710    -2.667050     5.244628      23.22
 C       0.713612     1.312785     3.973743      18.80
 O       2.088542     1.789845     4.529645     185.83
 H       2.136059     2.590776     3.911168      29.27
 C      -0.161777     2.323467     3.631352      57.64
 H       0.109757     3.553574     3.658833      22.01
 C      -1.847538     0.691730     3.054284       1.10
 C      -3.356865     0.383253     2.539894     122.80
 H      -3.864611     1.183687     2.888245      31.02
 O      -3.824626    -0.853698     3.027793     257.91
 H      -4.757753    -1.210956     3.015447      19.95
 C      -3.566696     0.490509     0.951965      68.88
 H      -3.293269     1.535099     0.733240      25.50
 C      -5.109069     0.364498     0.433716      98.06
 O      -5.816326    -0.766331     0.688520     205.36
 H      -5.230026    -1.511875     0.267201      24.64
 H      -5.251275     0.910457    -0.534731      26.54
 H      -5.669320     1.033820     1.268864      23.75
 C       0.662468     0.549986    -0.610721      73.06
 H       1.313089     1.416008    -0.834178      23.80
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 C       0.550081    -1.913451    -0.598536      23.64
 H       1.152983    -2.852160    -0.765535      24.40
 C      -0.925382    -1.837943    -0.470176       3.69
 O      -1.770493    -2.902678    -0.300075     162.57
 C      -1.490659    -3.835689    -1.362327     121.78
 H      -2.099726    -4.742171    -1.104064      28.26
 H      -1.818915    -3.498643    -2.286876      30.02
 H      -0.332436    -4.018894    -1.179447      23.51
 C      -1.437478    -0.549632    -0.222812      -4.02
 O      -2.752625    -0.567215     0.199462      33.68
 C      -0.620881     0.695472    -0.212965      65.84
 H      -1.015773     1.748654    -0.119221      22.94
 C       1.309486    -0.701588    -0.868630       4.61
 C       2.774562    -0.838478    -1.413035      65.90
 H       2.843567    -1.876044    -2.203269      20.04
 O       3.238111     0.082189    -2.423468     292.34
 H       3.242758     0.929028    -1.821226      24.66
 C       3.838674    -1.206506    -0.267283      81.89
 H       3.486470    -1.795101     0.586282      25.94
 O       4.996021    -1.836784    -0.630918     244.42
 H       5.369146    -1.317038    -1.480857      26.12
 C       4.348744     0.212810     0.560742      83.23
 O       4.723683     1.321363    -0.334965     310.38
 H       4.978044     2.114117     0.380962      24.83
 H       5.114780    -0.006604     1.270675      26.39
 H       3.499049     0.525665     1.136177      28.27
55
name = lig-Water-frame_181
 C      -1.442803     2.026153     3.191709      52.20
 H      -2.448756     2.700265     3.207699      23.60
 C      -0.934657    -0.264110     3.206475      51.83
 H      -1.131188    -1.253827     3.289851      25.42
 C       0.395957    -0.060435     3.799943      20.56
 O       1.282314    -0.977584     4.224094     211.76
 C       0.894992    -2.369120     4.176505     131.26
 H       1.702955    -3.228413     4.355751      26.69
 H       0.287309    -2.737166     3.425314      30.50
 H       0.303896    -2.605237     4.988595      29.07
 C       0.772797     1.297951     3.985196      -0.13
 O       2.090873     1.779920     4.477838     234.13
 H       2.256360     2.564619     3.931903      28.55
 C      -0.211934     2.353003     3.647029      50.80
 H       0.136412     3.273186     3.809795      24.48
 C      -1.924198     0.652068     3.070130      36.03
 C      -3.348022     0.402583     2.515302      75.91
 H      -3.960809     1.457331     2.999911      24.40
 O      -3.803369    -0.878402     3.060565     188.19
 H      -4.787106    -0.842369     2.954761      24.87
 C      -3.570647     0.505190     0.940554      65.11
 H      -3.461577     1.604922     0.595729      25.69
 C      -5.017529     0.407289     0.465759     101.46
 O      -5.795167    -0.823260     0.689508     152.05
 H      -5.354224    -1.629062     0.437782      26.76
 H      -5.171338     0.739478    -0.558674      27.68
 H      -5.410504     1.077837     1.309673      25.46
 C       0.661972     0.523531    -0.629551      53.90
 H       1.173558     1.470581    -0.747666      23.83
 C       0.517984    -1.966329    -0.644719      41.55
 H       1.221344    -2.800521    -0.763235      25.69
 C      -0.879810    -1.840726    -0.451753      17.91
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 O      -1.801659    -2.864433    -0.319368     158.02
 C      -1.481899    -3.855847    -1.353678     108.24
 H      -2.266263    -4.820920    -1.031405      24.11
 H      -1.862308    -3.513408    -2.451789      26.88
 H      -0.484482    -4.095866    -1.639525      25.45
 C      -1.420373    -0.514720    -0.215169       5.01
 O      -2.715903    -0.566164     0.179099       7.54
 C      -0.667403     0.693048    -0.229343      70.17
 H      -0.849284     1.801944    -0.078738      24.50
 C       1.333532    -0.698180    -0.896251      -6.34
 C       2.778749    -0.893822    -1.401706      83.44
 H       2.711447    -1.928042    -1.726889      22.88
 O       3.196456     0.062828    -2.463910     311.02
 H       3.235290     0.839590    -1.915275      28.78
 C       3.799035    -1.194611    -0.203924      72.46
 H       3.317712    -1.928661     0.674228      23.27
 O       4.972833    -1.810284    -0.643072     270.17
 H       5.144970    -1.523008    -1.516248      29.08
 C       4.312188     0.177219     0.526835      80.40
 O       4.725725     1.333897    -0.353233     319.20
 H       4.862422     2.068214     0.213133      30.70
 H       5.062462    -0.133834     1.376598      25.03
 H       3.574238     0.651562     1.328260      24.75
55
name = lig-Water-frame_182
 C      -1.508790     2.040967     3.125024      64.58
 H      -2.111246     2.863605     3.232957      28.29
 C      -0.870073    -0.249519     3.219347      55.84
 H      -1.393258    -1.324101     3.335693      25.53
 C       0.414515    -0.046721     3.765578      20.71
 O       1.328620    -0.994578     4.289747     172.95
 C       0.865086    -2.396370     4.142952     110.08
 H       1.649253    -2.967215     4.504862      29.65
 H       0.337416    -3.114954     3.263151      26.50
 H       0.081597    -2.471980     5.060474      25.44
 C       0.839414     1.340928     3.985168       0.43
 O       2.057144     1.742477     4.408211     222.98
 H       2.464080     2.619535     3.984930      24.94
 C      -0.204164     2.328927     3.680373      61.06
 H       0.182063     3.446974     3.998604      20.85
 C      -1.979335     0.673442     3.041730      37.17
 C      -3.330258     0.456344     2.503410      91.78
 H      -3.946078     1.163059     2.882486      31.45
 O      -3.794570    -0.891817     3.048858     169.84
 H      -4.773302    -0.636628     2.985060      25.11
 C      -3.534571     0.503341     0.917368      78.57
 H      -3.258074     1.531432     0.491365      25.95
 C      -4.934562     0.428128     0.531759      92.26
 O      -5.779194    -0.885391     0.696580      69.10
 H      -5.279430    -1.738985     0.371526      24.11
 H      -5.100519     0.640794    -0.584071      25.86
 H      -5.428665     1.324414     1.154774      25.05
 C       0.715941     0.505507    -0.666961      53.27
 H       1.190221     1.520821    -0.693367      24.51
 C       0.525680    -1.944735    -0.719316      35.95
 H       0.976573    -2.947990    -0.761723      25.33
 C      -0.797420    -1.790207    -0.414389     -16.19
 O      -1.794633    -2.851193    -0.356199     137.08
 C      -1.538014    -3.899613    -1.387360     124.83
 H      -2.092788    -4.842374    -1.044564      26.17
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 H      -1.963250    -3.485316    -2.263901      28.75
 H      -0.522177    -4.277564    -1.739314      24.21
 C      -1.412901    -0.452668    -0.173222      -9.11
 O      -2.736538    -0.551042     0.174398      49.62
 C      -0.692828     0.666907    -0.259190     105.48
 H      -1.043303     1.620471     0.046451      31.81
 C       1.302894    -0.727336    -0.900615       4.31
 C       2.759189    -0.966303    -1.355981      79.18
 H       2.677416    -2.172383    -1.788647      19.73
 O       3.155563     0.020356    -2.461171     244.33
 H       3.454831     0.921540    -2.084250      24.18
 C       3.773320    -1.090813    -0.117776      81.39
 H       3.143336    -1.801421     0.460625      26.35
 O       4.958584    -1.813574    -0.662547     221.57
 H       5.127817    -1.762712    -1.722224      24.20
 C       4.250372     0.160903     0.556254      95.25
 O       4.718602     1.299975    -0.374950     278.45
 H       4.722879     2.230157     0.212435      26.28
 H       5.163173    -0.242074     1.036581      24.03
 H       3.537361     0.600394     1.166411      28.41
55
name = lig-Water-frame_183
 C      -1.549392     2.054665     3.116070      93.17
 H      -2.024469     3.142588     3.070258      23.84
 C      -0.869714    -0.301785     3.266957      52.85
 H      -1.282335    -1.268255     3.218490      29.18
 C       0.447723     0.016653     3.752983      13.11
 O       1.354120    -1.025115     4.303279     140.71
 C       0.797596    -2.458387     4.179000     106.20
 H       1.843824    -2.792466     4.626404      25.54
 H       0.656129    -2.727457     3.180608      31.88
 H      -0.019600    -2.397206     4.831301      27.39
 C       0.826172     1.403276     3.934080      15.94
 O       2.060093     1.700111     4.346794     249.50
 H       2.308386     2.588135     4.033371      28.38
 C      -0.156355     2.304762     3.718247      78.31
 H      -0.071092     3.337061     3.991941      21.35
 C      -1.925155     0.759316     2.995013      34.19
 C      -3.285804     0.446800     2.470598      79.30
 H      -4.231008     1.204763     2.912725      22.74
 O      -3.800045    -0.873850     2.995540     184.54
 H      -4.768365    -0.898813     3.136596      23.79
 C      -3.429320     0.486658     0.902614      96.85
 H      -2.985492     1.441795     0.552708      24.19
 C      -4.927380     0.412793     0.566787     103.30
 O      -5.746201    -0.927367     0.718601     170.80
 H      -5.109028    -1.521096     0.216296      27.58
 H      -4.965547     0.601242    -0.469208      26.57
 H      -5.594184     1.314610     0.786441      24.45
 C       0.740664     0.528893    -0.688263      86.58
 H       1.397645     1.373071    -0.754702      28.26
 C       0.539957    -1.904448    -0.791287      59.73
 H       0.707724    -3.003572    -0.857484      27.86
 C      -0.784985    -1.722036    -0.370101     -11.13
 O      -1.727503    -2.850988    -0.400338     107.71
 C      -1.594218    -3.933038    -1.427401     123.88
 H      -2.141703    -5.029412    -1.000055      22.72
 H      -2.198144    -3.472632    -2.330499      25.48
 H      -0.551463    -4.275816    -1.473863      23.23
 C      -1.430264    -0.468359    -0.115867     -12.71
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 O      -2.791450    -0.532268     0.183277     105.81
 C      -0.637408     0.662334    -0.299777      89.04
 H      -1.288683     1.528225     0.163801      27.51
 C       1.284054    -0.773963    -0.908133      28.15
 C       2.728717    -1.020621    -1.311980      92.28
 H       2.887497    -1.875291    -1.986127      21.26
 O       3.114888    -0.045379    -2.431298     238.00
 H       3.763975     0.686632    -2.124160      24.91
 C       3.749529    -0.996066    -0.155301      77.96
 H       3.122111    -1.703877     0.614348      25.85
 O       4.941794    -1.830675    -0.675000     189.18
 H       5.086914    -1.823885    -1.654702      24.42
 C       4.230569     0.176786     0.575249      90.33
 O       4.692772     1.258851    -0.383922     286.21
 H       4.637068     2.066045     0.158149      29.17
 H       5.222460    -0.183363     0.936238      24.48
 H       3.320878     0.567717     1.248159      25.66
55
name = lig-Water-frame_184
 C      -1.492177     2.137137     3.174794      43.47
 H      -2.124044     2.918023     2.775926      19.61
 C      -0.890678    -0.304173     3.321489      37.72
 H      -1.108425    -1.420616     3.127331      26.17
 C       0.460578     0.027887     3.758736      25.57
 O       1.344696    -1.016484     4.274706     160.03
 C       0.801538    -2.464267     4.237314      87.55
 H       1.633872    -3.000183     4.684273      27.73
 H       0.920707    -2.382502     3.041080      27.60
 H      -0.257608    -2.605317     4.721553      27.38
 C       0.786468     1.405669     3.868417      33.61
 O       2.101908     1.666231     4.300789     188.31
 H       2.158303     2.630332     4.025913      30.89
 C      -0.205265     2.324474     3.711866      32.10
 H      -0.082178     3.416050     3.992286      25.95
 C      -1.826630     0.796854     2.951341      29.66
 C      -3.303565     0.424834     2.453173     109.77
 H      -3.883143     1.161548     2.714924      32.53
 O      -3.792768    -0.863399     2.937852     218.29
 H      -4.719248    -1.084372     3.146869      21.83
 C      -3.352956     0.483791     0.935886      83.89
 H      -2.890175     1.539403     0.664521      21.62
 C      -4.968329     0.387125     0.535848      85.55
 O      -5.676086    -0.923518     0.743900     181.26
 H      -5.120389    -1.502159     0.183455      28.22
 H      -4.822888     0.464826    -0.624973      24.34
 H      -5.679005     1.180251     0.850356      24.73
 C       0.749233     0.547494    -0.696410      57.94
 H       1.569200     1.293373    -0.856130      25.36
 C       0.478380    -1.895249    -0.830674      66.56
 H       0.823768    -2.883811    -1.081587      29.42
 C      -0.840359    -1.704537    -0.356726      28.77
 O      -1.644867    -2.857254    -0.432261     208.69
 C      -1.661494    -3.956346    -1.439426     128.07
 H      -2.211129    -4.815175    -0.956307      27.74
 H      -2.136499    -3.734726    -2.413680      28.85
 H      -0.601814    -4.184869    -1.487568      26.30
 C      -1.436884    -0.527470    -0.066548       0.34
 O      -2.828442    -0.539893     0.183822     116.66
 C      -0.590594     0.677198    -0.306405      66.00
 H      -1.002994     1.573857    -0.022784      26.70
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 C       1.308639    -0.790193    -0.930481     -13.30
 C       2.720670    -0.986927    -1.310758      99.89
 H       2.937307    -2.012090    -1.975875      21.30
 O       3.088620    -0.103359    -2.393153     285.11
 H       3.867757     0.289117    -2.043335      27.53
 C       3.720746    -1.014285    -0.244876      95.30
 H       3.484252    -1.481394     0.747374      26.99
 O       4.910285    -1.845153    -0.655790     179.56
 H       5.068621    -1.700589    -1.613257      25.08
 C       4.224451     0.235030     0.572638     103.95
 O       4.645336     1.210141    -0.388021     267.74
 H       4.706815     2.073415     0.143000      26.00
 H       5.110833    -0.071052     1.266046      26.64
 H       3.519737     0.491044     1.283220      30.02
55
name = lig-Water-frame_185
 C      -1.442840     2.171351     3.213615      63.94
 H      -2.211031     2.810986     2.720711      20.83
 C      -0.903471    -0.266302     3.363902      55.48
 H      -1.028122    -1.343754     3.067787      25.80
 C       0.425272    -0.024463     3.776752      30.70
 O       1.313523    -0.971133     4.251892     207.65
 C       0.822249    -2.407106     4.239713     107.49
 H       1.409688    -3.175257     4.754022      27.36
 H       0.890938    -2.666728     3.231210      33.24
 H      -0.185205    -2.787736     4.452743      29.97
 C       0.780750     1.343115     3.830521      16.65
 O       2.131573     1.654968     4.250508     180.34
 H       2.273180     2.663668     4.019925      25.89
 C      -0.263418     2.439277     3.699657      40.29
 H       0.201458     3.467659     3.969996      22.97
 C      -1.745338     0.747673     2.931084      31.78
 C      -3.269472     0.380941     2.438977      86.44
 H      -3.839511     1.514713     2.771655      27.96
 O      -3.760451    -0.870658     2.900929     186.74
 H      -4.780496    -0.939665     2.955443      22.19
 C      -3.374111     0.520895     0.985149      93.25
 H      -3.036922     1.476047     0.709045      25.24
 C      -4.983706     0.355356     0.439314      83.31
 O      -5.587989    -0.889264     0.771625     124.73
 H      -5.227326    -1.755473     0.282949      24.20
 H      -4.902536     0.415294    -0.587055      26.91
 H      -5.659149     1.100251     1.093534      24.04
 C       0.788134     0.519551    -0.708305      73.59
 H       1.413926     1.393927    -0.891145      25.60
 C       0.415980    -1.875000    -0.854715      58.12
 H       0.968603    -2.757519    -1.275416      25.24
 C      -0.887524    -1.783028    -0.407829      33.32
 O      -1.612679    -2.877837    -0.443587     225.45
 C      -1.679138    -3.943160    -1.427863     109.43
 H      -2.382596    -4.814786    -0.798601      24.71
 H      -2.089777    -3.798549    -2.515288      26.98
 H      -0.633558    -4.314188    -1.757264      26.09
 C      -1.431714    -0.517149    -0.029291     -52.00
 O      -2.819552    -0.570918     0.169774     100.74
 C      -0.563084     0.663936    -0.288105       7.68
 H      -0.726053     1.854613    -0.231387      22.31
 C       1.303572    -0.774295    -0.946362       3.74
 C       2.713296    -0.993088    -1.378059     112.06
 H       2.660550    -2.128700    -1.463005      26.91
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 O       3.077552    -0.135229    -2.362259     267.48
 H       4.028205     0.136415    -2.109941      26.47
 C       3.775440    -1.059832    -0.240080      89.09
 H       3.460445    -1.646993     0.690067      27.68
 O       4.868461    -1.854342    -0.633807     192.23
 H       5.224337    -1.577753    -1.614555      23.75
 C       4.241874     0.262603     0.549138     105.76
 O       4.595330     1.197441    -0.385361     228.60
 H       4.926800     2.124010     0.032479      23.04
 H       4.948586    -0.028558     1.353512      27.77
 H       3.419894     0.677878     1.329613      27.05
55
name = lig-Water-frame_186
 C      -1.484825     2.120600     3.185015      57.85
 H      -2.265384     2.966537     2.941590      25.65
 C      -0.899858    -0.257484     3.374908      79.57
 H      -1.214088    -1.239998     3.110363      29.37
 C       0.382798    -0.044175     3.813690      32.98
 O       1.272647    -0.951087     4.245491     209.39
 C       0.847762    -2.357056     4.189355     101.68
 H       1.455773    -3.000014     5.015792      25.02
 H       0.929729    -3.051562     3.174582      27.88
 H      -0.248510    -2.525969     4.419540      27.52
 C       0.775761     1.318414     3.823485      -6.23
 O       2.137011     1.653913     4.197062     199.37
 H       2.410633     2.493717     3.885857      25.02
 C      -0.161473     2.543559     3.715885      24.65
 H       0.262816     3.486426     3.870731      18.81
 C      -1.727059     0.705817     2.935771      50.96
 C      -3.195017     0.416291     2.459196     100.03
 H      -3.738292     1.123992     2.871208      29.66
 O      -3.734278    -0.877909     2.893869     210.80
 H      -4.655139    -0.693999     2.676517      26.39
 C      -3.489895     0.524793     0.971391      69.84
 H      -3.099714     1.600980     0.547193      22.43
 C      -4.954458     0.337095     0.399688     104.76
 O      -5.520718    -0.883617     0.806595     167.02
 H      -5.155829    -1.696337     0.442572      23.84
 H      -5.089888     0.593286    -0.758271      25.04
 H      -5.492076     1.054807     0.939446      27.21
 C       0.810161     0.483185    -0.713359      84.49
 H       1.224525     1.483192    -0.883508      27.29
 C       0.422873    -1.842190    -0.896056      65.08
 H       0.804978    -2.766709    -1.311478      25.89
 C      -0.885238    -1.829877    -0.490078     -20.19
 O      -1.653342    -2.940073    -0.441564     213.17
 C      -1.665251    -3.960275    -1.430906     130.68
 H      -2.344431    -4.697548    -0.879476      26.85
 H      -2.222041    -3.560600    -2.327890      29.10
 H      -0.811306    -4.508322    -1.724253      27.84
 C      -1.409811    -0.476252    -0.028191     -77.33
 O      -2.778405    -0.585495     0.166209      83.28
 C      -0.541828     0.663215    -0.263351      69.48
 H      -0.796109     1.666891    -0.286719      29.10
 C       1.273468    -0.740765    -0.954625      62.28
 C       2.683706    -1.056765    -1.359493      82.79
 H       2.580234    -2.290862    -1.508509      24.83
 O       3.097218    -0.144529    -2.370547     232.86
 H       4.056335     0.116208    -2.397918      27.64
 C       3.828530    -1.084105    -0.139296      91.17
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 H       3.132180    -1.851830     0.415247      27.91
 O       4.864833    -1.869922    -0.643222     239.63
 H       5.322534    -1.645005    -1.413253      29.65
 C       4.198440     0.252884     0.570097     111.36
 O       4.582290     1.239731    -0.414307     266.03
 H       4.939021     1.961802     0.040527      29.80
 H       5.097382    -0.033915     1.278617      27.57
 H       3.351447     0.714832     0.965854      29.53
55
name = lig-Water-frame_187
 C      -1.483873     2.094844     3.169720      49.91
 H      -2.190244     2.876113     3.175826      26.19
 C      -0.899876    -0.309724     3.357555      52.48
 H      -1.480706    -1.347321     3.262246      26.08
 C       0.356384    -0.001141     3.855141      19.32
 O       1.249685    -0.968812     4.236561     179.96
 C       0.859223    -2.359162     4.148643     121.04
 H       1.418222    -2.546422     5.026559      27.83
 H       1.139119    -2.934015     3.320939      30.46
 H      -0.175801    -2.096036     4.489367      27.06
 C       0.778166     1.401564     3.846098      14.22
 O       2.131448     1.626181     4.151498     208.48
 H       2.423233     2.443410     3.537876      23.31
 C      -0.064510     2.501462     3.694049      43.26
 H       0.227923     3.684895     3.758461      19.69
 C      -1.782188     0.753525     2.944476      47.70
 C      -3.106141     0.429553     2.468703      79.09
 H      -3.931594     1.095205     3.207775      21.84
 O      -3.700697    -0.871987     2.903132     188.23
 H      -4.604891    -0.782338     2.512297      24.52
 C      -3.573764     0.532879     0.868987      90.70
 H      -3.215413     1.369247     0.527979      27.01
 C      -4.900711     0.342013     0.375323     113.78
 O      -5.490392    -0.889709     0.851636     202.11
 H      -4.860697    -1.638524     0.423675      20.35
 H      -5.106294     0.631263    -0.613093      26.70
 H      -5.567847     1.288248     0.828405      24.44
 C       0.769265     0.523251    -0.692188      77.84
 H       1.342599     1.456846    -0.907407      25.13
 C       0.437580    -1.849407    -0.953139      61.49
 H       0.687226    -2.870486    -1.277611      23.93
 C      -0.871889    -1.791299    -0.551215     -56.54
 O      -1.713176    -2.998935    -0.414877     156.20
 C      -1.679400    -3.969352    -1.454490     116.16
 H      -2.467742    -4.913034    -0.940804      23.24
 H      -2.274019    -3.424676    -2.246044      26.92
 H      -0.725613    -4.640164    -1.609426      22.86
 C      -1.371206    -0.485369    -0.080720     -64.19
 O      -2.732309    -0.568530     0.184307      90.13
 C      -0.541927     0.625050    -0.241921      90.76
 H      -1.133288     1.643691    -0.128970      27.18
 C       1.290618    -0.745683    -0.980588      45.50
 C       2.692661    -1.127927    -1.289782      85.52
 H       2.812875    -2.028553    -1.944216      23.04
 O       3.109998    -0.152537    -2.415047     252.60
 H       4.033391    -0.028068    -2.519522      30.83
 C       3.787364    -1.121545    -0.075227      90.59
 H       3.186488    -1.785135     0.516635      28.62
 O       4.895244    -1.914927    -0.626645     218.17
 H       5.376185    -1.576790    -1.514447      26.03
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 C       4.160459     0.211996     0.576575      93.14
 O       4.591010     1.279016    -0.470673     237.62
 H       4.920659     2.039993     0.245909      24.90
 H       5.018192     0.097540     1.190363      27.10
 H       3.133028     0.621090     0.972901      26.65
55
name = lig-Water-frame_188
 C      -1.385285     2.103447     3.192950      61.19
 H      -2.303080     2.900443     3.309781      24.23
 C      -0.949287    -0.356976     3.322743      43.54
 H      -1.336295    -1.276083     3.423509      25.75
 C       0.329103     0.049675     3.874789     -10.92
 O       1.265596    -0.938190     4.204962     151.87
 C       0.849989    -2.320557     4.178239     114.98
 H       1.450275    -2.612545     5.220188      24.65
 H       1.275029    -2.828169     3.194859      27.05
 H      -0.213509    -2.361643     4.418945      27.97
 C       0.803187     1.478925     3.894235      20.97
 O       2.142361     1.612911     4.097282     291.14
 H       2.375431     2.261139     3.377564      25.31
 C      -0.068538     2.434373     3.618950      72.34
 H       0.152619     3.385707     3.677202      29.85
 C      -1.806620     0.801878     2.972021       1.58
 C      -3.180922     0.448511     2.487785      96.77
 H      -3.712377     1.124333     2.954201      31.76
 O      -3.645796    -0.867001     2.917863     203.05
 H      -4.537916    -1.117735     2.500680      24.77
 C      -3.518076     0.521783     0.798314      80.76
 H      -3.122992     1.581134     0.371517      25.95
 C      -4.939098     0.391077     0.399183     111.24
 O      -5.464129    -0.897727     0.879544     172.21
 H      -4.867354    -1.587980     0.475469      24.99
 H      -4.963275     0.447282    -0.778085      27.41
 H      -5.474465     1.149653     0.791370      30.19
 C       0.745973     0.584951    -0.674110      42.39
 H       1.475382     1.345220    -0.858424      23.98
 C       0.436187    -1.902201    -1.016899      51.59
 H       0.832917    -2.922751    -1.227035      25.65
 C      -0.893099    -1.749881    -0.581396      -1.22
 O      -1.750689    -3.013610    -0.365560     144.15
 C      -1.733775    -4.022122    -1.454751     128.13
 H      -2.403801    -4.855040    -1.284615      28.68
 H      -2.064393    -3.568488    -2.490175      27.43
 H      -0.762718    -4.372891    -1.595989      26.96
 C      -1.353564    -0.559199    -0.162749      41.63
 O      -2.701199    -0.540701     0.209918     108.55
 C      -0.592520     0.623095    -0.220788      73.81
 H      -1.191928     1.464625     0.104332      28.35
 C       1.315710    -0.774870    -1.007677     -17.28
 C       2.765374    -1.124809    -1.275188      81.36
 H       2.926323    -2.018808    -1.982374      20.99
 O       3.106638    -0.158239    -2.457648     186.11
 H       4.120523    -0.223475    -2.519676      28.24
 C       3.723887    -1.180572    -0.093646      78.34
 H       3.493904    -1.742369     1.000026      23.84
 O       4.941318    -1.964718    -0.591241     179.15
 H       5.148115    -1.561924    -1.495202      25.92
 C       4.090805     0.195678     0.527008      88.29
 O       4.605847     1.309342    -0.487941     262.74
 H       4.748479     2.083416     0.097708      27.31
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 H       4.932636     0.195069     1.392100      25.50
 H       3.251915     0.439151     1.158812      29.53
55
name = lig-Water-frame_189
 C      -1.349246     2.129542     3.224515      79.81
 H      -2.042294     2.827858     3.229199      29.21
 C      -0.971644    -0.292134     3.309634      54.03
 H      -1.239638    -1.453463     3.458009      23.12
 C       0.294324     0.081493     3.863024       4.60
 O       1.286510    -0.865980     4.168455     153.09
 C       0.869078    -2.289227     4.260441     141.64
 H       1.304981    -2.902788     4.983008      29.86
 H       1.218956    -2.677951     3.290283      29.30
 H      -0.171376    -2.840497     4.212436      26.93
 C       0.820379     1.413640     3.946124      36.32
 O       2.181203     1.616103     4.041437     208.17
 H       2.500355     2.271669     3.412871      29.45
 C      -0.121915     2.399858     3.529645      60.25
 H       0.250125     3.563558     3.662018      25.12
 C      -1.803795     0.771347     3.005892       0.08
 C      -3.302084     0.457575     2.450521      85.07
 H      -3.988236     1.528249     2.788457      25.89
 O      -3.579442    -0.868628     2.945263     177.98
 H      -4.393016    -1.218534     2.556606      25.14
 C      -3.354336     0.547293     0.786172      98.63
 H      -3.037092     1.477764     0.404335      28.74
 C      -4.972545     0.393302     0.386228      82.32
 O      -5.453461    -0.885320     0.906146     172.42
 H      -5.037789    -1.699605     0.434157      25.83
 H      -4.878288     0.206500    -0.666413      28.58
 H      -5.649162     1.286557     0.947826      24.64
 C       0.751381     0.570523    -0.668341      19.89
 H       1.493338     1.447784    -0.695992      24.25
 C       0.445591    -1.946241    -1.066024      53.01
 H       0.956585    -2.875738    -1.201283      25.64
 C      -0.912513    -1.833335    -0.623650       1.79
 O      -1.780061    -2.994513    -0.328138     130.30
 C      -1.760811    -4.024225    -1.493130      90.98
 H      -2.586521    -5.031735    -1.301478      23.55
 H      -1.888569    -3.699998    -2.549607      25.62
 H      -0.618895    -4.257544    -1.603052      22.68
 C      -1.395845    -0.582336    -0.224372      46.55
 O      -2.694120    -0.533906     0.228026     134.26
 C      -0.623778     0.624769    -0.207963      46.79
 H      -1.061628     1.540177     0.254937      26.63
 C       1.295467    -0.800545    -1.020886     -32.19
 C       2.816393    -1.091517    -1.329356      84.65
 H       2.800536    -2.270077    -1.599810      22.55
 O       3.126520    -0.170110    -2.471231     221.25
 H       4.115779    -0.270761    -2.607006      27.89
 C       3.737219    -1.233979    -0.084705      88.38
 H       3.605078    -1.664258     0.819703      27.53
 O       4.960375    -1.998056    -0.537315     204.03
 H       5.147110    -1.761997    -1.445981      29.01
 C       4.070927     0.215630     0.479515      96.07
 O       4.590318     1.299860    -0.476968     277.40
 H       4.679582     2.221408     0.006277      25.64
 H       4.746401     0.058499     1.240880      28.83
 H       3.183815     0.525353     1.168818      28.39
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name = lig-Water-frame_190
 C      -1.424248     2.089365     3.217737      41.90
 H      -2.099401     3.138210     2.989486      22.75
 C      -0.960136    -0.229409     3.343961      83.92
 H      -1.184215    -1.220811     3.229006      30.09
 C       0.295394     0.089034     3.847467      33.07
 O       1.283085    -0.820803     4.156337     184.28
 C       0.883681    -2.287082     4.292518     119.68
 H       1.471406    -3.066607     5.030584      25.12
 H       1.306309    -2.677066     3.282541      26.75
 H      -0.079604    -2.686612     4.123058      27.02
 C       0.795744     1.334180     3.942553      23.94
 O       2.232558     1.614408     4.000209      95.93
 H       2.506448     2.539960     3.510153      27.29
 C      -0.042792     2.435751     3.500891      60.77
 H       0.229216     3.414955     3.582035      29.31
 C      -1.864615     0.746134     3.026653      13.88
 C      -3.371506     0.529811     2.400153     101.77
 H      -4.092799     1.163890     2.592480      29.96
 O      -3.524698    -0.855732     2.980097     177.98
 H      -4.390600    -1.146205     2.562681      23.86
 C      -3.257636     0.568617     0.845382      93.92
 H      -2.797841     1.511097     0.469107      25.34
 C      -4.948430     0.373741     0.400678      93.52
 O      -5.460655    -0.870098     0.946253     171.92
 H      -5.264603    -1.658974     0.300063      25.11
 H      -5.029874     0.305503    -0.722973      28.09
 H      -5.548713     1.092631     0.714145      29.05
 C       0.760503     0.491504    -0.660050      59.07
 H       1.275928     1.399202    -0.517452      26.45
 C       0.446489    -1.961366    -1.084723      52.50
 H       0.985632    -2.946365    -1.255352      24.46
 C      -0.924631    -1.960526    -0.664391     -30.11
 O      -1.807762    -2.971929    -0.337671     163.41
 C      -1.743387    -4.034262    -1.522923      92.68
 H      -2.421556    -4.824785    -1.177771      25.28
 H      -1.999564    -3.524953    -2.558600      24.61
 H      -0.785924    -4.458858    -1.434533      24.30
 C      -1.448204    -0.554162    -0.268623     -14.47
 O      -2.701798    -0.569239     0.233127     126.29
 C      -0.603291     0.609333    -0.221094      44.52
 H      -0.813919     1.614578     0.305322      24.88
 C       1.266875    -0.789604    -1.030095      19.82
 C       2.785579    -1.095305    -1.379320      83.83
 H       2.714637    -2.232221    -1.555946      23.79
 O       3.170429    -0.210985    -2.456254     270.91
 H       4.070840    -0.187780    -2.721110      29.38
 C       3.826747    -1.194110    -0.129212      59.93
 H       3.205905    -1.922195     0.772580      23.96
 O       4.960478    -2.020954    -0.465287     200.81
 H       5.349527    -2.039091    -1.490801      24.86
 C       4.064052     0.261503     0.445027      92.82
 O       4.554084     1.261816    -0.451913     265.83
 H       4.655443     2.188417     0.047549      25.75
 H       4.943517    -0.112322     1.211433      23.66
 H       3.121271     0.679373     0.804543      26.47
55
name = lig-Water-frame_191
 C      -1.498198     2.111830     3.187379      48.40
 H      -2.000997     2.862793     2.823540      23.51
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 C      -0.954386    -0.185397     3.383177      58.24
 H      -1.225360    -1.244440     2.991497      29.07
 C       0.326226     0.043179     3.844061      27.37
 O       1.272222    -0.837817     4.174291     188.89
 C       0.952909    -2.315372     4.260145     103.86
 H       1.485743    -2.572553     5.114674      27.93
 H       1.444467    -2.719900     3.333557      27.95
 H      -0.238952    -2.247561     4.276154      22.78
 C       0.805436     1.396141     3.877787      22.17
 O       2.262104     1.620596     3.965005     124.02
 H       2.242898     2.538711     3.737245      29.81
 C      -0.000881     2.409469     3.502182      86.61
 H       0.342024     3.553638     3.506918      27.95
 C      -1.984191     0.814919     3.037030      20.37
 C      -3.299865     0.533354     2.373332     105.98
 H      -4.408438     1.100301     2.759161      21.94
 O      -3.512394    -0.830416     2.998650     178.03
 H      -4.395930    -1.097742     2.617583      25.12
 C      -3.277547     0.574502     0.899206      84.87
 H      -2.605562     1.485120     0.581922      22.33
 C      -4.849986     0.331976     0.384559      89.51
 O      -5.483681    -0.854575     0.983949     193.87
 H      -5.293543    -1.511837     0.322067      28.77
 H      -5.109092     0.502581    -0.702658      26.59
 H      -5.612360     1.280309     0.720338      25.14
 C       0.743345     0.388132    -0.639955      80.23
 H       1.327291     1.344775    -0.450250      25.72
 C       0.423418    -1.989333    -1.078749      50.07
 H       0.869243    -2.904186    -1.355437      25.87
 C      -0.930694    -1.970417    -0.675257     -27.95
 O      -1.825380    -2.977077    -0.399951     185.05
 C      -1.717644    -4.001657    -1.517122      89.73
 H      -2.597926    -4.892102    -1.069135      21.33
 H      -2.064163    -3.467897    -2.352283      25.72
 H      -0.779889    -4.673662    -1.423903      22.30
 C      -1.450410    -0.552607    -0.312003     -25.97
 O      -2.717701    -0.625819     0.239567     100.13
 C      -0.563352     0.565287    -0.247426      79.52
 H      -0.750884     1.474575     0.207723      26.48
 C       1.270985    -0.779252    -1.051188      45.33
 C       2.741041    -1.111613    -1.393797      86.60
 H       2.742182    -2.192078    -1.953593      21.56
 O       3.200317    -0.256352    -2.445855     252.47
 H       4.189349    -0.217503    -2.673069      29.08
 C       3.846942    -1.141341    -0.200025      97.67
 H       3.175580    -1.663371     0.337668      29.11
 O       4.975434    -2.050105    -0.402288     250.58
 H       5.321412    -2.026717    -1.270592      30.68
 C       4.104941     0.260015     0.443897     113.52
 O       4.530346     1.233095    -0.445040     297.52
 H       4.675696     1.969835     0.131158      28.99
 H       4.795658     0.141086     1.193018      29.57
 H       3.079803     0.628838     0.730658      26.92
55
name = lig-Water-frame_192
 C      -1.481074     2.152512     3.163296      48.36
 H      -2.192823     3.029345     2.608844      22.63
 C      -1.007369    -0.179632     3.391063      24.85
 H      -1.205215    -1.166727     2.930815      26.40
 C       0.352500     0.028464     3.835133      24.40
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 O       1.288459    -0.882497     4.197729     183.19
 C       1.000044    -2.290674     4.212204     107.75
 H       1.423461    -2.264606     5.342116      22.10
 H       1.418241    -2.881431     3.380570      27.68
 H      -0.006995    -2.209035     4.516357      25.02
 C       0.869810     1.454107     3.800401       9.96
 O       2.232201     1.627120     3.942236     195.25
 H       2.293254     2.649713     3.822194      27.51
 C      -0.069982     2.414448     3.497445      61.29
 H       0.374703     3.414053     3.364608      25.42
 C      -2.021546     0.919783     3.074743      31.36
 C      -3.255439     0.492635     2.437563     122.45
 H      -3.964744     1.077841     2.800375      31.80
 O      -3.531048    -0.813779     3.001864     204.96
 H      -4.395682    -1.096487     2.682604      25.18
 C      -3.356550     0.542947     0.885181      95.74
 H      -2.857947     1.414413     0.616431      26.50
 C      -4.786107     0.388437     0.390752     108.12
 O      -5.503008    -0.817075     1.004357     175.05
 H      -5.194033    -1.642067     0.404176      25.69
 H      -4.868284     0.386127    -0.671111      29.43
 H      -5.245703     1.143426     0.845788      29.99
 C       0.762966     0.350477    -0.609983      64.82
 H       1.500630     1.111785    -0.538704      23.66
 C       0.389927    -2.001342    -1.066805      44.46
 H       0.803497    -2.974483    -1.476354      22.35
 C      -0.935470    -1.863444    -0.660256       3.05
 O      -1.819226    -2.999021    -0.487098     207.39
 C      -1.731781    -4.022312    -1.429689     122.77
 H      -2.624378    -4.641519    -1.304380      25.94
 H      -2.054652    -3.501943    -2.473020      25.98
 H      -0.800414    -4.571125    -1.663978      25.72
 C      -1.432064    -0.605026    -0.332310      18.57
 O      -2.720284    -0.676510     0.249467      95.03
 C      -0.568300     0.478164    -0.279246      69.43
 H      -0.927449     1.523061     0.177600      23.63
 C       1.293441    -0.863534    -1.088654      -2.67
 C       2.752320    -1.129735    -1.447493     107.19
 H       2.766317    -2.130727    -2.001886      21.40
 O       3.219736    -0.269622    -2.468845     261.01
 H       4.208329    -0.422509    -2.400537      28.73
 C       3.828044    -1.091706    -0.299213      73.42
 H       3.054650    -1.645355     0.607081      24.05
 O       4.984351    -2.071581    -0.330487     173.83
 H       5.332818    -1.892675    -1.324514      26.43
 C       4.106857     0.211557     0.441018      98.26
 O       4.531849     1.229394    -0.472259     227.36
 H       4.827530     2.055983     0.194842      22.53
 H       4.729149     0.338957     1.497218      24.58
 H       3.099655     0.386494     0.948210      26.70
55
name = lig-Water-frame_193
 C      -1.458442     2.272727     3.112533      63.51
 H      -2.029365     3.039123     2.783539      29.47
 C      -1.047482    -0.157556     3.390815      36.95
 H      -1.275813    -1.173277     3.069845      23.72
 C       0.349362     0.082199     3.800858      13.17
 O       1.330543    -0.890242     4.187470     208.80
 C       1.045488    -2.234606     4.265873     123.63
 H       1.458321    -2.661209     5.144998      26.78
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 H       1.291230    -3.082001     3.481244      27.26
 H      -0.075874    -2.599808     4.491263      24.54
 C       0.881185     1.420496     3.726828      16.14
 O       2.179153     1.664563     3.930041     233.70
 H       2.625567     2.554542     3.724288      25.85
 C      -0.159007     2.442966     3.475637      51.66
 H       0.265171     3.460528     3.247942      18.87
 C      -1.928965     0.941083     3.133269      44.16
 C      -3.225761     0.426779     2.505949      87.40
 H      -3.993276     1.457978     2.920609      24.20
 O      -3.561737    -0.819614     3.011850     189.22
 H      -4.481431    -1.037712     2.656518      25.45
 C      -3.413355     0.447488     0.866364      77.15
 H      -3.138326     1.565190     0.441023      21.96
 C      -4.746046     0.430197     0.427573      79.51
 O      -5.507156    -0.776616     0.994160     189.75
 H      -5.114056    -1.603906     0.666157      28.73
 H      -4.635954     0.226053    -0.720788      24.92
 H      -5.242572     1.394686     1.007249      25.07
 C       0.828367     0.310974    -0.603774       8.80
 H       1.600402     1.120510    -0.592577      18.24
 C       0.387652    -2.010774    -1.080538      67.33
 H       0.643991    -2.979506    -1.449952      21.54
 C      -0.938025    -1.815485    -0.660752      19.63
 O      -1.789997    -2.986833    -0.546837     204.01
 C      -1.761860    -4.020983    -1.443783     122.33
 H      -2.816874    -4.802825    -1.307082      22.75
 H      -1.899983    -3.697487    -2.449638      27.95
 H      -0.757430    -4.487635    -1.654132      24.34
 C      -1.460017    -0.655788    -0.296052      36.11
 O      -2.708916    -0.707668     0.256277     112.85
 C      -0.594292     0.445978    -0.291777      81.63
 H      -1.017022     1.300391     0.014628      26.75
 C       1.294368    -0.984680    -1.110663       0.39
 C       2.786595    -1.148872    -1.514978      96.96
 H       2.832600    -2.355694    -1.772315      22.74
 O       3.248812    -0.259875    -2.512431     288.70
 H       4.167726    -0.451580    -2.431969      30.33
 C       3.762503    -1.127004    -0.275066      88.22
 H       3.361487    -1.540802     0.570144      28.68
 O       4.979756    -2.062078    -0.302070     155.56
 H       5.442799    -1.958287    -1.210193      28.65
 C       4.089671     0.178565     0.474818      99.27
 O       4.548101     1.258583    -0.480310     299.27
 H       4.819276     2.052366    -0.063134      28.36
 H       4.686836     0.100765     1.296121      28.05
 H       3.103302     0.375419     0.956998      27.86
55
name = lig-Water-frame_194
 C      -1.452979     2.339274     3.077556      75.51
 H      -2.101975     3.339918     2.863843      24.51
 C      -1.011841    -0.117190     3.407060      62.44
 H      -1.454494    -1.212248     3.402792      22.85
 C       0.342046     0.129407     3.757748      18.98
 O       1.366800    -0.860883     4.153466     193.83
 C       1.029204    -2.283660     4.356043     107.78
 H       1.695627    -2.972776     5.058351      24.66
 H       1.318494    -2.819504     3.425779      28.84
 H       0.049240    -2.653976     4.319053      28.27
 C       0.791223     1.400680     3.646787      19.96
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 O       2.161057     1.698694     3.934699     238.43
 H       2.518457     2.453236     3.387451      26.66
 C      -0.146180     2.493537     3.444322      46.48
 H       0.186713     3.603546     3.257170      16.61
 C      -1.824129     0.895313     3.153821      48.67
 C      -3.231806     0.469665     2.563691      98.99
 H      -3.862329     1.165276     2.750283      30.06
 O      -3.614403    -0.846212     3.036885     203.08
 H      -4.514820    -0.916331     2.632096      26.86
 C      -3.364285     0.390063     0.896856     101.66
 H      -3.111323     1.245957     0.449192      26.58
 C      -4.793741     0.427257     0.469301     108.41
 O      -5.515503    -0.719581     0.988905     275.51
 H      -5.011009    -1.522669     0.670652      28.01
 H      -4.758669     0.366170    -0.559929      29.29
 H      -5.277569     1.326894     0.668759      28.69
 C       0.868145     0.247445    -0.623916      39.36
 H       1.449664     1.174817    -0.614440      18.85
 C       0.375799    -2.046483    -1.114104      73.86
 H       0.592817    -3.088892    -1.404833      21.21
 C      -0.926777    -1.903402    -0.698474      17.50
 O      -1.769738    -2.941413    -0.568953     215.91
 C      -1.797571    -4.057051    -1.530338     113.34
 H      -2.483134    -4.830794    -1.139032      25.44
 H      -1.905079    -3.709635    -2.653221      25.85
 H      -0.822634    -4.604781    -1.287206      23.46
 C      -1.494581    -0.645812    -0.219714       8.76
 O      -2.721537    -0.724376     0.267338     160.65
 C      -0.563835     0.425639    -0.310570      54.89
 H      -1.074270     1.472640    -0.021126      21.07
 C       1.319972    -1.024874    -1.110871      29.80
 C       2.814226    -1.219208    -1.530893      92.53
 H       2.950018    -2.341404    -1.758795      23.08
 O       3.272168    -0.256346    -2.561240     241.29
 H       4.285364    -0.337561    -2.756704      27.62
 C       3.733646    -1.175399    -0.212538      59.99
 H       3.236323    -1.848774     0.789995      22.60
 O       4.970721    -2.039661    -0.301271     170.46
 H       5.463307    -2.002542    -1.113253      30.82
 C       4.055577     0.187324     0.459802      67.99
 O       4.552336     1.260481    -0.485532     258.59
 H       4.741621     2.185113     0.023509      25.31
 H       4.968147    -0.254194     1.194818      21.92
 H       3.089999     0.643763     0.864383      22.07
55
name = lig-Water-frame_195
 C      -1.468208     2.339671     3.060604      68.51
 H      -2.154529     3.199123     2.994003      25.63
 C      -0.933039    -0.147715     3.461991      71.08
 H      -1.427268    -1.002511     3.674160      26.38
 C       0.365634     0.094998     3.734082      20.29
 O       1.377328    -0.816931     4.126226     156.64
 C       1.038387    -2.385726     4.383920      85.19
 H       1.797079    -2.726056     5.101986      25.95
 H       1.422862    -2.410398     3.294157      25.01
 H      -0.111712    -2.490434     4.457241      25.05
 C       0.731672     1.466669     3.583333      -2.63
 O       2.135636     1.727675     3.932022     256.98
 H       2.214863     2.362628     3.132854      25.18
 C      -0.084391     2.578865     3.388615      27.45
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 H       0.317463     3.548917     3.426545      19.49
 C      -1.830700     0.919365     3.103637      21.91
 C      -3.184088     0.490217     2.569688      74.35
 H      -4.220610     1.291673     2.837055      22.43
 O      -3.677648    -0.865684     3.073453     159.29
 H      -4.563759    -0.918566     2.682963      27.22
 C      -3.291573     0.371439     0.974438      76.83
 H      -2.679302     1.312019     0.449280      23.89
 C      -4.852196     0.386105     0.494250      91.07
 O      -5.538172    -0.671960     0.994272     256.22
 H      -5.029951    -1.452836     0.529227      24.74
 H      -4.952252     0.473362    -0.694282      25.47
 H      -5.445872     1.414254     0.621379      25.08
 C       0.845958     0.190902    -0.659847      51.99
 H       1.375068     1.134824    -0.678276      21.68
 C       0.374675    -2.119574    -1.165785      65.94
 H       0.736019    -3.144539    -1.389534      24.92
 C      -0.929054    -1.954741    -0.722360      11.46
 O      -1.802694    -2.935131    -0.592377     205.44
 C      -1.762963    -4.081946    -1.596828     108.70
 H      -2.614742    -4.936172    -1.037480      23.15
 H      -1.940960    -3.788333    -2.572412      28.05
 H      -0.935745    -4.628766    -1.329286      25.52
 C      -1.431391    -0.651383    -0.174788     -14.08
 O      -2.766026    -0.747792     0.290271     125.18
 C      -0.536221     0.430806    -0.311094      66.93
 H      -0.732006     1.435224    -0.112178      24.55
 C       1.374420    -1.006291    -1.112401      21.53
 C       2.854383    -1.288066    -1.495220      67.28
 H       3.068917    -2.348278    -2.090709      20.60
 O       3.283677    -0.268848    -2.601951     229.63
 H       4.208635    -0.372098    -2.955186      29.10
 C       3.704226    -1.249180    -0.128708      84.27
 H       3.102335    -1.792859     0.510693      27.18
 O       4.954410    -2.018640    -0.291396     150.64
 H       5.383497    -1.840204    -1.305717      25.15
 C       4.055499     0.208785     0.431766     105.35
 O       4.553834     1.253199    -0.478675     305.84
 H       4.541656     2.006282     0.194818      28.01
 H       4.838738    -0.135967     0.982001      24.89
 H       3.286271     0.703736     0.972568      25.37
55
name = lig-Water-frame_196
 C      -1.453427     2.282011     3.070122      68.51
 H      -2.297650     3.036526     2.993279      25.60
 C      -0.914415    -0.164229     3.511615      35.54
 H      -1.453599    -1.174635     3.906209      26.00
 C       0.436175     0.059889     3.723605      20.28
 O       1.375129    -0.761170     4.123882     146.46
 C       1.053458    -2.407720     4.328489      92.69
 H       1.720414    -2.518194     5.218434      26.37
 H       1.338464    -2.670449     3.351384      28.16
 H       0.048876    -2.409696     4.781988      25.58
 C       0.749958     1.531033     3.569015       4.16
 O       2.074466     1.755492     3.897415     220.42
 H       2.417759     2.449893     3.222119      22.36
 C      -0.063790     2.636765     3.309826      41.98
 H       0.533292     3.641779     3.668317      20.05
 C      -1.865362     0.971869     3.042356      25.31
 C      -3.210498     0.502861     2.561037     107.90
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 H      -3.888105     1.117883     2.864582      30.35
 O      -3.723459    -0.863832     3.121698     137.74
 H      -4.646046    -0.957556     2.720085      25.44
 C      -3.240490     0.442879     1.015130      81.81
 H      -2.645364     1.209879     0.765033      29.35
 C      -4.875874     0.438770     0.465243      93.85
 O      -5.573728    -0.674283     1.003442     285.14
 H      -5.297819    -1.454325     0.539815      29.81
 H      -4.902754     0.372649    -0.564373      28.93
 H      -5.391140     1.275366     0.969168      27.43
 C       0.812199     0.171826    -0.709748      49.58
 H       1.496614     1.056406    -0.777317      23.81
 C       0.426653    -2.170032    -1.215573      45.70
 H       0.845590    -3.129938    -1.425701      27.57
 C      -0.915157    -1.930389    -0.722973       7.48
 O      -1.883279    -2.987583    -0.636709     151.73
 C      -1.754046    -4.122479    -1.564708     121.37
 H      -2.693865    -4.642351    -1.334746      26.94
 H      -2.003777    -3.800306    -2.670793      26.48
 H      -0.678250    -4.696977    -1.669244      22.83
 C      -1.345304    -0.699702    -0.161289      -5.05
 O      -2.780360    -0.783528     0.314772      71.93
 C      -0.498541     0.411268    -0.302631      65.84
 H      -0.565609     1.530685    -0.066492      24.63
 C       1.396586    -1.040503    -1.135360     -13.99
 C       2.909141    -1.323094    -1.487065      84.82
 H       3.007667    -2.261899    -2.086414      22.98
 O       3.270716    -0.293353    -2.622054     227.65
 H       4.133864    -0.586684    -2.890747      29.99
 C       3.697897    -1.280202    -0.127849      78.31
 H       2.797286    -1.857801     0.588619      24.44
 O       4.942989    -1.996068    -0.301687     168.69
 H       5.115895    -1.699658    -1.157951      29.68
 C       4.052764     0.210501     0.383781      95.46
 O       4.536800     1.230237    -0.463220     279.11
 H       4.559569     2.010566     0.111120      28.46
 H       4.999396     0.050194     1.208087      24.67
 H       3.338045     0.584418     1.263961      24.49
55
name = lig-Water-frame_197
 C      -1.433301     2.259071     3.080826      62.84
 H      -2.362151     2.965569     2.882481      22.00
 C      -0.966567    -0.165579     3.554567      54.18
 H      -1.289006    -1.082813     3.809822      29.50
 C       0.439735     0.111984     3.689888      12.82
 O       1.404218    -0.752814     4.142563     116.58
 C       1.077904    -2.332740     4.291007      90.46
 H       1.781968    -2.488400     5.217273      25.39
 H       1.170579    -3.212385     3.441162      26.02
 H       0.127232    -2.494558     4.822647      26.16
 C       0.797968     1.553110     3.568636      18.33
 O       2.050132     1.793630     3.853742     146.12
 H       2.599255     2.576860     3.537495      24.41
 C      -0.056133     2.660012     3.259030      57.90
 H       0.273183     3.538019     3.590339      26.30
 C      -1.843184     0.919275     3.032556      23.76
 C      -3.234055     0.446550     2.549022      82.05
 H      -4.038508     1.428551     3.001612      22.72
 O      -3.753835    -0.838590     3.174402     192.96
 H      -4.614881    -0.920434     2.703302      26.36
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 C      -3.269998     0.485923     1.021551      60.21
 H      -2.619200     1.493578     0.770720      22.81
 C      -4.837759     0.508112     0.492940      71.46
 O      -5.620095    -0.692916     1.020753     276.77
 H      -5.454034    -1.569731     0.514083      26.58
 H      -4.801468     0.432295    -0.653563      24.97
 H      -5.314829     1.316501     1.121232      24.88
 C       0.843737     0.173342    -0.784709      48.52
 H       1.545252     0.967201    -0.842400      25.65
 C       0.489296    -2.164736    -1.237132      63.30
 H       0.816576    -3.217576    -1.505577      26.72
 C      -0.882706    -1.947499    -0.728670     -11.23
 O      -1.942959    -3.040513    -0.692724     132.60
 C      -1.728074    -4.130594    -1.584805     118.17
 H      -2.846681    -4.840119    -1.424715      22.54
 H      -1.938690    -3.745997    -2.537824      28.28
 H      -0.849051    -4.594874    -1.759000      26.36
 C      -1.321631    -0.757758    -0.150341     -18.12
 O      -2.734009    -0.797090     0.341138      31.01
 C      -0.451435     0.398799    -0.283191      55.14
 H      -0.738240     1.419118     0.088057      25.53
 C       1.371077    -1.127656    -1.176310      20.25
 C       2.911081    -1.284462    -1.499762      89.45
 H       2.912872    -2.481400    -1.918603      22.55
 O       3.251635    -0.340075    -2.611275     225.95
 H       4.169013    -0.768920    -2.821346      26.44
 C       3.670565    -1.269100    -0.146937      93.20
 H       3.128671    -1.712538     0.584157      29.74
 O       4.917818    -1.984729    -0.294667     114.70
 H       5.253297    -1.684379    -1.284540      25.22
 C       4.081089     0.179142     0.452700     115.58
 O       4.497520     1.201864    -0.464716     283.13
 H       4.701841     2.185363    -0.070132      23.54
 H       4.849174     0.061988     1.096462      29.68
 H       3.276957     0.425279     1.084111      29.84
55
name = lig-Water-frame_198
 C      -1.434141     2.248611     3.064615      51.17
 H      -2.146539     2.987009     2.822644      21.58
 C      -0.982612    -0.113811     3.569819      63.45
 H      -1.311785    -1.259388     3.645905      25.53
 C       0.374784     0.213866     3.651707      11.88
 O       1.440695    -0.795057     4.152145     148.97
 C       1.115772    -2.241537     4.289489     121.83
 H       1.891899    -2.551708     4.955297      28.11
 H       1.088652    -3.093687     3.692552      29.69
 H       0.071861    -2.435455     4.715559      26.34
 C       0.811243     1.558781     3.545571      25.56
 O       2.116641     1.818585     3.840468     117.07
 H       2.377072     2.850365     3.672344      23.96
 C      -0.096750     2.595669     3.229677      59.03
 H       0.036764     3.817097     3.426607      25.03
 C      -1.806421     0.791490     3.070205      29.09
 C      -3.281039     0.435207     2.591934     101.12
 H      -3.837211     1.198326     2.788990      29.92
 O      -3.772372    -0.786148     3.214185     248.09
 H      -4.593779    -0.915138     2.661652      27.03
 C      -3.333274     0.508075     0.994220      71.51
 H      -2.949674     1.415662     0.637068      24.80
 C      -4.762833     0.526852     0.556608      89.99
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 O      -5.657139    -0.696184     1.033204     296.31
 H      -5.345121    -1.471799     0.461822      27.09
 H      -4.829136     0.743495    -0.523614      26.67
 H      -5.300709     1.478359     0.955883      25.20
 C       0.896375     0.163015    -0.860359      43.35
 H       1.602480     1.045662    -0.898792      24.52
 C       0.480141    -2.197084    -1.234361      81.00
 H       0.702113    -3.169299    -1.538879      25.93
 C      -0.862063    -2.033047    -0.742758     -12.65
 O      -1.948802    -3.059575    -0.732419     148.25
 C      -1.791906    -4.128924    -1.645021     107.90
 H      -2.369889    -5.056358    -1.489023      26.05
 H      -1.928762    -3.632044    -2.689490      25.26
 H      -0.724631    -4.713382    -1.517468      22.56
 C      -1.335413    -0.788119    -0.140620     -23.58
 O      -2.642350    -0.772109     0.370062      35.78
 C      -0.416192     0.354769    -0.254286      47.30
 H      -0.854290     1.242118     0.177325      25.28
 C       1.361351    -1.149264    -1.223606      35.82
 C       2.824128    -1.263879    -1.510318     109.67
 H       2.992005    -2.351560    -1.732116      24.73
 O       3.246886    -0.422953    -2.577063     258.38
 H       4.175320    -0.643489    -2.835180      28.52
 C       3.700627    -1.179924    -0.201476      71.54
 H       3.280939    -1.794336     0.852356      24.26
 O       4.905689    -1.983320    -0.312800     168.64
 H       5.482930    -1.927394    -1.108624      29.52
 C       4.082135     0.144408     0.527419      79.06
 O       4.455911     1.187425    -0.490832     241.63
 H       4.660076     1.997294    -0.033375      28.27
 H       5.023767    -0.183019     1.262608      24.46
 H       3.002194     0.498938     0.905276      24.44
55
name = lig-Water-frame_199
 C      -1.448126     2.162168     3.027663      28.28
 H      -2.101100     3.167447     2.720299      18.45
 C      -0.948703    -0.146974     3.579983      55.21
 H      -1.255483    -1.150684     3.454618      30.48
 C       0.360552     0.268880     3.656235       5.19
 O       1.451700    -0.819227     4.125918     131.12
 C       1.121967    -2.141105     4.337538     102.88
 H       2.049657    -2.653510     4.926170      24.59
 H       1.172657    -2.758084     3.202418      24.86
 H       0.169863    -2.178161     4.806880      26.30
 C       0.830604     1.565596     3.525133      17.84
 O       2.205574     1.852609     3.843951     198.34
 H       2.145589     2.735130     3.577384      30.89
 C      -0.160513     2.560992     3.230336      32.31
 H       0.021975     3.542201     3.095372      27.49
 C      -1.864836     0.765825     3.094954      32.86
 C      -3.247507     0.419243     2.619650      88.82
 H      -4.066503     1.448193     2.876171      23.14
 O      -3.795947    -0.726665     3.233102     251.73
 H      -4.619258    -0.997399     2.701318      25.66
 C      -3.380861     0.461877     0.991270      64.85
 H      -3.018416     1.473705     0.484728      21.32
 C      -4.755559     0.527530     0.610668     108.12
 O      -5.656423    -0.664325     1.024765     310.79
 H      -5.211341    -1.324231     0.489369      29.22
 H      -4.889542     0.805641    -0.456625      27.03
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 H      -5.208318     1.437608     0.961784      27.29
 C       0.914170     0.163230    -0.901015      68.02
 H       1.554126     1.012295    -0.971089      24.59
 C       0.399749    -2.258389    -1.215358      74.45
 H       0.740365    -3.262608    -1.600888      23.11
 C      -0.892256    -2.119387    -0.737888       8.51
 O      -1.924636    -3.053374    -0.751190     211.59
 C      -1.780839    -4.133344    -1.745914     110.87
 H      -2.465620    -5.152822    -1.461204      24.49
 H      -1.881145    -3.836042    -2.763039      27.43
 H      -0.865970    -4.442536    -1.460758      26.89
 C      -1.310206    -0.803870    -0.158383      -2.07
 O      -2.555726    -0.725271     0.403274      63.16
 C      -0.390120     0.254677    -0.239379      51.18
 H      -0.775920     1.274219     0.225118      23.20
 C       1.349250    -1.089941    -1.266591      13.57
 C       2.747894    -1.272788    -1.494251      94.96
 H       3.176719    -2.422964    -1.717759      21.00
 O       3.235706    -0.494445    -2.558592     267.56
 H       4.181489    -0.547819    -2.675042      30.87
 C       3.754312    -1.101103    -0.192234      92.65
 H       3.269991    -1.644958     0.502061      29.81
 O       4.915283    -2.012074    -0.322098     162.11
 H       5.426035    -1.917124    -1.154937      29.35
 C       4.056116     0.128079     0.562253     115.43
 O       4.422325     1.155066    -0.506542     257.28
 H       4.580324     1.952849     0.156198      24.90
 H       4.745855    -0.163706     1.289375      29.43
 H       3.210247     0.536145     0.964763      28.36
55
name = lig-Water-frame_200
 C      -1.510818     2.086090     2.968416      52.93
 H      -2.123789     2.804997     2.710714      33.78
 C      -0.921597    -0.191811     3.551415      26.94
 H      -1.157672    -1.292872     3.444877      24.83
 C       0.429390     0.222034     3.716538       5.54
 O       1.460236    -0.749080     4.080150     166.02
 C       1.142894    -2.101627     4.320524     125.75
 H       1.867195    -2.548669     4.878718      28.63
 H       1.069123    -2.211851     3.318594      27.22
 H       0.192591    -2.162175     5.002427      23.65
 C       0.870850     1.573392     3.529089      14.44
 O       2.242074     1.866173     3.844057     188.74
 H       2.429068     2.859736     3.365198      26.04
 C      -0.179730     2.496317     3.234739      53.63
 H       0.216069     3.580915     2.847915      16.30
 C      -1.948258     0.813068     3.122957      41.62
 C      -3.257340     0.484035     2.619570     117.97
 H      -3.832954     1.202712     2.922799      30.39
 O      -3.821289    -0.692489     3.244553     278.18
 H      -4.624583    -0.941652     2.787905      27.07
 C      -3.330761     0.418526     1.019093      76.85
 H      -2.903142     1.348180     0.609018      26.36
 C      -4.843945     0.501107     0.622739      85.78
 O      -5.624239    -0.602048     1.004074     295.15
 H      -5.181200    -1.435256     0.535509      25.79
 H      -4.936183     0.589560    -0.525165      25.48
 H      -5.153844     1.438882     1.346396      24.49
 C       0.870954     0.169606    -0.902234      70.49
 H       1.542031     1.050035    -1.013451      22.00
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 C       0.351898    -2.292901    -1.206145      65.76
 H       0.803332    -3.203727    -1.559037      24.25
 C      -0.952149    -2.152641    -0.714662      32.40
 O      -1.917521    -3.050019    -0.774938     199.00
 C      -1.756807    -4.160503    -1.813319     108.99
 H      -2.751278    -4.699712    -1.445238      24.53
 H      -1.890556    -3.948975    -2.913716      25.79
 H      -0.635070    -4.488348    -1.645027      23.70
 C      -1.250764    -0.823332    -0.193844       8.84
 O      -2.513785    -0.689026     0.444010      71.28
 C      -0.361442     0.189523    -0.234864      78.03
 H      -0.542273     1.116257     0.128743      27.45
 C       1.274895    -1.079538    -1.296221     -33.65
 C       2.798752    -1.326362    -1.470840      87.32
 H       2.965158    -2.394504    -1.720092      22.34
 O       3.208900    -0.533555    -2.579070     247.70
 H       4.241186    -0.549500    -2.375032      25.35
 C       3.775601    -1.093311    -0.183521      80.48
 H       2.902519    -1.753191     0.463364      24.25
 O       4.939188    -2.042264    -0.327363     118.94
 H       5.178043    -1.742275    -1.341424      24.38
 C       4.020981     0.154909     0.522613      94.82
 O       4.406997     1.130226    -0.473864     265.95
 H       4.561700     2.024984     0.033248      25.74
 H       4.815543    -0.019085     1.452229      24.50
 H       3.151510     0.579973     1.263933      24.26
55
name = lig-Water-frame_201
 C      -1.529210     2.054386     2.927327      60.10
 H      -2.502030     2.774053     2.542836      25.97
 C      -0.913744    -0.207427     3.488538      52.51
 H      -1.071076    -1.333638     3.596949      21.52
 C       0.505015     0.133509     3.793453      19.58
 O       1.489132    -0.599912     4.052354     151.97
 C       1.111294    -2.045070     4.303456      92.19
 H       2.053766    -2.593152     4.864002      24.65
 H       0.750175    -2.513600     3.188430      26.79
 H       0.270944    -2.237856     4.883804      24.73
 C       0.901530     1.571141     3.558625       7.58
 O       2.242901     1.902456     3.813167     278.25
 H       2.809845     2.542073     3.365095      26.01
 C      -0.140728     2.452654     3.207397      52.66
 H       0.208431     3.389141     2.854422      20.93
 C      -1.940770     0.782717     3.183672      58.63
 C      -3.287126     0.501894     2.586427      68.99
 H      -4.035278     1.522141     2.981959      24.80
 O      -3.834430    -0.682798     3.259256     202.19
 H      -4.734651    -0.789660     2.820898      24.82
 C      -3.246291     0.396597     1.053793      84.41
 H      -2.743269     1.368956     0.749690      27.31
 C      -4.901074     0.492060     0.625618     101.62
 O      -5.597948    -0.580054     0.993371     306.42
 H      -5.352064    -1.439329     0.662390      28.38
 H      -4.991840     0.633652    -0.404797      28.45
 H      -5.191577     1.224764     1.279295      28.40
 C       0.829466     0.163993    -0.902952      71.68
 H       1.466941     1.041206    -0.981018      23.06
 C       0.357049    -2.258369    -1.204669      80.63
 H       0.792616    -3.212621    -1.466851      27.66
 C      -0.968717    -2.115927    -0.702296      42.25
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 O      -1.940546    -3.078817    -0.820041     162.50
 C      -1.723934    -4.157997    -1.845967     118.36
 H      -2.769714    -4.691204    -1.532808      24.27
 H      -1.918926    -3.769798    -2.866095      26.50
 H      -0.849346    -4.828819    -1.885960      24.94
 C      -1.246057    -0.857727    -0.200189       6.68
 O      -2.505445    -0.689580     0.486533      71.73
 C      -0.319028     0.188431    -0.244053      55.75
 H      -0.588895     1.255765     0.262814      26.03
 C       1.213120    -1.150276    -1.307899     -38.67
 C       2.852454    -1.358380    -1.455482      75.30
 H       2.698822    -2.557833    -1.724152      21.22
 O       3.205292    -0.560137    -2.609415     277.42
 H       4.163851    -0.407517    -2.480491      28.22
 C       3.689833    -1.218726    -0.148625      84.61
 H       3.099423    -1.644254     0.526424      29.98
 O       4.952870    -2.032900    -0.357869     178.06
 H       5.184884    -1.876624    -1.254349      30.09
 C       3.995105     0.225890     0.543077     105.37
 O       4.399934     1.131515    -0.429250     335.92
 H       4.587779     2.019108    -0.123608      29.78
 H       4.870713     0.145796     1.152767      26.72
 H       3.151154     0.425372     1.125576      29.45
55
name = lig-Water-frame_202
 C      -1.518432     2.088403     2.908047      52.78
 H      -2.213664     2.677437     2.565964      26.87
 C      -0.865664    -0.224568     3.456759      55.98
 H      -1.179812    -1.206503     3.657764      22.12
 C       0.459112     0.190036     3.809288      18.06
 O       1.571297    -0.548878     4.064444     139.46
 C       1.112280    -2.021663     4.236588     110.62
 H       1.972158    -2.430904     4.521082      30.03
 H       0.795541    -2.710658     3.536523      31.28
 H       0.186300    -2.109065     4.939145      25.11
 C       0.896483     1.545149     3.590873      10.56
 O       2.233864     1.902566     3.795373     240.33
 H       2.759103     2.513144     3.152534      23.91
 C      -0.117599     2.413249     3.147052      47.69
 H       0.192394     3.508642     2.898839      24.65
 C      -1.887016     0.707230     3.230066      12.19
 C      -3.332107     0.509187     2.612068      85.53
 H      -3.894509     1.333582     2.668851      30.68
 O      -3.856951    -0.678784     3.259765     176.53
 H      -4.809344    -0.696274     2.950129      25.49
 C      -3.192013     0.424068     1.064105      69.82
 H      -2.691513     1.430271     0.792175      26.42
 C      -4.840637     0.495346     0.602518      76.04
 O      -5.626997    -0.618974     1.025497     297.22
 H      -5.359430    -1.473383     0.566655      26.85
 H      -5.023732     0.941850    -0.508492      24.17
 H      -5.401907     1.442175     1.232702      24.09
 C       0.838436     0.122706    -0.931848      69.12
 H       1.477169     0.999603    -0.967934      25.98
 C       0.371044    -2.218518    -1.208107      83.64
 H       0.684231    -3.296599    -1.326811      27.99
 C      -0.953978    -2.076419    -0.724534      19.25
 O      -1.951521    -3.126942    -0.866792     143.78
 C      -1.751225    -4.135446    -1.869418     120.16
 H      -2.636008    -4.995810    -1.836874      24.43
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 H      -1.864262    -3.526624    -2.773266      25.48
 H      -0.996070    -4.987899    -1.879573      23.39
 C      -1.301874    -0.846554    -0.150582      -3.83
 O      -2.512197    -0.736331     0.524323      98.36
 C      -0.354505     0.269549    -0.209663      53.14
 H      -0.695760     1.062730     0.287191      30.11
 C       1.238883    -1.200474    -1.300946     -11.52
 C       2.805614    -1.406173    -1.467713      88.99
 H       2.907476    -2.414293    -1.694496      23.51
 O       3.209012    -0.583979    -2.632648     270.99
 H       4.142850    -0.302027    -2.726005      27.69
 C       3.629214    -1.327656    -0.129024      52.62
 H       3.218908    -1.885423     0.950629      24.94
 O       4.945396    -2.014938    -0.367588     137.80
 H       5.338363    -1.954997    -1.346659      26.87
 C       3.987092     0.241712     0.542682      70.59
 O       4.386166     1.154364    -0.430906     246.60
 H       4.618406     2.154110    -0.001732      23.31
 H       4.986907     0.042087     1.183449      23.90
 H       2.921966     0.488480     1.056256      25.39
55
name = lig-Water-frame_203
 C      -1.422161     2.057096     2.947977      45.57
 H      -2.138609     2.997414     2.500858      22.09
 C      -0.816932    -0.238444     3.467752      29.56
 H      -1.293137    -1.302822     3.681061      22.26
 C       0.418518     0.305191     3.786468      16.92
 O       1.631763    -0.590136     4.078074     108.02
 C       1.118171    -1.982535     4.205605     102.43
 H       2.186386    -2.468064     4.563770      25.48
 H       0.788246    -2.719873     3.257789      27.80
 H       0.465261    -1.840043     5.034398      28.07
 C       0.853784     1.540971     3.600828      33.52
 O       2.226360     1.884216     3.776517     174.73
 H       2.216362     2.580556     3.042172      26.31
 C      -0.113646     2.429864     3.062831      64.27
 H       0.153641     3.528651     3.029491      24.53
 C      -1.849567     0.711306     3.209889     -21.26
 C      -3.279984     0.443741     2.653756      76.25
 H      -4.029805     1.511495     2.690805      23.24
 O      -3.898795    -0.672083     3.256629     149.68
 H      -4.835513    -0.753029     3.064631      26.99
 C      -3.199482     0.469445     1.055650      73.96
 H      -2.727433     1.366699     0.698697      27.02
 C      -4.766151     0.558536     0.572463      96.27
 O      -5.659766    -0.667737     1.057855     309.87
 H      -5.305188    -1.392539     0.411424      26.55
 H      -4.903416     0.841913    -0.388507      28.33
 H      -5.207465     1.320255     1.049100      28.73
 C       0.842687     0.086658    -0.938263      64.29
 H       1.597319     0.908216    -1.020088      27.65
 C       0.351648    -2.251522    -1.205453      73.04
 H       0.623410    -3.263438    -1.282468      29.99
 C      -0.960113    -2.060247    -0.769411      -7.80
 O      -1.941523    -3.164085    -0.876057     162.06
 C      -1.803673    -4.128213    -1.928830     100.16
 H      -2.740912    -4.933801    -2.007117      24.15
 H      -1.679848    -3.531900    -2.894565      23.69
 H      -0.842395    -4.715778    -1.723996      22.50
 C      -1.352504    -0.788943    -0.085894     -10.74
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 O      -2.541231    -0.802440     0.565159      92.64
 C      -0.429311     0.295709    -0.194014      44.20
 H      -0.761839     1.294505     0.388961      26.58
 C       1.341286    -1.184744    -1.285050      -4.63
 C       2.725759    -1.444914    -1.482465      75.96
 H       3.258607    -2.534551    -1.856449      20.14
 O       3.188575    -0.601364    -2.650838     187.16
 H       4.247293    -0.423799    -2.715398      23.62
 C       3.623732    -1.379559    -0.072466      71.19
 H       3.356434    -1.961760     0.670671      29.46
 O       4.935091    -2.008685    -0.371284     120.96
 H       5.233516    -1.749590    -1.319036      26.52
 C       3.968499     0.187075     0.537672      97.12
 O       4.376179     1.214845    -0.453308     325.28
 H       4.519801     1.963932     0.099521      29.14
 H       4.635628    -0.125324     1.357459      27.61
 H       3.115616     0.602018     0.996786      29.12
55
name = lig-Water-frame_204
 C      -1.368808     2.047076     2.972267      73.81
 H      -1.943022     2.843974     2.699382      24.25
 C      -0.847790    -0.243334     3.508497      51.50
 H      -1.009693    -1.236894     3.621979      26.72
 C       0.466201     0.277959     3.779396      -1.64
 O       1.632303    -0.631281     4.063680     162.54
 C       1.208779    -1.966541     4.186402     129.03
 H       1.964630    -2.517330     4.611050      29.58
 H       0.802287    -2.193107     3.257344      31.79
 H       0.533552    -1.901003     5.056375      26.38
 C       0.822904     1.610205     3.589378      24.73
 O       2.181650     1.874723     3.728153     137.68
 H       2.103013     2.705392     3.216889      24.53
 C      -0.069817     2.487160     3.015921      85.94
 H       0.148884     3.544848     2.981429      27.44
 C      -1.824634     0.750986     3.146051      32.61
 C      -3.222018     0.435301     2.670378     100.82
 H      -3.773018     1.231294     3.033705      27.85
 O      -3.931559    -0.680714     3.270339     168.24
 H      -4.884869    -0.759707     2.917894      23.52
 C      -3.271500     0.464797     1.057979      56.27
 H      -2.646438     1.363562     0.539106      23.58
 C      -4.683001     0.557769     0.572014      71.79
 O      -5.654139    -0.674016     1.059829     239.23
 H      -5.376798    -1.376686     0.460206      27.26
 H      -4.757210     0.532506    -0.630381      22.95
 H      -5.121401     1.564135     1.223515      23.05
 C       0.835083     0.081641    -0.902735      71.21
 H       1.561111     0.856409    -1.025299      27.16
 C       0.340578    -2.280158    -1.195391      35.76
 H       0.691173    -3.346393    -1.412936      23.29
 C      -1.001429    -2.049882    -0.805124     -21.05
 O      -1.933619    -3.160895    -0.852912     179.90
 C      -1.802802    -4.109980    -2.005740      99.41
 H      -2.916601    -4.601074    -2.078414      23.84
 H      -1.594128    -3.743255    -2.984419      24.80
 H      -0.872962    -4.541104    -1.717933      23.61
 C      -1.371846    -0.756313    -0.061224     -31.61
 O      -2.596129    -0.853851     0.612625      73.57
 C      -0.492093     0.306908    -0.198068      66.30
 H      -0.529844     1.294339     0.162666      26.82
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 C       1.343377    -1.187204    -1.248615      -9.49
 C       2.774412    -1.511250    -1.515016      94.08
 H       2.964436    -2.418833    -1.851051      27.60
 O       3.170707    -0.605545    -2.660117     218.25
 H       4.093268    -0.722874    -2.527874      27.65
 C       3.670859    -1.334366    -0.081360      67.36
 H       3.081319    -2.170992     0.696708      25.56
 O       4.925691    -2.000051    -0.382768     149.78
 H       5.155233    -1.523823    -1.194472      28.66
 C       3.920681     0.088262     0.507121      94.18
 O       4.369361     1.228281    -0.473701     252.89
 H       4.494605     2.110329     0.199408      22.85
 H       4.567950    -0.129213     1.474604      25.91
 H       3.043209     0.631800     1.073787      24.49
55
name = lig-Water-frame_205
 C      -1.348422     2.062287     2.977711      50.85
 H      -2.244255     2.879049     2.753180      21.00
 C      -0.857242    -0.197113     3.561749      59.73
 H      -0.887667    -1.373076     3.543747      23.85
 C       0.534209     0.165845     3.777092       9.43
 O       1.614821    -0.606955     4.041942     199.44
 C       1.279704    -1.947035     4.204827     106.05
 H       2.094202    -2.753267     4.523158      25.73
 H       0.720367    -2.050184     3.125435      26.06
 H       0.332318    -2.219721     4.827417      25.44
 C       0.835960     1.646990     3.571500      19.29
 O       2.128119     1.893068     3.665676     144.67
 H       2.549229     2.849846     3.497510      24.96
 C      -0.013261     2.552176     3.013808      68.92
 H       0.191370     3.709795     2.776595      26.52
 C      -1.780646     0.739668     3.086774      49.13
 C      -3.174107     0.441501     2.671456      79.42
 H      -3.759828     1.401279     3.276240      23.07
 O      -3.953256    -0.712241     3.288521     203.15
 H      -4.705463    -0.679357     2.610062      24.62
 C      -3.308913     0.422627     1.079329      83.06
 H      -2.765997     1.174513     0.665354      25.17
 C      -4.665695     0.530247     0.583625     111.13
 O      -5.620306    -0.618266     1.056085     264.46
 H      -5.388237    -1.493501     0.535013      25.79
 H      -4.648070     0.377316    -0.433937      27.28
 H      -4.988720     1.376024     0.938554      28.88
 C       0.806560     0.074063    -0.839675      49.95
 H       1.438793     1.004579    -0.947221      22.65
 C       0.344374    -2.288482    -1.184260      56.26
 H       0.652528    -3.231796    -1.556559      19.82
 C      -1.041499    -2.042084    -0.812097     -19.50
 O      -1.934049    -3.114281    -0.836119     162.23
 C      -1.792242    -4.056708    -2.057492      82.32
 H      -2.865714    -4.539487    -2.062542      23.74
 H      -1.589207    -3.639553    -3.122910      22.83
 H      -0.994923    -4.966993    -1.752171      21.60
 C      -1.403702    -0.791990    -0.076222     -30.63
 O      -2.651016    -0.877725     0.653507      81.08
 C      -0.475130     0.300690    -0.254206      62.47
 H      -0.519970     1.388092     0.074292      23.27
 C       1.255944    -1.224995    -1.193711      18.72
 C       2.826642    -1.502198    -1.524976      79.58
 H       2.634723    -2.714327    -1.856437      23.22
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 O       3.155731    -0.623433    -2.645563     195.98
 H       4.203672    -0.804722    -2.673325      23.05
 C       3.678680    -1.311888    -0.123475      98.45
 H       3.039622    -1.778954     0.471277      30.06
 O       4.921698    -1.987272    -0.393957     144.57
 H       5.412402    -1.373576    -1.150728      26.53
 C       3.854628     0.028738     0.504580      93.91
 O       4.362005     1.201489    -0.461946     297.55
 H       4.514092     2.047785    -0.040596      27.14
 H       4.699492     0.032215     1.249218      25.47
 H       2.894005     0.341760     0.951224      26.68
55
name = lig-Water-frame_206
 C      -1.375994     2.138604     2.949707      32.55
 H      -2.309665     2.681403     2.816059      20.35
 C      -0.784008    -0.203866     3.612149      74.98
 H      -1.166002    -1.195726     3.475424      28.15
 C       0.543234     0.158296     3.753978      25.22
 O       1.619717    -0.562755     4.053837     219.51
 C       1.279097    -2.004128     4.176563     123.79
 H       2.205605    -2.567512     4.197437      27.95
 H       1.009813    -2.412366     3.236157      31.05
 H       0.429897    -2.285488     4.712599      29.11
 C       0.865594     1.617083     3.538236      10.89
 O       2.159521     1.931464     3.616394     205.21
 H       2.679266     2.725709     3.695189      27.85
 C      -0.024246     2.626722     3.025476      46.72
 H       0.269303     3.544591     2.705892      30.24
 C      -1.710081     0.716144     3.055498      36.74
 C      -3.180073     0.472369     2.704135      91.43
 H      -3.691636     1.382495     2.983024      27.06
 O      -3.954274    -0.735400     3.276654     243.01
 H      -4.567965    -0.806334     2.531528      28.90
 C      -3.295055     0.333725     1.158356      75.54
 H      -2.700627     1.330775     0.726933      21.94
 C      -4.696215     0.420145     0.583414      98.82
 O      -5.577446    -0.535232     1.057354     231.38
 H      -5.264927    -1.390031     0.650891      25.29
 H      -4.614093     0.398180    -0.571317      25.56
 H      -5.225570     1.601097     0.726434      23.62
 C       0.776749     0.072370    -0.773439      66.29
 H       1.338514     0.969203    -0.867511      24.86
 C       0.309586    -2.267728    -1.173672      69.42
 H       0.569668    -3.242585    -1.649612      20.11
 C      -1.053239    -2.028276    -0.781990       6.52
 O      -1.940627    -3.069592    -0.853318     168.58
 C      -1.770096    -4.027177    -2.072137     100.23
 H      -2.899432    -4.582888    -2.084781      23.12
 H      -1.595290    -3.426738    -2.898061      26.27
 H      -1.331752    -4.943115    -1.939404      25.26
 C      -1.442656    -0.857957    -0.116613      -9.38
 O      -2.680893    -0.883826     0.674242      68.48
 C      -0.455779     0.287942    -0.310284      59.61
 H      -0.823369     1.292386     0.065387      24.35
 C       1.209449    -1.239209    -1.143944      22.29
 C       2.779186    -1.472736    -1.514000      97.89
 H       2.805241    -2.454012    -1.708555      28.82
 O       3.173469    -0.667060    -2.621501     259.31
 H       4.073347    -0.636317    -3.007129      28.77
 C       3.679265    -1.284496    -0.258636      81.64
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 H       2.962787    -1.835228     0.663893      25.72
 O       4.943855    -1.966929    -0.403883     213.32
 H       5.513984    -1.544284    -0.992106      31.74
 C       3.818701     0.057311     0.480539      87.75
 O       4.336415     1.112151    -0.465867     272.04
 H       4.524355     2.028240     0.071395      24.60
 H       4.701899     0.005352     1.154187      24.43
 H       2.751309     0.178041     0.889648      26.32
55
name = lig-Water-frame_207
 C      -1.406613     2.172776     2.916432      37.55
 H      -2.306545     2.864042     2.720591      24.71
 C      -0.746638    -0.226976     3.612217      67.97
 H      -1.280623    -1.200831     3.613082      29.32
 C       0.544585     0.267526     3.720868      21.82
 O       1.634701    -0.567105     4.086101     144.82
 C       1.301099    -2.070853     4.088923      96.28
 H       2.401526    -2.373268     4.307698      25.97
 H       1.190644    -2.673443     3.074306      27.20
 H       0.551585    -2.254745     5.018395      25.65
 C       0.871600     1.606550     3.476722      30.37
 O       2.257656     1.928435     3.586407     175.41
 H       2.419802     2.925622     3.645642      27.41
 C      -0.085266     2.616844     3.066984      57.44
 H       0.455553     3.642848     2.666917      18.76
 C      -1.637625     0.749311     3.071360      30.63
 C      -3.182629     0.452598     2.720860      79.27
 H      -3.861422     1.499800     2.800788      25.29
 O      -3.924026    -0.740186     3.256494     212.85
 H      -4.681951    -1.030146     2.623284      25.72
 C      -3.249518     0.312291     1.221703     100.75
 H      -2.828654     1.131009     0.880270      27.72
 C      -4.730754     0.404199     0.532766     111.96
 O      -5.562599    -0.484664     1.075824     233.91
 H      -5.229775    -1.325564     0.673478      25.43
 H      -4.544140     0.361997    -0.559889      28.03
 H      -5.169502     1.248005     0.660726      30.38
 C       0.781033     0.067852    -0.728274      40.99
 H       1.488015     0.922815    -0.845959      23.57
 C       0.253436    -2.247885    -1.177300      71.49
 H       0.477922    -3.235268    -1.595873      24.35
 C      -1.049556    -2.041060    -0.740159      11.20
 O      -1.962861    -3.065590    -0.891342     194.61
 C      -1.821114    -3.970497    -2.038377      93.03
 H      -2.945036    -4.392501    -2.213416      23.64
 H      -1.519444    -3.218504    -2.872528      24.80
 H      -1.108128    -5.015110    -2.004770      22.13
 C      -1.463671    -0.871631    -0.151552       7.68
 O      -2.672520    -0.896943     0.669221      85.06
 C      -0.567743     0.244229    -0.308983      86.40
 H      -0.976159     1.151448     0.002558      27.38
 C       1.238120    -1.212618    -1.115109       1.23
 C       2.709196    -1.408240    -1.474885     109.05
 H       3.048892    -2.636372    -1.747745      23.50
 O       3.155257    -0.689754    -2.632697     226.69
 H       4.102936    -0.715135    -2.885863      28.73
 C       3.645546    -1.272054    -0.337146      93.97
 H       3.408270    -1.900263     0.410626      30.58
 O       4.964187    -1.967516    -0.394983     121.67
 H       5.543214    -1.554746    -1.144266      26.11
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 C       3.805669     0.110816     0.410704      97.09
 O       4.296826     1.029926    -0.466004     330.20
 H       4.502290     1.748408     0.164544      27.82
 H       4.473925    -0.217269     1.353038      25.51
 H       2.801363     0.313460     0.927913      27.32
55
name = lig-Water-frame_208
 C      -1.429501     2.176745     2.891387      88.29
 H      -2.095634     3.077175     2.530724      28.42
 C      -0.771090    -0.204939     3.556151      47.98
 H      -1.012979    -1.279815     3.957298      23.84
 C       0.584228     0.331346     3.709273       4.93
 O       1.626461    -0.592188     4.102749     112.56
 C       1.388100    -2.128488     4.023186     118.60
 H       2.301957    -2.294314     4.634531      27.04
 H       1.116615    -2.522810     3.104174      31.84
 H       0.832703    -2.286859     4.838801      30.95
 C       0.899006     1.648661     3.404072      19.39
 O       2.349663     1.930847     3.563423     225.09
 H       2.082722     2.899733     3.394080      27.66
 C      -0.098022     2.589068     3.101324      24.53
 H       0.244481     3.500832     2.880483      13.87
 C      -1.653245     0.809665     3.124256      33.08
 C      -3.194770     0.416914     2.718364      90.98
 H      -3.898272     1.286191     2.821134      27.69
 O      -3.872584    -0.746829     3.257655     191.24
 H      -4.708040    -0.908910     2.784915      25.96
 C      -3.245978     0.309622     1.223149      76.25
 H      -2.649516     1.302114     0.768338      26.07
 C      -4.661799     0.437571     0.475922      80.39
 O      -5.599507    -0.509578     1.105739     184.51
 H      -5.407035    -1.447364     0.683406      25.08
 H      -4.497131     0.195426    -0.579182      28.38
 H      -5.207810     1.575823     0.783805      24.45
 C       0.778597     0.071214    -0.697014      36.61
 H       1.509892     0.875056    -0.768539      20.81
 C       0.237002    -2.220652    -1.189686      61.14
 H       0.491144    -3.216367    -1.511136      27.10
 C      -1.049674    -2.103263    -0.713767      12.26
 O      -2.005438    -3.088911    -0.915506     244.19
 C      -1.861974    -3.908032    -2.016869     123.49
 H      -2.979317    -4.162257    -2.454665      23.92
 H      -1.472395    -3.375699    -2.843604      28.63
 H      -1.113319    -4.559108    -1.919284      28.17
 C      -1.494630    -0.840512    -0.149445      25.15
 O      -2.634080    -0.921907     0.644669      52.54
 C      -0.692840     0.188306    -0.289017      72.58
 H      -1.027416     1.294075    -0.008098      24.41
 C       1.260772    -1.185416    -1.099332      18.82
 C       2.684038    -1.429919    -1.474478     115.43
 H       2.836876    -2.380983    -1.752581      26.66
 O       3.110873    -0.684100    -2.676788     203.18
 H       4.123043    -0.939137    -2.473060      21.30
 C       3.645794    -1.241834    -0.325760      73.73
 H       3.287302    -2.076576     0.500725      25.55
 O       5.002681    -1.957103    -0.413412     124.36
 H       5.375562    -1.618384    -1.336349      27.14
 C       3.771144     0.068260     0.378969     108.23
 O       4.275141     0.986245    -0.471477     345.99
 H       4.600296     1.790225     0.049285      28.26
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 H       4.297141    -0.201641     1.319547      26.08
 H       2.843533     0.555187     0.864244      24.47
55
name = lig-Water-frame_209
 C      -1.407244     2.190307     2.875170      73.90
 H      -2.021980     2.931319     2.460178      26.82
 C      -0.754335    -0.130244     3.516286      48.76
 H      -0.818685    -1.034100     4.017423      24.78
 C       0.602538     0.285653     3.703667       5.41
 O       1.604331    -0.604914     4.096842     155.43
 C       1.511912    -2.110468     4.023893      97.05
 H       2.402991    -2.562395     4.502218      26.46
 H       1.116275    -2.430724     2.957891      28.26
 H       0.529977    -2.495548     4.737726      24.97
 C       0.981852     1.659844     3.360541      18.53
 O       2.367126     1.958891     3.527161     224.03
 H       2.537474     2.892841     3.161103      25.37
 C      -0.085913     2.547106     3.127143      29.97
 H       0.049151     3.763326     3.044427      19.75
 C      -1.791961     0.829474     3.178635      38.91
 C      -3.192739     0.372650     2.699836      80.52
 H      -3.945662     1.305984     3.031489      26.14
 O      -3.805436    -0.764177     3.291873     165.75
 H      -4.709334    -0.624195     2.841690      24.51
 C      -3.236031     0.356819     1.124072      96.57
 H      -2.653566     1.103942     0.819851      29.92
 C      -4.587956     0.499979     0.484637      92.25
 O      -5.651895    -0.553605     1.127327     199.94
 H      -5.535261    -1.401799     0.717998      28.55
 H      -4.532732     0.142041    -0.607028      28.13
 H      -4.905126     1.418148     0.639038      31.07
 C       0.719408     0.067347    -0.670121      45.75
 H       1.319249     0.981376    -0.636084      23.28
 C       0.261245    -2.205669    -1.197244      53.86
 H       0.642255    -3.222824    -1.517461      24.98
 C      -1.062257    -2.149058    -0.695768       9.91
 O      -2.068618    -3.090064    -0.897098     208.87
 C      -1.909374    -3.830258    -2.064427      92.37
 H      -2.931519    -4.237934    -2.428858      24.89
 H      -1.412099    -3.309661    -2.965028      25.60
 H      -1.025125    -4.717691    -1.696184      22.28
 C      -1.545755    -0.883540    -0.131829      15.32
 O      -2.612988    -0.942429     0.628013      74.61
 C      -0.695396     0.242589    -0.283883      77.85
 H      -0.964881     1.167428    -0.015270      27.49
 C       1.224674    -1.158186    -1.080657      42.00
 C       2.660711    -1.443333    -1.498216      75.06
 H       2.568984    -2.704856    -1.849600      23.07
 O       3.078917    -0.682498    -2.707165     203.43
 H       4.062589    -0.810118    -2.644612      24.27
 C       3.637432    -1.294184    -0.223459      91.76
 H       2.948967    -1.771385     0.427784      28.05
 O       5.029428    -1.924647    -0.466940     174.40
 H       5.290550    -1.695991    -1.318008      31.51
 C       3.703529     0.007741     0.414185      93.90
 O       4.297721     0.990969    -0.509266     302.37
 H       4.682429     1.886792    -0.146113      26.71
 H       4.462421    -0.055865     1.348888      23.94
 H       2.736115     0.536077     0.692714      23.45
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name = lig-Water-frame_210
 C      -1.378668     2.143596     2.889653      41.56
 H      -2.235952     2.891085     2.382122      22.31
 C      -0.723976    -0.011795     3.503485      36.92
 H      -1.005729    -1.099303     3.983181      20.93
 C       0.615205     0.240831     3.667258      20.30
 O       1.600076    -0.622381     4.092619     214.21
 C       1.542409    -2.081264     4.049406     134.81
 H       2.474764    -2.732052     4.127842      27.56
 H       1.466623    -2.293496     3.002602      31.77
 H       0.702929    -2.507686     4.350281      31.51
 C       1.076192     1.635197     3.352993      -1.50
 O       2.363627     2.007542     3.475347     214.21
 H       2.992960     2.689058     3.049611      20.36
 C      -0.042128     2.572046     3.133890      46.92
 H       0.026211     3.599108     3.213095      23.72
 C      -1.912995     0.826645     3.209564      43.51
 C      -3.189674     0.383697     2.678736      83.14
 H      -3.836717     1.218183     3.073786      27.28
 O      -3.748467    -0.784580     3.325724     177.14
 H      -4.717865    -0.608219     3.052938      23.51
 C      -3.221053     0.359074     1.042100      81.83
 H      -2.492698     1.253273     0.708393      24.06
 C      -4.544970     0.459729     0.489737      88.90
 O      -5.690576    -0.545542     1.149139     189.96
 H      -5.433238    -1.418309     0.635851      24.18
 H      -4.574379     0.305615    -0.534246      28.51
 H      -4.935565     1.678388     0.588906      25.16
 C       0.619927     0.097018    -0.643196      55.84
 H       1.139214     1.072783    -0.570646      24.92
 C       0.285014    -2.228296    -1.188409      61.87
 H       0.709135    -3.111158    -1.576775      24.91
 C      -1.074820    -2.144839    -0.685833      19.22
 O      -2.137159    -3.068234    -0.862675     189.57
 C      -1.892320    -3.817354    -2.129847     106.71
 H      -2.897548    -4.524143    -2.251621      23.93
 H      -1.493970    -3.177717    -2.898269      27.42
 H      -1.435786    -4.662569    -1.876035      27.24
 C      -1.512349    -0.937406    -0.141328       6.35
 O      -2.649833    -0.952376     0.638525      56.70
 C      -0.643606     0.267737    -0.288522      62.53
 H      -0.980062     1.339988     0.097846      24.01
 C       1.166303    -1.137045    -1.075605      41.54
 C       2.642648    -1.484784    -1.541490      88.99
 H       2.524524    -2.462549    -1.731879      27.77
 O       3.043642    -0.690433    -2.721626     237.75
 H       4.035741    -0.596359    -3.014513      26.17
 C       3.609920    -1.384084    -0.175606      73.38
 H       2.874595    -1.912066     0.612633      27.15
 O       5.011473    -1.895813    -0.484259     137.22
 H       5.213411    -1.582816    -1.503277      25.18
 C       3.694712     0.045464     0.467754      96.28
 O       4.336315     0.999440    -0.571155     282.78
 H       4.578639     1.788935    -0.072292      27.32
 H       4.368784     0.011328     1.292226      28.58
 H       2.619816     0.238717     0.711333      27.94
55
name = lig-Water-frame_211
 C      -1.405220     2.095281     2.910474      39.65
 H      -2.054402     2.780012     2.593965      27.53
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 C      -0.772109     0.023151     3.540118      63.28
 H      -1.120209    -0.909046     3.674231      26.35
 C       0.657665     0.258722     3.607672      -8.33
 O       1.625170    -0.640252     4.110855     138.17
 C       1.567534    -2.054584     3.988282     109.68
 H       2.510698    -2.471529     4.283378      26.62
 H       1.681905    -2.202232     2.814916      27.77
 H       0.568849    -2.640424     4.411908      22.26
 C       1.091550     1.626429     3.343613     -25.84
 O       2.392966     2.029451     3.449003     245.99
 H       2.933795     2.640809     2.766879      18.71
 C       0.009589     2.557076     3.134438      39.51
 H       0.265141     3.705324     3.226412      23.15
 C      -1.868812     0.842613     3.216615      80.16
 C      -3.201408     0.406508     2.649593      78.85
 H      -3.952607     1.314562     2.895609      26.55
 O      -3.705629    -0.794152     3.351167     228.22
 H      -4.652221    -0.875504     3.333290      24.97
 C      -3.165339     0.340988     1.025684      90.11
 H      -2.658183     1.205157     0.613558      28.93
 C      -4.607703     0.445295     0.496427      93.27
 O      -5.685005    -0.500628     1.144603     250.16
 H      -5.339117    -1.345591     0.731782      26.73
 H      -4.630359     0.358276    -0.673025      26.29
 H      -4.956257     1.408084     0.712837      29.02
 C       0.601161     0.154337    -0.649094      36.79
 H       1.210148     1.035661    -0.653525      27.00
 C       0.277867    -2.250417    -1.158268      66.63
 H       0.669617    -3.178241    -1.684091      21.84
 C      -1.082409    -2.136288    -0.697726       8.01
 O      -2.176463    -3.053436    -0.847697     153.41
 C      -1.930093    -3.829069    -2.146173      84.97
 H      -2.955394    -4.352339    -2.335454      24.49
 H      -1.630601    -3.118662    -2.950822      26.76
 H      -1.188489    -4.882698    -2.047795      23.51
 C      -1.437310    -0.921283    -0.137965       3.74
 O      -2.693976    -0.952921     0.643966      55.19
 C      -0.697018     0.260194    -0.244109      89.89
 H      -0.930812     1.220797     0.103075      29.39
 C       1.126611    -1.122597    -1.096580      19.51
 C       2.635600    -1.456128    -1.530585      73.41
 H       2.659219    -2.721222    -1.836439      23.51
 O       2.988295    -0.698236    -2.735054     207.65
 H       4.000831    -0.612139    -3.081180      25.88
 C       3.570911    -1.444909    -0.168826      73.81
 H       3.356471    -2.205161     0.588263      27.89
 O       4.959343    -1.873939    -0.497126     171.64
 H       5.062015    -1.445370    -1.365697      29.31
 C       3.707335     0.089861     0.447945      89.39
 O       4.353252     0.983173    -0.607096     247.65
 H       4.479776     1.821727     0.011173      24.55
 H       4.331779     0.050927     1.508409      27.78
 H       2.606615     0.140085     0.811218      29.97
55
name = lig-Water-frame_212
 C      -1.361592     2.127803     2.954276      56.23
 H      -2.122099     3.094137     2.726139      23.74
 C      -0.798051    -0.010784     3.595197      40.05
 H      -1.121922    -1.184237     3.478316      29.93
 C       0.677401     0.294159     3.559531     -30.75
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 O       1.649011    -0.623967     4.138881     136.35
 C       1.569294    -2.056029     3.869586     119.19
 H       2.445320    -2.189866     4.691396      22.79
 H       1.678214    -2.286389     2.834555      28.36
 H       0.817348    -2.498193     4.394455      24.88
 C       1.053567     1.627972     3.327460      -4.13
 O       2.449179     2.030688     3.428713     215.26
 H       2.443425     2.649686     2.706530      27.08
 C       0.030383     2.529045     3.126738      61.17
 H       0.444902     3.548504     3.026741      26.44
 C      -1.765866     0.856675     3.190752      25.62
 C      -3.233038     0.435457     2.635810      86.79
 H      -4.031121     1.286231     2.590692      24.54
 O      -3.643775    -0.788001     3.369582     269.50
 H      -4.632722    -0.995951     3.473560      23.53
 C      -3.181257     0.291539     1.059302      93.58
 H      -2.706761     1.197106     0.547603      26.70
 C      -4.708649     0.408042     0.498474      79.96
 O      -5.635661    -0.433945     1.117250     257.57
 H      -5.398425    -1.380670     0.912440      27.55
 H      -4.695845     0.315079    -0.541972      27.49
 H      -5.146423     1.535020     0.916934      24.80
 C       0.650838     0.177832    -0.698210      33.47
 H       1.375686     1.030924    -0.791018      26.73
 C       0.243376    -2.277474    -1.133712      64.89
 H       0.515673    -3.166219    -1.645432      24.38
 C      -1.082374    -2.139838    -0.722682      -1.97
 O      -2.166089    -3.055771    -0.865367     173.75
 C      -1.970589    -3.888105    -2.126666     108.64
 H      -3.120083    -4.010637    -2.527847      23.24
 H      -1.736836    -3.165388    -2.959911      28.04
 H      -1.160777    -4.446806    -2.159186      28.09
 C      -1.435762    -0.888674    -0.085059      11.41
 O      -2.690487    -0.950119     0.616955      75.26
 C      -0.748014     0.247036    -0.186008      78.69
 H      -1.083076     1.232379     0.213575      27.37
 C       1.116583    -1.114723    -1.131483      11.48
 C       2.613954    -1.470562    -1.488215      91.91
 H       2.790208    -2.400024    -1.859226      28.53
 O       2.929888    -0.697061    -2.745602     244.54
 H       3.856246    -0.844397    -2.763546      30.24
 C       3.588311    -1.433177    -0.189807      94.29
 H       3.436166    -2.146706     0.589266      28.45
 O       4.892847    -1.856414    -0.514937     179.87
 H       5.180930    -1.357427    -1.324172      29.01
 C       3.720753     0.068341     0.425604     111.57
 O       4.341739     0.955791    -0.587384     283.09
 H       4.480558     1.894260    -0.254406      26.18
 H       4.251670     0.094366     1.312222      31.52
 H       2.743451     0.502065     0.732766      30.13
55
name = lig-Water-frame_213
 C      -1.290247     2.289457     3.001246      68.53
 H      -1.975432     2.974945     2.890836      27.29
 C      -0.753928    -0.135141     3.622574      40.11
 H      -0.903003    -1.127588     3.553264      31.02
 C       0.649838     0.280677     3.564601     -17.68
 O       1.644611    -0.560633     4.135698     142.05
 C       1.621941    -2.031874     3.819407     119.60
 H       2.270079    -2.332036     4.592159      27.09
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 H       1.745148    -2.471544     2.759673      26.56
 H       0.618925    -2.503169     4.348351      23.55
 C       1.046011     1.593738     3.338125      29.36
 O       2.466543     2.013985     3.396490     122.03
 H       2.253040     2.858589     2.804217      24.64
 C       0.026844     2.519596     3.092453      73.38
 H       0.384583     3.543760     2.824805      25.93
 C      -1.729887     0.860278     3.134309     -39.18
 C      -3.232358     0.450963     2.624536      94.13
 H      -4.014137     1.304642     2.728264      24.04
 O      -3.570775    -0.766545     3.384196     254.08
 H      -4.568010    -0.806198     3.421824      24.73
 C      -3.280679     0.251711     1.099415      93.20
 H      -2.741893     1.152575     0.617269      25.30
 C      -4.781441     0.425185     0.536492     105.02
 O      -5.609985    -0.399150     1.106794     274.11
 H      -5.438624    -1.401145     1.015661      25.37
 H      -4.780199     0.332196    -0.611817      25.71
 H      -5.081609     1.418269     0.810796      27.76
 C       0.681969     0.158653    -0.759753      54.25
 H       1.329342     1.002931    -0.868792      25.93
 C       0.200114    -2.278470    -1.122018      55.93
 H       0.509864    -3.237025    -1.594955      24.41
 C      -1.101221    -2.126452    -0.727567       5.04
 O      -2.119494    -3.069324    -0.901686     221.93
 C      -2.070497    -3.852371    -2.127084     100.16
 H      -3.034151    -4.185873    -2.428332      25.34
 H      -1.739160    -3.130121    -2.890827      28.05
 H      -0.980396    -4.551751    -2.127552      23.05
 C      -1.501920    -0.911433    -0.020996      14.89
 O      -2.659162    -0.954013     0.573403      89.04
 C      -0.682712     0.283841    -0.152274      58.88
 H      -1.206233     1.193448     0.315850      25.44
 C       1.120352    -1.130168    -1.153161      31.68
 C       2.556867    -1.449473    -1.431624      66.70
 H       2.715082    -2.656391    -1.868522      23.70
 O       2.882317    -0.692802    -2.729415     190.54
 H       3.917679    -0.971296    -2.643970      23.60
 C       3.606801    -1.326314    -0.220703     100.18
 H       3.012503    -1.854418     0.684355      26.60
 O       4.853393    -1.852587    -0.553570     193.51
 H       5.424032    -1.323357    -1.268575      26.06
 C       3.706877     0.048818     0.384209     101.43
 O       4.335512     0.917342    -0.575219     274.07
 H       4.441287     1.864089    -0.331011      28.38
 H       4.485585     0.015991     1.367161      25.08
 H       2.875451     0.808733     0.578340      22.91
55
name = lig-Water-frame_214
 C      -1.270298     2.336700     3.059186      28.88
 H      -2.133142     3.206060     2.907740      20.52
 C      -0.704378    -0.181272     3.581705      45.90
 H      -0.873995    -1.364056     3.737437      25.81
 C       0.613122     0.227704     3.626423      24.14
 O       1.639471    -0.509291     4.098626     172.83
 C       1.617669    -2.012468     3.833029     123.08
 H       2.424195    -2.661208     4.425928      25.80
 H       1.887475    -2.374381     2.801984      28.08
 H       0.630461    -2.338249     3.919755      26.94
 C       1.069402     1.555932     3.359070      24.27
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 O       2.415193     1.993561     3.344524     142.92
 H       2.689007     2.969470     3.154545      25.36
 C       0.088474     2.568986     3.046057      50.52
 H       0.306127     3.650638     2.690654      24.41
 C      -1.702857     0.869066     3.083197     -27.10
 C      -3.174063     0.456693     2.630987     102.13
 H      -3.830867     1.303331     3.173735      22.89
 O      -3.510236    -0.725926     3.395229     248.71
 H      -4.449987    -0.637060     3.347577      26.02
 C      -3.395855     0.252211     1.107799      97.20
 H      -2.854047     1.104415     0.743463      25.67
 C      -4.746161     0.460698     0.519010      96.76
 O      -5.673163    -0.432648     1.155469     239.35
 H      -5.297539    -1.308685     0.877476      25.89
 H      -4.791814     0.429987    -0.566857      25.41
 H      -5.069984     1.665972     0.756447      24.14
 C       0.650795     0.122732    -0.799227      47.88
 H       1.268428     1.041926    -0.921191      23.16
 C       0.191211    -2.254677    -1.134514      53.63
 H       0.567436    -3.229393    -1.483691      24.32
 C      -1.145636    -2.093920    -0.709443      10.65
 O      -2.081416    -3.089637    -0.922776     225.00
 C      -2.084416    -3.792550    -2.141576     110.33
 H      -3.007921    -4.673419    -2.153080      22.81
 H      -1.831574    -3.073657    -2.986562      27.29
 H      -1.509091    -4.608000    -2.056341      27.69
 C      -1.479660    -0.910115    -0.016795      10.68
 O      -2.687893    -0.961954     0.564495     108.79
 C      -0.588612     0.277655    -0.133988      57.86
 H      -0.940897     1.172285     0.254711      25.90
 C       1.098769    -1.175060    -1.146189      39.62
 C       2.512954    -1.458721    -1.436183      90.84
 H       2.451608    -2.486493    -1.504298      26.23
 O       2.871583    -0.710622    -2.673468     266.91
 H       3.816116    -0.750121    -2.967018      27.93
 C       3.534769    -1.191387    -0.247533      92.98
 H       2.969429    -1.699978     0.454129      28.89
 O       4.843312    -1.873569    -0.581405     213.12
 H       5.265479    -1.318252    -1.205438      31.26
 C       3.739596     0.112503     0.378347     113.76
 O       4.366157     0.879191    -0.608350     336.27
 H       4.370783     1.823478    -0.133505      24.49
 H       4.338713    -0.131251     1.183696      26.63
 H       2.787277     0.510279     0.718502      26.24
55
name = lig-Water-frame_215
 C      -1.320677     2.284593     3.099450      44.19
 H      -1.934675     3.101538     2.900001      17.11
 C      -0.716219    -0.180268     3.484259      56.75
 H      -1.045237    -1.123456     3.877331      25.69
 C       0.611017     0.213431     3.700146      22.36
 O       1.677629    -0.529109     4.069260     165.16
 C       1.623065    -1.986907     3.836469     132.03
 H       2.295286    -2.615232     4.403490      29.20
 H       1.998097    -1.974772     2.733873      26.49
 H       0.540351    -2.357416     3.759167      27.33
 C       1.064677     1.606803     3.349888      15.76
 O       2.378631     1.948845     3.305813     184.96
 H       2.780900     2.798516     3.379011      23.87
 C       0.165882     2.637036     3.004171      66.02
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 H       0.472482     3.611424     2.749949      26.79
 C      -1.651729     0.879673     3.054304      15.04
 C      -3.074239     0.474431     2.696905     126.23
 H      -3.623170     1.281100     3.165899      26.87
 O      -3.462441    -0.690593     3.410555     203.25
 H      -4.485750    -0.682629     3.331035      25.21
 C      -3.436031     0.292056     1.102771      74.22
 H      -2.798955     1.242018     0.689431      21.91
 C      -4.734642     0.525633     0.515986      98.09
 O      -5.751599    -0.483057     1.204970     187.48
 H      -5.309748    -1.291554     0.789961      25.33
 H      -4.727621     0.433740    -0.595211      25.72
 H      -5.025466     1.550254     0.763468      26.68
 C       0.606704     0.097857    -0.819561      48.68
 H       1.224846     0.968024    -0.982045      21.55
 C       0.187663    -2.231069    -1.148630      52.67
 H       0.547400    -3.208713    -1.414414      21.74
 C      -1.157219    -2.069533    -0.706303      15.90
 O      -2.072620    -3.098295    -0.901538     198.73
 C      -2.114347    -3.784495    -2.163946     111.66
 H      -3.013302    -4.344851    -2.030693      25.84
 H      -2.083138    -3.246204    -3.091946      28.58
 H      -1.396209    -4.808479    -2.095237      23.79
 C      -1.411646    -0.863170    -0.045484       7.90
 O      -2.769641    -0.957509     0.588982      79.52
 C      -0.525849     0.209501    -0.124597      70.10
 H      -0.625261     1.352027     0.233669      19.92
 C       1.056576    -1.196832    -1.129959      36.26
 C       2.514852    -1.420961    -1.460682      76.68
 H       2.488883    -2.725803    -1.447713      21.79
 O       2.853599    -0.731628    -2.629356     258.32
 H       3.716639    -0.692385    -3.020725      28.99
 C       3.433474    -1.123615    -0.305175      69.09
 H       3.087050    -1.930146     0.538507      24.01
 O       4.807217    -1.895904    -0.581473     104.76
 H       5.079571    -1.320934    -1.386956      26.78
 C       3.752943     0.175065     0.368079      80.83
 O       4.412596     0.896886    -0.638883     328.62
 H       4.535203     1.770696    -0.245573      25.40
 H       4.417432    -0.206575     1.345751      21.84
 H       2.715256     0.237275     0.906134      23.12
55
name = lig-Water-frame_216
 C      -1.277285     2.201378     3.099027      61.32
 H      -2.047816     3.043526     2.848409      22.50
 C      -0.726034    -0.118246     3.388833      38.56
 H      -1.272615    -1.011573     3.832342      26.76
 C       0.628312     0.269000     3.741384      12.69
 O       1.732591    -0.578369     4.079195     113.20
 C       1.605584    -1.947733     3.766769     146.04
 H       2.190127    -2.454125     4.628991      30.58
 H       2.089221    -1.785236     2.777272      26.68
 H       0.597981    -2.447247     3.784598      29.64
 C       1.022956     1.687977     3.332183      16.51
 O       2.389489     1.850339     3.281481     139.25
 H       2.555060     2.918317     3.425556      17.35
 C       0.151500     2.649154     2.996643      54.84
 H       0.714240     3.705016     2.851874      21.16
 C      -1.596374     0.886433     3.045243      31.83
 C      -2.989700     0.501319     2.753497     111.12
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 H      -3.691564     1.517286     2.954096      26.55
 O      -3.435301    -0.676619     3.442604     183.45
 H      -4.398296    -0.822614     3.276068      25.81
 C      -3.338145     0.372904     1.107598      72.95
 H      -2.833107     1.142717     0.633825      27.65
 C      -4.790518     0.543251     0.545540      73.59
 O      -5.798198    -0.511966     1.222277     152.19
 H      -5.534055    -1.451258     0.886086      24.89
 H      -4.698685     0.348139    -0.567955      25.45
 H      -5.172049     1.652388     0.880189      24.72
 C       0.625697     0.068763    -0.853980      59.96
 H       1.272577     0.924669    -1.033338      22.92
 C       0.154464    -2.246642    -1.153159      69.73
 H       0.497022    -3.283392    -1.451041      24.17
 C      -1.127684    -2.059954    -0.725373      20.81
 O      -2.073498    -3.080758    -0.858349     192.30
 C      -2.123251    -3.865703    -2.159988      97.33
 H      -3.382750    -3.940922    -2.069347      21.42
 H      -2.209870    -3.270092    -3.156947      26.67
 H      -1.316157    -4.446159    -2.304482      27.04
 C      -1.439624    -0.835911    -0.050217     -19.19
 O      -2.831875    -0.923567     0.611558      39.83
 C      -0.523102     0.211384    -0.087985      68.69
 H      -0.618848     1.132220     0.279346      28.03
 C       1.055251    -1.182836    -1.142064      21.30
 C       2.516158    -1.440218    -1.475033     105.39
 H       2.778586    -2.400097    -1.716359      24.02
 O       2.809051    -0.733272    -2.627285     247.09
 H       3.875435    -0.884836    -2.805905      23.67
 C       3.386359    -1.181890    -0.298267      86.07
 H       3.157932    -1.762705     0.493361      27.59
 O       4.745514    -1.882035    -0.590559     117.55
 H       5.022691    -1.680215    -1.590403      25.46
 C       3.750591     0.150745     0.399718      91.08
 O       4.453742     0.947202    -0.658185     325.94
 H       4.761192     1.949577    -0.417041      25.30
 H       4.432963     0.013813     1.142235      25.31
 H       2.861085     0.630704     0.834951      26.93
55
name = lig-Water-frame_217
 C      -1.185405     2.227687     3.041520      64.26
 H      -2.151980     2.795389     2.892988      25.40
 C      -0.658987    -0.078684     3.359376       2.07
 H      -1.252759    -1.045517     3.574544      27.57
 C       0.644486     0.350644     3.729536      29.57
 O       1.741529    -0.569251     4.117671     151.47
 C       1.611810    -1.936979     3.697403     130.07
 H       2.117223    -2.345645     4.622031      33.12
 H       2.161028    -2.199349     2.719813      30.08
 H       0.604211    -2.381882     3.736278      31.58
 C       1.017375     1.659888     3.342022      15.04
 O       2.417956     1.783634     3.274961     166.60
 H       2.468977     2.725932     3.203331      24.33
 C       0.083548     2.674169     3.015523      40.21
 H       0.447944     3.604956     2.915903      24.82
 C      -1.574467     0.890622     3.046967       3.20
 C      -2.996312     0.572785     2.744020     104.45
 H      -3.619499     1.379645     2.906071      30.76
 O      -3.411630    -0.669722     3.485340     202.69
 H      -4.288003    -0.839816     3.130968      28.16
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 C      -3.230083     0.425349     1.140507      60.78
 H      -2.670248     1.288530     0.461738      26.37
 C      -4.857246     0.511282     0.630333      82.60
 O      -5.815304    -0.517013     1.220489     169.43
 H      -5.594332    -1.420935     0.998157      27.37
 H      -4.824250     0.365799    -0.413453      27.83
 H      -5.391270     1.505699     0.896522      26.30
 C       0.669753     0.075789    -0.868560      76.13
 H       1.353307     0.931419    -1.024808      28.93
 C       0.153330    -2.293526    -1.163096     112.28
 H       0.417869    -3.242764    -1.521193      31.74
 C      -1.130356    -2.055132    -0.733049      20.54
 O      -2.076281    -3.056915    -0.821167     157.77
 C      -2.216327    -3.871451    -2.152100     103.10
 H      -3.163689    -4.187566    -2.195584      29.21
 H      -2.069872    -3.083103    -2.887092      28.94
 H      -1.236580    -4.563057    -2.414400      23.12
 C      -1.543997    -0.848303    -0.036038     -12.54
 O      -2.840298    -0.866201     0.614435      31.36
 C      -0.556764     0.223957    -0.064869      15.83
 H      -0.854466     1.225111     0.540088      30.51
 C       1.086558    -1.215531    -1.189762       3.29
 C       2.488096    -1.453403    -1.483411      81.59
 H       2.857879    -2.617575    -1.936679      22.31
 O       2.804281    -0.707201    -2.672476     218.79
 H       3.711024    -0.902067    -2.654945      27.53
 C       3.437563    -1.246971    -0.253076      82.72
 H       2.896329    -1.823348     0.712841      28.62
 O       4.675188    -1.866070    -0.616389     182.94
 H       4.973053    -1.948550    -1.490501      27.65
 C       3.744611     0.165927     0.377191      89.23
 O       4.491697     0.992958    -0.688087     274.18
 H       4.620473     1.904811    -0.253801      28.22
 H       4.637959     0.058844     1.212762      24.60
 H       3.065708     1.036148     0.657026      23.23
55
name = lig-Water-frame_219
 C      -1.278265     2.285091     2.884735      26.56
 H      -1.910988     3.316255     2.808525      20.58
 C      -0.576898    -0.064735     3.388057      73.84
 H      -0.436602    -1.222104     3.150837      26.90
 C       0.721259     0.307796     3.650645       9.87
 O       1.679287    -0.489287     4.130456     130.45
 C       1.615064    -1.976665     3.664331     106.92
 H       2.071030    -2.711501     4.442341      28.27
 H       1.995321    -2.182035     2.608611      31.19
 H       0.618837    -2.160238     3.612624      25.06
 C       1.130676     1.676564     3.347801      -5.92
 O       2.464270     1.742104     3.262788     163.29
 H       2.957354     2.520073     2.781335      22.94
 C       0.138521     2.699652     3.112883      63.48
 H       0.214350     3.700644     2.974726      29.70
 C      -1.564255     0.919373     3.068174      39.76
 C      -3.022377     0.621024     2.688847     108.16
 H      -3.581802     1.326550     3.059624      34.88
 O      -3.374543    -0.608885     3.493714     236.20
 H      -4.236884    -0.950680     3.177221      28.24
 C      -3.278701     0.484057     1.190364      73.37
 H      -2.748138     1.478862     0.685207      28.94
 C      -4.912967     0.437187     0.813882     105.04
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 O      -5.782459    -0.535201     1.252586     222.25
 H      -5.413409    -1.394571     0.970259      27.54
 H      -4.920183     0.466850    -0.216536      30.62
 H      -5.293611     1.507865     1.223734      27.84
 C       0.616381     0.075670    -0.742382      41.67
 H       1.332691     0.925755    -0.815163      31.13
 C       0.148525    -2.323632    -1.188111      42.10
 H       0.373770    -3.269248    -1.599667      22.67
 C      -1.224990    -2.075653    -0.706391     -19.05
 O      -2.174077    -3.118387    -0.762261     166.49
 C      -2.259884    -3.773773    -2.094985     105.41
 H      -3.085364    -4.287719    -2.180234      30.23
 H      -2.192345    -3.076088    -2.939916      29.08
 H      -1.432120    -4.638714    -2.037319      22.98
 C      -1.571670    -0.855500    -0.065861      26.89
 O      -2.770168    -0.754619     0.599194      64.22
 C      -0.641237     0.199537    -0.110137      87.26
 H      -0.787653     1.188674     0.466119      34.13
 C       1.037708    -1.239290    -1.255828     -36.68
 C       2.501866    -1.513132    -1.552071      79.78
 H       2.422680    -2.808950    -1.684915      24.52
 O       2.840426    -0.648311    -2.756138     137.49
 H       3.796696    -0.445463    -3.107210      23.68
 C       3.436371    -1.251064    -0.218155      58.25
 H       2.923176    -1.945875     0.657907      30.95
 O       4.644490    -1.930060    -0.571527     135.70
 H       4.637457    -1.723072    -1.538510      25.23
 C       3.864073     0.264097     0.235704     115.74
 O       4.543420     0.993155    -0.739039     243.97
 H       4.731773     1.997924    -0.452641      24.27
 H       4.417284    -0.050718     1.286616      28.54
 H       2.841666     0.575217     0.676583      31.58
55
name = lig-Water-frame_220
 C      -1.269738     2.330881     2.865887      60.18
 H      -1.869595     3.103866     2.674386      26.58
 C      -0.573851    -0.064772     3.381884      71.04
 H      -0.746498    -1.026531     3.098993      30.11
 C       0.754408     0.309961     3.603439     -16.83
 O       1.687815    -0.522093     4.117000     113.57
 C       1.601897    -1.993857     3.670163      92.53
 H       2.069885    -2.584253     4.372980      26.98
 H       1.954146    -1.590093     2.675355      27.21
 H       0.444196    -2.392826     3.680564      22.75
 C       1.162297     1.768266     3.330693     -19.36
 O       2.547968     1.753897     3.252490     225.55
 H       2.825115     2.516524     2.807428      26.12
 C       0.167955     2.665113     3.149864      65.26
 H       0.616363     3.790470     3.028597      26.36
 C      -1.601868     0.940719     3.048332      29.14
 C      -3.003360     0.559440     2.717590      85.58
 H      -3.687947     1.639897     3.050026      25.32
 O      -3.359907    -0.579146     3.463104     226.86
 H      -4.254644    -0.910713     3.366133      26.35
 C      -3.409349     0.487576     1.210633      94.47
 H      -3.011644     1.305912     0.788083      29.99
 C      -4.854403     0.509915     0.868675     100.96
 O      -5.752591    -0.599763     1.308145     189.48
 H      -5.527889    -1.522955     0.969519      25.59
 H      -4.884045     0.583126    -0.324431      26.28
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 H      -5.165754     1.473334     1.372206      28.30
 C       0.566892     0.009606    -0.672284      46.75
 H       1.190789     0.879257    -0.655312      28.09
 C       0.061869    -2.296234    -1.192627      36.87
 H       0.393218    -3.310174    -1.564992      20.82
 C      -1.243850    -2.125985    -0.699136      -2.00
 O      -2.251991    -3.153194    -0.735373     219.34
 C      -2.234811    -3.752209    -2.034307      92.92
 H      -3.527677    -3.998029    -2.026238      21.11
 H      -2.263450    -3.292367    -3.073720      26.74
 H      -1.322672    -4.314733    -2.075691      24.06
 C      -1.518071    -0.847260    -0.100530       6.71
 O      -2.748645    -0.720860     0.598035      61.29
 C      -0.642543     0.188854    -0.160528     104.36
 H      -0.794880     1.206292     0.289311      28.73
 C       0.991001    -1.173399    -1.250921      17.06
 C       2.496367    -1.509709    -1.558069      93.87
 H       2.729403    -2.455663    -1.836946      29.21
 O       2.857279    -0.642432    -2.789977     202.58
 H       3.758509    -0.543504    -2.957960      31.14
 C       3.392644    -1.205739    -0.280988      81.48
 H       3.085649    -1.617764     0.610975      29.73
 O       4.684611    -1.998416    -0.555135     117.81
 H       4.866680    -1.643345    -1.432216      29.23
 C       3.862115     0.215913     0.211976     116.28
 O       4.573046     0.976639    -0.775138     270.37
 H       4.736482     1.902190    -0.456518      26.33
 H       4.506087     0.183512     1.014521      29.66
 H       2.838216     0.550481     0.521060      29.33
55
name = lig-Water-frame_221
 C      -1.166443     2.331857     2.901293      58.39
 H      -2.111080     3.029819     2.495323      22.50
 C      -0.598102    -0.018927     3.347793      17.37
 H      -1.245122    -1.045712     3.226270      24.31
 C       0.761294     0.375851     3.557091       1.58
 O       1.702004    -0.567689     4.123271     148.49
 C       1.536819    -1.958651     3.655821      63.46
 H       2.429557    -2.495751     4.287956      21.10
 H       1.990438    -1.786868     2.697947      28.65
 H       0.665758    -2.451835     3.697590      29.44
 C       1.186455     1.716438     3.341705     -10.66
 O       2.634315     1.792903     3.242783     175.75
 H       2.800954     2.797781     2.870628      21.72
 C       0.177451     2.701696     3.147098      69.70
 H       0.732474     3.581532     3.060446      23.76
 C      -1.599037     0.987159     3.009207      17.94
 C      -3.044218     0.555774     2.747047     113.24
 H      -3.550580     1.357292     2.984353      30.64
 O      -3.342898    -0.581764     3.454501     204.19
 H      -4.383358    -0.652293     3.421690      23.98
 C      -3.468526     0.438351     1.247385      82.84
 H      -3.039122     1.368017     0.725198      23.33
 C      -4.818202     0.555680     0.870684     101.73
 O      -5.717625    -0.645332     1.380206     177.76
 H      -5.491562    -1.542035     0.898619      24.19
 H      -4.974715     0.741664    -0.121715      30.00
 H      -5.324179     1.454283     1.543024      25.97
 C       0.601385    -0.028491    -0.644896      44.47
 H       1.223037     0.875115    -0.565114      23.19
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 C      -0.006023    -2.260159    -1.212060      59.62
 H       0.385801    -3.226200    -1.507643      22.48
 C      -1.267034    -2.167518    -0.672805      10.95
 O      -2.302270    -3.128562    -0.704969     242.92
 C      -2.299780    -3.757001    -2.003477     101.14
 H      -3.184568    -4.162427    -1.980080      27.02
 H      -2.192677    -3.042168    -2.852752      28.20
 H      -1.409368    -4.506711    -2.152622      24.80
 C      -1.548725    -0.856060    -0.106811       6.83
 O      -2.743255    -0.716322     0.588422     124.83
 C      -0.679530     0.223774    -0.183894      74.58
 H      -0.972433     1.174160     0.177589      23.90
 C       0.960316    -1.189933    -1.242646      42.21
 C       2.473073    -1.410785    -1.556461      74.50
 H       2.921293    -2.519805    -1.999011      23.02
 O       2.854118    -0.647114    -2.807083     152.86
 H       3.916903    -0.786606    -2.699824      23.53
 C       3.429265    -1.163055    -0.365632      84.63
 H       2.952264    -1.530713     0.679252      25.06
 O       4.712270    -2.054507    -0.547769      57.28
 H       5.413999    -1.714326    -1.299277      23.41
 C       3.824653     0.160866     0.162054     102.51
 O       4.603445     0.950480    -0.841505     218.11
 H       4.584945     1.875530    -0.205959      22.38
 H       4.634467     0.180246     1.044579      23.02
 H       2.940401     0.855515     0.410441      21.59
55
name = lig-Water-frame_222
 C      -1.108106     2.344227     2.929105      60.21
 H      -1.810431     2.955208     2.575602      26.85
 C      -0.676500     0.043103     3.292646      40.57
 H      -1.061668    -0.866089     3.623403      26.60
 C       0.745989     0.374254     3.539851      16.94
 O       1.681451    -0.582816     4.127234     185.74
 C       1.577230    -1.912168     3.643445     102.59
 H       2.383370    -2.345803     4.055155      26.45
 H       1.872477    -2.350933     2.526147      26.37
 H       0.538132    -2.543886     3.796965      26.54
 C       1.220837     1.614093     3.355013       3.54
 O       2.684510     1.878032     3.227299     159.67
 H       2.904930     2.840617     3.127776      27.53
 C       0.225725     2.724618     3.125967      61.03
 H       0.585481     3.828021     2.978795      19.57
 C      -1.539432     1.018059     2.970628      31.72
 C      -3.051881     0.578107     2.729771      93.65
 H      -3.827364     1.510447     3.235450      23.89
 O      -3.361887    -0.622633     3.479074     205.62
 H      -4.310223    -0.457529     3.440077      28.58
 C      -3.378772     0.399783     1.262280      89.71
 H      -2.900275     1.319471     0.784336      23.77
 C      -4.901676     0.552650     0.914089     100.39
 O      -5.671895    -0.659155     1.443106     206.54
 H      -5.367509    -1.411557     0.945911      28.19
 H      -5.146064     0.843646    -0.216286      27.21
 H      -5.332686     1.343281     1.481369      29.24
 C       0.647816     0.015066    -0.627312      26.47
 H       1.412733     0.798954    -0.594789      22.60
 C      -0.024548    -2.248838    -1.246821      64.45
 H       0.320453    -3.229065    -1.579933      24.27
 C      -1.312634    -2.157257    -0.619641      22.07
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 O      -2.321360    -3.078792    -0.669667     192.16
 C      -2.333073    -3.769728    -1.994785      80.90
 H      -3.316229    -4.662086    -2.116835      22.09
 H      -2.193261    -2.815226    -2.534535      25.23
 H      -1.712494    -4.686648    -2.127099      23.87
 C      -1.629800    -0.855785    -0.091195      12.90
 O      -2.780047    -0.746487     0.581444     170.24
 C      -0.724797     0.241647    -0.201613      57.75
 H      -1.196516     1.292346     0.146820      21.18
 C       0.964185    -1.264688    -1.227994      30.41
 C       2.458481    -1.340496    -1.599253     100.08
 H       2.566662    -2.378278    -1.731265      28.79
 O       2.872086    -0.652609    -2.798605     222.12
 H       3.856029    -0.881736    -2.785833      25.11
 C       3.492082    -1.162459    -0.407242      86.26
 H       2.883990    -1.693566     0.297469      28.19
 O       4.736395    -2.086436    -0.545251     165.30
 H       5.529052    -1.792485    -0.967359      27.49
 C       3.834638     0.170772     0.101739     125.47
 O       4.629196     0.945568    -0.885985     250.92
 H       4.647460     1.774378    -0.506924      29.77
 H       4.325357    -0.118100     1.010172      27.89
 H       3.103651     0.960415     0.406920      22.64
55
name = lig-Water-frame_223
 C      -1.041285     2.370409     2.945324      64.55
 H      -1.730105     3.343669     2.632935      19.55
 C      -0.663706     0.074572     3.291932      54.41
 H      -0.829224    -0.902928     3.903760      25.05
 C       0.707058     0.294168     3.545560      17.21
 O       1.630164    -0.574808     4.096637     205.57
 C       1.609840    -1.943923     3.590273     116.23
 H       2.476717    -2.495089     4.225835      25.79
 H       1.534566    -2.273093     2.606388      30.84
 H       0.752942    -2.305459     4.058657      29.19
 C       1.283088     1.639555     3.333140      -3.60
 O       2.692503     1.941083     3.232738      80.71
 H       2.870874     2.927614     3.218776      30.63
 C       0.322226     2.717047     3.098108      56.01
 H       0.314181     3.806602     2.935338      20.95
 C      -1.541732     1.044204     2.929069      40.95
 C      -3.038027     0.647602     2.749342     111.94
 H      -3.618408     1.305501     3.091307      31.46
 O      -3.392373    -0.660038     3.511260     171.80
 H      -4.382874    -0.569872     3.537759      28.33
 C      -3.277824     0.413731     1.226189      91.89
 H      -2.803409     1.279299     0.815736      25.84
 C      -4.994225     0.496946     0.950803      92.75
 O      -5.620789    -0.631485     1.495269     212.58
 H      -5.217699    -1.485761     1.014194      24.17
 H      -5.179473     0.641452    -0.084540      29.33
 H      -5.317799     1.541557     1.599599      26.74
 C       0.633644     0.057595    -0.626009      35.35
 H       1.458528     0.756006    -0.658647      24.32
 C      -0.035206    -2.280747    -1.270586      42.43
 H       0.158450    -3.276528    -1.766740      23.20
 C      -1.328643    -2.098125    -0.581506       7.14
 O      -2.343167    -3.062115    -0.627731     188.66
 C      -2.415233    -3.828516    -1.973848     100.41
 H      -3.276915    -4.236763    -2.161020      29.31
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 H      -2.308091    -2.987385    -2.712626      26.89
 H      -1.536200    -4.538506    -2.046879      25.66
 C      -1.673897    -0.830287    -0.077274      11.69
 O      -2.872444    -0.799581     0.596220     172.81
 C      -0.748714     0.260194    -0.217695      72.60
 H      -1.073029     1.160918     0.047427      25.52
 C       0.985553    -1.250679    -1.177018      -0.55
 C       2.450229    -1.313460    -1.637664      88.38
 H       2.351489    -2.651059    -1.693460      23.78
 O       2.890480    -0.657461    -2.795073     200.35
 H       3.844896    -0.820162    -3.046261      24.88
 C       3.519835    -1.203296    -0.477691      73.43
 H       2.932193    -1.882103     0.241974      28.90
 O       4.732465    -2.100753    -0.529017     169.21
 H       5.509708    -1.637101    -0.860064      27.26
 C       3.878085     0.222293     0.050772     111.93
 O       4.666914     0.919110    -0.927444     205.39
 H       4.759989     2.008012    -0.719286      22.55
 H       4.317248    -0.202170     1.085133      26.56
 H       3.001218     0.774918     0.425502      26.15
55
name = lig-Water-frame_224
 C      -1.009647     2.423294     2.928922      53.74
 H      -1.529075     3.337589     2.868850      26.35
 C      -0.579104     0.034339     3.357405      48.25
 H      -0.962922    -0.907146     3.822948      26.73
 C       0.717352     0.297740     3.533991      13.17
 O       1.593424    -0.569114     4.045741     196.51
 C       1.639516    -2.011341     3.616778     101.72
 H       2.436992    -2.488993     4.102349      28.56
 H       1.357254    -1.914919     2.439559      28.64
 H       0.741354    -2.363726     4.319226      26.41
 C       1.333720     1.719144     3.285436     -10.51
 O       2.672756     1.965640     3.260942     128.80
 H       2.737428     3.039807     3.083805      26.22
 C       0.394404     2.671375     3.069634      42.55
 H       0.585991     3.751614     2.962220      26.22
 C      -1.588856     1.089152     2.915138      10.36
 C      -2.970465     0.637799     2.754068      93.80
 H      -3.772000     1.640557     3.083655      23.67
 O      -3.416790    -0.669391     3.537970     127.80
 H      -4.435491    -0.728055     3.553306      25.07
 C      -3.275098     0.455401     1.188577      69.89
 H      -2.730124     1.354669     0.595852      24.76
 C      -4.993995     0.487936     1.015837     101.37
 O      -5.576403    -0.624386     1.546577     224.22
 H      -5.200060    -1.460732     1.222500      27.64
 H      -5.219005     0.458011    -0.148109      27.92
 H      -5.295857     1.329656     1.490687      31.26
 C       0.565480     0.047903    -0.648360      70.00
 H       1.272112     0.912867    -0.678445      27.01
 C      -0.050455    -2.296364    -1.261484      47.06
 H       0.062969    -3.153397    -1.871606      25.27
 C      -1.304257    -2.056388    -0.601861      -6.90
 O      -2.372061    -3.068391    -0.601545     148.56
 C      -2.442595    -3.829309    -1.940539      94.40
 H      -3.723863    -4.090284    -2.058821      22.28
 H      -2.379948    -3.311903    -2.944875      26.04
 H      -1.423777    -4.321528    -1.950284      23.31
 C      -1.682010    -0.795337    -0.059746      -4.45
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 O      -2.967047    -0.847285     0.618731     109.22
 C      -0.739094     0.252347    -0.234295      71.84
 H      -0.964335     1.405285     0.101010      26.30
 C       0.986409    -1.173002    -1.120282     -16.85
 C       2.476163    -1.418380    -1.660175     104.24
 H       2.471548    -2.359681    -1.936262      28.78
 O       2.886220    -0.647527    -2.815861     233.74
 H       3.899239    -0.851780    -3.152768      24.49
 C       3.505885    -1.269715    -0.531299      95.08
 H       3.066208    -1.670613     0.434473      30.27
 O       4.722979    -2.088413    -0.525573     169.15
 H       5.429254    -1.396500    -0.909834      26.00
 C       3.921695     0.230407     0.040830     102.47
 O       4.718911     0.913644    -0.964326     240.14
 H       4.676799     1.860674    -0.663352      27.53
 H       4.572915     0.167381     0.909486      29.98
 H       2.855533     0.591454     0.315080      28.50
55
name = lig-Water-frame_225
 C      -0.995778     2.429711     2.913633      64.31
 H      -1.666067     3.392354     2.946467      26.51
 C      -0.581555     0.024746     3.406576      30.98
 H      -1.097075    -0.924329     3.609039      32.37
 C       0.800826     0.391915     3.504262      17.00
 O       1.620167    -0.584548     4.015151     166.50
 C       1.574174    -2.030610     3.660629     126.55
 H       2.680368    -2.463379     3.842870      27.56
 H       1.423493    -1.911990     2.655833      30.10
 H       0.842570    -2.665394     4.138022      29.32
 C       1.343814     1.716059     3.238687      14.07
 O       2.654058     1.989334     3.296891     185.60
 H       2.870166     2.866821     2.942466      27.68
 C       0.415302     2.668668     3.029170      56.06
 H       1.077677     3.624409     3.022682      19.93
 C      -1.538343     1.114355     2.972164      -2.05
 C      -2.982921     0.646808     2.743818     105.65
 H      -3.518853     1.401328     2.954778      30.29
 O      -3.417330    -0.646591     3.552051     218.12
 H      -4.367796    -0.641413     3.387417      25.65
 C      -3.360357     0.504682     1.161646      87.20
 H      -2.926934     1.171314     0.547728      29.69
 C      -4.882367     0.483537     1.005809      96.76
 O      -5.556296    -0.650559     1.633550     174.11
 H      -5.140991    -1.482965     1.253666      26.04
 H      -5.170332     0.465408    -0.042224      29.02
 H      -5.494850     1.499627     1.526437      25.48
 C       0.510481     0.052194    -0.685890      61.20
 H       0.987565     1.008841    -0.695213      28.06
 C      -0.045945    -2.232683    -1.212082      51.61
 H       0.148912    -3.085122    -1.948018      25.01
 C      -1.293672    -2.054425    -0.653325      -2.14
 O      -2.384369    -3.056902    -0.614426     176.14
 C      -2.498544    -3.794539    -1.904764     125.83
 H      -3.371162    -4.286422    -1.722517      29.95
 H      -2.410396    -3.319927    -2.904474      27.52
 H      -1.732661    -4.602871    -1.871682      26.90
 C      -1.693124    -0.786498    -0.031943     -26.18
 O      -3.008962    -0.862236     0.626372      77.91
 C      -0.775992     0.292551    -0.209656      83.64
 H      -0.869040     1.237552     0.104999      30.91
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 C       0.983165    -1.165552    -1.117673      -4.85
 C       2.505783    -1.501758    -1.669310      77.49
 H       2.645884    -2.682877    -2.239081      22.56
 O       2.878871    -0.625494    -2.856683     217.66
 H       3.763528    -0.911685    -2.950770      29.15
 C       3.505057    -1.297949    -0.480695     106.56
 H       3.020275    -1.491752     0.504229      28.90
 O       4.729154    -2.045732    -0.551324     202.24
 H       5.310182    -1.468077    -1.030026      30.33
 C       3.938333     0.185872    -0.001448     107.12
 O       4.757528     0.919856    -0.996395     220.59
 H       4.651193     1.849125    -0.553385      27.00
 H       4.690022     0.356987     0.884444      27.03
 H       3.021520     0.696037     0.151946      28.22
55
name = lig-Water-frame_226
 C      -0.990851     2.452128     2.905238      55.86
 H      -1.822041     3.226274     2.862516      24.12
 C      -0.609604     0.109708     3.419543      41.10
 H      -0.978636    -1.020107     3.375564      29.11
 C       0.853864     0.428186     3.484976       7.08
 O       1.694326    -0.607868     4.016108     136.37
 C       1.534128    -2.026543     3.699534     121.34
 H       2.608006    -2.230310     3.584218      26.86
 H       1.371736    -2.198238     2.480180      28.05
 H       0.844124    -2.858877     4.094250      25.51
 C       1.325986     1.641641     3.199403      33.46
 O       2.663744     1.981603     3.342626     159.68
 H       3.073131     2.847914     2.855717      19.67
 C       0.412687     2.721148     2.979021      45.59
 H       0.939065     3.608729     3.002611      20.68
 C      -1.434812     1.081094     3.067542      19.78
 C      -2.976311     0.624474     2.704791      79.47
 H      -3.751418     1.614056     3.143492      23.64
 O      -3.388237    -0.578370     3.534880     216.48
 H      -4.367622    -0.516994     3.263237      21.51
 C      -3.460164     0.486754     1.187269      78.54
 H      -3.003949     1.319932     0.407349      24.11
 C      -4.824704     0.517686     1.001457     112.07
 O      -5.529130    -0.685405     1.724242     153.71
 H      -5.149240    -1.486178     1.188651      24.66
 H      -5.081090     0.541543    -0.113803      28.69
 H      -5.234819     1.310110     1.356028      31.98
 C       0.473484     0.087101    -0.728606      20.04
 H       1.044596     1.051170    -0.795526      26.19
 C      -0.003527    -2.158059    -1.181356      68.94
 H       0.256422    -3.002693    -1.755351      27.26
 C      -1.342830    -2.048620    -0.677091      13.90
 O      -2.361285    -3.017289    -0.660828     195.32
 C      -2.510558    -3.790152    -1.837397     119.64
 H      -3.512819    -4.606663    -1.547384      22.13
 H      -2.505637    -3.111692    -2.701504      26.91
 H      -2.064185    -4.830779    -1.881666      24.50
 C      -1.721305    -0.818545    -0.005529     -11.16
 O      -2.991939    -0.842652     0.615846      98.85
 C      -0.851156     0.291857    -0.166111      53.50
 H      -1.025484     1.387014     0.278104      25.71
 C       0.994350    -1.224699    -1.169180      12.17
 C       2.505890    -1.572477    -1.698132      82.16
 H       2.663425    -2.522724    -1.948624      28.80
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 O       2.854351    -0.616714    -2.868867     187.66
 H       3.912966    -0.857584    -2.940095      24.54
 C       3.525458    -1.272409    -0.380389      89.61
 H       2.868008    -1.670212     0.510018      28.53
 O       4.740341    -2.014811    -0.585226     195.65
 H       5.294433    -1.561871    -1.243226      30.23
 C       3.961056     0.145244    -0.074169     115.98
 O       4.785210     0.937590    -1.027727     143.29
 H       4.741141     1.925164    -0.545397      25.28
 H       4.394885     0.092775     0.972842      28.58
 H       3.121054     0.952505     0.077094      24.23
55
name = lig-Water-frame_227
 C      -0.982062     2.463484     2.903704      53.22
 H      -1.803878     3.158528     2.716416      24.68
 C      -0.532977     0.140782     3.423153      89.94
 H      -0.730357    -0.838522     3.341774      31.62
 C       0.837216     0.336958     3.502177      -2.47
 O       1.761635    -0.618371     4.021315     158.28
 C       1.516993    -2.022210     3.628156     114.79
 H       2.589233    -2.341512     3.689302      27.20
 H       1.154805    -2.290483     2.704276      31.50
 H       0.942074    -2.662878     4.408158      26.04
 C       1.332249     1.646147     3.154751       1.63
 O       2.699799     1.944401     3.387664     172.46
 H       2.889656     2.818502     3.023245      27.85
 C       0.370586     2.749103     2.928524      59.05
 H       0.599451     3.925348     2.906660      20.52
 C      -1.436397     1.087812     3.117638      29.70
 C      -2.979597     0.664945     2.713587     103.34
 H      -3.518095     1.364078     3.086941      32.34
 O      -3.347270    -0.478019     3.481147     242.35
 H      -4.347461    -0.591292     3.381799      23.08
 C      -3.411321     0.456287     1.213585     101.29
 H      -3.126983     1.260903     0.696939      30.49
 C      -4.885768     0.489134     0.975780      78.87
 O      -5.487275    -0.701747     1.777335     166.87
 H      -5.274173    -1.458399     1.233284      28.08
 H      -5.044699     0.477266    -0.159900      27.45
 H      -5.234694     1.650869     1.502609      25.15
 C       0.447049     0.127304    -0.767756      24.62
 H       1.168651     0.913829    -0.919534      27.18
 C       0.001059    -2.150695    -1.166126      47.44
 H       0.288142    -3.199987    -1.534518      26.37
 C      -1.385100    -2.010007    -0.677454      29.47
 O      -2.317881    -2.979237    -0.695938     226.21
 C      -2.581553    -3.867729    -1.754915     138.37
 H      -3.566311    -4.105965    -1.702429      28.61
 H      -2.712543    -3.144262    -2.600041      27.75
 H      -1.770007    -4.594656    -2.009460      26.11
 C      -1.754880    -0.859903     0.006195      24.55
 O      -2.953741    -0.804185     0.602684     125.47
 C      -0.886098     0.285811    -0.124682      59.61
 H      -1.233017     1.204485     0.327265      29.55
 C       1.018912    -1.209515    -1.228016      -4.28
 C       2.478297    -1.515664    -1.671018      64.58
 H       2.627714    -2.815469    -1.836418      25.64
 O       2.849712    -0.649363    -2.847471     186.55
 H       3.784114    -0.606548    -3.108445      30.05
 C       3.515791    -1.247776    -0.343671      79.83
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 H       3.037756    -1.814158     0.428491      31.28
 O       4.762196    -2.005490    -0.605716     125.93
 H       5.161521    -1.637836    -1.532526      27.40
 C       3.938785     0.176148    -0.115739     136.13
 O       4.821117     0.955247    -1.040517     170.59
 H       4.768733     1.802016    -0.671293      31.98
 H       4.304823    -0.129668     0.979585      29.90
 H       3.131703     0.785397     0.057382      29.89
55
name = lig-Water-frame_228
 C      -1.012425     2.422593     2.909848      50.92
 H      -1.725880     3.314542     2.498545      23.55
 C      -0.430153     0.111406     3.423388      44.45
 H      -0.795534    -1.071957     3.479694      27.43
 C       0.870573     0.288597     3.529674       9.92
 O       1.802722    -0.619543     4.000465     181.24
 C       1.541008    -2.025631     3.606407      97.54
 H       2.474826    -2.696735     3.806820      27.59
 H       0.855469    -2.176504     2.626906      30.49
 H       1.025248    -2.293679     4.613315      25.80
 C       1.344143     1.697268     3.144526     -13.63
 O       2.714507     1.887757     3.424838     122.07
 H       2.812426     2.912641     3.232146      20.17
 C       0.347204     2.775682     2.889495      65.39
 H       0.435390     3.787208     2.749991      24.74
 C      -1.512169     1.147128     3.107798      20.61
 C      -2.930058     0.690442     2.731903      97.89
 H      -3.639062     1.763435     3.111489      25.35
 O      -3.300374    -0.406641     3.441050     225.87
 H      -4.229494    -0.575680     3.508963      26.42
 C      -3.328462     0.425108     1.250117      90.72
 H      -2.944755     1.451390     0.732012      26.92
 C      -4.973788     0.469508     1.005073      97.71
 O      -5.456066    -0.684183     1.795204     198.31
 H      -5.360161    -1.524341     1.221289      27.35
 H      -5.208945     0.354165    -0.065654      29.05
 H      -5.279486     1.285025     1.373845      32.58
 C       0.426068     0.135165    -0.799431      48.46
 H       1.127348     0.980932    -0.950320      27.63
 C      -0.023704    -2.216616    -1.163714      18.95
 H       0.190883    -3.268886    -1.256699      26.64
 C      -1.354797    -1.975838    -0.697019      20.13
 O      -2.293387    -2.965636    -0.683350     217.23
 C      -2.627431    -3.900362    -1.741073     113.99
 H      -3.877224    -4.039352    -1.673553      21.15
 H      -2.758679    -3.348962    -2.715073      26.18
 H      -1.642197    -4.324531    -2.037842      21.55
 C      -1.737874    -0.842190    -0.005423      35.64
 O      -2.938646    -0.765228     0.607974     110.05
 C      -0.853612     0.239710    -0.117703      70.67
 H      -1.253623     1.175788     0.315660      30.45
 C       0.988752    -1.120970    -1.264965     -34.99
 C       2.473560    -1.457069    -1.607964     100.11
 H       2.441398    -2.431269    -1.831956      29.35
 O       2.819178    -0.693056    -2.816308     189.41
 H       3.810619    -0.643396    -3.000205      29.84
 C       3.503340    -1.251561    -0.436125      83.54
 H       3.203525    -1.818588     0.593697      28.89
 O       4.790627    -2.000096    -0.643808     190.71
 H       4.902788    -1.790493    -1.547489      32.38
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 C       3.906370     0.219400    -0.096505     107.61
 O       4.850983     0.930487    -1.038991     147.03
 H       4.654919     1.979767    -0.624045      23.89
 H       4.541774     0.104941     0.827228      30.61
 H       2.869289     0.742780     0.110695      28.61
55
name = lig-Water-frame_229
 C      -1.072606     2.412614     2.881674      64.18
 H      -1.604419     3.199499     2.521289      27.04
 C      -0.470267     0.034533     3.405403      10.49
 H      -0.859668    -0.824727     3.704875      28.21
 C       0.965062     0.348369     3.537671       2.51
 O       1.860411    -0.613106     3.945538     159.77
 C       1.544339    -2.051648     3.648685     111.64
 H       2.319849    -2.731107     3.596201      32.35
 H       0.880149    -2.007517     2.820781      32.92
 H       0.849735    -2.145866     4.544154      30.30
 C       1.338321     1.740237     3.184977      17.34
 O       2.701993     1.857799     3.442142     224.12
 H       3.037228     2.828923     3.458720      14.09
 C       0.358324     2.726921     2.872750      71.39
 H       0.675184     3.822217     2.557063      24.14
 C      -1.525498     1.138580     3.087118      10.82
 C      -2.915264     0.793317     2.757912     125.13
 H      -3.445209     1.598589     2.806929      33.17
 O      -3.244238    -0.390529     3.456994     210.02
 H      -4.276926    -0.370728     3.478500      24.93
 C      -3.293096     0.493252     1.248138      89.37
 H      -2.838423     1.251406     0.701137      30.30
 C      -4.968990     0.386095     1.053668      82.02
 O      -5.448997    -0.670900     1.795572     200.11
 H      -5.374310    -1.485240     1.224053      28.03
 H      -5.402162     0.227269    -0.057289      26.62
 H      -5.600962     1.438931     1.512891      24.25
 C       0.422036     0.135596    -0.827231      82.88
 H       0.878404     1.130041    -0.884282      29.59
 C      -0.024052    -2.249174    -1.158186      11.44
 H       0.215674    -3.333836    -1.172769      24.98
 C      -1.301285    -1.987446    -0.734005       0.27
 O      -2.304972    -2.971278    -0.643079     193.58
 C      -2.680857    -3.856796    -1.789082     104.70
 H      -3.494139    -4.503026    -1.438845      25.83
 H      -2.740057    -3.386165    -2.785253      27.26
 H      -1.878599    -4.654290    -1.898527      24.09
 C      -1.680726    -0.781885    -0.034471       0.71
 O      -2.931106    -0.745853     0.623287      79.21
 C      -0.779342     0.205854    -0.134773      87.09
 H      -1.029906     1.290756     0.239491      31.50
 C       0.891666    -1.061713    -1.265571     -23.92
 C       2.442408    -1.355726    -1.535133      81.26
 H       2.358923    -2.605097    -1.928484      22.68
 O       2.790258    -0.727238    -2.794692     142.27
 H       3.818770    -0.859259    -2.712508      27.68
 C       3.521390    -1.260729    -0.503393     110.85
 H       3.176129    -1.540183     0.421572      31.39
 O       4.798497    -1.997242    -0.698168     177.83
 H       4.963051    -1.966338    -1.708801      27.58
 C       3.872979     0.251112    -0.062565     109.76
 O       4.841355     0.928520    -1.012750     210.26
 H       4.677322     1.780219    -0.724363      32.89
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 H       4.573389     0.382420     0.846153      29.09
 H       2.979572     0.787337     0.112009      31.31
55
name = lig-Water-frame_230
 C      -1.051611     2.419957     2.838525      54.66
 H      -1.877616     3.313549     2.506252      23.00
 C      -0.516942     0.045070     3.384064      10.58
 H      -0.999875    -0.918460     3.969536      23.69
 C       0.956260     0.417298     3.519005     -13.80
 O       1.950467    -0.593809     3.872473      97.13
 C       1.481372    -2.022337     3.735973     109.68
 H       2.439483    -2.699226     3.360273      27.27
 H       0.876561    -2.012806     2.738113      30.50
 H       0.747647    -2.445098     4.473899      31.22
 C       1.333851     1.743706     3.263676      34.32
 O       2.700147     1.851156     3.457065     206.75
 H       3.113062     2.686902     3.420838      19.60
 C       0.375825     2.677327     2.860383      75.64
 H       0.901270     3.526331     2.503519      28.44
 C      -1.448888     1.067025     3.069586      12.68
 C      -2.885694     0.843083     2.734544      84.99
 H      -3.696488     1.897180     2.876722      26.66
 O      -3.227628    -0.390203     3.514740     174.70
 H      -4.199417    -0.254700     3.442246      27.59
 C      -3.316955     0.572514     1.216559      74.16
 H      -2.850044     1.355297     0.478122      27.69
 C      -4.943670     0.388812     1.092391     112.21
 O      -5.465162    -0.699108     1.811034     226.54
 H      -5.321418    -1.469628     1.291191      30.47
 H      -5.234059     0.275401     0.081651      30.29
 H      -5.350447     1.196809     1.418900      32.13
 C       0.425702     0.175315    -0.849078      82.29
 H       0.874723     1.153832    -0.923226      30.53
 C       0.015266    -2.236378    -1.155834      39.73
 H       0.409135    -3.269829    -1.311823      23.63
 C      -1.310933    -2.022976    -0.741075      -6.63
 O      -2.333168    -2.987494    -0.610357     163.92
 C      -2.671158    -3.846012    -1.817293     100.07
 H      -3.344408    -4.627828    -1.306575      23.33
 H      -2.868688    -3.288597    -2.751553      27.38
 H      -2.099927    -4.780764    -1.818672      23.80
 C      -1.653512    -0.767235    -0.071922     -38.26
 O      -2.891560    -0.746050     0.634090      40.94
 C      -0.714150     0.266045    -0.143440      85.86
 H      -0.817050     1.209553     0.202644      34.39
 C       0.837961    -1.094426    -1.252211      21.86
 C       2.344215    -1.341606    -1.529586      78.69
 H       2.408915    -2.341214    -1.640915      29.21
 O       2.785558    -0.750416    -2.772920     182.41
 H       3.732373    -0.866141    -2.840371      30.99
 C       3.579387    -1.201231    -0.514662      93.83
 H       2.944766    -1.590211     0.481092      29.58
 O       4.778187    -1.997886    -0.773287     186.08
 H       5.189074    -2.112262    -1.719184      24.33
 C       3.894989     0.260716    -0.049821     110.24
 O       4.809344     0.909051    -0.995631     144.27
 H       4.720339     1.953023    -0.712384      26.82
 H       4.260325     0.353709     1.077830      29.05
 H       2.975574     0.959633     0.045037      28.53
55
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name = lig-Water-frame_231
 C      -0.990675     2.439414     2.778777      24.53
 H      -1.724438     3.046086     2.611011      23.00
 C      -0.516184     0.066994     3.408758      88.65
 H      -0.850804    -0.796916     3.859185      30.31
 C       0.859653     0.403931     3.508453      -2.41
 O       2.002471    -0.566972     3.797018     111.27
 C       1.419956    -1.976444     3.753632     117.89
 H       2.294017    -2.403316     3.561915      30.71
 H       0.916142    -2.079280     2.777752      32.63
 H       0.932821    -2.712178     4.520293      27.22
 C       1.339517     1.701186     3.355069      18.96
 O       2.712070     1.843728     3.473607     112.18
 H       3.029855     2.845993     3.167874      24.83
 C       0.387571     2.644963     2.846315      88.23
 H       0.911418     3.565699     2.465430      31.99
 C      -1.370656     1.051536     3.027293      31.78
 C      -2.888947     0.879865     2.699254     101.06
 H      -3.404190     1.574299     3.137216      30.17
 O      -3.243441    -0.364971     3.571667     220.65
 H      -4.215396    -0.406462     3.553123      26.41
 C      -3.355532     0.620684     1.166133      72.35
 H      -3.159320     1.459256     0.468290      26.00
 C      -4.852887     0.406723     1.108245      72.89
 O      -5.491244    -0.746272     1.842068     192.10
 H      -5.218736    -1.600432     1.327215      27.56
 H      -4.999796     0.363874    -0.121417      25.67
 H      -5.341726     1.506866     1.578312      24.11
 C       0.459133     0.218227    -0.885883      65.99
 H       1.203082     1.037112    -1.102120      29.25
 C       0.042582    -2.220066    -1.157292      63.38
 H       0.525651    -3.113628    -1.508797      26.41
 C      -1.360311    -2.051859    -0.709621      15.46
 O      -2.353721    -3.010857    -0.602008     163.25
 C      -2.647758    -3.874151    -1.780769      83.65
 H      -3.748691    -4.200123    -1.360793      22.54
 H      -3.041156    -3.280138    -2.613124      26.91
 H      -1.716764    -4.557155    -2.090312      22.40
 C      -1.646254    -0.788987    -0.105643      -5.85
 O      -2.822482    -0.740913     0.641604      55.01
 C      -0.711704     0.345584    -0.142548      41.44
 H      -0.882139     1.413503     0.455851      25.82
 C       0.867001    -1.130643    -1.240813      -7.21
 C       2.290273    -1.337879    -1.539181      48.83
 H       2.407721    -2.668132    -1.523155      26.38
 O       2.763351    -0.757494    -2.780660     127.40
 H       3.773886    -0.849762    -3.004543      23.41
 C       3.574526    -1.113808    -0.461419      80.31
 H       3.213199    -1.713625     0.279113      30.78
 O       4.744916    -2.013082    -0.833893     185.27
 H       5.106663    -1.910583    -1.691887      25.86
 C       3.905478     0.280282    -0.032498     125.70
 O       4.781866     0.902997    -0.975658     179.78
 H       4.786798     1.890049    -0.610123      26.19
 H       4.134652     0.173836     1.103364      27.74
 H       2.975744     0.839577    -0.139801      27.46
55
name = lig-Water-frame_232
 C      -0.887764     2.371452     2.732571      42.45
 H      -1.781696     3.241442     2.513665      20.98
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 C      -0.474989     0.084206     3.448013      79.23
 H      -0.825885    -1.002795     3.707559      26.97
 C       0.824016     0.345186     3.531178      15.29
 O       1.952690    -0.538374     3.730159     179.41
 C       1.401746    -1.942020     3.735481     105.58
 H       2.526077    -2.483857     3.734137      24.13
 H       0.790870    -2.113911     2.822382      29.46
 H       1.059437    -2.388366     4.686248      26.27
 C       1.329455     1.657239     3.411113      13.36
 O       2.731487     1.873569     3.479846     139.86
 H       2.756147     2.706999     3.018300      23.95
 C       0.453227     2.657661     2.836868      83.06
 H       0.702175     3.718456     2.547912      30.98
 C      -1.365676     1.114970     2.949144      34.98
 C      -2.851235     0.817815     2.684326      85.28
 H      -3.380945     1.731334     3.416383      22.96
 O      -3.263851    -0.327047     3.612662     218.80
 H      -4.261251    -0.548833     3.631250      24.62
 C      -3.376991     0.614177     1.163310      76.29
 H      -3.269220     1.483007     0.504617      24.43
 C      -4.799724     0.462890     1.095485     106.19
 O      -5.500792    -0.778477     1.850422     199.29
 H      -5.155973    -1.613155     1.437780      28.89
 H      -5.011936     0.395969     0.110600      30.46
 H      -5.264578     1.252608     1.526977      29.07
 C       0.510468     0.236619    -0.919921      68.17
 H       1.337641     0.868850    -1.166858      28.52
 C       0.005473    -2.216715    -1.154636      19.04
 H       0.442927    -3.147645    -1.663091      24.18
 C      -1.366136    -2.066438    -0.677923      23.49
 O      -2.360508    -3.036010    -0.600887     203.78
 C      -2.651882    -3.881185    -1.731585     119.33
 H      -3.714135    -4.179596    -1.558665      24.45
 H      -2.969402    -3.178465    -2.551981      26.84
 H      -1.760842    -4.243771    -2.194377      25.03
 C      -1.624874    -0.776679    -0.118273       0.37
 O      -2.756234    -0.711176     0.654066      71.94
 C      -0.736235     0.433765    -0.144204      50.02
 H      -1.017073     1.180462     0.426000      24.91
 C       0.915809    -1.094456    -1.225440     -40.54
 C       2.356445    -1.415352    -1.546706      79.33
 H       2.356236    -2.384156    -1.631136      30.41
 O       2.721705    -0.756478    -2.820349     162.01
 H       3.712886    -0.938819    -2.881702      24.64
 C       3.530527    -1.089647    -0.443716      79.22
 H       3.408152    -1.840310     0.525035      25.27
 O       4.695184    -2.016819    -0.881205     155.80
 H       4.958074    -1.520584    -1.804383      22.94
 C       3.877813     0.282841    -0.025971     115.22
 O       4.785406     0.906946    -0.946732     232.71
 H       4.777936     1.799017    -0.498282      26.57
 H       4.295701     0.192222     1.085098      26.82
 H       2.875079     0.752479    -0.089804      27.32
55
name = lig-Water-frame_233
 C      -0.843247     2.349563     2.670901      55.58
 H      -1.334759     3.155354     2.375450      23.50
 C      -0.508717     0.070798     3.477004      52.41
 H      -0.862370    -0.993431     3.350325      29.26
 C       0.899909     0.317616     3.579581      14.96
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 O       1.837843    -0.533394     3.669224     209.18
 C       1.489902    -1.934879     3.726348     113.52
 H       2.268503    -2.572647     3.695530      28.50
 H       0.671764    -2.249732     2.968704      26.73
 H       0.983456    -1.744007     4.789757      23.12
 C       1.323248     1.663472     3.408950      31.18
 O       2.721237     1.896955     3.483296     147.68
 H       2.829514     2.781114     2.992778      21.80
 C       0.549404     2.684371     2.857331      71.81
 H       0.720899     3.729033     2.743513      30.00
 C      -1.385380     1.110130     2.890050      22.87
 C      -2.844688     0.766443     2.743503     117.94
 H      -3.284286     1.675235     2.943874      28.65
 O      -3.265756    -0.301230     3.640954     248.42
 H      -4.227285    -0.398250     3.491295      25.66
 C      -3.327284     0.567837     1.221184      83.39
 H      -3.015137     1.487531     0.538380      23.77
 C      -4.820068     0.439283     1.102005      80.67
 O      -5.486586    -0.777591     1.839605     177.26
 H      -5.115545    -1.600926     1.492839      28.42
 H      -5.342146     0.338164    -0.050086      24.95
 H      -5.417763     1.374948     1.643415      24.53
 C       0.536248     0.232896    -0.913238      64.83
 H       1.281509     1.060132    -1.086720      27.96
 C      -0.045743    -2.209217    -1.166775      23.37
 H       0.150899    -3.159469    -1.580371      27.06
 C      -1.320233    -2.063130    -0.662593      14.06
 O      -2.359089    -3.054045    -0.572076     198.06
 C      -2.678180    -3.795606    -1.728201     113.31
 H      -3.501695    -4.770065    -1.684474      23.59
 H      -2.811442    -3.026943    -2.507173      26.61
 H      -1.778132    -4.447072    -2.195717      23.49
 C      -1.580843    -0.704838    -0.107536       4.34
 O      -2.720152    -0.663501     0.676042     118.02
 C      -0.733729     0.416299    -0.221987      56.12
 H      -1.155806     1.348023     0.448199      19.95
 C       0.933476    -1.063148    -1.203180     -28.85
 C       2.439436    -1.433593    -1.538907      61.13
 H       2.456862    -2.731753    -1.854621      22.77
 O       2.684461    -0.764780    -2.853361     177.07
 H       3.629932    -0.942839    -2.953441      23.93
 C       3.481047    -1.206099    -0.414749      96.36
 H       3.245262    -1.489398     0.541542      28.23
 O       4.639070    -1.975375    -0.953163     203.99
 H       4.981898    -1.438973    -1.713433      25.65
 C       3.835236     0.264362    -0.022069      99.70
 O       4.800558     0.914181    -0.914439     215.81
 H       4.769921     1.928153    -0.407220      21.24
 H       4.385341     0.354237     0.988453      25.46
 H       2.874585     0.855914     0.217642      25.48
55
name = lig-Water-frame_234
 C      -0.771214     2.357236     2.606158      56.97
 H      -1.332056     3.330551     2.086433      22.76
 C      -0.545562     0.068562     3.454774      54.30
 H      -0.908966    -0.922887     3.223336      33.81
 C       0.874518     0.375829     3.607443       2.44
 O       1.808620    -0.578626     3.591409     173.86
 C       1.499401    -1.909243     3.780413     134.51
 H       2.384362    -2.738778     3.681607      25.57
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 H       0.744987    -2.295492     3.136137      28.53
 H       0.953640    -1.812456     4.672799      26.97
 C       1.373949     1.707982     3.379462      32.47
 O       2.702165     1.912053     3.484477     149.07
 H       3.099170     2.847229     3.215945      23.69
 C       0.577262     2.677248     2.898503      50.96
 H       1.012894     3.763796     2.957138      26.73
 C      -1.372469     1.037219     2.884916       4.83
 C      -2.844415     0.730523     2.766115      97.82
 H      -3.499685     1.866864     2.733156      24.14
 O      -3.259136    -0.274264     3.658267     225.04
 H      -4.212477    -0.226597     3.402948      24.53
 C      -3.243048     0.512418     1.280207     105.78
 H      -2.844875     1.340006     0.781107      28.23
 C      -4.937514     0.389425     1.097288     104.06
 O      -5.455714    -0.748959     1.823338     196.26
 H      -5.051315    -1.642315     1.442281      24.87
 H      -5.257366     0.385666     0.178234      32.27
 H      -5.298766     1.296214     1.598540      28.58
 C       0.546350     0.242229    -0.875629      46.63
 H       1.037521     1.202969    -0.920174      26.76
 C      -0.066321    -2.176392    -1.187380      41.10
 H       0.082031    -3.272993    -1.509490      26.74
 C      -1.297794    -2.009484    -0.632450       2.72
 O      -2.346583    -3.059025    -0.508976     210.06
 C      -2.661010    -3.753048    -1.796093     129.06
 H      -3.179851    -4.593348    -1.636068      29.28
 H      -2.930332    -3.009568    -2.576239      27.81
 H      -1.856416    -4.451282    -1.996279      25.74
 C      -1.559058    -0.653340    -0.082629      15.76
 O      -2.703517    -0.625260     0.697014     162.52
 C      -0.729087     0.386809    -0.309095      85.64
 H      -0.911274     1.349976     0.029119      27.70
 C       0.949897    -1.101368    -1.194143     -13.50
 C       2.439721    -1.485868    -1.556407      84.42
 H       2.558768    -2.411673    -1.802950      26.98
 O       2.663958    -0.780239    -2.860055     188.34
 H       3.648953    -0.854931    -3.248820      23.82
 C       3.462978    -1.299965    -0.426784      93.86
 H       2.887580    -1.570311     0.633215      26.16
 O       4.587491    -1.926670    -0.992399     235.39
 H       5.042976    -1.470088    -1.710040      26.47
 C       3.799330     0.243688    -0.006505     103.75
 O       4.804666     0.945548    -0.877904     240.86
 H       4.736192     1.821266    -0.532066      28.12
 H       4.419004     0.254530     1.013824      25.80
 H       2.993133     0.886819     0.291312      26.33
55
name = lig-Water-frame_235
 C      -0.736655     2.390843     2.534485      49.17
 H      -1.395093     3.042485     2.033869      28.57
 C      -0.530607     0.080678     3.409172      48.20
 H      -0.886814    -1.069174     3.369525      28.84
 C       0.788328     0.455704     3.599947     -30.43
 O       1.858505    -0.616557     3.502180      85.29
 C       1.468091    -1.941490     3.858277     121.12
 H       2.438205    -2.451929     3.833584      28.40
 H       0.752683    -2.359602     3.003641      29.36
 H       0.962585    -2.350883     4.899252      26.47
 C       1.437258     1.712458     3.361572       3.64
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 O       2.737010     1.913617     3.503403     165.33
 H       3.011124     2.814620     3.383506      26.11
 C       0.548590     2.706597     2.941051      51.01
 H       1.035921     3.598126     2.947938      23.23
 C      -1.341424     1.042178     2.896753      39.61
 C      -2.852608     0.777461     2.735404     110.81
 H      -3.425356     1.566888     2.981767      30.90
 O      -3.263055    -0.244813     3.674714     216.51
 H      -4.287133    -0.283978     3.598843      23.74
 C      -3.216001     0.458427     1.327033      90.05
 H      -2.798028     1.509273     0.870364      26.00
 C      -4.974633     0.348884     1.131648      84.60
 O      -5.425479    -0.736549     1.807101     179.57
 H      -5.081008    -1.550712     1.427004      26.59
 H      -5.184623     0.425367    -0.151605      26.53
 H      -5.360224     1.332460     1.633005      26.58
 C       0.556307     0.209425    -0.841982      38.98
 H       1.085391     1.174821    -0.877899      25.76
 C      -0.043012    -2.155619    -1.211926      50.90
 H       0.263713    -3.133244    -1.459899      28.26
 C      -1.330181    -1.926720    -0.580789       7.96
 O      -2.317365    -3.035961    -0.454808     174.60
 C      -2.587576    -3.697634    -1.855639      90.85
 H      -3.574140    -4.473288    -1.347755      24.05
 H      -3.086012    -3.146736    -2.667970      27.44
 H      -1.541548    -4.215393    -2.067518      23.71
 C      -1.592408    -0.679942    -0.050811      33.19
 O      -2.688750    -0.629618     0.706654     191.88
 C      -0.706586     0.387835    -0.404777      77.92
 H      -0.864688     1.530806    -0.238669      26.82
 C       0.974068    -1.157825    -1.202715      11.50
 C       2.372073    -1.474374    -1.582624      72.45
 H       2.528240    -2.774663    -1.834245      25.25
 O       2.660633    -0.786991    -2.871947     183.24
 H       3.570585    -0.841500    -3.170728      27.29
 C       3.421837    -1.284730    -0.448334      99.30
 H       3.020212    -1.971723     0.247399      30.28
 O       4.562967    -1.919674    -0.979017     162.77
 H       4.976888    -1.367221    -1.824715      23.48
 C       3.815972     0.197043     0.027925     104.91
 O       4.794274     0.938088    -0.858758     183.53
 H       4.611879     2.022221    -0.515115      21.38
 H       4.303346    -0.051668     1.060357      26.18
 H       2.885561     0.891785     0.163224      23.68
55
name = lig-Water-frame_236
 C      -0.759793     2.359246     2.498570      58.08
 H      -1.539495     3.055607     1.984783      26.35
 C      -0.503612     0.063351     3.364932      43.11
 H      -0.734444    -0.882572     3.636679      25.04
 C       0.812404     0.469248     3.565519       6.61
 O       1.886807    -0.623634     3.451941       7.36
 C       1.414797    -2.024941     3.923136     124.14
 H       2.536755    -2.420220     3.923544      27.07
 H       0.945037    -2.410070     3.095076      31.29
 H       1.128920    -2.386231     4.836702      30.05
 C       1.422779     1.689425     3.356690       8.36
 O       2.808958     1.887441     3.541985     116.73
 H       2.883321     2.958358     3.353155      22.51
 C       0.521905     2.736877     2.974232      47.18
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 H       0.904493     3.840062     2.721146      19.02
 C      -1.327110     1.135672     2.890231      55.89
 C      -2.833311     0.803860     2.727298      88.70
 H      -3.456516     1.773714     3.263585      24.50
 O      -3.268511    -0.239707     3.705674     224.09
 H      -4.208123    -0.275093     3.852296      29.03
 C      -3.262335     0.499887     1.326370     101.89
 H      -3.054419     1.363583     0.812258      28.55
 C      -4.908623     0.377702     1.106788     101.41
 O      -5.424531    -0.754747     1.802404     217.20
 H      -5.071840    -1.612032     1.393082      25.82
 H      -5.054295     0.342672     0.153647      31.37
 H      -5.501077     1.277546     1.558956      27.37
 C       0.600512     0.134177    -0.838600      43.10
 H       1.358759     0.924841    -1.007460      25.32
 C      -0.020791    -2.122406    -1.202784      50.12
 H       0.410902    -3.130736    -1.496906      26.16
 C      -1.345012    -1.911863    -0.565202      16.24
 O      -2.272607    -2.976866    -0.441729     196.82
 C      -2.534094    -3.678609    -1.830013     124.93
 H      -3.317532    -4.158729    -1.526128      29.85
 H      -3.041389    -3.109596    -2.647886      28.72
 H      -1.647098    -3.995544    -2.276711      26.98
 C      -1.612315    -0.688642    -0.040278      20.50
 O      -2.698908    -0.668228     0.726304     174.02
 C      -0.720593     0.429656    -0.462200      74.39
 H      -1.111462     1.485696    -0.388791      27.70
 C       0.964757    -1.178910    -1.212246      49.29
 C       2.313888    -1.509890    -1.643066     107.42
 H       2.289569    -2.471257    -1.746416      32.15
 O       2.650123    -0.788650    -2.881561     133.75
 H       3.675581    -0.920820    -2.907100      26.29
 C       3.374664    -1.232339    -0.527314      91.33
 H       3.210127    -2.186537     0.185440      26.47
 O       4.588228    -1.925877    -0.967185     200.09
 H       4.771211    -1.457403    -1.738366      30.63
 C       3.822988     0.141562     0.064988     123.86
 O       4.761460     0.928656    -0.825086     226.14
 H       4.573280     1.737816    -0.447834      28.41
 H       4.152067    -0.226457     1.132525      27.26
 H       2.960388     0.676847     0.103940      27.88
55
name = lig-Water-frame_237
 C      -0.814963     2.344018     2.489197      61.91
 H      -1.450267     3.202572     2.079986      26.23
 C      -0.467806     0.113879     3.325021      39.05
 H      -0.812438    -0.908595     3.921447      23.93
 C       0.927019     0.381223     3.501306      15.25
 O       1.869559    -0.624021     3.455770      59.19
 C       1.459078    -2.089870     3.937374      94.21
 H       2.491317    -2.590250     3.951472      27.41
 H       0.886881    -2.668349     3.055314      27.73
 H       0.973695    -2.081846     5.075539      25.91
 C       1.400548     1.720171     3.359571       5.24
 O       2.849979     1.875046     3.580725     175.06
 H       3.049776     2.777437     3.272224      25.08
 C       0.508696     2.781192     2.963291      57.56
 H       0.663425     3.735017     2.611356      21.35
 C      -1.338624     1.166007     2.888602      57.31
 C      -2.841938     0.858847     2.791914      94.33
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 H      -3.254190     1.796271     3.045747      30.15
 O      -3.238945    -0.255763     3.740863     191.25
 H      -4.231750     0.001008     3.902225      24.44
 C      -3.373377     0.570584     1.305075      75.81
 H      -3.187390     1.452516     0.470372      24.88
 C      -4.796752     0.406636     1.132617      86.32
 O      -5.438343    -0.788804     1.796920     185.24
 H      -5.067379    -1.656847     1.384193      23.50
 H      -5.029422     0.227786    -0.147439      24.07
 H      -5.408652     1.269278     1.450049      26.95
 C       0.633181     0.093476    -0.854275      51.19
 H       1.447147     0.728955    -1.148290      27.90
 C      -0.036567    -2.140614    -1.165347      67.22
 H       0.225480    -3.126800    -1.527441      27.87
 C      -1.290876    -1.962822    -0.600253      18.69
 O      -2.226203    -2.918322    -0.474420     193.38
 C      -2.476947    -3.591559    -1.780759      97.65
 H      -3.359645    -4.638044    -1.615828      23.56
 H      -2.850276    -2.760934    -2.435357      27.65
 H      -1.622887    -4.124901    -2.453746      24.06
 C      -1.590046    -0.635798    -0.062598     -15.53
 O      -2.744917    -0.704621     0.768524      60.64
 C      -0.757949     0.449831    -0.485028      88.46
 H      -1.226067     1.428302    -0.397754      31.65
 C       0.921930    -1.158220    -1.212476      63.22
 C       2.274312    -1.488629    -1.685074      83.37
 H       2.231795    -2.803768    -1.880381      25.62
 O       2.660093    -0.799439    -2.894325     114.01
 H       3.683456    -0.877520    -2.834750      25.92
 C       3.355951    -1.258514    -0.600396      95.76
 H       3.052971    -1.714202     0.339446      30.31
 O       4.632806    -1.937143    -0.965643     154.16
 H       4.963186    -1.566067    -1.896510      25.74
 C       3.808066     0.050615     0.083166     109.83
 O       4.720160     0.871402    -0.773770     175.01
 H       4.555745     1.897510    -0.256749      21.22
 H       4.215765    -0.102876     1.120668      28.51
 H       2.823470     0.721648     0.272792      26.19
55
name = lig-Water-frame_238
 C      -0.832401     2.405721     2.516007      63.61
 H      -1.415811     3.245493     2.169174      29.48
 C      -0.424554     0.159054     3.336777      89.89
 H      -0.911423    -0.604771     3.743452      32.40
 C       1.007558     0.298746     3.402996       2.48
 O       1.858784    -0.668125     3.491760     146.91
 C       1.508374    -2.127712     3.947760     116.44
 H       2.457503    -2.717801     4.054505      27.36
 H       0.821084    -2.618781     3.360532      30.30
 H       0.955874    -1.781874     4.730409      29.11
 C       1.428599     1.776513     3.362562      -9.80
 O       2.842983     1.851844     3.614739     217.04
 H       3.282629     2.757297     3.236413      22.17
 C       0.466825     2.757351     2.911579      71.08
 H       0.781021     3.834007     2.632972      28.17
 C      -1.366976     1.103074     2.898837      57.57
 C      -2.835863     0.895108     2.830265      80.34
 H      -3.390957     1.999448     3.040639      25.54
 O      -3.221126    -0.241507     3.761714     213.09
 H      -4.113248     0.196551     3.903280      23.52
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 C      -3.406848     0.644807     1.264727      77.87
 H      -3.164350     1.360533     0.603517      28.81
 C      -4.781042     0.360250     1.100257     111.47
 O      -5.444085    -0.802401     1.784296     259.45
 H      -5.097704    -1.586679     1.371635      27.47
 H      -4.894257     0.283693     0.151618      28.85
 H      -5.333510     1.415252     1.370033      25.90
 C       0.597796     0.141262    -0.877177      34.51
 H       1.342082     0.919350    -1.201854      27.38
 C      -0.063715    -2.218119    -1.134218      91.30
 H       0.041853    -3.202628    -1.583147      27.99
 C      -1.220658    -1.951762    -0.610996      15.09
 O      -2.196894    -2.910884    -0.520919     229.80
 C      -2.455379    -3.548092    -1.760148     139.22
 H      -2.972711    -4.352900    -1.705318      32.31
 H      -2.791326    -2.631568    -2.248866      28.78
 H      -1.655271    -4.044842    -2.173165      28.46
 C      -1.580035    -0.609634    -0.092793     -25.80
 O      -2.781923    -0.710097     0.799203     -10.75
 C      -0.774761     0.439462    -0.484354      93.27
 H      -1.121619     1.572207    -0.292006      32.33
 C       0.887489    -1.168847    -1.224238      43.82
 C       2.265911    -1.526236    -1.715358      97.11
 H       2.351850    -2.460501    -1.957666      32.65
 O       2.681443    -0.811529    -2.914542     194.10
 H       3.625156    -0.729427    -3.037010      29.37
 C       3.385586    -1.302293    -0.630689      90.31
 H       2.777238    -1.567451     0.395500      28.95
 O       4.671484    -1.955134    -0.976199     192.10
 H       5.177892    -1.744144    -1.838865      26.23
 C       3.741250     0.013579     0.073592     120.36
 O       4.669937     0.841677    -0.690075     210.26
 H       4.618460     1.705262    -0.374153      30.73
 H       4.431584    -0.086481     1.047777      27.10
 H       2.967599     0.576128     0.441721      29.76
55
name = lig-Water-frame_239
 C      -0.852475     2.447924     2.578878      53.06
 H      -1.603485     3.317769     2.192522      23.92
 C      -0.387945     0.197085     3.354587      59.33
 H      -1.001875    -0.825850     3.629741      28.04
 C       1.001915     0.336824     3.296021      -0.35
 O       1.911542    -0.766472     3.524185     143.24
 C       1.538014    -2.094943     3.951520     110.17
 H       2.487764    -2.793282     4.314747      24.29
 H       0.668870    -2.591824     3.322730      26.72
 H       0.907698    -1.770653     4.909545      25.04
 C       1.475430     1.758565     3.347946       6.33
 O       2.816421     1.841651     3.639860     176.05
 H       3.213629     2.730111     3.343466      24.38
 C       0.473392     2.728675     2.841939      64.88
 H       0.967401     3.701172     2.865447      28.22
 C      -1.351414     1.104244     2.891247      40.25
 C      -2.841233     0.934040     2.825725     108.49
 H      -3.448955     1.754396     3.205033      26.09
 O      -3.220046    -0.176151     3.759260     216.87
 H      -4.163705     0.038064     4.038481      24.54
 C      -3.333277     0.639504     1.295218      66.11
 H      -2.949563     1.604846     0.638927      23.67
 C      -4.872313     0.323571     1.098217      91.33
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 O      -5.440042    -0.778420     1.769588     247.43
 H      -5.114968    -1.622126     1.241902      24.59
 H      -4.986596     0.235565    -0.214822      22.73
 H      -5.348821     1.238847     1.367048      27.22
 C       0.519019     0.212206    -0.928087      17.76
 H       1.066456     1.113507    -1.121004      24.65
 C      -0.011651    -2.295799    -1.142578      59.70
 H       0.085827    -3.299604    -1.638153      23.72
 C      -1.244997    -1.887855    -0.555055      10.62
 O      -2.182160    -2.929299    -0.518364     204.09
 C      -2.410856    -3.461729    -1.767390      90.27
 H      -3.346119    -4.462793    -1.589664      23.07
 H      -2.927652    -2.789436    -2.564209      26.41
 H      -1.317208    -3.851606    -2.093980      22.23
 C      -1.618885    -0.642471    -0.096953       6.69
 O      -2.775606    -0.677669     0.794127      20.33
 C      -0.768592     0.470690    -0.455299      85.74
 H      -0.893160     1.439963    -0.192305      31.54
 C       0.887273    -1.194514    -1.255189      -6.24
 C       2.318885    -1.509794    -1.725232      78.73
 H       2.434435    -2.791252    -2.049185      24.97
 O       2.680047    -0.806278    -2.963477     143.04
 H       3.719535    -0.667466    -3.119965      22.43
 C       3.416245    -1.332685    -0.612024      87.95
 H       2.906048    -2.004231     0.080778      30.15
 O       4.695339    -2.004844    -0.957600     213.42
 H       5.022806    -1.641760    -1.755291      28.28
 C       3.727943     0.004947     0.071554     121.49
 O       4.631512     0.810644    -0.638548     209.15
 H       4.486544     1.848504    -0.312945      22.98
 H       4.322390    -0.435936     0.924896      28.36
 H       2.789258     0.543919     0.561806      26.85
55
name = lig-Water-frame_240
 C      -0.898742     2.472532     2.646711      52.32
 H      -1.546847     3.161523     2.336892      24.76
 C      -0.416516     0.165828     3.361192      56.93
 H      -0.607919    -0.856559     3.451462      29.07
 C       0.994680     0.387369     3.231587     -13.67
 O       1.991738    -0.830132     3.531125      91.48
 C       1.485249    -2.040606     4.018172     136.06
 H       2.334453    -2.614516     4.274238      28.32
 H       0.932424    -2.523742     3.248396      29.44
 H       1.073267    -2.139056     5.002384      28.89
 C       1.476592     1.662959     3.287658      18.81
 O       2.789734     1.845184     3.666281     141.75
 H       3.048298     2.798737     3.387393      26.01
 C       0.568309     2.695588     2.809733      54.70
 H       0.942261     3.714843     2.935449      25.70
 C      -1.306793     1.190902     2.883097      33.43
 C      -2.860852     0.910958     2.810620     117.05
 H      -3.441441     1.837846     3.259657      24.20
 O      -3.223573    -0.101459     3.750281     250.43
 H      -4.205674    -0.154895     3.969405      26.26
 C      -3.253525     0.613591     1.334678      99.86
 H      -2.967580     1.448418     0.846725      27.49
 C      -4.942997     0.320912     1.019918      93.23
 O      -5.429860    -0.768489     1.747484     247.66
 H      -5.236176    -1.570998     1.215958      28.29
 H      -5.101148     0.214541     0.072860      29.69
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 H      -5.645456     1.232206     1.482726      25.18
 C       0.431113     0.221664    -1.008057      25.40
 H       1.019605     1.174440    -1.099816      27.04
 C       0.047044    -2.284372    -1.143857      43.16
 H       0.316912    -3.247018    -1.510782      26.24
 C      -1.273538    -1.891730    -0.521296       7.36
 O      -2.192791    -2.932997    -0.467376     203.98
 C      -2.406104    -3.454660    -1.821151     121.15
 H      -3.086057    -4.086421    -1.606015      31.62
 H      -2.875227    -2.983199    -2.674336      29.05
 H      -1.527049    -3.750650    -2.241900      27.97
 C      -1.674327    -0.644734    -0.064209      31.64
 O      -2.733757    -0.618714     0.767612     103.99
 C      -0.771428     0.468095    -0.400585      32.66
 H      -0.886628     1.608065     0.060075      24.42
 C       0.927694    -1.196873    -1.305714     -85.52
 C       2.412910    -1.531903    -1.759408     115.37
 H       2.365063    -2.497184    -1.877171      29.41
 O       2.676983    -0.784078    -3.026364     204.38
 H       3.640246    -0.797827    -3.010579      26.09
 C       3.429411    -1.397891    -0.611658      79.84
 H       3.173468    -2.373783     0.042852      24.98
 O       4.702628    -2.056503    -0.930412     201.81
 H       4.897871    -1.432987    -1.770376      24.11
 C       3.709610    -0.030396     0.124944     129.30
 O       4.604311     0.827916    -0.604073     247.91
 H       4.259494     1.751086    -0.284240      24.37
 H       4.104350    -0.714697     0.979395      27.26
 H       2.814017     0.413636     0.435412      29.02
55
name = lig-Water-frame_241
 C      -0.832056     2.490738     2.720181      54.44
 H      -1.648189     3.380145     2.398019      18.94
 C      -0.410605     0.139028     3.311190      54.59
 H      -0.555191    -1.010888     3.382882      25.75
 C       0.973509     0.324670     3.231476      -3.43
 O       2.051905    -0.805654     3.526041      59.31
 C       1.426377    -2.013423     4.095120     108.34
 H       2.545185    -2.649377     4.024359      24.01
 H       1.024666    -2.588271     3.185879      26.51
 H       0.938644    -2.226553     5.118748      26.24
 C       1.472465     1.610599     3.191005      19.64
 O       2.766721     1.859843     3.689488     108.71
 H       2.949269     2.861167     3.357438      24.50
 C       0.644959     2.667018     2.809543      61.09
 H       0.860542     3.783040     2.866469      26.53
 C      -1.310940     1.220599     2.915657      30.98
 C      -2.878885     0.889889     2.810051     114.27
 H      -3.261586     1.995364     2.918563      27.43
 O      -3.217974    -0.062291     3.754705     268.52
 H      -4.198296    -0.071109     3.640164      27.55
 C      -3.265700     0.572722     1.370223      89.24
 H      -2.948673     1.539862     0.720415      22.13
 C      -4.974265     0.391545     1.019241      83.59
 O      -5.431500    -0.789709     1.732632     188.49
 H      -5.277650    -1.605149     1.197642      26.99
 H      -5.218124     0.218412    -0.268465      23.59
 H      -5.551396     1.151597     1.326754      29.00
 C       0.389547     0.184337    -1.101131      43.78
 H       1.114705     0.978870    -1.204883      28.86
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 C       0.066314    -2.179472    -1.112702      30.88
 H       0.482326    -3.245749    -1.247465      26.22
 C      -1.251718    -1.955094    -0.530602       7.22
 O      -2.216442    -2.927123    -0.425103     169.04
 C      -2.405194    -3.447669    -1.880147      69.64
 H      -3.224744    -4.519410    -1.561990      22.26
 H      -2.882935    -2.632580    -2.602339      24.79
 H      -1.490987    -3.982770    -2.441100      24.04
 C      -1.660166    -0.606409    -0.041971      22.37
 O      -2.705227    -0.563765     0.759578     127.42
 C      -0.806709     0.469902    -0.308024      67.54
 H      -0.994428     1.347272     0.078690      24.76
 C       0.979379    -1.147503    -1.359869     -53.29
 C       2.447174    -1.496657    -1.778736      70.97
 H       2.356884    -2.800629    -2.004631      21.80
 O       2.682564    -0.773217    -3.061831     172.27
 H       3.702831    -0.837146    -3.175009      23.11
 C       3.434544    -1.504149    -0.604124      88.21
 H       3.104522    -2.175459     0.206424      27.63
 O       4.715556    -2.071468    -0.948094     233.55
 H       5.201863    -1.548588    -1.650632      26.20
 C       3.686093    -0.155256     0.191116     100.97
 O       4.565934     0.851755    -0.560548     233.30
 H       4.288772     1.753741    -0.312947      26.05
 H       4.136699    -0.400888     1.205408      27.32
 H       2.695431     0.420988     0.379350      25.55
55
name = lig-Water-frame_242
 C      -0.725928     2.527749     2.772322      28.06
 H      -1.289096     3.314029     2.606762      17.96
 C      -0.387258     0.088116     3.219377      54.84
 H      -0.929604    -0.895624     3.366662      24.62
 C       0.982680     0.204414     3.271008      22.06
 O       2.042996    -0.725130     3.532655     169.92
 C       1.461016    -2.057291     4.114253     113.19
 H       2.306909    -2.604914     4.110577      28.43
 H       0.815805    -2.543955     3.369611      27.41
 H       0.837982    -1.921506     4.997387      28.26
 C       1.502443     1.603895     3.104801      23.21
 O       2.739520     1.883360     3.694038     203.92
 H       3.034628     2.725797     3.365460      27.51
 C       0.639812     2.676990     2.817649      20.09
 H       1.018025     3.655265     2.775430      26.32
 C      -1.344330     1.176094     2.973965      37.99
 C      -2.824013     0.925664     2.779490     106.00
 H      -3.316884     1.985757     2.790548      25.07
 O      -3.231031    -0.040512     3.766721     261.82
 H      -4.200238    -0.044099     3.537198      27.20
 C      -3.346937     0.594595     1.332966      95.83
 H      -3.067391     1.425674     0.759877      24.61
 C      -4.942262     0.416964     0.984849      92.22
 O      -5.450038    -0.810970     1.720336     210.49
 H      -5.146377    -1.650772     1.136590      22.41
 H      -5.052540     0.364850    -0.000200      29.75
 H      -5.544276     1.483149     1.314018      26.07
 C       0.393624     0.146829    -1.168831      61.42
 H       1.137720     0.940219    -1.371006      27.68
 C       0.064215    -2.100591    -1.055506      53.88
 H       0.391987    -3.099374    -0.994163      26.91
 C      -1.203313    -1.966386    -0.536285      15.40
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 O      -2.229734    -2.943485    -0.432882     194.89
 C      -2.456383    -3.506565    -1.912034     102.82
 H      -3.022641    -4.278938    -1.851356      29.56
 H      -2.805486    -2.564820    -2.237824      25.79
 H      -1.591685    -3.957296    -2.298975      27.86
 C      -1.583189    -0.613469    -0.048757      15.07
 O      -2.709536    -0.550846     0.778025     134.22
 C      -0.791009     0.425705    -0.273236      49.31
 H      -1.107474     1.531618     0.146676      18.70
 C       0.989126    -1.061341    -1.398993      -7.09
 C       2.411408    -1.514578    -1.811023      84.85
 H       2.451375    -2.418037    -2.153438      25.43
 O       2.719163    -0.772970    -3.062713     219.17
 H       3.667183    -0.816384    -3.433750      26.02
 C       3.478601    -1.550129    -0.577883      84.64
 H       2.832207    -2.096847     0.307789      25.83
 O       4.743745    -2.097271    -0.974521     274.42
 H       5.341420    -1.629848    -1.521209      29.39
 C       3.652945    -0.248677     0.254055     106.21
 O       4.520941     0.839449    -0.514444     220.03
 H       4.347506     1.916225    -0.226431      19.96
 H       4.148820     0.009180     1.238349      26.04
 H       2.677835     0.244083     0.325548      27.20
55
name = lig-Water-frame_243
 C      -0.671624     2.475529     2.825237      44.91
 H      -1.255656     3.565021     2.739445      24.10
 C      -0.428943     0.024989     3.122765      52.69
 H      -1.087827    -0.794770     3.349555      24.79
 C       1.042395     0.172504     3.301246      22.67
 O       1.985332    -0.671290     3.557074     128.05
 C       1.480221    -2.056917     4.088081      91.74
 H       2.413797    -2.904886     4.504858      23.24
 H       0.630666    -2.446537     3.479948      25.96
 H       0.928671    -1.580342     4.943853      27.83
 C       1.522603     1.565246     3.062881      15.54
 O       2.717800     1.882938     3.687627     178.52
 H       3.215520     2.772454     3.283176      23.20
 C       0.654561     2.680312     2.829146      50.64
 H       1.252786     3.637085     2.694118      17.66
 C      -1.303809     1.165040     3.012756      42.20
 C      -2.764989     0.991740     2.737083      96.09
 H      -3.457880     1.894731     3.024308      23.99
 O      -3.256646    -0.018008     3.767108     210.12
 H      -4.255540    -0.151169     3.755020      26.17
 C      -3.430443     0.627727     1.268598      69.81
 H      -3.141834     1.605706     0.645524      22.29
 C      -4.880712     0.451725     1.039684      96.44
 O      -5.470767    -0.811953     1.683121     222.77
 H      -5.046317    -1.547232     1.243438      26.36
 H      -4.937137     0.380859    -0.272672      23.29
 H      -5.336034     1.271763     1.325325      29.10
 C       0.426810     0.209445    -1.192690      63.72
 H       0.948239     1.122850    -1.528360      28.17
 C       0.077704    -2.079788    -0.992696      47.46
 H       0.381650    -3.176237    -0.973972      23.66
 C      -1.204669    -1.923036    -0.513417      24.35
 O      -2.213361    -2.982011    -0.467617     172.29
 C      -2.473311    -3.520533    -1.878818      74.34
 H      -3.492971    -4.439041    -2.059725      22.03
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 H      -2.861090    -2.482485    -2.348767      23.85
 H      -1.427736    -3.787375    -2.275917      23.73
 C      -1.552735    -0.675724    -0.029371       3.12
 O      -2.717103    -0.588831     0.789507     112.57
 C      -0.699071     0.431957    -0.306697      59.44
 H      -0.974157     1.394523    -0.042565      22.12
 C       0.956599    -1.040573    -1.417343      12.82
 C       2.386050    -1.473275    -1.837131      59.46
 H       2.408019    -2.690319    -2.286117      20.93
 O       2.755963    -0.754107    -3.063657     219.23
 H       3.691710    -0.907714    -3.274097      27.69
 C       3.527639    -1.535209    -0.530243      83.54
 H       2.903303    -2.266713     0.001306      27.44
 O       4.756357    -2.167770    -0.975982     199.61
 H       5.276188    -1.375938    -1.511713      25.05
 C       3.633209    -0.233520     0.285501     109.12
 O       4.475952     0.825098    -0.473687     242.54
 H       4.313979     1.641436    -0.115742      26.28
 H       4.050990    -0.237644     1.283878      28.82
 H       2.540503     0.045095     0.351136      26.56
55
name = lig-Water-frame_244
 C      -0.706149     2.455007     2.868863      38.61
 H      -1.287268     3.306945     2.873141      26.61
 C      -0.455902    -0.008417     3.050168      49.61
 H      -1.008817    -1.029819     3.357337      21.67
 C       1.009402     0.256334     3.281138      15.33
 O       1.971234    -0.705972     3.592956     133.21
 C       1.492906    -2.022147     4.108991     128.92
 H       2.101286    -2.642168     4.458642      30.49
 H       0.690267    -2.454591     3.438789      27.36
 H       1.095835    -1.599797     5.036086      28.40
 C       1.522867     1.520131     3.071307      24.25
 O       2.739300     1.873817     3.668014     174.52
 H       3.067632     2.663301     3.269675      29.69
 C       0.736521     2.645008     2.834364      50.65
 H       1.133801     3.624067     2.684599      16.93
 C      -1.215565     1.190512     3.004331      27.66
 C      -2.801525     1.041127     2.734379      88.45
 H      -3.284736     1.939482     3.134701      26.43
 O      -3.265336    -0.010177     3.760516     209.24
 H      -4.238400    -0.029700     3.882953      27.18
 C      -3.395394     0.686781     1.212712      68.08
 H      -3.233893     1.552061     0.572356      25.08
 C      -4.826925     0.407092     1.049064     103.09
 O      -5.487387    -0.765870     1.635695     223.31
 H      -4.946277    -1.617288     1.290862      23.56
 H      -4.962861     0.381914     0.040938      28.65
 H      -5.484736     1.369885     1.531625      24.67
 C       0.465132     0.342661    -1.192559      53.93
 H       0.799259     1.266137    -1.651284      22.17
 C       0.116525    -2.121517    -0.944617      50.75
 H       0.437224    -3.128645    -1.158710      23.37
 C      -1.252215    -1.911866    -0.488486       7.53
 O      -2.181482    -3.029717    -0.503673     209.28
 C      -2.511947    -3.499750    -1.857410     130.58
 H      -3.236303    -4.105640    -1.916450      30.02
 H      -2.852942    -2.789938    -2.586271      28.33
 H      -1.553694    -3.730442    -2.346236      25.78
 C      -1.562438    -0.677454     0.029122      10.80
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 O      -2.721891    -0.638931     0.785022     127.54
 C      -0.604025     0.406634    -0.385504      55.60
 H      -0.893338     1.514780    -0.144530      22.86
 C       0.927828    -1.083559    -1.419611       9.09
 C       2.380920    -1.464064    -1.884176      80.83
 H       2.265447    -2.450046    -1.957018      27.30
 O       2.792586    -0.722618    -3.055183     234.79
 H       3.802332    -0.967726    -3.005886      23.97
 C       3.544846    -1.520208    -0.532154      58.71
 H       3.100935    -2.493868    -0.024696      25.39
 O       4.769306    -2.212558    -0.976840     236.56
 H       5.065029    -1.433687    -1.430342      30.21
 C       3.619877    -0.182733     0.292058     107.82
 O       4.423014     0.765744    -0.431508     235.01
 H       4.208723     1.719666     0.090477      20.10
 H       3.945788    -0.700017     1.304115      26.03
 H       2.510912     0.002099     0.442614      25.19
55
name = lig-Water-frame_245
 C      -0.677354     2.459276     2.901407      60.86
 H      -1.533859     3.292139     2.914172      20.10
 C      -0.423860    -0.022537     3.026941      68.82
 H      -0.695734    -0.973582     3.181377      25.79
 C       0.912153     0.284131     3.239774      12.40
 O       1.982477    -0.763671     3.618192     128.56
 C       1.428907    -1.912485     4.146451     109.81
 H       2.505729    -2.772824     4.344160      23.19
 H       0.857118    -2.493811     3.440150      27.47
 H       0.956469    -1.877726     5.194569      26.26
 C       1.545300     1.533202     3.123862      25.56
 O       2.786359     1.827216     3.643503     109.21
 H       3.011314     2.784064     3.225216      23.73
 C       0.733979     2.597289     2.826508      70.07
 H       1.030039     3.656211     2.765730      26.35
 C      -1.207789     1.165110     2.947098      15.14
 C      -2.851453     1.050148     2.765122      71.52
 H      -3.084863     2.216226     3.067306      24.49
 O      -3.258705    -0.003217     3.739578     203.54
 H      -4.242134     0.288233     3.855990      24.36
 C      -3.281956     0.717847     1.222003      63.04
 H      -3.097379     1.533012     0.418184      24.61
 C      -4.851641     0.386710     1.105252      97.39
 O      -5.482108    -0.723497     1.590349     215.44
 H      -5.088777    -1.572085     1.302954      25.35
 H      -5.146560     0.398208    -0.187904      24.07
 H      -5.347457     1.152139     1.494885      28.92
 C       0.533890     0.390505    -1.215775      41.01
 H       0.883816     1.313283    -1.752167      21.42
 C       0.128125    -2.160178    -0.926399      37.12
 H       0.475950    -3.145665    -1.299929      23.40
 C      -1.269381    -1.952508    -0.482102      -6.09
 O      -2.149964    -3.058201    -0.534566     181.92
 C      -2.484183    -3.422670    -1.865441      97.38
 H      -3.381357    -4.479034    -1.546661      21.48
 H      -2.941616    -2.749639    -2.732601      24.94
 H      -1.669504    -4.005366    -2.418084      24.89
 C      -1.549414    -0.642951     0.075821       3.64
 O      -2.730976    -0.651345     0.779686     106.92
 C      -0.613075     0.418791    -0.418113      54.39
 H      -0.927107     1.471711    -0.177184      25.96
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 C       0.934982    -1.078410    -1.412529       2.36
 C       2.359801    -1.428082    -1.865838      67.43
 H       2.249878    -2.698072    -1.994084      23.97
 O       2.844326    -0.706913    -3.026013     220.73
 H       3.855476    -0.762306    -3.100379      24.80
 C       3.490496    -1.546227    -0.578838      63.80
 H       3.174683    -2.315461     0.208213      27.25
 O       4.775088    -2.216769    -0.979206     203.02
 H       5.287963    -1.596019    -1.576626      29.03
 C       3.597157    -0.227325     0.306858     116.32
 O       4.362061     0.726150    -0.355810     275.09
 H       4.310402     1.667554    -0.054708      24.74
 H       4.010836    -0.641625     1.186210      29.60
 H       2.616151     0.208431     0.504445      27.31
55
name = lig-Water-frame_246
 C      -0.663875     2.449692     2.915253      60.54
 H      -1.413056     3.274944     2.863799      22.41
 C      -0.376177     0.017067     3.023102      64.22
 H      -0.638077    -1.186267     2.946599      24.06
 C       0.920325     0.248768     3.216078      17.99
 O       1.963707    -0.769001     3.627465     153.93
 C       1.421490    -1.905531     4.222601     143.25
 H       2.259936    -2.373478     4.152917      30.26
 H       0.903647    -2.552126     3.419978      27.65
 H       0.810579    -2.052145     5.108537      29.52
 C       1.559070     1.563198     3.200874      12.64
 O       2.855204     1.779235     3.596855     133.79
 H       3.094590     2.743542     3.378079      25.16
 C       0.667271     2.608614     2.819765      65.10
 H       1.106340     3.642279     2.908601      27.81
 C      -1.285887     1.108867     2.866283      29.86
 C      -2.806812     1.061553     2.788438      99.92
 H      -3.156237     2.025752     2.926258      28.26
 O      -3.280164     0.039438     3.698766     254.64
 H      -4.195813     0.363859     3.917145      26.43
 C      -3.207045     0.695567     1.267259      74.00
 H      -2.850934     1.418644     0.467893      25.09
 C      -4.862061     0.405016     1.058387      98.61
 O      -5.485724    -0.717899     1.581645     203.95
 H      -5.164860    -1.547840     1.104181      25.01
 H      -5.092660     0.548368     0.091700      28.81
 H      -5.419870     1.394398     1.603096      25.19
 C       0.581640     0.322044    -1.239372      53.44
 H       1.090555     1.151870    -1.696198      24.20
 C       0.105051    -2.161695    -0.948659      34.29
 H       0.413280    -3.171672    -1.302034      24.20
 C      -1.205454    -1.981081    -0.478801      -1.85
 O      -2.115862    -3.051732    -0.552890     206.39
 C      -2.499866    -3.453510    -1.907531     128.64
 H      -3.095176    -4.177442    -1.561015      29.16
 H      -2.971500    -2.641547    -2.382197      29.17
 H      -1.812704    -4.193737    -2.336802      25.98
 C      -1.493705    -0.651967     0.063510     -25.08
 O      -2.731743    -0.610636     0.784756      87.24
 C      -0.691112     0.465142    -0.418159      42.67
 H      -1.050734     1.459898    -0.133070      27.02
 C       0.969969    -1.016127    -1.392604      19.42
 C       2.363607    -1.478501    -1.807431      90.15
 H       2.395210    -2.366560    -2.295649      28.39
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 O       2.887453    -0.690499    -2.988865     237.39
 H       3.861426    -0.619999    -3.191657      25.34
 C       3.412856    -1.553526    -0.631199      79.35
 H       2.972975    -2.175631     0.249919      27.12
 O       4.765057    -2.190117    -0.981956     178.66
 H       5.459054    -1.886110    -1.713076      25.86
 C       3.561889    -0.314850     0.312550     108.40
 O       4.347269     0.709261    -0.308175     257.13
 H       4.258657     1.661093    -0.055945      26.67
 H       4.203217    -0.439198     1.314209      25.93
 H       2.627468     0.291788     0.626639      25.80
55
name = lig-Water-frame_247
 C      -0.736157     2.380809     2.895817      52.67
 H      -1.272909     3.380833     2.808930      21.34
 C      -0.393764     0.011043     3.003744      49.50
 H      -0.700403    -0.909849     2.803559      27.19
 C       1.077134     0.236637     3.229574      20.24
 O       1.901394    -0.708424     3.626539     156.59
 C       1.387560    -1.976865     4.246883      92.65
 H       2.588947    -2.601021     4.360355      23.03
 H       0.825751    -2.473127     3.498893      26.95
 H       0.750013    -1.863520     5.173964      27.18
 C       1.526774     1.577975     3.263702      17.04
 O       2.927536     1.731241     3.545326     120.63
 H       3.208249     2.647293     3.421608      26.81
 C       0.671539     2.651942     2.856661      56.51
 H       1.090755     3.605779     2.961776      28.34
 C      -1.324958     1.098237     2.808678      46.60
 C      -2.721474     1.022159     2.758981     109.35
 H      -3.444206     2.030501     2.914803      22.95
 O      -3.319470     0.096011     3.663999     253.06
 H      -4.247877     0.260850     3.969573      29.12
 C      -3.197522     0.630873     1.310781      85.56
 H      -2.784945     1.463750     0.682903      24.75
 C      -4.842923     0.528138     1.056023      80.11
 O      -5.489166    -0.747338     1.586510     133.68
 H      -5.220548    -1.419845     0.826341      24.80
 H      -5.055601     0.717718    -0.227050      24.56
 H      -5.288547     1.290462     1.560933      29.02
 C       0.547801     0.230207    -1.214416      52.82
 H       1.297173     1.007456    -1.537971      26.32
 C       0.102030    -2.125623    -1.015956      43.44
 H       0.347861    -3.140760    -1.246520      26.83
 C      -1.109398    -1.985355    -0.472031      29.79
 O      -2.069537    -3.024095    -0.545546     209.03
 C      -2.495095    -3.506529    -1.928984      80.44
 H      -3.604839    -4.281940    -1.590287      21.33
 H      -2.972376    -2.487590    -2.270264      24.88
 H      -1.700704    -4.039158    -2.499189      24.63
 C      -1.447957    -0.668335     0.013550     -17.10
 O      -2.694222    -0.563738     0.787213     108.36
 C      -0.751384     0.486970    -0.433804      40.92
 H      -1.114549     1.570414    -0.080597      22.53
 C       1.007994    -1.011538    -1.352531      17.67
 C       2.424576    -1.500925    -1.781118      86.30
 H       2.388070    -2.517043    -2.429244      22.79
 O       2.900526    -0.650204    -2.957060     171.30
 H       3.966849    -0.675418    -3.018219      21.25
 C       3.358912    -1.542839    -0.647740      79.07
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 H       2.781680    -2.356802    -0.016681      26.40
 O       4.732371    -2.178404    -0.966720     200.49
 H       5.128462    -1.855852    -1.757198      28.42
 C       3.551683    -0.343630     0.346154     119.89
 O       4.375716     0.708063    -0.303127     238.49
 H       3.981310     1.663189     0.109143      22.00
 H       4.069207    -0.594829     1.224245      29.17
 H       2.579472    -0.066859     0.688032      28.15
55
name = lig-Water-frame_248
 C      -0.787351     2.360735     2.843775      64.57
 H      -1.345087     3.387578     2.761294      19.74
 C      -0.372517     0.040423     2.976983      41.65
 H      -0.878865    -1.042092     2.760054      24.32
 C       1.113124     0.268558     3.243215      20.86
 O       1.875184    -0.690590     3.647330     134.40
 C       1.414511    -2.066049     4.260145     103.53
 H       2.113261    -2.597750     4.647321      29.35
 H       0.675661    -2.552185     3.518531      24.96
 H       0.930172    -1.582037     5.122052      27.31
 C       1.529358     1.606464     3.298669      26.60
 O       2.978619     1.679256     3.494488      18.88
 H       3.267913     2.713392     3.289296      24.02
 C       0.682207     2.646780     2.941905      67.85
 H       0.993638     3.769630     2.949937      28.23
 C      -1.251738     1.113233     2.802302      39.21
 C      -2.789394     0.981021     2.701942     118.29
 H      -3.151129     1.901666     2.866887      28.92
 O      -3.347443     0.114613     3.665073     259.64
 H      -4.348907     0.353424     3.798077      27.96
 C      -3.231807     0.593612     1.316859      92.82
 H      -2.931476     1.634205     0.862219      23.90
 C      -4.789351     0.629471     1.030508      84.36
 O      -5.474639    -0.752882     1.553264      99.71
 H      -5.250591    -1.354609     0.848526      29.12
 H      -4.924694     0.703639     0.019061      28.16
 H      -5.345189     1.493899     1.674184      25.66
 C       0.473641     0.216861    -1.144090      42.93
 H       1.216831     0.975554    -1.297290      25.32
 C       0.160260    -2.096663    -1.113298      41.86
 H       0.418865    -3.193865    -1.303746      25.88
 C      -1.072054    -1.966835    -0.463202      31.73
 O      -2.018898    -3.009412    -0.521679     195.57
 C      -2.551206    -3.539173    -1.903450     105.84
 H      -3.395010    -4.108370    -1.867846      28.40
 H      -2.830120    -2.693349    -2.472187      28.19
 H      -1.712549    -3.749356    -2.636602      26.25
 C      -1.459616    -0.642622    -0.033473       7.94
 O      -2.616885    -0.562209     0.769706     122.57
 C      -0.757928     0.482724    -0.469690      72.77
 H      -0.992336     1.425300    -0.199451      25.95
 C       1.045617    -1.117241    -1.315473      10.10
 C       2.475789    -1.492891    -1.853921      95.62
 H       2.300441    -2.569454    -1.980966      25.34
 O       2.915091    -0.604151    -2.917270     209.12
 H       3.841996    -0.686928    -2.906860      26.06
 C       3.360961    -1.569342    -0.617124      72.31
 H       2.830728    -2.504189    -0.154919      26.34
 O       4.664486    -2.168350    -0.938879     195.55
 H       4.766847    -1.677902    -1.822307      26.04
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 C       3.552765    -0.368400     0.346905     115.64
 O       4.377347     0.720242    -0.283165     249.45
 H       4.029727     1.483802     0.035957      27.42
 H       4.042426    -0.983072     1.261022      26.75
 H       2.445055    -0.255251     0.688205      25.62
55
name = lig-Water-frame_249
 C      -0.738864     2.449115     2.786086      45.58
 H      -1.520360     3.182048     2.707363      23.27
 C      -0.308584     0.040064     2.944986      73.43
 H      -0.720910    -0.929239     2.959561      24.82
 C       0.977858     0.302568     3.252168       7.61
 O       1.930069    -0.748487     3.681210     128.05
 C       1.368912    -2.057838     4.253566      93.25
 H       2.208213    -2.854399     4.919941      22.12
 H       0.708430    -2.649146     3.679338      26.38
 H       0.873508    -1.550403     5.092477      25.41
 C       1.594489     1.635191     3.310824      -3.94
 O       3.006123     1.668607     3.438784     213.54
 H       3.211973     2.517097     3.127206      34.25
 C       0.641009     2.654531     3.043203      80.10
 H       0.897235     3.649242     2.950916      26.10
 C      -1.208023     1.094329     2.813504      23.88
 C      -2.853958     0.919952     2.656096      73.81
 H      -2.972367     2.150043     2.859399      20.76
 O      -3.387060     0.105906     3.695839     264.30
 H      -4.292299     0.430973     3.663506      29.56
 C      -3.281974     0.629040     1.280171      90.08
 H      -3.038992     1.557046     0.733252      23.59
 C      -4.736075     0.663676     1.079098      89.80
 O      -5.450699    -0.701051     1.507268      85.93
 H      -5.131093    -1.475984     0.843986      23.30
 H      -4.959528     0.743319    -0.164570      23.87
 H      -5.254399     1.503226     1.575243      26.89
 C       0.456744     0.199602    -1.063578      48.82
 H       1.030355     1.156378    -1.152020      23.83
 C       0.188208    -2.167747    -1.187977      31.01
 H       0.495220    -3.135142    -1.451591      26.31
 C      -1.074197    -1.928212    -0.487934      16.73
 O      -1.988723    -3.021736    -0.499669     199.71
 C      -2.525124    -3.471481    -1.887987      78.00
 H      -3.480953    -4.482150    -1.968440      22.82
 H      -2.921974    -2.635088    -2.610958      25.62
 H      -1.713664    -3.864334    -2.481400      27.56
 C      -1.512950    -0.620317    -0.073718      26.14
 O      -2.546217    -0.587738     0.744983     107.74
 C      -0.722107     0.437770    -0.518908      64.80
 H      -0.962245     1.620173    -0.262686      21.28
 C       1.091186    -1.145062    -1.316392       5.61
 C       2.471904    -1.456349    -1.887664      94.05
 H       2.365493    -2.636033    -2.049644      23.57
 O       2.909864    -0.575395    -2.874281     193.14
 H       3.993485    -0.549782    -3.045526      20.69
 C       3.386249    -1.616668    -0.571192      72.54
 H       2.862637    -2.465401     0.066377      25.96
 O       4.595686    -2.147863    -0.935675     204.68
 H       4.836897    -1.628973    -1.832706      24.46
 C       3.543562    -0.442234     0.352811     118.80
 O       4.357391     0.682427    -0.247212     242.37
 H       4.090084     1.720638     0.030346      21.61
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 H       4.062230    -0.943010     1.137456      28.74
 H       2.623833    -0.023372     0.655465      26.64
55
name = lig-Water-frame_250
 C      -0.681417     2.480506     2.748691      43.70
 H      -1.632482     3.195908     2.630148      23.59
 C      -0.297285     0.030778     2.924461      62.17
 H      -0.563150    -1.067982     3.113923      24.49
 C       0.955377     0.313534     3.311193      -2.03
 O       1.988644    -0.821834     3.694890      86.07
 C       1.340233    -2.016020     4.317565     117.48
 H       2.095327    -2.541762     4.564803      30.42
 H       0.742649    -2.728869     3.626842      26.95
 H       0.580127    -1.786676     5.127013      27.66
 C       1.616169     1.614188     3.298333      -1.88
 O       2.999144     1.674977     3.381481     196.70
 H       3.313516     2.591524     2.947927      24.51
 C       0.618133     2.686465     3.135185      57.08
 H       1.031370     3.763057     3.040365      21.17
 C      -1.224464     1.097985     2.804759      24.94
 C      -2.807063     0.934266     2.661062      89.13
 H      -3.176358     1.858689     2.816195      26.10
 O      -3.426082     0.094323     3.719776     247.60
 H      -4.445967     0.353076     3.831959      26.76
 C      -3.286203     0.682036     1.213194      68.59
 H      -2.906024     1.469682     0.409381      21.76
 C      -4.746822     0.595661     1.059804     115.17
 O      -5.414708    -0.619534     1.451329     219.93
 H      -4.957735    -1.354948     0.981861      26.54
 H      -5.005749     0.827700     0.031517      27.86
 H      -5.201070     1.514522     1.606870      26.32
 C       0.573628     0.170284    -1.024033      54.38
 H       0.989741     1.161487    -1.189324      22.31
 C       0.167022    -2.237235    -1.213674      10.03
 H       0.476515    -3.263998    -1.640971      23.44
 C      -1.077207    -1.919442    -0.570558       1.93
 O      -1.990109    -3.048314    -0.489578     248.19
 C      -2.493461    -3.412777    -1.897735     105.73
 H      -3.138063    -4.267072    -1.718934      27.74
 H      -3.027724    -2.613401    -2.347884      27.35
 H      -1.629986    -4.068172    -2.246020      24.91
 C      -1.538517    -0.631324    -0.140229      18.46
 O      -2.546832    -0.611739     0.750144     105.54
 C      -0.738642     0.444331    -0.524550      74.55
 H      -0.956416     1.388016    -0.382667      25.85
 C       1.098387    -1.085701    -1.351896       1.36
 C       2.449279    -1.462569    -1.832478      95.86
 H       2.558104    -2.336218    -2.525921      22.75
 O       2.924781    -0.538482    -2.856855     248.87
 H       3.837246    -0.475897    -3.119148      26.64
 C       3.361119    -1.646630    -0.544768      83.82
 H       2.834907    -2.363103     0.257323      25.84
 O       4.581659    -2.140092    -0.966711     269.54
 H       5.073065    -1.732255    -1.608711      29.78
 C       3.544822    -0.460521     0.359596     108.93
 O       4.335433     0.630402    -0.207690     274.33
 H       4.206447     1.617299    -0.023522      24.54
 H       4.200713    -0.758752     1.316032      25.01
 H       2.672817     0.162080     0.750072      23.56
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name = lig-Water-frame_251
 C      -0.705632     2.437221     2.739010      50.74
 H      -1.252294     3.307392     2.602754      27.73
 C      -0.354164     0.007272     2.937428      20.56
 H      -0.543895    -1.102725     3.110723      26.47
 C       1.092365     0.300601     3.397369      -8.28
 O       1.993056    -0.868606     3.699152      87.28
 C       1.268652    -1.956951     4.356555     114.77
 H       2.425761    -2.567203     4.528329      23.63
 H       0.913448    -2.534394     3.505862      27.53
 H       0.514771    -1.950031     5.148317      27.16
 C       1.564141     1.581316     3.272106       1.17
 O       2.977201     1.708520     3.316663     176.05
 H       3.340882     2.604520     2.963438      22.15
 C       0.676548     2.745069     3.197159      35.51
 H       1.121672     3.722271     3.255815      19.44
 C      -1.255940     1.123978     2.779632      44.54
 C      -2.734144     0.964427     2.673727      72.82
 H      -3.453115     1.952310     2.894314      23.60
 O      -3.458618     0.074008     3.731425     216.32
 H      -4.389818     0.269737     3.946833      28.05
 C      -3.206556     0.701268     1.124532      78.48
 H      -2.848094     1.402020     0.455846      27.43
 C      -4.801965     0.541636     1.026421     103.36
 O      -5.379696    -0.543055     1.410614     235.02
 H      -4.835739    -1.309846     1.031216      25.96
 H      -5.119246     0.887358    -0.165344      25.55
 H      -5.132828     1.396705     1.734529      25.69
 C       0.684651     0.181244    -1.003464      38.90
 H       1.324739     1.024404    -1.321866      22.59
 C       0.150646    -2.233039    -1.221512      60.48
 H       0.300652    -3.186098    -1.649995      27.71
 C      -1.085792    -1.979317    -0.682083      -4.68
 O      -2.000900    -3.053696    -0.489860     203.86
 C      -2.418667    -3.388692    -1.860432     103.61
 H      -3.245637    -4.238955    -1.246281      21.29
 H      -3.005475    -2.531839    -2.284193      26.44
 H      -1.595274    -3.882548    -2.390131      24.36
 C      -1.533621    -0.659373    -0.212760      -0.56
 O      -2.601915    -0.635485     0.767620     109.25
 C      -0.727234     0.414738    -0.531538      53.30
 H      -1.087808     1.574696    -0.360097      26.21
 C       1.043781    -1.079156    -1.403602      36.89
 C       2.461086    -1.468203    -1.784754      86.82
 H       2.526155    -2.302007    -2.485600      26.49
 O       2.919962    -0.462396    -2.851746     198.30
 H       3.944319    -0.563801    -2.994919      24.82
 C       3.313873    -1.641188    -0.543644      83.09
 H       2.866534    -2.412218     0.214612      27.83
 O       4.604599    -2.187021    -0.983135     194.44
 H       5.245267    -1.521176    -1.494682      25.72
 C       3.562733    -0.387149     0.427163     120.03
 O       4.348701     0.564190    -0.202205     312.53
 H       4.110726     1.489432     0.021000      25.70
 H       4.074787    -0.686656     1.336899      28.88
 H       2.586287    -0.097931     0.828145      30.23
55
name = lig-Water-frame_252
 C      -0.674754     2.415273     2.784871      58.92
 H      -1.092161     3.502343     2.542137      24.90
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 C      -0.346128     0.014508     3.015434      15.58
 H      -0.789916    -0.977227     2.982038      28.27
 C       1.155736     0.215267     3.442150       9.20
 O       1.956719    -0.843025     3.708302     164.98
 C       1.296818    -1.967233     4.349546     125.56
 H       1.982926    -2.528536     4.766568      32.96
 H       0.877446    -2.461002     3.455197      28.07
 H       0.600933    -1.796172     5.216239      28.28
 C       1.547058     1.603189     3.255284       4.35
 O       2.949272     1.747853     3.256099     202.42
 H       3.175566     2.647872     3.070326      24.05
 C       0.712451     2.723557     3.208360      35.78
 H       1.119751     3.739335     3.399187      18.18
 C      -1.258116     1.127466     2.770593      38.28
 C      -2.769357     1.028173     2.668932      75.90
 H      -3.162876     1.959154     2.889981      28.57
 O      -3.437768     0.034153     3.728929     172.17
 H      -4.419486     0.382176     3.801442      24.05
 C      -3.138108     0.644482     1.087125      75.65
 H      -2.750189     1.641613     0.461538      26.04
 C      -4.798342     0.631413     0.935884     105.48
 O      -5.368978    -0.558316     1.397874     215.31
 H      -4.889318    -1.399466     1.030527      25.63
 H      -5.126028     0.874917    -0.051061      29.07
 H      -5.185297     1.368031     1.683382      27.40
 C       0.717607     0.227830    -1.001415      23.76
 H       1.599549     0.844034    -1.296934      23.58
 C       0.139055    -2.171786    -1.241606      53.35
 H       0.317934    -3.214091    -1.633980      25.41
 C      -1.130924    -2.021597    -0.740130      14.04
 O      -1.986243    -3.031542    -0.498556     247.59
 C      -2.406120    -3.417108    -1.762219     125.26
 H      -3.216182    -4.177798    -1.540667      26.97
 H      -2.871034    -2.587471    -2.348434      26.98
 H      -1.666933    -3.663718    -2.628024      24.31
 C      -1.527312    -0.712688    -0.256930     -16.15
 O      -2.649451    -0.654790     0.748116      98.39
 C      -0.655967     0.428064    -0.549347      59.90
 H      -1.037127     1.353979    -0.299080      30.08
 C       0.993065    -1.139898    -1.450924      30.51
 C       2.462277    -1.440711    -1.789560      73.14
 H       2.391708    -2.603587    -2.084350      26.48
 O       2.925758    -0.379892    -2.833177     164.27
 H       3.933415    -0.646358    -2.819126      22.37
 C       3.324400    -1.607136    -0.528396      60.93
 H       2.849290    -2.542198     0.039892      28.57
 O       4.646685    -2.246828    -0.999224     190.55
 H       5.050040    -1.327938    -1.184434      26.34
 C       3.545026    -0.356196     0.502592     109.55
 O       4.381960     0.516749    -0.220604     255.24
 H       4.015478     1.539522     0.037511      21.11
 H       4.045304    -0.850730     1.449188      27.34
 H       2.479562    -0.181177     0.786299      30.20
55
name = lig-Water-frame_253
 C      -0.602583     2.472396     2.860873      44.53
 H      -1.237858     3.244681     2.574412      25.36
 C      -0.293846     0.045967     3.129744      37.98
 H      -1.008912    -0.861859     2.884426      31.07
 C       1.060665     0.170793     3.418871      32.90
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 O       1.944205    -0.798155     3.735420     199.10
 C       1.305780    -1.983280     4.324081     108.81
 H       2.005493    -2.797038     5.044299      26.41
 H       0.639473    -2.589152     3.627885      25.42
 H       0.636546    -1.436313     5.024720      28.39
 C       1.591784     1.589776     3.268622      -0.63
 O       2.922814     1.784254     3.202626     136.09
 H       3.045931     2.865861     3.182097      24.26
 C       0.697684     2.643394     3.179505      22.21
 H       1.030844     3.703344     3.383565      23.52
 C      -1.210212     1.127100     2.794336     -22.71
 C      -2.809456     1.029951     2.635621      66.51
 H      -3.054053     2.215292     2.875628      25.35
 O      -3.392812     0.024232     3.697947     200.85
 H      -4.356490     0.295003     3.619005      23.75
 C      -3.132526     0.631650     1.093878     100.06
 H      -2.744503     1.403930     0.603544      28.81
 C      -4.731162     0.732082     0.871989      74.70
 O      -5.372216    -0.613794     1.395211     156.33
 H      -4.977614    -1.379916     0.925235      27.07
 H      -5.129905     0.982904    -0.298757      25.47
 H      -5.280621     1.555448     1.553897      25.62
 C       0.700792     0.218468    -1.037195      30.27
 H       1.520457     0.926651    -1.094275      27.40
 C       0.109155    -2.165028    -1.296816      31.96
 H       0.503500    -3.160623    -1.536594      26.27
 C      -1.181631    -1.964020    -0.727001      38.48
 O      -1.964659    -3.033181    -0.494914     235.64
 C      -2.440805    -3.459151    -1.739144     128.69
 H      -3.220296    -4.378574    -2.145150      25.43
 H      -2.918018    -2.582269    -2.229359      28.01
 H      -1.662319    -3.661444    -2.474411      26.13
 C      -1.506708    -0.745479    -0.276583     -16.85
 O      -2.656153    -0.666560     0.676587      92.55
 C      -0.562083     0.410280    -0.556077      49.93
 H      -0.945424     1.438118    -0.155746      27.33
 C       1.003259    -1.136674    -1.471305      34.00
 C       2.426482    -1.422667    -1.814477      91.52
 H       2.453651    -2.467666    -2.031636      30.24
 O       2.938344    -0.351508    -2.778604     185.15
 H       3.871450    -0.456986    -2.923314      25.20
 C       3.367906    -1.593993    -0.484607      62.33
 H       2.757027    -2.528405    -0.141127      30.06
 O       4.669250    -2.260734    -0.998222     207.49
 H       5.126125    -1.450506    -1.027071      29.64
 C       3.511516    -0.434565     0.555884     110.31
 O       4.398283     0.513328    -0.226589     221.27
 H       4.293250     1.424653    -0.136592      27.57
 H       4.020708    -0.854982     1.454162      29.22
 H       2.532600     0.108074     0.704884      30.23
55
name = lig-Water-frame_254
 C      -0.627857     2.468428     2.923802      48.00
 H      -1.443249     3.239005     2.703665      19.43
 C      -0.345689     0.065501     3.209452      74.18
 H      -0.716612    -0.880194     3.101338      30.49
 C       0.973465     0.224122     3.365765      21.67
 O       1.965807    -0.788763     3.759235     156.43
 C       1.284526    -2.000385     4.347570     119.17
 H       1.983575    -2.588443     4.802163      30.80
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 H       0.626928    -2.633645     3.794809      26.40
 H       0.581774    -1.396809     4.918094      27.07
 C       1.608829     1.504578     3.298234       8.13
 O       2.921083     1.840494     3.164631     125.11
 H       3.071931     2.774577     3.150310      34.88
 C       0.717041     2.594661     3.150371      82.34
 H       1.056903     3.584616     3.212669      31.44
 C      -1.131504     1.167550     2.851022      14.15
 C      -2.785635     1.000886     2.611289      90.57
 H      -3.163869     2.006303     2.739272      28.83
 O      -3.334121     0.058585     3.626897     245.17
 H      -4.325233     0.019334     3.636457      24.62
 C      -3.194881     0.634792     1.145252      81.60
 H      -2.540266     1.444968     0.437233      22.76
 C      -4.685924     0.778249     0.817965      94.60
 O      -5.373745    -0.620491     1.383426     128.04
 H      -4.931044    -1.343732     0.726385      23.17
 H      -4.871073     0.893952    -0.253837      27.96
 H      -5.139810     1.579124     1.327442      28.93
 C       0.682230     0.175619    -1.096839      65.04
 H       1.271630     1.116964    -0.944343      27.95
 C       0.082949    -2.170893    -1.360393      22.25
 H       0.520773    -3.162010    -1.467922      27.92
 C      -1.173748    -1.921002    -0.718965      -1.79
 O      -1.968236    -3.083368    -0.459381     169.01
 C      -2.504666    -3.505542    -1.842072      88.88
 H      -3.105665    -4.421837    -1.981724      28.54
 H      -3.092059    -2.582961    -2.094713      26.35
 H      -1.469768    -3.739646    -2.298971      23.30
 C      -1.492988    -0.663517    -0.251223      14.75
 O      -2.632221    -0.669660     0.576192      86.05
 C      -0.544809     0.387227    -0.513590      43.36
 H      -0.664036     1.412125    -0.063616      25.29
 C       1.039825    -1.087444    -1.475999     -18.13
 C       2.437278    -1.377761    -1.822025      92.11
 H       2.649351    -2.370637    -2.503563      22.94
 O       2.929211    -0.354681    -2.714725     176.43
 H       3.943176    -0.312281    -3.013301      18.75
 C       3.384679    -1.621357    -0.477720      79.96
 H       2.774008    -2.466919     0.048287      28.88
 O       4.659352    -2.240298    -0.970006     168.32
 H       5.505912    -1.593970    -1.022050      23.45
 C       3.495305    -0.496152     0.546299     111.62
 O       4.426365     0.478482    -0.228587     177.68
 H       4.373162     1.585772    -0.092836      21.78
 H       3.993900    -0.760160     1.542718      28.66
 H       2.695986     0.176056     0.752198      29.28
55
name = lig-Water-frame_255
 C      -0.715015     2.448704     2.968352      50.61
 H      -1.306111     3.359335     2.944468      23.72
 C      -0.443689     0.065844     3.258475      50.12
 H      -0.571476    -1.110622     3.404216      23.58
 C       1.026637     0.268706     3.347339       0.34
 O       1.963883    -0.796689     3.758098     148.63
 C       1.232905    -1.947918     4.369079      92.83
 H       2.246179    -2.545076     4.814751      24.74
 H       0.721098    -2.680535     3.597945      24.08
 H       0.487071    -1.689493     5.233667      26.71
 C       1.577660     1.480769     3.303498       8.96
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 O       2.949898     1.850425     3.145045     101.69
 H       3.077725     2.875325     3.008671      26.09
 C       0.750117     2.576523     3.126796      77.84
 H       1.279494     3.615840     3.001146      25.22
 C      -1.153820     1.188498     2.915641      44.85
 C      -2.720445     0.930896     2.591671     109.18
 H      -3.364614     1.991431     2.700461      24.86
 O      -3.262896     0.100942     3.550067     259.78
 H      -4.256975    -0.120782     3.606021      24.03
 C      -3.194770     0.675162     1.147000      91.42
 H      -2.754329     1.350605     0.596374      27.90
 C      -4.639667     0.721509     0.798680      81.91
 O      -5.358267    -0.569803     1.341754     168.23
 H      -4.940351    -1.259677     0.798366      27.81
 H      -4.709131     0.750804    -0.420185      25.26
 H      -5.121579     1.762286     1.290985      25.56
 C       0.654862     0.181597    -1.136185      64.17
 H       1.229821     1.086397    -1.086225      28.04
 C       0.081943    -2.136378    -1.401133      47.66
 H       0.367401    -3.234851    -1.485778      25.19
 C      -1.124124    -1.945889    -0.731596     -41.52
 O      -1.986888    -3.134854    -0.424410     112.62
 C      -2.536708    -3.531435    -1.947921      72.84
 H      -3.049453    -4.546143    -1.391771      22.02
 H      -3.165325    -2.751709    -2.289325      26.04
 H      -1.545237    -3.700924    -2.406290      23.53
 C      -1.494309    -0.554558    -0.202546      20.76
 O      -2.618362    -0.650686     0.487324     114.90
 C      -0.575371     0.381001    -0.435397      81.02
 H      -0.572447     1.359827     0.014262      26.91
 C       1.064133    -1.091018    -1.495541       5.12
 C       2.535632    -1.369482    -1.851477     102.40
 H       2.617793    -2.150089    -2.524168      26.73
 O       2.922224    -0.326842    -2.674488     220.18
 H       3.906600    -0.427290    -2.767335      24.20
 C       3.377902    -1.672306    -0.505472      87.68
 H       2.954526    -2.439106     0.284426      27.11
 O       4.641433    -2.214450    -0.923830     236.42
 H       5.506177    -1.744220    -0.986491      25.79
 C       3.540214    -0.491899     0.495626      99.31
 O       4.470778     0.452460    -0.225815     243.36
 H       4.148977     1.297613     0.131737      24.53
 H       3.961887    -0.742969     1.548489      27.25
 H       2.541337     0.034051     0.815446      26.47
55
name = lig-Water-frame_256
 C      -0.700580     2.490567     3.022386      34.94
 H      -1.238125     3.440323     3.061803      20.88
 C      -0.417301     0.023099     3.308258      43.60
 H      -0.875263    -0.902870     3.547844      27.13
 C       1.062118     0.215175     3.375620       2.70
 O       1.912192    -0.798808     3.751050     206.41
 C       1.225019    -1.924861     4.403666     129.03
 H       2.118819    -2.422442     4.729694      28.55
 H       0.931258    -2.465928     3.582410      28.45
 H       0.629830    -1.945328     5.280781      29.62
 C       1.595087     1.575627     3.264374       2.26
 O       2.987622     1.826603     3.143021     120.54
 H       3.002117     2.816510     2.826692      26.25
 C       0.715388     2.610025     3.090067      34.24
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 H       1.223104     3.476271     2.902527      29.43
 C      -1.310763     1.140435     2.969500      18.21
 C      -2.688324     0.932687     2.566961     127.22
 H      -3.209065     1.862258     2.685838      26.67
 O      -3.193482     0.089396     3.518574     280.84
 H      -4.156116     0.079992     3.362673      28.77
 C      -3.137591     0.674172     1.130165      72.28
 H      -2.766563     1.727303     0.494585      22.52
 C      -4.636160     0.640588     0.790974     112.94
 O      -5.337515    -0.462360     1.293807     208.66
 H      -4.899288    -1.320556     0.856904      25.86
 H      -4.618395     0.585468    -0.342176      26.75
 H      -5.061300     1.473918     1.119471      30.18
 C       0.616705     0.201158    -1.150083      50.83
 H       1.403521     0.980753    -1.379927      27.30
 C       0.096049    -2.122607    -1.407382      60.18
 H       0.263012    -3.140849    -1.643057      27.46
 C      -1.094856    -1.957816    -0.717831     -21.58
 O      -1.989174    -3.136585    -0.440291      87.65
 C      -2.554379    -3.601726    -1.938058      73.83
 H      -2.963157    -4.385958    -1.483713      26.78
 H      -3.282076    -2.916422    -2.566197      24.18
 H      -1.743385    -3.752756    -2.720190      24.82
 C      -1.488449    -0.592086    -0.189365      21.63
 O      -2.651510    -0.596100     0.442026     102.83
 C      -0.568336     0.437579    -0.370224      60.02
 H      -0.693654     1.503468     0.176796      22.68
 C       1.082245    -1.116046    -1.528960     -27.34
 C       2.587703    -1.386562    -1.843208      88.24
 H       2.546050    -2.488687    -2.423892      25.26
 O       2.953122    -0.261815    -2.648754     209.45
 H       3.926951    -0.372177    -2.647789      24.48
 C       3.385670    -1.696380    -0.508487      87.93
 H       2.942341    -2.532403     0.119439      28.81
 O       4.629993    -2.229266    -0.880904     256.13
 H       5.299357    -1.579983    -0.864573      28.77
 C       3.588551    -0.462835     0.426336     125.20
 O       4.491358     0.412883    -0.198933     276.80
 H       4.130099     1.302713     0.145021      22.39
 H       4.024162    -0.871761     1.378556      28.61
 H       2.587504    -0.210233     0.620572      28.86
55
name = lig-Water-frame_257
 C      -0.686096     2.498164     3.070650      29.28
 H      -1.327791     3.430395     3.020800      19.10
 C      -0.358088     0.031034     3.343088      50.90
 H      -1.097955    -0.830392     3.586771      25.23
 C       1.033775     0.192627     3.423503      21.08
 O       1.851922    -0.785546     3.763368     239.48
 C       1.278070    -1.931095     4.412724     105.87
 H       2.234558    -2.598890     4.777459      24.86
 H       0.788240    -2.525386     3.507454      25.04
 H       0.518127    -1.808773     5.308435      27.20
 C       1.628399     1.620584     3.202355      -6.40
 O       3.005205     1.793734     3.141693     176.69
 H       3.173050     2.676109     2.819474      27.96
 C       0.655806     2.652740     3.049344      54.95
 H       1.062271     3.744554     2.872676      29.94
 C      -1.348800     1.128485     3.032651      -0.65
 C      -2.680146     0.975205     2.532510      98.19
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 H      -3.142117     2.130745     2.713292      22.90
 O      -3.173504     0.021593     3.518375     230.71
 H      -4.120510     0.217332     3.334444      27.52
 C      -3.047630     0.700610     1.050412     105.11
 H      -2.856039     1.557845     0.617696      27.24
 C      -4.596165     0.559486     0.766029      89.98
 O      -5.330695    -0.390825     1.262639     254.32
 H      -4.943275    -1.244590     0.928374      27.66
 H      -4.639183     0.536066    -0.431819      24.64
 H      -5.263848     1.610060     1.077722      24.24
 C       0.614614     0.211718    -1.152087      43.89
 H       1.360366     0.908405    -1.526427      28.48
 C       0.119392    -2.137754    -1.391319      37.07
 H       0.323964    -3.153799    -1.911334      27.55
 C      -1.105352    -1.941437    -0.675073      50.56
 O      -1.973195    -3.093697    -0.527955     116.29
 C      -2.550627    -3.639156    -1.906560      90.94
 H      -3.185233    -4.782018    -1.728433      24.51
 H      -3.317195    -3.062605    -2.351503      26.30
 H      -1.898616    -3.934997    -2.803828      26.19
 C      -1.440918    -0.711506    -0.205759       5.62
 O      -2.709116    -0.516681     0.432382      94.52
 C      -0.534194     0.523399    -0.326261      46.96
 H      -0.799664     1.392288     0.103733      22.27
 C       1.068826    -1.115177    -1.549693     -74.43
 C       2.547792    -1.446159    -1.831253      82.66
 H       2.641123    -2.393786    -2.230442      26.57
 O       3.015461    -0.211812    -2.621413     192.62
 H       4.071156    -0.084069    -2.786466      21.83
 C       3.396618    -1.697021    -0.509925      77.64
 H       2.655478    -2.584116    -0.185576      27.22
 O       4.653707    -2.271405    -0.847315     209.15
 H       5.120433    -1.310683    -0.776001      23.96
 C       3.614375    -0.507181     0.361463     117.52
 O       4.496999     0.395471    -0.167903     228.42
 H       4.438049     1.482584    -0.132263      18.38
 H       4.097134    -1.028310     1.301323      27.03
 H       2.539634    -0.076534     0.499456      27.37
55
name = lig-Water-frame_258
 C      -0.761976     2.449413     3.097520      66.31
 H      -1.401564     3.276094     2.924014      21.17
 C      -0.384937     0.084620     3.361555      79.51
 H      -0.824491    -0.949221     3.555741      27.07
 C       0.981385     0.275338     3.461424      14.59
 O       1.832958    -0.781270     3.800129     191.51
 C       1.327124    -1.991081     4.398672     126.11
 H       2.147815    -2.662904     4.784324      27.48
 H       0.664205    -2.557875     3.829822      30.43
 H       0.641177    -1.548766     5.064971      28.40
 C       1.610537     1.603957     3.138936       7.81
 O       3.006661     1.743680     3.143016     167.03
 H       3.433020     2.702168     2.889276      21.96
 C       0.679018     2.720506     3.009431      84.76
 H       0.817500     3.766637     2.982240      23.35
 C      -1.198987     1.190724     3.095843      28.08
 C      -2.689771     1.046095     2.533682      91.57
 H      -3.122396     2.004959     2.688840      27.65
 O      -3.209546    -0.051403     3.501454     180.29
 H      -4.236218     0.093797     3.686778      22.91
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 C      -3.021217     0.715562     1.004698      87.38
 H      -2.666383     1.756432     0.320177      23.25
 C      -4.555817     0.643115     0.688537     103.85
 O      -5.362058    -0.401520     1.280303     244.63
 H      -4.991727    -1.249336     0.902732      27.59
 H      -4.641311     0.570495    -0.449639      26.28
 H      -5.026575     1.449428     0.942017      29.96
 C       0.631500     0.230733    -1.136061      48.73
 H       1.242399     1.087603    -1.449506      29.95
 C       0.148948    -2.175981    -1.380466      63.49
 H       0.347698    -3.031583    -1.935877      30.59
 C      -1.102965    -1.981842    -0.678436      56.56
 O      -1.967719    -3.055495    -0.657528     186.21
 C      -2.574330    -3.734986    -1.863424     112.36
 H      -3.016487    -4.596171    -1.779435      32.73
 H      -3.405491    -2.928674    -2.039916      24.04
 H      -1.786768    -3.953951    -2.586059      28.41
 C      -1.397073    -0.717236    -0.174286     -24.01
 O      -2.713671    -0.473846     0.409639      87.14
 C      -0.488754     0.479373    -0.347421      20.33
 H      -0.922940     1.571171     0.036769      20.64
 C       1.023567    -1.105947    -1.546734     -26.79
 C       2.507791    -1.428578    -1.823604      62.80
 H       2.781225    -2.438866    -2.499776      24.07
 O       3.081813    -0.178325    -2.599652     216.35
 H       3.982841    -0.151405    -2.865587      25.10
 C       3.348570    -1.730243    -0.565265      92.36
 H       2.650959    -2.440984    -0.094643      29.11
 O       4.696158    -2.290241    -0.811000     212.39
 H       5.244815    -1.485583    -0.916887      26.86
 C       3.564513    -0.566432     0.363341     119.93
 O       4.548427     0.401555    -0.177351     253.86
 H       4.357607     1.327016    -0.125648      26.33
 H       3.982473    -0.951897     1.310770      29.19
 H       2.756880     0.052738     0.596869      29.44
55
name = lig-Water-frame_259
 C      -0.759947     2.470300     3.097975      70.07
 H      -1.566434     3.224629     2.816396      25.72
 C      -0.406855     0.117233     3.383970      83.65
 H      -0.591918    -0.935165     3.443604      31.05
 C       0.970656     0.372352     3.493224      -3.15
 O       1.855100    -0.763907     3.815203      96.52
 C       1.332324    -2.024490     4.394525     100.74
 H       2.190153    -2.639186     4.822170      27.27
 H       0.555558    -2.716185     3.828129      27.48
 H       0.749967    -1.486170     5.287703      24.71
 C       1.563803     1.615985     3.091311      18.16
 O       3.005610     1.684042     3.142601     181.22
 H       3.278858     2.599762     3.036923      24.52
 C       0.684264     2.743269     2.995180      66.19
 H       0.957573     3.837627     3.032755      20.90
 C      -1.135629     1.206358     3.112537      40.10
 C      -2.671861     1.049579     2.581622      61.25
 H      -3.340722     2.064083     2.776111      24.83
 O      -3.279297    -0.103754     3.471527     205.00
 H      -4.126193     0.000021     3.885897      23.10
 C      -3.036263     0.802654     0.963731      79.32
 H      -2.592604     1.449111     0.366719      29.19
 C      -4.528006     0.739116     0.603259      73.35
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 O      -5.388034    -0.425879     1.307322     165.06
 H      -5.009871    -1.293700     0.819995      22.86
 H      -4.592588     0.636329    -0.538721      24.67
 H      -5.012659     1.862682     1.007683      24.35
 C       0.668657     0.254547    -1.117578      60.52
 H       1.198097     1.228094    -1.276462      29.00
 C       0.156475    -2.186929    -1.360099      93.83
 H       0.402568    -3.188212    -1.880235      26.15
 C      -1.068008    -2.043825    -0.741697     -17.63
 O      -1.984736    -3.048564    -0.747068     205.77
 C      -2.582433    -3.745362    -1.834569     113.86
 H      -3.042515    -4.890948    -1.353215      23.61
 H      -3.321561    -3.034542    -2.185148      25.54
 H      -1.657135    -3.762523    -2.538728      23.85
 C      -1.372195    -0.639088    -0.111199     -76.04
 O      -2.644633    -0.490766     0.365385      73.06
 C      -0.495134     0.382605    -0.380904     106.53
 H      -0.724564     1.325922    -0.216538      35.06
 C       1.007225    -1.078871    -1.531264       1.82
 C       2.522586    -1.380695    -1.893442      93.98
 H       2.611452    -2.094158    -2.613153      30.69
 O       3.100846    -0.163408    -2.570172     181.00
 H       4.114178    -0.485679    -2.870855      21.75
 C       3.296310    -1.755864    -0.625198      84.12
 H       2.848649    -2.485982     0.244306      27.95
 O       4.719905    -2.314645    -0.781486     206.28
 H       5.386133    -1.693152    -1.051000      27.87
 C       3.522828    -0.572541     0.385362      91.79
 O       4.616574     0.365211    -0.206361     208.51
 H       4.055832     1.296880     0.074274      22.12
 H       3.893114    -0.925742     1.472210      28.58
 H       2.660070     0.119408     0.738725      30.31
55
name = lig-Water-frame_260
 C      -0.684792     2.588966     3.061531      63.11
 H      -1.467735     3.252852     2.835270      25.67
 C      -0.352966     0.122194     3.421374      42.82
 H      -0.709779    -1.045160     3.261885      30.59
 C       1.001272     0.403122     3.521591      11.25
 O       1.887931    -0.724953     3.800673     105.55
 C       1.282003    -2.008903     4.440142     111.17
 H       2.334742    -2.524619     4.718060      26.75
 H       0.751086    -2.597848     3.756178      30.11
 H       0.903797    -1.904997     5.417030      29.57
 C       1.543817     1.646495     3.085930      22.83
 O       2.967891     1.620579     3.140453     181.19
 H       3.144767     2.614002     3.091829      23.06
 C       0.660520     2.760991     3.002031      69.03
 H       1.265540     3.700301     2.973747      23.79
 C      -1.251970     1.176948     3.078311      -8.51
 C      -2.688599     1.014639     2.659169      73.53
 H      -3.347513     1.858313     2.921972      25.02
 O      -3.322088    -0.141134     3.424259     182.80
 H      -4.226194     0.215221     3.823091      18.89
 C      -3.065866     0.832338     0.967327      44.54
 H      -2.396035     1.671922     0.294141      24.49
 C      -4.558885     0.853806     0.580058      87.15
 O      -5.378258    -0.413933     1.299988     174.87
 H      -5.055921    -1.193302     0.845933      24.32
 H      -4.620332     0.713993    -0.595682      23.68
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 H      -4.934962     1.689057     0.879755      29.39
 C       0.720379     0.239510    -1.107115      94.99
 H       1.316212     1.111868    -1.187592      29.71
 C       0.173082    -2.201247    -1.361646      87.71
 H       0.480121    -3.182707    -1.642831      29.07
 C      -1.046771    -2.033508    -0.795532     -42.05
 O      -2.018135    -3.041254    -0.754426     226.87
 C      -2.559237    -3.775145    -1.825431     119.25
 H      -2.816680    -4.536468    -1.321007      29.48
 H      -3.446419    -3.288216    -2.530049      24.88
 H      -1.875489    -3.894534    -2.643041      25.60
 C      -1.360016    -0.659055    -0.095119     -46.15
 O      -2.565288    -0.523081     0.342344      48.94
 C      -0.502961     0.302771    -0.424888      94.38
 H      -0.712297     1.479064    -0.218810      30.90
 C       1.066159    -1.028017    -1.520294      23.90
 C       2.524255    -1.293314    -1.972145      88.84
 H       2.392227    -2.148711    -2.861453      27.09
 O       3.123170    -0.174061    -2.539298     220.03
 H       4.008400    -0.506179    -2.795325      26.58
 C       3.303731    -1.763542    -0.596811      76.48
 H       2.948632    -2.562761    -0.026968      31.25
 O       4.708109    -2.361346    -0.755913     157.55
 H       5.399445    -1.685519    -1.219487      25.95
 C       3.512523    -0.537332     0.418139     113.39
 O       4.625739     0.315626    -0.212825     237.07
 H       4.374109     1.232294     0.025114      27.09
 H       3.852159    -0.985781     1.320152      32.34
 H       2.588414    -0.044421     0.589864      33.68
55
name = lig-Water-frame_261
 C      -0.680548     2.629388     3.003407      38.00
 H      -1.299875     3.601641     2.901011      24.37
 C      -0.351037     0.120112     3.420419      42.40
 H      -0.750482    -0.783191     3.313316      34.23
 C       1.048317     0.369867     3.539166      30.78
 O       1.901453    -0.676689     3.794951     118.53
 C       1.311450    -1.963186     4.480569     110.15
 H       2.273550    -2.462136     4.511220      29.92
 H       0.803140    -2.497844     3.599143      28.96
 H       0.783173    -2.138996     5.525660      27.73
 C       1.541326     1.626722     3.135721      29.03
 O       2.903031     1.595282     3.131138     213.60
 H       3.291275     2.590271     3.064553      20.73
 C       0.711004     2.778500     3.009811      31.40
 H       1.226550     3.672864     2.874402      21.51
 C      -1.335909     1.195666     3.046480     -10.63
 C      -2.745707     0.921731     2.717267      80.63
 H      -3.330885     1.918697     3.058774      23.07
 O      -3.363920    -0.152447     3.378723     235.11
 H      -4.229925     0.294442     3.522297      21.11
 C      -3.048100     0.842717     0.968266      47.70
 H      -2.596395     1.683725     0.613635      27.53
 C      -4.585053     0.859641     0.576631      75.68
 O      -5.348139    -0.331406     1.268883     217.74
 H      -4.985694    -1.222898     0.779130      22.20
 H      -4.701636     0.807175    -0.498363      25.27
 H      -5.214998     1.919158     0.993496      22.78
 C       0.757286     0.196277    -1.093181      64.38
 H       1.545166     1.017553    -1.180358      28.82
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 C       0.234313    -2.173912    -1.373967       5.65
 H       0.603063    -3.220257    -1.544418      27.06
 C      -1.065077    -1.972238    -0.815721       0.33
 O      -2.048339    -3.001292    -0.717405     178.63
 C      -2.535872    -3.762349    -1.897062      96.09
 H      -2.878965    -4.853595    -1.263134      22.85
 H      -3.478220    -3.590847    -2.385395      26.98
 H      -1.862757    -4.290963    -2.740921      23.47
 C      -1.322006    -0.785565    -0.164221     -20.57
 O      -2.556671    -0.532742     0.372446      24.35
 C      -0.478726     0.356562    -0.467665      48.77
 H      -0.812966     1.272290    -0.063646      32.16
 C       1.160267    -1.025508    -1.524302      43.23
 C       2.497755    -1.274291    -2.032279     101.45
 H       2.452282    -2.105440    -2.606901      29.68
 O       3.134460    -0.168789    -2.520061     215.44
 H       4.158330    -0.271401    -2.814943      22.79
 C       3.373503    -1.745402    -0.566815      58.02
 H       2.658179    -2.768254    -0.387620      28.54
 O       4.685553    -2.403752    -0.747339     207.56
 H       5.142738    -1.715414    -1.226436      30.00
 C       3.529319    -0.516798     0.391855     110.42
 O       4.609134     0.247695    -0.200293     177.52
 H       4.572707     1.339887    -0.070938      23.16
 H       3.943994    -1.092664     1.395182      29.22
 H       2.523749    -0.027594     0.445250      31.84
55
name = lig-Water-frame_262
 C      -0.738600     2.614813     2.935725      90.44
 H      -1.074715     3.623903     2.976196      32.08
 C      -0.396885     0.202261     3.380950      51.87
 H      -0.879762    -0.972567     3.520353      26.84
 C       1.022485     0.318858     3.537612      35.08
 O       1.909286    -0.645280     3.827127     171.23
 C       1.367854    -1.925896     4.472412     115.83
 H       2.374866    -2.629764     4.417612      27.24
 H       0.730015    -2.306447     3.667330      29.90
 H       0.723802    -1.898047     5.297070      29.97
 C       1.540259     1.594573     3.219439      35.11
 O       2.877654     1.608860     3.116374     241.25
 H       3.287836     2.414792     3.004406      32.64
 C       0.766536     2.753546     3.013239      86.06
 H       1.064321     3.866207     2.786884      12.67
 C      -1.290936     1.254914     3.043254      31.01
 C      -2.822035     0.874300     2.715842     101.97
 H      -3.223036     1.885563     2.993281      25.64
 O      -3.412009    -0.162824     3.343773     263.25
 H      -4.375356     0.000891     3.406169      24.74
 C      -3.053358     0.802215     1.018983      47.60
 H      -2.552142     1.884243     0.655692      24.86
 C      -4.633533     0.841843     0.639380      96.56
 O      -5.298774    -0.223004     1.208366     270.33
 H      -4.987201    -1.036248     0.815429      26.47
 H      -4.791287     0.878510    -0.576785      24.57
 H      -5.102097     1.621424     1.027514      28.50
 C       0.796521     0.204314    -1.069863      34.14
 H       1.519554     0.951538    -1.185225      27.75
 C       0.309378    -2.122716    -1.385364      21.39
 H       0.632290    -3.161053    -1.583409      26.10
 C      -1.062399    -1.969081    -0.857050      30.84
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 O      -2.072962    -2.957083    -0.697314     144.97
 C      -2.512816    -3.869836    -1.935499      99.22
 H      -2.805914    -4.696618    -1.536883      30.01
 H      -3.576917    -3.419731    -2.231730      24.27
 H      -1.732283    -4.235848    -2.516935      25.32
 C      -1.286168    -0.800114    -0.257153     -34.23
 O      -2.584636    -0.524209     0.429918      -2.24
 C      -0.458276     0.387711    -0.484703      43.42
 H      -0.849784     1.291002     0.076787      27.17
 C       1.197598    -1.099160    -1.535082      73.74
 C       2.545101    -1.302457    -2.008181      81.70
 H       2.702860    -2.360659    -2.616893      25.96
 O       3.145105    -0.119458    -2.544334     214.46
 H       4.168660    -0.117866    -2.719425      24.14
 C       3.400485    -1.782974    -0.580342      90.50
 H       2.670898    -2.411820    -0.362066      32.47
 O       4.643875    -2.433990    -0.749974     232.85
 H       5.151035    -1.746650    -1.221440      28.97
 C       3.554820    -0.552662     0.367116     128.23
 O       4.607738     0.198143    -0.183204     233.06
 H       4.339256     1.234669    -0.126791      25.02
 H       3.828523    -0.839076     1.333266      33.09
 H       2.661633     0.074836     0.489389      30.53
55
name = lig-Water-frame_263
 C      -0.722266     2.563513     2.884347      78.92
 H      -1.295977     3.537677     2.918801      30.71
 C      -0.451931     0.226727     3.350366      76.15
 H      -0.839033    -0.598309     3.633196      27.90
 C       0.921365     0.304297     3.519649      50.74
 O       1.924847    -0.645879     3.891067     183.43
 C       1.449731    -1.895409     4.387452     119.78
 H       2.177558    -2.578145     4.592121      29.13
 H       0.637811    -2.295026     3.708997      28.10
 H       0.802246    -1.497770     5.327325      25.91
 C       1.534600     1.600479     3.297674      18.95
 O       2.904271     1.603594     3.105762      67.62
 H       3.191144     2.652664     2.954319      27.73
 C       0.728072     2.714413     3.003515      54.82
 H       1.053015     3.681432     2.860611      20.66
 C      -1.245322     1.316747     3.041774      52.99
 C      -2.844702     0.911767     2.634666      94.83
 H      -3.419682     1.901149     2.897667      24.67
 O      -3.464285    -0.207801     3.341047     260.09
 H      -4.474335    -0.306204     3.350249      23.32
 C      -3.064747     0.778747     1.087994      83.62
 H      -2.579304     1.586697     0.618939      27.73
 C      -4.613207     0.825115     0.663140      89.08
 O      -5.284472    -0.149529     1.168144     252.12
 H      -4.939999    -1.035523     0.754226      23.57
 H      -4.729338     0.900603    -0.395882      26.64
 H      -5.090555     1.891722     1.268500      23.77
 C       0.826405     0.212630    -1.055132      18.68
 H       1.493069     1.122225    -1.193652      24.26
 C       0.315985    -2.137236    -1.392539      61.66
 H       0.626882    -3.110753    -1.739852      25.36
 C      -1.025950    -2.026300    -0.921812     -16.61
 O      -2.083680    -2.938873    -0.705377     112.77
 C      -2.507919    -3.936391    -1.929851      83.71
 H      -2.891806    -5.014843    -1.384827      21.35
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 H      -3.202319    -3.154463    -2.337992      21.95
 H      -1.489578    -3.869072    -2.561634      21.86
 C      -1.317363    -0.659594    -0.311142     -62.04
 O      -2.594105    -0.511667     0.480880      39.35
 C      -0.441704     0.378033    -0.475542      80.73
 H      -0.662566     1.381785     0.056305      26.73
 C       1.199799    -1.121067    -1.542920      48.88
 C       2.702487    -1.387994    -1.951752      94.28
 H       2.867082    -2.132909    -2.625011      30.38
 O       3.130299    -0.055484    -2.584388     232.76
 H       4.106391    -0.262931    -2.656936      25.19
 C       3.389075    -1.780059    -0.616705      82.07
 H       2.564844    -2.464909     0.123564      26.96
 O       4.601846    -2.465113    -0.765343     211.12
 H       5.385038    -1.853505    -1.169121      25.59
 C       3.561942    -0.607891     0.338930     111.73
 O       4.632789     0.189293    -0.176488     259.19
 H       4.192427     1.073298    -0.138207      26.66
 H       3.741953    -0.744727     1.561042      27.91
 H       2.721622     0.077643     0.479265      28.22
55
name = lig-Water-frame_264
 C      -0.676761     2.560641     2.850815      34.34
 H      -1.514432     3.237169     2.682669      23.27
 C      -0.478135     0.222941     3.341436      68.42
 H      -1.144096    -0.771733     3.769274      22.51
 C       0.881661     0.333779     3.507914      38.38
 O       1.938298    -0.631658     3.928930     217.41
 C       1.441234    -1.832265     4.330045     125.58
 H       2.230663    -2.636152     4.858018      24.67
 H       0.682362    -2.425544     3.747113      27.13
 H       1.095316    -1.514342     5.273542      27.61
 C       1.517986     1.600854     3.339959      13.08
 O       2.950484     1.633012     3.101668      54.68
 H       3.017191     2.605224     3.058751      25.63
 C       0.648344     2.658081     2.997531      89.29
 H       1.224415     3.654083     2.952460      31.62
 C      -1.299449     1.324517     3.018054      47.68
 C      -2.851011     0.995120     2.554934      83.16
 H      -3.650356     1.787001     2.804370      23.68
 O      -3.478888    -0.270656     3.351302     205.65
 H      -4.446591    -0.197220     3.203911      25.20
 C      -3.080757     0.737667     1.130118      90.52
 H      -2.474509     1.564993     0.474432      22.78
 C      -4.525013     0.944903     0.708059     100.27
 O      -5.336009    -0.177553     1.165849     240.31
 H      -4.943619    -1.016774     0.716612      24.02
 H      -4.571097     1.035374    -0.508619      25.24
 H      -4.826588     1.783387     1.131771      29.72
 C       0.865337     0.196290    -1.072356      57.27
 H       1.408844     1.116059    -1.171014      24.99
 C       0.261441    -2.225440    -1.412137      68.26
 H       0.626849    -3.174079    -1.935874      24.89
 C      -1.020307    -2.009249    -0.936587     -30.18
 O      -2.073639    -2.948243    -0.725850     150.91
 C      -2.444928    -3.942262    -1.889565     111.28
 H      -2.796999    -4.836316    -1.548441      26.83
 H      -3.076607    -3.279222    -2.571505      24.05
 H      -1.656725    -3.836600    -2.505840      25.52
 C      -1.414919    -0.559936    -0.348119     -52.85
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 O      -2.567272    -0.509049     0.513412      83.93
 C      -0.403868     0.399802    -0.450667      76.19
 H      -0.492333     1.375874    -0.072222      27.37
 C       1.238940    -1.061324    -1.546621      -0.80
 C       2.804683    -1.413346    -1.879132      79.79
 H       2.976316    -2.140934    -2.825825      23.89
 O       3.116068    -0.029061    -2.600637     192.60
 H       4.163873    -0.255389    -2.825445      21.13
 C       3.338943    -1.779945    -0.580033     103.10
 H       2.908567    -2.429247     0.012316      29.81
 O       4.589229    -2.519773    -0.787360     234.32
 H       5.325071    -1.989468    -0.985063      29.93
 C       3.569601    -0.631534     0.367387     121.41
 O       4.679583     0.196284    -0.168373     223.90
 H       4.196943     1.255112    -0.231844      21.14
 H       3.722708    -0.980343     1.311655      29.73
 H       2.603898    -0.052048     0.302894      25.58
55
name = lig-Water-frame_265
 C      -0.736093     2.550379     2.813604      38.94
 H      -1.399663     3.334151     2.378550      15.21
 C      -0.559381     0.154082     3.377984      49.90
 H      -1.051883    -0.693091     3.588289      24.58
 C       0.929885     0.359533     3.523538      30.82
 O       1.939619    -0.572204     3.905736     218.05
 C       1.422174    -1.847310     4.373782     116.93
 H       2.266427    -2.366834     4.570741      26.71
 H       0.803218    -2.426919     3.696602      27.07
 H       0.866646    -1.749836     5.447420      26.15
 C       1.503201     1.573106     3.329849       8.29
 O       2.950064     1.673471     3.121381      -3.57
 H       3.225213     2.708842     3.118913      25.18
 C       0.663594     2.655428     3.004971      83.40
 H       1.159877     3.626559     2.984248      37.42
 C      -1.396752     1.269656     2.975471      55.99
 C      -2.847986     1.040300     2.557878      81.69
 H      -3.575072     1.824380     2.804925      25.14
 O      -3.452775    -0.304242     3.342883     188.55
 H      -4.361510    -0.019898     3.152343      23.61
 C      -3.042109     0.731399     1.073330      97.66
 H      -2.511830     1.551841     0.574369      22.31
 C      -4.429633     1.011060     0.697767      80.77
 O      -5.401600    -0.208068     1.164102     222.27
 H      -4.974758    -0.997499     0.740929      25.31
 H      -4.433861     1.150119    -0.317480      27.89
 H      -4.865893     2.087102     1.228020      24.06
 C       0.879195     0.168657    -1.101597      37.52
 H       1.538069     1.048719    -1.183113      20.18
 C       0.239303    -2.269006    -1.461732      42.57
 H       0.481054    -3.179083    -1.927706      23.62
 C      -1.071519    -1.928939    -0.905480     -24.37
 O      -2.055676    -2.977103    -0.756792     173.09
 C      -2.360919    -3.828924    -1.859972     101.44
 H      -2.770895    -4.927431    -1.521896      23.55
 H      -3.275438    -3.684218    -2.619187      23.27
 H      -1.380789    -4.192824    -2.578760      23.11
 C      -1.489658    -0.531122    -0.375089     -16.50
 O      -2.523440    -0.523191     0.534889     147.31
 C      -0.376666     0.417281    -0.434565      40.18
 H      -0.472607     1.578448    -0.074901      18.11
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 C       1.273498    -1.068304    -1.552078       1.96
 C       2.774353    -1.367640    -1.896335      87.02
 H       2.958105    -2.146026    -2.579273      25.13
 O       3.147512    -0.050251    -2.588692     262.92
 H       4.015677    -0.034120    -2.980877      27.12
 C       3.387438    -1.777045    -0.533459      63.55
 H       2.681606    -2.786017    -0.078536      22.36
 O       4.588534    -2.602428    -0.799862     192.40
 H       5.309262    -1.912339    -0.866649      27.98
 C       3.572126    -0.608268     0.364883      98.89
 O       4.709331     0.235376    -0.148478     262.72
 H       4.495744     1.082687    -0.221772      29.72
 H       3.860311    -1.288568     1.370571      22.54
 H       2.623740    -0.149967     0.349936      23.03
55
name = lig-Water-frame_266
 C      -0.828257     2.517523     2.767757     105.64
 H      -1.056709     3.486586     2.257279      18.37
 C      -0.589441     0.137677     3.411705      47.20
 H      -1.018594    -1.028269     3.511358      22.03
 C       0.939075     0.331879     3.557425      23.01
 O       1.901096    -0.521818     3.872760     183.56
 C       1.397113    -1.870188     4.467473      90.51
 H       2.520125    -2.336857     4.322370      22.74
 H       0.891886    -2.334505     3.522693      25.75
 H       0.669065    -1.972431     5.232784      28.02
 C       1.524136     1.604058     3.268608      -1.77
 O       2.917621     1.717494     3.164735     177.04
 H       3.339620     2.630673     3.117717      24.38
 C       0.672246     2.678992     3.012640      60.94
 H       1.018738     3.710827     2.919221      23.71
 C      -1.442214     1.202678     2.942096      57.63
 C      -2.829025     0.991629     2.606182      89.72
 H      -3.389508     2.036921     2.901690      24.96
 O      -3.398060    -0.281411     3.305922     210.04
 H      -4.428791    -0.085884     3.322174      21.98
 C      -2.968317     0.760779     1.017523      84.18
 H      -2.394193     1.698630     0.543045      21.28
 C      -4.420071     1.031803     0.703164      77.71
 O      -5.447940    -0.182108     1.148060     189.21
 H      -4.952261    -1.066792     0.796758      22.35
 H      -4.514234     1.216674    -0.509567      24.87
 H      -4.837697     1.834655     1.274683      26.96
 C       0.857359     0.160364    -1.117315      19.87
 H       1.700057     0.892152    -1.193132      17.49
 C       0.219518    -2.186378    -1.495159      41.43
 H       0.316270    -3.287428    -1.858378      21.60
 C      -1.116097    -1.841298    -0.886298     -11.34
 O      -2.034440    -2.989611    -0.785935     203.62
 C      -2.272189    -3.805383    -1.891443     133.23
 H      -2.535482    -4.674995    -1.264262      25.33
 H      -3.190393    -3.620980    -2.436834      26.62
 H      -1.485980    -4.263318    -2.296433      28.09
 C      -1.459256    -0.546003    -0.400681       4.50
 O      -2.491394    -0.538349     0.558232     165.74
 C      -0.379162     0.449605    -0.437041      55.18
 H      -0.533610     1.363097    -0.092341      20.92
 C       1.256846    -1.176879    -1.567516      12.46
 C       2.692160    -1.277948    -1.932977      83.40
 H       2.857363    -2.306752    -2.530171      22.75
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 O       3.164887    -0.087053    -2.552592     248.96
 H       4.149647    -0.109039    -3.026952      22.34
 C       3.431677    -1.849845    -0.529592      79.15
 H       2.642340    -2.387693    -0.308308      28.87
 O       4.601725    -2.671162    -0.802497     206.11
 H       5.344254    -1.907739    -0.786686      26.68
 C       3.622644    -0.615787     0.398404     105.11
 O       4.740276     0.227472    -0.111251     247.22
 H       4.442901     1.365574    -0.157338      20.19
 H       3.950813    -0.946261     1.292103      26.25
 H       2.662602    -0.027962     0.663630      21.27
55
name = lig-Water-frame_267
 C      -0.827147     2.471002     2.737079      86.71
 H      -1.159260     3.411787     2.286035      26.31
 C      -0.551215     0.115195     3.445578      71.79
 H      -0.824000    -0.929977     3.430186      26.39
 C       0.863723     0.348889     3.564774      18.64
 O       1.845478    -0.528858     3.881305     174.65
 C       1.431160    -1.903841     4.442211     109.67
 H       2.316862    -2.450078     4.592395      27.74
 H       0.974679    -2.269565     3.586064      28.90
 H       0.641341    -1.971956     5.284532      26.08
 C       1.529165     1.672497     3.195391       6.79
 O       2.888494     1.721612     3.223117     195.96
 H       3.115444     2.735728     3.057259      25.04
 C       0.601548     2.694796     3.002354      37.54
 H       0.921304     3.792254     2.803325      18.10
 C      -1.390901     1.162255     2.938783      46.00
 C      -2.839014     0.906140     2.638033     107.12
 H      -3.257794     1.816535     2.907008      28.15
 O      -3.349674    -0.213895     3.259868     295.85
 H      -4.266961    -0.272937     3.525598      22.93
 C      -2.910913     0.821267     0.998702      82.09
 H      -2.310657     1.650515     0.514507      23.96
 C      -4.468720     0.966323     0.656231      84.10
 O      -5.451327    -0.123559     1.112570     266.56
 H      -5.034148    -0.957147     0.906127      28.46
 H      -4.672610     1.164080    -0.313436      29.63
 H      -4.887335     1.865485     1.399205      25.24
 C       0.824497     0.132262    -1.118505      34.43
 H       1.625419     0.820535    -1.154835      22.81
 C       0.163200    -2.079844    -1.510661      70.21
 H       0.245782    -3.097770    -1.698710      26.40
 C      -1.118973    -1.806843    -0.921971      12.37
 O      -1.987756    -2.931308    -0.780795     157.19
 C      -2.215763    -3.850253    -1.878334      97.54
 H      -2.556626    -4.710918    -1.122946      23.39
 H      -3.098147    -3.258820    -2.520204      23.82
 H      -1.203983    -4.208067    -2.467056      23.55
 C      -1.371982    -0.574805    -0.390605      11.92
 O      -2.464112    -0.530094     0.573892     135.23
 C      -0.377158     0.432183    -0.489541      51.15
 H      -0.629072     1.503720     0.069473      20.22
 C       1.172733    -1.238339    -1.572823       7.79
 C       2.647476    -1.274465    -1.969991      98.08
 H       2.714974    -2.142594    -2.612919      25.90
 O       3.187852    -0.116080    -2.531949     258.30
 H       4.068909    -0.493380    -2.694395      24.13
 C       3.462556    -1.854746    -0.580925      68.09
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 H       2.399898    -2.393076    -0.123938      25.74
 O       4.617842    -2.709868    -0.791461     226.67
 H       5.365011    -2.178888    -0.785762      30.91
 C       3.693098    -0.618284     0.442554      96.17
 O       4.763482     0.253611    -0.075274     286.77
 H       4.282287     1.054155    -0.045569      28.71
 H       4.161748    -0.759901     1.591281      24.01
 H       2.872640    -0.025324     0.749615      25.81
55
name = lig-Water-frame_268
 C      -0.781816     2.412124     2.724253      61.89
 H      -1.612770     3.137428     2.408586      26.01
 C      -0.470257     0.121667     3.459287      72.07
 H      -0.832868    -0.976687     3.488973      25.87
 C       0.811584     0.428676     3.543482      23.77
 O       1.797039    -0.580346     3.928164     168.18
 C       1.445633    -1.911454     4.383690     109.45
 H       2.302810    -2.567715     4.931463      24.98
 H       0.887719    -2.527142     3.530342      26.12
 H       0.840927    -1.735502     5.317337      26.23
 C       1.451796     1.684017     3.157958      13.76
 O       2.864336     1.731236     3.282831     227.35
 H       2.992065     2.704505     2.988394      27.29
 C       0.519116     2.729225     2.958496      41.81
 H       0.863668     3.672110     2.760382      18.34
 C      -1.302883     1.140293     2.957862      43.68
 C      -2.814880     0.852012     2.599086      87.66
 H      -3.500709     1.843585     2.972119      24.27
 O      -3.300143    -0.194358     3.242014     252.26
 H      -4.247971    -0.158424     3.561205      22.42
 C      -2.924955     0.841815     1.011928      75.35
 H      -2.324155     1.651497     0.499303      23.69
 C      -4.541953     0.894045     0.664873      88.54
 O      -5.432213    -0.043995     1.076625     271.84
 H      -5.018608    -1.004935     0.889528      23.61
 H      -4.807534     1.170339    -0.504008      24.89
 H      -4.773768     1.855916     1.227583      26.46
 C       0.803159     0.091717    -1.117291      48.54
 H       1.549990     0.955875    -1.122436      23.84
 C       0.060166    -2.048298    -1.522383      56.45
 H       0.331446    -3.142137    -1.710464      25.72
 C      -1.107521    -1.821443    -0.991126      37.78
 O      -1.929921    -2.843903    -0.749086     212.08
 C      -2.158110    -3.890969    -1.853063     114.79
 H      -2.741842    -4.811454    -1.489754      26.65
 H      -2.739433    -3.366417    -2.552839      28.72
 H      -1.369237    -3.957757    -2.499438      26.02
 C      -1.317944    -0.584149    -0.319103     -19.40
 O      -2.420882    -0.498409     0.567374      96.49
 C      -0.391895     0.438574    -0.530788      72.73
 H      -0.471389     1.295558    -0.038047      26.61
 C       1.123714    -1.137154    -1.570976      52.41
 C       2.604652    -1.356967    -1.961979      89.08
 H       2.709879    -2.143411    -2.864868      24.57
 O       3.208839    -0.149549    -2.513392     225.08
 H       4.173773    -0.493654    -2.575732      23.71
 C       3.414887    -1.814443    -0.594885      79.40
 H       2.914549    -2.487529    -0.020986      29.91
 O       4.607616    -2.749180    -0.779866     179.94
 H       5.511269    -2.291399    -0.784841      27.54
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 C       3.819974    -0.642467     0.524225      98.58
 O       4.783816     0.271187    -0.043709     296.59
 H       4.240981     1.208571    -0.097168      22.28
 H       4.119218    -1.024568     1.420709      28.19
 H       2.825319    -0.061482     0.612803      24.74
55
name = lig-Water-frame_269
 C      -0.821235     2.366535     2.708084      57.47
 H      -1.745407     2.898500     2.615045      27.72
 C      -0.456648     0.115808     3.442065      55.07
 H      -0.878979    -0.953577     3.740340      25.34
 C       0.891533     0.463385     3.537304      32.07
 O       1.774525    -0.621576     3.966853     171.87
 C       1.427535    -1.922453     4.344230     135.47
 H       2.300064    -2.318073     4.870120      29.22
 H       0.952588    -2.630578     3.773920      30.49
 H       0.772493    -1.657163     5.238906      27.84
 C       1.360689     1.657739     3.168144      40.41
 O       2.802150     1.745866     3.331235     253.68
 H       3.218018     2.649782     3.070831      25.16
 C       0.498999     2.760631     2.893100      42.76
 H       0.913199     3.854313     2.706397      12.72
 C      -1.262196     1.102050     2.977645      49.80
 C      -2.754386     0.928921     2.530940      95.25
 H      -3.383923     1.664664     2.819702      29.88
 O      -3.278773    -0.258592     3.267805     223.95
 H      -4.217500     0.107850     3.397718      24.64
 C      -2.998604     0.801706     1.028528      67.83
 H      -2.493696     1.754708     0.502399      23.74
 C      -4.560677     0.902280     0.612886     103.77
 O      -5.423390    -0.022528     1.066610     293.84
 H      -5.066040    -0.889582     0.789108      28.03
 H      -4.602050     1.044505    -0.397531      28.09
 H      -4.836541     1.962009     1.148567      25.81
 C       0.819747     0.153105    -1.111374      61.19
 H       1.478191     0.951565    -1.152094      22.80
 C       0.081794    -2.090814    -1.588216      45.54
 H       0.391823    -3.085261    -1.842801      25.99
 C      -1.138220    -1.798084    -1.013946      19.13
 O      -1.927732    -2.825014    -0.707561     156.60
 C      -2.122722    -3.878391    -1.823621      91.55
 H      -2.697417    -4.803002    -1.672315      27.49
 H      -2.808941    -3.366272    -2.746669      24.35
 H      -1.101550    -4.056742    -2.445621      22.01
 C      -1.309770    -0.575856    -0.235573      22.50
 O      -2.374102    -0.462646     0.549512      95.20
 C      -0.427738     0.421225    -0.555569      68.38
 H      -0.375237     1.492265    -0.002238      22.04
 C       1.115369    -1.044731    -1.599835      59.50
 C       2.578588    -1.467693    -1.934536      81.98
 H       2.687065    -2.190135    -2.749049      26.36
 O       3.227409    -0.196985    -2.484780     229.27
 H       4.236949    -0.130879    -2.710849      26.00
 C       3.404539    -1.771308    -0.578622      61.70
 H       2.986103    -2.664107     0.123382      26.46
 O       4.594899    -2.782567    -0.783108     146.85
 H       5.521484    -2.281088    -0.822522      26.31
 C       3.890174    -0.661164     0.521479      91.61
 O       4.802630     0.298559    -0.002251     288.49
 H       4.493975     1.298248    -0.193901      22.97
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 H       4.178749    -1.459854     1.428925      24.83
 H       2.905584    -0.250009     0.641528      26.58
55
name = lig-Water-frame_270
 C      -0.881593     2.367845     2.703793      71.84
 H      -1.653555     3.188786     2.629167      24.21
 C      -0.448223     0.077150     3.439012      69.99
 H      -0.822706    -0.813359     3.856995      28.67
 C       0.956690     0.352637     3.562821      37.14
 O       1.794852    -0.609425     3.964061     220.89
 C       1.376030    -1.901713     4.390986     121.98
 H       2.437373    -2.228598     4.731915      27.96
 H       0.932105    -2.729732     3.640789      28.28
 H       0.522019    -1.905721     5.164762      28.18
 C       1.371479     1.708530     3.193760      40.37
 O       2.719647     1.751452     3.374417     249.60
 H       3.210222     2.623531     3.215956      12.02
 C       0.504024     2.789098     2.811733     -31.73
 H       0.843957     3.747467     2.732036      19.53
 C      -1.302765     1.055860     2.964581      59.36
 C      -2.661407     0.955165     2.486154      70.35
 H      -3.351155     1.969283     2.844733      23.96
 O      -3.280471    -0.315351     3.292308     187.84
 H      -4.188430    -0.010386     3.334841      25.81
 C      -3.072645     0.766020     1.023902      89.65
 H      -2.692133     1.674648     0.540556      26.55
 C      -4.501578     0.975469     0.571261      91.43
 O      -5.447073    -0.044870     1.080263     254.83
 H      -5.115219    -0.917174     0.684519      26.92
 H      -4.371122     0.951120    -0.635437      24.33
 H      -5.000374     1.964090     0.958344      25.64
 C       0.830995     0.279230    -1.108712      36.45
 H       1.635892     1.090166    -1.185449      21.04
 C       0.179030    -2.084227    -1.665015      41.68
 H       0.414977    -3.099384    -2.041751      24.83
 C      -1.133031    -1.754316    -1.000345      -5.12
 O      -1.992396    -2.888861    -0.672832     134.72
 C      -2.079841    -3.800249    -1.869196     107.14
 H      -2.615219    -4.807190    -1.413197      25.05
 H      -2.687304    -3.395989    -2.545279      28.43
 H      -1.109229    -4.259394    -1.986428      24.13
 C      -1.304663    -0.571426    -0.215014      28.52
 O      -2.377028    -0.434926     0.554427      91.69
 C      -0.438264     0.470712    -0.533534      66.36
 H      -0.541681     1.447502    -0.087794      26.10
 C       1.132475    -1.071322    -1.666073      42.62
 C       2.606865    -1.506629    -1.874160      67.53
 H       2.653944    -2.484771    -2.554656      25.98
 O       3.223402    -0.232236    -2.462349     242.38
 H       4.140773    -0.240918    -2.743756      28.67
 C       3.431911    -1.813288    -0.527827      77.16
 H       2.628063    -2.302854    -0.002360      30.74
 O       4.589733    -2.795527    -0.805932     200.13
 H       5.316987    -2.261086    -0.913670      31.58
 C       3.899031    -0.712079     0.467480     111.83
 O       4.856610     0.311638     0.047254     314.79
 H       4.404853     1.146843    -0.007081      26.55
 H       4.375288    -1.318299     1.173883      28.22
 H       2.971044    -0.260423     0.994799      27.81
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name = lig-Water-frame_271
 C      -0.898359     2.429989     2.713976      52.26
 H      -1.412773     3.373902     2.498693      18.52
 C      -0.401075     0.041657     3.437778      54.82
 H      -0.914243    -0.977917     3.972343      23.92
 C       0.914482     0.269688     3.558848      34.95
 O       1.851588    -0.588803     3.956201     181.59
 C       1.313060    -1.922364     4.450632     119.23
 H       2.314312    -2.419264     4.732200      26.51
 H       1.096717    -2.319117     3.496859      29.28
 H       0.549820    -2.033144     5.189052      28.04
 C       1.398415     1.744933     3.229154      16.80
 O       2.676725     1.759501     3.423345     142.11
 H       2.952495     2.727294     3.272660      17.45
 C       0.485998     2.733059     2.749835      71.40
 H       0.835814     3.840365     2.714286      33.83
 C      -1.335352     1.063731     2.922657      57.64
 C      -2.690080     0.938218     2.506883     105.86
 H      -3.044835     1.810461     2.796936      28.02
 O      -3.280832    -0.341574     3.299758     191.65
 H      -4.287398    -0.299590     3.367321      23.70
 C      -3.083202     0.768492     1.026443      80.30
 H      -2.578083     1.726092     0.444758      21.57
 C      -4.469778     0.988799     0.503914      98.75
 O      -5.467446    -0.061229     1.084544     284.38
 H      -5.181231    -0.956407     0.640870      25.30
 H      -4.397060     0.911743    -0.520680      27.49
 H      -4.948316     1.975708     0.806363      25.83
 C       0.846231     0.358870    -1.137493      25.12
 H       1.610648     1.108422    -1.169705      21.76
 C       0.218566    -2.038567    -1.703512      54.28
 H       0.381680    -3.019875    -2.222644      22.44
 C      -1.079017    -1.771262    -0.969805     -28.34
 O      -2.055149    -2.945134    -0.660839     100.95
 C      -2.041242    -3.778148    -1.811825      95.29
 H      -2.612842    -4.513959    -1.286182      25.36
 H      -2.666780    -3.234612    -2.825951      21.77
 H      -1.051502    -4.283940    -1.910049      22.47
 C      -1.293585    -0.567802    -0.266053       1.21
 O      -2.434842    -0.433867     0.575694      62.85
 C      -0.398227     0.553813    -0.503701      55.71
 H      -0.792362     1.555279    -0.064848      20.57
 C       1.185919    -1.079806    -1.703542     -17.40
 C       2.679407    -1.483660    -1.828264      79.00
 H       2.669434    -2.529327    -2.222821      24.54
 O       3.197121    -0.279612    -2.452958     239.87
 H       4.168125    -0.636641    -2.707101      21.27
 C       3.441166    -1.868356    -0.500679      82.99
 H       2.452850    -2.199136     0.038500      26.71
 O       4.546443    -2.793343    -0.827515     167.45
 H       5.295176    -2.117527    -1.052756      26.82
 C       3.885066    -0.745438     0.408877     106.02
 O       4.913671     0.304612     0.095709     291.47
 H       4.162788     1.127650     0.232185      18.66
 H       4.688157    -1.270920     1.208716      20.64
 H       3.275004    -0.330012     1.211191      24.28
55
name = lig-Water-frame_272
 C      -0.873193     2.472044     2.723563      50.75
 H      -1.499700     3.300213     2.348096      18.30
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 C      -0.451991    -0.003539     3.434218      57.23
 H      -0.838806    -0.831894     3.727458      27.33
 C       0.878358     0.310437     3.522236      13.84
 O       1.917928    -0.586614     3.987750     122.48
 C       1.312137    -1.947342     4.457208      98.72
 H       2.085501    -2.604725     4.872847      26.32
 H       1.002990    -2.164426     3.384460      25.04
 H       0.507383    -1.928194     5.368498      25.23
 C       1.335209     1.677045     3.259136       6.57
 O       2.697500     1.806040     3.476929     172.06
 H       2.943644     2.780649     3.311516      18.94
 C       0.503820     2.662343     2.729641      77.65
 H       0.801148     3.705081     2.654779      32.84
 C      -1.292079     1.113425     2.887788      42.28
 C      -2.809584     0.838146     2.554444      99.72
 H      -3.273002     1.957696     2.977458      23.28
 O      -3.281084    -0.344176     3.296986     237.24
 H      -4.281424    -0.448385     3.307899      23.75
 C      -3.017249     0.825561     1.014618      90.56
 H      -2.466082     1.618314     0.544695      21.05
 C      -4.491231     0.916261     0.477590      78.51
 O      -5.471623    -0.051829     1.069986     334.85
 H      -5.212118    -0.895937     0.720684      28.82
 H      -4.544690     0.859918    -0.695786      23.65
 H      -4.823713     2.092434     0.772295      23.88
 C       0.852637     0.358305    -1.178329      33.36
 H       1.595150     1.184619    -1.183331      23.94
 C       0.177067    -1.992836    -1.707432      59.14
 H       0.360879    -2.882384    -2.250351      28.04
 C      -1.011833    -1.832755    -0.920736     -10.33
 O      -2.061668    -2.923454    -0.661188     149.25
 C      -2.042104    -3.783222    -1.759733     122.53
 H      -2.975584    -4.567970    -1.480886      23.72
 H      -2.251820    -3.395204    -2.640773      28.51
 H      -1.036334    -4.189075    -2.108459      24.42
 C      -1.298665    -0.537014    -0.329661     -25.43
 O      -2.489425    -0.473078     0.569395      46.20
 C      -0.350420     0.620336    -0.476773      40.93
 H      -0.857467     1.588307    -0.131553      16.79
 C       1.250486    -1.008062    -1.673196     -30.96
 C       2.707895    -1.428509    -1.772108      85.48
 H       2.791724    -2.464232    -2.372604      21.32
 O       3.217738    -0.363268    -2.472394     259.15
 H       4.152376    -0.609068    -2.722126      23.98
 C       3.399083    -1.878915    -0.485564      87.42
 H       2.767617    -2.525573     0.181740      26.02
 O       4.486887    -2.772041    -0.846460     173.23
 H       5.259612    -2.150431    -1.166619      27.24
 C       3.975030    -0.795873     0.452516     103.48
 O       4.913211     0.316045     0.129570     316.86
 H       4.529738     1.174955     0.182930      26.66
 H       4.602670    -1.402514     1.036562      23.19
 H       3.233748    -0.410325     1.185721      24.41
55
name = lig-Water-frame_273
 C      -0.852498     2.458447     2.707602      42.22
 H      -1.673000     3.079464     2.286324      19.34
 C      -0.538125     0.051256     3.383620      41.62
 H      -1.010472    -1.155814     3.508886      23.67
 C       0.895990     0.352024     3.511745       9.73
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 O       1.952635    -0.590010     4.047654     142.24
 C       1.315094    -1.928228     4.429723     107.68
 H       2.042283    -2.737740     4.916579      25.47
 H       0.694653    -2.428752     3.640481      27.75
 H       0.600985    -1.668617     5.136951      29.03
 C       1.308599     1.577165     3.280280      15.75
 O       2.718973     1.864516     3.530725     195.60
 H       3.107670     2.761957     3.319970      22.95
 C       0.534210     2.615480     2.743934      63.25
 H       0.968259     3.601614     2.569071      30.62
 C      -1.284598     1.133531     2.879835      33.72
 C      -2.924586     0.804313     2.635331     113.34
 H      -3.558465     1.479644     2.978630      28.21
 O      -3.282999    -0.349654     3.288219     240.43
 H      -4.233150    -0.348899     3.165730      24.52
 C      -2.986594     0.833832     1.003315      57.57
 H      -2.246527     1.764986     0.620328      18.71
 C      -4.522207     0.848855     0.458359     103.76
 O      -5.461393    -0.007526     1.054853     315.80
 H      -5.154345    -0.991596     0.775723      24.15
 H      -4.613406     0.806029    -0.609485      26.05
 H      -4.817737     1.815895     0.788817      26.62
 C       0.875161     0.332967    -1.205685      54.91
 H       1.586392     1.189676    -1.248912      23.38
 C       0.140523    -1.929671    -1.679985      44.25
 H       0.405859    -2.904526    -2.242514      24.99
 C      -0.972685    -1.869536    -0.852600       6.03
 O      -2.011241    -2.842243    -0.663013     136.37
 C      -2.082811    -3.863633    -1.726111     117.17
 H      -2.853418    -4.521627    -1.805302      27.92
 H      -2.149789    -3.169303    -2.838682      23.36
 H      -1.106222    -4.337633    -1.918319      25.27
 C      -1.312203    -0.489860    -0.358196     -10.48
 O      -2.499874    -0.526791     0.518259      40.61
 C      -0.354616     0.605603    -0.478521      52.01
 H      -0.576853     1.632472    -0.217962      20.90
 C       1.239095    -0.916303    -1.587336       8.40
 C       2.667991    -1.427039    -1.746135      91.20
 H       2.784204    -2.153886    -2.549702      20.88
 O       3.293107    -0.417292    -2.522636     268.16
 H       4.259099    -0.426796    -2.766395      25.74
 C       3.378848    -1.862946    -0.461963      87.38
 H       2.937087    -2.686672     0.187347      25.17
 O       4.443013    -2.750538    -0.879557     212.10
 H       5.156630    -2.318364    -1.227224      31.68
 C       4.069688    -0.817291     0.552837      70.39
 O       4.915141     0.303725     0.141573     286.59
 H       4.549798     1.307027     0.105900      22.43
 H       4.695764    -1.669693     1.168148      21.75
 H       3.102391    -0.483124     1.020826      23.80
55
name = lig-Water-frame_274
 C      -0.845545     2.406584     2.661156      50.27
 H      -1.599874     3.092478     2.319609      22.38
 C      -0.582429     0.083400     3.320517      61.82
 H      -0.952795    -0.784287     3.252866      31.40
 C       0.889835     0.262984     3.552844      21.24
 O       1.936056    -0.605509     4.090038     148.76
 C       1.313375    -1.901735     4.403688     102.81
 H       2.078519    -2.469860     4.758914      27.81
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 H       0.639995    -2.577395     3.800731      26.51
 H       0.527323    -1.391732     5.193325      23.53
 C       1.407520     1.593459     3.282873       5.35
 O       2.720964     1.890290     3.588020     137.47
 H       3.050728     2.799744     3.233570      27.79
 C       0.543638     2.604567     2.775152      55.64
 H       1.220162     3.495406     2.460216      23.91
 C      -1.383563     1.112759     2.910955      42.56
 C      -2.932460     0.820207     2.656641      98.57
 H      -3.913536     1.523964     3.024464      21.61
 O      -3.301730    -0.400636     3.284588     190.27
 H      -4.298204    -0.360507     3.131715      21.35
 C      -2.998138     0.792196     0.997640      67.51
 H      -2.442125     1.589172     0.706588      25.87
 C      -4.506488     0.817028     0.449372      82.56
 O      -5.447023    -0.001190     1.052104     291.99
 H      -5.177127    -0.927215     0.905116      26.88
 H      -4.539340     0.756086    -0.681224      25.03
 H      -5.013042     1.934567     0.887687      22.71
 C       0.882912     0.361801    -1.186778      62.58
 H       1.612027     1.123456    -1.288970      24.69
 C       0.156539    -1.891784    -1.635432      61.07
 H       0.422748    -2.785269    -2.082331      26.99
 C      -0.967217    -1.835959    -0.795394       7.85
 O      -1.953565    -2.770382    -0.667372     122.13
 C      -2.070594    -3.870190    -1.785406      96.70
 H      -3.103066    -4.617033    -1.839445      23.66
 H      -2.125508    -3.296392    -2.537115      27.40
 H      -1.215112    -4.631301    -1.484628      23.01
 C      -1.325977    -0.464059    -0.333867      26.10
 O      -2.466367    -0.548070     0.439662      82.82
 C      -0.389258     0.537494    -0.521346      69.24
 H      -0.255849     1.690934    -0.219999      22.27
 C       1.183620    -0.907952    -1.512066      18.34
 C       2.610670    -1.420698    -1.769114      66.65
 H       2.521574    -2.355981    -2.454166      22.65
 O       3.381452    -0.405485    -2.591425     232.00
 H       4.457520    -0.519422    -2.624270      22.56
 C       3.427647    -1.843993    -0.440007      75.16
 H       2.625096    -2.485200     0.158493      25.98
 O       4.415048    -2.762184    -0.924841     185.99
 H       5.206116    -2.299425    -1.410758      27.59
 C       4.111645    -0.833886     0.655768      89.79
 O       4.929627     0.276719     0.144576     301.22
 H       4.169176     1.021422     0.139459      21.70
 H       4.712045    -1.453271     1.343440      24.92
 H       3.237426    -0.445275     1.136142      26.82
55
name = lig-Water-frame_275
 C      -0.846797     2.347347     2.607771      61.48
 H      -1.369493     3.334071     2.349091      25.99
 C      -0.523393     0.108785     3.273393      45.27
 H      -1.079745    -1.051619     3.157508      22.43
 C       0.885701     0.214290     3.590899       4.24
 O       1.863440    -0.621200     4.079160     163.30
 C       1.265997    -1.844093     4.446137     110.41
 H       2.308766    -2.353590     4.828166      22.97
 H       0.789375    -2.444461     3.594683      27.39
 H       0.673001    -1.704526     5.266181      27.01
 C       1.493715     1.614128     3.291094     -24.23
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 O       2.729242     1.900987     3.640761     170.44
 H       2.920181     2.777185     3.221047      30.34
 C       0.573865     2.596448     2.803251      53.14
 H       1.052275     3.435571     2.416193      20.22
 C      -1.523989     1.132246     2.957829      56.68
 C      -2.924618     0.856101     2.628381      92.55
 H      -3.505233     1.666407     2.814194      29.55
 O      -3.339087    -0.472260     3.279826     183.75
 H      -4.339027    -0.555007     3.251213      24.65
 C      -3.077769     0.682749     1.018423      56.76
 H      -2.478515     1.700498     0.517016      24.96
 C      -4.476182     0.870761     0.456731     102.85
 O      -5.448173    -0.027916     1.071443     257.85
 H      -5.143548    -0.983776     0.940434      26.14
 H      -4.402700     0.755208    -0.659510      26.67
 H      -4.853359     1.822396     0.690834      28.29
 C       0.858025     0.396956    -1.133623      46.62
 H       1.675017     1.198711    -1.240714      21.76
 C       0.182661    -1.882271    -1.546791      65.11
 H       0.475795    -2.900598    -2.010148      23.48
 C      -0.967538    -1.740197    -0.790189      16.59
 O      -1.928082    -2.742855    -0.670128     133.81
 C      -2.061492    -3.911427    -1.771725      91.54
 H      -3.012153    -4.211441    -1.558952      27.27
 H      -1.901455    -3.265676    -2.925933      21.44
 H      -1.425956    -4.642338    -1.447828      26.85
 C      -1.315123    -0.491563    -0.291262      48.99
 O      -2.441464    -0.518906     0.379209      69.37
 C      -0.387934     0.546879    -0.575220      82.91
 H      -0.503285     1.444168    -0.101902      28.49
 C       1.172984    -0.951255    -1.485817       2.27
 C       2.583492    -1.392768    -1.822120      58.05
 H       2.338915    -2.471283    -2.034627      23.05
 O       3.457015    -0.391342    -2.650897     215.20
 H       4.314166    -0.742156    -2.543830      24.97
 C       3.474960    -1.815776    -0.428904      70.28
 H       2.565620    -2.240569     0.098473      27.30
 O       4.407664    -2.796388    -0.968647     157.93
 H       5.072872    -2.243907    -1.536217      27.19
 C       4.111846    -0.839944     0.718443     100.12
 O       4.912216     0.237127     0.150809     288.73
 H       4.238391     0.853639     0.085060      27.85
 H       4.801042    -1.382836     1.532281      25.04
 H       3.376230    -0.336436     1.470433      25.81
55
name = lig-Water-frame_276
 C      -0.842503     2.331647     2.576835      53.23
 H      -1.198837     3.304849     2.355077      24.70
 C      -0.481259     0.054029     3.237178      29.73
 H      -0.837005    -0.885470     3.341955      24.03
 C       0.880849     0.304804     3.585917      12.70
 O       1.760584    -0.618893     4.043433     174.10
 C       1.288078    -1.854383     4.509728     116.79
 H       2.081228    -2.391745     4.815722      27.29
 H       0.975304    -2.218257     3.539179      29.13
 H       0.572313    -2.065556     5.490257      23.79
 C       1.460594     1.581324     3.311834       5.69
 O       2.770021     1.907757     3.689359     167.01
 H       3.026878     2.819147     3.322135      27.41
 C       0.592675     2.546205     2.822342      52.56
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 H       0.793685     3.637754     2.382514      18.79
 C      -1.541018     1.168616     3.002209      19.01
 C      -2.918624     0.814406     2.546299      65.11
 H      -3.399663     1.969182     2.780948      23.19
 O      -3.382051    -0.517130     3.274039     181.77
 H      -4.336725    -0.575665     3.343194      25.86
 C      -3.113862     0.635199     1.014500     108.83
 H      -2.686012     1.419402     0.589121      28.67
 C      -4.448983     0.868197     0.468951      81.54
 O      -5.459162    -0.056801     1.091897     238.38
 H      -5.005261    -0.979889     0.864067      23.82
 H      -4.358198     0.743384    -0.603046      25.36
 H      -4.735886     2.131224     0.599592      23.85
 C       0.864999     0.393960    -1.089025      58.40
 H       1.516467     1.204555    -1.095236      23.43
 C       0.221295    -1.939154    -1.451704      64.88
 H       0.399297    -2.901124    -1.841743      26.42
 C      -0.983954    -1.687465    -0.835284      43.41
 O      -1.917777    -2.747788    -0.682367     157.35
 C      -2.039623    -3.855185    -1.766223      99.44
 H      -3.207365    -3.844589    -1.377869      21.11
 H      -1.746642    -3.765789    -2.691464      27.32
 H      -1.341399    -4.801914    -1.536296      23.91
 C      -1.245295    -0.506162    -0.269872       5.66
 O      -2.479130    -0.466570     0.369043      88.30
 C      -0.412298     0.604641    -0.587128      61.28
 H      -0.957213     1.469084     0.067095      23.36
 C       1.223532    -0.925280    -1.496329      28.96
 C       2.596852    -1.341583    -1.823761      65.93
 H       2.553727    -2.423493    -2.104082      23.77
 O       3.462638    -0.410550    -2.691834     174.11
 H       4.427693    -0.895918    -2.680052      22.62
 C       3.497183    -1.763637    -0.420725      60.81
 H       2.632513    -2.368597     0.159478      27.08
 O       4.403653    -2.822261    -0.998174     175.32
 H       4.945797    -2.346124    -1.549190      30.92
 C       4.107690    -0.838955     0.778878     106.87
 O       4.898539     0.181609     0.163312     237.38
 H       4.367328     1.156511    -0.112744      20.01
 H       4.844142    -1.499510     1.364572      26.32
 H       3.424875    -0.430026     1.477309      25.93
55
name = lig-Water-frame_277
 C      -0.808501     2.335755     2.592118      64.18
 H      -1.414349     3.246740     2.241274      23.25
 C      -0.471826     0.060929     3.229509      12.16
 H      -0.776276    -1.102592     3.568195      20.53
 C       0.845267     0.406561     3.560680      13.35
 O       1.683300    -0.587062     4.034332     157.50
 C       1.284412    -1.921810     4.572677     104.91
 H       2.243119    -2.598075     4.835563      24.71
 H       0.875763    -2.428933     3.595072      27.88
 H       0.519672    -1.986407     5.241452      27.78
 C       1.425171     1.593555     3.340165      17.44
 O       2.811218     1.900202     3.731102     162.24
 H       3.089550     2.806359     3.421715      25.13
 C       0.553935     2.528977     2.797661      61.07
 H       0.839916     3.493369     2.621147      24.47
 C      -1.428249     1.134584     3.007670       2.05
 C      -2.937236     0.770366     2.486618      80.41
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 H      -3.516444     1.575161     2.765519      28.83
 O      -3.413428    -0.517690     3.262549     191.15
 H      -4.428689    -0.388767     3.350874      25.31
 C      -3.097029     0.627913     1.019137      87.02
 H      -2.519942     1.710416     0.582736      23.55
 C      -4.485623     0.865332     0.487128     105.43
 O      -5.457626    -0.072597     1.092912     279.37
 H      -5.061635    -0.907906     0.870107      28.92
 H      -4.454775     0.677916    -0.654990      25.49
 H      -4.663150     1.789022     0.715383      30.40
 C       0.869783     0.387690    -1.045475      56.11
 H       1.550612     1.308685    -1.007363      22.18
 C       0.292260    -1.981747    -1.366939      48.97
 H       0.426514    -3.038129    -1.738824      24.26
 C      -0.995523    -1.736658    -0.903922       8.38
 O      -1.896018    -2.751407    -0.709766     209.17
 C      -2.045840    -3.810528    -1.668603     120.04
 H      -3.064062    -3.982200    -1.791298      28.06
 H      -1.668788    -3.778274    -2.924369      23.62
 H      -1.560524    -4.660749    -1.372175      27.87
 C      -1.205069    -0.453386    -0.247865      -4.95
 O      -2.533159    -0.448963     0.374428      80.57
 C      -0.493051     0.670018    -0.522373      74.76
 H      -0.848202     1.581147    -0.208616      25.63
 C       1.261058    -0.873867    -1.514813      41.63
 C       2.688483    -1.297544    -1.785983      76.19
 H       2.819508    -2.180892    -2.498274      22.19
 O       3.436151    -0.462857    -2.712458     262.19
 H       4.356723    -0.670460    -2.984245      29.16
 C       3.473066    -1.742264    -0.402449      70.27
 H       2.837027    -2.499655     0.135180      29.00
 O       4.390139    -2.833989    -0.994550     103.78
 H       5.086353    -2.413686    -1.676936      26.76
 C       4.110816    -0.845547     0.763646     110.97
 O       4.902562     0.167144     0.171366     262.48
 H       4.501377     0.977448    -0.052652      27.86
 H       4.865553    -1.637551     1.197559      25.84
 H       3.210900    -0.547084     1.447879      25.92
55
name = lig-Water-frame_278
 C      -0.817159     2.354417     2.624467      79.10
 H      -1.554053     2.975664     2.192535      23.87
 C      -0.508880     0.070019     3.266516      92.89
 H      -0.757647    -0.933926     3.625241      25.67
 C       0.808426     0.394804     3.557256       1.81
 O       1.648635    -0.567375     4.057763     134.66
 C       1.282466    -2.014009     4.547005      96.96
 H       2.220225    -2.374846     4.889458      25.58
 H       0.808334    -2.696393     3.882070      28.61
 H       0.372391    -1.756207     5.306448      23.44
 C       1.450039     1.687556     3.368443      10.42
 O       2.816151     1.873655     3.762141     137.92
 H       3.025632     2.798147     3.426529      25.93
 C       0.523233     2.560045     2.770312      77.95
 H       1.117220     3.587871     2.741392      24.14
 C      -1.326576     1.039294     2.941501       9.76
 C      -2.913822     0.685075     2.507052      88.75
 H      -3.819182     1.428661     2.855887      22.49
 O      -3.445899    -0.483722     3.239975     222.89
 H      -4.391196    -0.222555     3.315133      24.75
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 C      -3.036120     0.722694     0.980933      98.67
 H      -2.585929     1.560816     0.749408      27.87
 C      -4.535173     0.799081     0.485930      87.16
 O      -5.459702    -0.068677     1.089785     262.45
 H      -5.150761    -1.080194     0.887821      25.11
 H      -4.598684     0.751733    -0.554727      26.34
 H      -4.948298     1.966810     1.002468      23.37
 C       0.850463     0.424109    -0.997803      46.91
 H       1.583800     1.206345    -1.030131      23.76
 C       0.375084    -2.002663    -1.318534      40.23
 H       0.669027    -3.024431    -1.636637      24.09
 C      -0.955479    -1.770150    -0.938664     -15.79
 O      -1.893390    -2.746333    -0.737242     191.46
 C      -2.047259    -3.788839    -1.649821     110.12
 H      -3.128840    -4.184833    -2.114006      24.58
 H      -1.653950    -3.413062    -2.484860      26.14
 H      -1.665166    -4.728492    -1.020997      23.89
 C      -1.272862    -0.433523    -0.233920     -23.03
 O      -2.550639    -0.475806     0.364922      97.64
 C      -0.498417     0.710453    -0.470055      61.72
 H      -0.641994     1.891200    -0.414864      23.94
 C       1.275815    -0.848647    -1.509173      25.36
 C       2.822181    -1.291300    -1.759688      80.59
 H       2.666660    -2.153411    -2.403479      25.28
 O       3.392915    -0.455518    -2.737446     279.61
 H       4.339085    -0.612705    -2.957614      28.63
 C       3.450715    -1.760863    -0.424446      73.07
 H       2.787509    -2.586663     0.160213      27.24
 O       4.396121    -2.829473    -0.979346     114.60
 H       5.119656    -2.496588    -1.599660      28.11
 C       4.084623    -0.875913     0.685248     112.88
 O       4.943054     0.157557     0.192914     231.84
 H       4.270737     0.981772     0.015771      24.47
 H       4.802999    -1.655285     1.192964      26.04
 H       3.296668    -0.641811     1.340499      28.33
55
name = lig-Water-frame_279
 C      -0.873807     2.328024     2.655575      65.19
 H      -1.610722     3.011049     2.144912      22.89
 C      -0.501525     0.039911     3.350523      76.34
 H      -0.940750    -1.003573     3.614805      27.80
 C       0.837270     0.358169     3.573126      14.42
 O       1.650180    -0.589872     4.089159     131.65
 C       1.228336    -2.025907     4.528874     100.35
 H       2.217507    -2.214187     5.064864      23.92
 H       0.797279    -2.918657     3.886015      25.13
 H       0.671967    -1.726877     5.384053      26.18
 C       1.444981     1.720075     3.400485      13.43
 O       2.783609     1.856329     3.772187     151.49
 H       3.072168     2.777983     3.473564      25.16
 C       0.579863     2.673890     2.774383      66.04
 H       1.010766     3.643840     2.591538      25.67
 C      -1.359172     1.008095     2.811209       1.61
 C      -2.878125     0.633245     2.575760     103.75
 H      -3.538313     1.498925     2.813590      25.62
 O      -3.465981    -0.456933     3.212233     258.13
 H      -4.408105    -0.265581     3.331798      25.49
 C      -3.044249     0.775010     0.953662      48.75
 H      -2.385194     1.832412     0.586213      20.18
 C      -4.586134     0.817221     0.533256     113.85
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 O      -5.473984    -0.105694     1.095647     326.75
 H      -5.195994    -0.994172     0.903674      29.65
 H      -4.707432     0.937395    -0.630517      24.43
 H      -4.992330     1.624011     0.841374      28.58
 C       0.825653     0.438025    -0.970928      50.40
 H       1.596099     1.236077    -1.074807      22.56
 C       0.457342    -1.986977    -1.304501      19.51
 H       0.905183    -2.943145    -1.554929      23.90
 C      -0.885922    -1.738710    -0.911568     -28.34
 O      -1.932108    -2.718367    -0.726374     149.83
 C      -2.065331    -3.832975    -1.648154     103.99
 H      -3.042533    -3.952840    -1.974316      27.93
 H      -1.256624    -3.296667    -2.501153      19.76
 H      -1.686349    -4.707788    -1.177191      27.93
 C      -1.375728    -0.452520    -0.266322     -31.59
 O      -2.534852    -0.509465     0.344647      41.10
 C      -0.435095     0.740367    -0.446340      56.90
 H      -0.609639     1.815993    -0.401630      25.80
 C       1.293590    -0.842622    -1.450798      19.17
 C       2.849529    -1.308104    -1.751723      72.79
 H       2.468707    -2.375715    -2.019221      24.73
 O       3.368200    -0.399094    -2.764441     260.79
 H       4.396992    -0.652284    -2.712534      25.39
 C       3.463342    -1.823298    -0.476748      84.90
 H       2.637043    -2.346491     0.037569      28.75
 O       4.421138    -2.836035    -0.945987     158.64
 H       5.071144    -2.429004    -1.453300      31.08
 C       4.074196    -0.946998     0.583013     112.72
 O       4.970389     0.179176     0.214761     239.21
 H       4.209039     0.909955     0.086560      24.50
 H       4.708343    -1.594141     1.252145      26.31
 H       3.316742    -0.524650     1.374127      25.90
55
name = lig-Water-frame_280
 C      -0.904386     2.310839     2.652684      44.85
 H      -1.457727     3.160708     2.246447      23.39
 C      -0.490376     0.007598     3.432576      25.68
 H      -1.043213    -1.039868     3.515715      28.90
 C       0.877061     0.331175     3.603585      22.73
 O       1.688359    -0.646368     4.114717     152.48
 C       1.206933    -1.989877     4.547082     113.24
 H       2.176447    -2.339194     5.030444      24.88
 H       0.907428    -2.655421     3.831452      28.65
 H       0.564510    -1.881711     5.485579      25.88
 C       1.391603     1.702623     3.415405      18.17
 O       2.740480     1.851607     3.769392     164.26
 H       3.146490     2.724931     3.580145      26.68
 C       0.602541     2.754254     2.810863      43.80
 H       0.810456     3.788918     2.401748      22.09
 C      -1.424178     0.987995     2.719220     -10.47
 C      -2.826669     0.670331     2.577732      95.23
 H      -3.233349     1.784686     2.917703      21.46
 O      -3.469705    -0.460937     3.195923     251.64
 H      -4.481078    -0.351152     3.342778      21.85
 C      -3.087270     0.810630     0.938750      76.92
 H      -2.610435     1.514501     0.513232      26.59
 C      -4.597079     0.851140     0.536632      85.83
 O      -5.503029    -0.163920     1.114135     270.15
 H      -5.081754    -1.077417     0.836581      24.73
 H      -4.678076     0.939851    -0.506064      27.03
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 H      -5.133353     2.014998     0.934842      23.21
 C       0.851583     0.434473    -0.976574      80.80
 H       1.488887     1.337015    -1.100227      29.62
 C       0.502283    -1.930325    -1.298883      25.73
 H       0.943376    -2.970002    -1.494169      23.94
 C      -0.855393    -1.692870    -0.828818     -44.09
 O      -1.970537    -2.676819    -0.689194      90.47
 C      -2.007316    -3.817201    -1.693504     101.43
 H      -3.180651    -3.687316    -1.937864      22.92
 H      -1.307276    -3.872216    -2.465723      25.20
 H      -1.616384    -4.845121    -1.336770      27.32
 C      -1.366674    -0.457004    -0.366588      -3.11
 O      -2.536431    -0.518560     0.335624      19.95
 C      -0.401064     0.693054    -0.436217       1.48
 H      -0.743877     1.733127    -0.168495      21.84
 C       1.335690    -0.841490    -1.354666      27.69
 C       2.730057    -1.319199    -1.758338      87.13
 H       2.647793    -2.323948    -2.157178      23.09
 O       3.378686    -0.371759    -2.758190     282.65
 H       4.312890    -0.486344    -2.721093      29.86
 C       3.520940    -1.869053    -0.533724      87.49
 H       2.448241    -2.182881    -0.062600      25.80
 O       4.447105    -2.868550    -0.893250     149.10
 H       5.180403    -2.254762    -1.381366      25.52
 C       4.080387    -0.989904     0.535963     117.47
 O       4.969487     0.199085     0.228255     242.39
 H       4.468942     0.973876     0.039315      30.56
 H       4.698284    -1.616488     1.374973      25.57
 H       3.327308    -0.489368     1.103711      27.34
55
name = lig-Water-frame_281
 C      -0.862755     2.324792     2.622461      39.29
 H      -1.450351     3.226335     2.363972      24.73
 C      -0.524381     0.024666     3.442439      51.57
 H      -0.831670    -0.999479     3.553546      33.43
 C       0.866319     0.298139     3.648838      -8.89
 O       1.753588    -0.700081     4.141955     142.63
 C       1.227797    -1.922029     4.617385     107.65
 H       2.096029    -2.556722     4.877306      25.62
 H       0.877114    -2.403841     3.564848      26.44
 H       0.263734    -2.110087     5.254034      24.26
 C       1.351718     1.705473     3.406877       2.12
 O       2.697237     1.837894     3.766675     139.90
 H       3.063106     2.775896     3.628240      26.69
 C       0.527079     2.733798     2.870488      56.51
 H       0.734873     3.759786     2.379409      22.33
 C      -1.364039     0.945533     2.736126       2.44
 C      -2.851923     0.786543     2.503236     100.78
 H      -3.132671     1.706126     3.082254      22.08
 O      -3.452431    -0.464864     3.186912     257.38
 H      -4.413400    -0.293384     3.247209      22.37
 C      -3.184980     0.753888     0.968496      74.55
 H      -2.603249     1.701235     0.279660      22.21
 C      -4.637713     0.937188     0.575615      99.30
 O      -5.515864    -0.221430     1.119638     231.47
 H      -4.974472    -1.052030     0.825203      23.90
 H      -4.664471     0.847536    -0.583703      26.02
 H      -4.884628     1.766309     0.952973      30.73
 C       0.909932     0.462161    -0.991904      94.90
 H       1.472873     1.355246    -1.102679      33.16
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 C       0.458487    -1.892812    -1.267891      61.11
 H       0.725897    -2.875029    -1.467674      29.10
 C      -0.856581    -1.695551    -0.749166      -7.90
 O      -1.952757    -2.647179    -0.669170      72.18
 C      -1.970488    -3.806214    -1.718033      90.72
 H      -3.000873    -3.676813    -2.066995      25.02
 H      -1.315020    -3.962064    -2.791083      23.30
 H      -1.910073    -4.772213    -1.145154      27.05
 C      -1.288660    -0.419533    -0.451579      14.08
 O      -2.551348    -0.498419     0.328875      13.26
 C      -0.419732     0.600380    -0.442156      31.10
 H      -0.791234     1.533329     0.146953      27.02
 C       1.392765    -0.834662    -1.269197       7.39
 C       2.648025    -1.309078    -1.800161      91.98
 H       2.705782    -2.122538    -2.643349      18.48
 O       3.370692    -0.357190    -2.723880     256.69
 H       4.376182    -0.400149    -2.771754      25.96
 C       3.535102    -1.871655    -0.570937      81.40
 H       2.769304    -2.422673    -0.030690      30.13
 O       4.489826    -2.904748    -0.856676     187.10
 H       5.274053    -2.432221    -1.221519      25.87
 C       4.104566    -0.961595     0.541861     114.46
 O       4.984686     0.184309     0.233262     238.56
 H       4.546316     1.162708    -0.090087      25.15
 H       4.630447    -1.552414     1.239630      28.98
 H       3.096074    -0.539260     0.931341      28.97
55
name = lig-Water-frame_282
 C      -0.804911     2.327182     2.588161      60.60
 H      -1.606867     3.068072     2.388836      25.43
 C      -0.533460     0.048455     3.413897      72.68
 H      -0.698641    -1.141688     3.675136      25.33
 C       0.836991     0.297516     3.700179     -44.08
 O       1.818536    -0.688299     4.182135     166.44
 C       1.216731    -1.923094     4.604833     108.34
 H       1.989604    -2.762045     4.866470      25.84
 H       0.868969    -2.214678     3.674443      31.92
 H       0.297690    -1.957822     5.135056      23.80
 C       1.338603     1.673300     3.407183     -18.54
 O       2.658973     1.835198     3.760789     168.24
 H       2.880041     2.792966     3.622794      22.86
 C       0.411379     2.655268     2.925241      79.76
 H       0.850859     3.580971     2.653182      27.59
 C      -1.267519     0.959270     2.797039      54.81
 C      -2.889450     0.857651     2.435680      88.53
 H      -3.434764     1.712579     3.048988      25.23
 O      -3.409166    -0.436482     3.168518     231.36
 H      -4.374964    -0.261816     3.160620      24.21
 C      -3.223677     0.727036     0.954513     108.88
 H      -2.886630     1.553382     0.574242      30.48
 C      -4.676706     0.907202     0.592015      79.80
 O      -5.510167    -0.243718     1.107969     224.10
 H      -4.990438    -1.051867     0.916539      26.58
 H      -4.751983     0.925711    -0.491993      27.19
 H      -4.983872     2.049837     1.218602      24.62
 C       0.952999     0.495335    -0.988733      65.52
 H       1.645483     1.410365    -1.068888      29.20
 C       0.357949    -1.870432    -1.198292      41.13
 H       0.603407    -2.957084    -1.567120      26.86
 C      -0.875593    -1.743893    -0.717818      34.38
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 O      -1.882684    -2.640906    -0.683857     149.43
 C      -1.952011    -3.806316    -1.740248      97.87
 H      -3.013128    -3.730776    -2.257801      25.02
 H      -1.359573    -3.627563    -2.616648      25.41
 H      -2.112415    -4.612670    -1.026984      25.57
 C      -1.292483    -0.407479    -0.446622      14.02
 O      -2.561841    -0.451445     0.314317      56.16
 C      -0.394091     0.574486    -0.448057      68.66
 H      -0.638386     1.362329     0.164754      30.99
 C       1.396588    -0.818867    -1.222378     -28.20
 C       2.707935    -1.318297    -1.887470      93.50
 H       2.354630    -1.997054    -2.662610      22.73
 O       3.353030    -0.311029    -2.676022     229.57
 H       4.371324    -0.554898    -2.690888      25.00
 C       3.532829    -1.877808    -0.601375      62.94
 H       3.062918    -2.740386     0.095390      26.84
 O       4.549046    -2.945518    -0.843085     202.57
 H       5.408245    -2.688617    -1.138193      26.19
 C       4.069147    -0.848083     0.525810      96.71
 O       5.012389     0.172718     0.224372     294.32
 H       4.438801     0.866932    -0.026617      31.24
 H       4.674352    -1.600521     1.322379      25.07
 H       3.094467    -0.620551     0.970611      30.23
55
name = lig-Water-frame_283
 C      -0.860652     2.279221     2.549672      67.37
 H      -1.643207     2.941807     2.267850      26.24
 C      -0.471163    -0.024224     3.418344      36.05
 H      -0.903118    -0.896053     3.599659      25.53
 C       0.849266     0.331308     3.747130       1.34
 O       1.860101    -0.618890     4.233354      95.46
 C       1.202023    -1.972210     4.536614      91.14
 H       1.885782    -2.604481     4.980263      27.25
 H       0.728883    -2.432817     3.557113      29.90
 H       0.419677    -1.595285     5.399593      21.54
 C       1.311460     1.569644     3.436570      -1.34
 O       2.624848     1.856207     3.749960     183.88
 H       2.857702     2.803673     3.584615      21.07
 C       0.424140     2.587548     2.993245      58.15
 H       1.016546     3.626553     3.036655      23.89
 C      -1.295705     1.050759     2.821104      25.73
 C      -2.885540     0.845299     2.441172      84.64
 H      -3.675281     1.710742     2.667584      26.19
 O      -3.351748    -0.374894     3.140355     207.56
 H      -4.377842    -0.390378     3.151791      25.43
 C      -3.223898     0.709726     0.939157      83.03
 H      -2.788357     1.884032     0.544832      24.82
 C      -4.741556     0.858870     0.651301     109.75
 O      -5.510583    -0.229202     1.087055     244.22
 H      -4.966114    -1.148522     1.019516      23.57
 H      -4.916564     1.122675    -0.461324      27.31
 H      -5.087455     1.628038     1.088333      32.03
 C       0.994593     0.508985    -0.967946      62.74
 H       1.669975     1.294132    -0.981406      27.14
 C       0.345615    -1.889785    -1.148737      64.67
 H       0.596207    -2.785506    -1.585397      29.57
 C      -0.938851    -1.741151    -0.716314      41.38
 O      -1.833261    -2.687648    -0.719999     205.15
 C      -1.995963    -3.755653    -1.732246      95.82
 H      -2.962625    -3.651873    -2.314389      25.97
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 H      -1.053065    -3.528074    -2.444013      24.84
 H      -2.012467    -4.803839    -1.096128      25.29
 C      -1.367395    -0.436320    -0.363191      10.70
 O      -2.570291    -0.389643     0.289704     107.30
 C      -0.319557     0.618193    -0.459147      33.24
 H      -0.530449     1.643272     0.175063      26.48
 C       1.358569    -0.819759    -1.227641     -34.11
 C       2.761954    -1.335950    -1.929605      86.67
 H       2.183346    -2.198787    -2.473766      23.03
 O       3.364902    -0.255895    -2.617386     258.63
 H       4.221921    -0.629199    -2.680513      27.92
 C       3.569700    -1.928001    -0.611812      62.84
 H       2.824408    -2.439676    -0.068965      29.79
 O       4.614879    -2.988209    -0.848858     166.87
 H       5.615843    -2.776926    -1.164882      23.88
 C       4.032259    -0.803755     0.517885     110.33
 O       5.028890     0.155845     0.207686     263.64
 H       4.362993     0.960411    -0.016044      25.88
 H       4.483339    -1.378817     1.200226      28.64
 H       3.170409    -0.381799     1.161813      27.90
55
name = lig-Water-frame_284
 C      -0.910987     2.285574     2.529803      43.58
 H      -1.558713     3.093945     2.047434      23.92
 C      -0.435046    -0.037279     3.404419      -2.28
 H      -1.241454    -0.965977     3.571444      22.62
 C       0.880688     0.266055     3.798594      20.29
 O       1.864160    -0.551670     4.273769     112.36
 C       1.166685    -1.971449     4.472211     105.11
 H       2.037176    -2.479901     5.112243      26.08
 H       0.700774    -2.554974     3.723456      30.74
 H       0.638504    -1.691834     5.231031      30.16
 C       1.298799     1.539592     3.470293      28.63
 O       2.605246     1.879519     3.745596     167.57
 H       2.869707     2.816506     3.462582      20.54
 C       0.507151     2.559114     3.062323      64.85
 H       0.822110     3.512383     3.192568      26.91
 C      -1.409925     1.045351     2.850090      -9.69
 C      -2.873854     0.784959     2.451685      97.22
 H      -3.514074     1.755902     2.583968      26.46
 O      -3.297658    -0.315069     3.124572     250.27
 H      -4.236807    -0.480214     3.160114      27.53
 C      -3.174942     0.793801     0.905865      99.55
 H      -2.816649     1.599512     0.509286      30.61
 C      -4.766967     0.780012     0.655885      89.44
 O      -5.530783    -0.251400     1.074238     245.21
 H      -5.025090    -1.052913     0.983045      27.64
 H      -4.984257     1.152830    -0.366950      26.68
 H      -5.342041     1.771895     1.383953      24.06
 C       1.008793     0.472132    -0.931282      44.52
 H       1.759389     1.333205    -0.920996      22.15
 C       0.405301    -1.878249    -1.120882      44.29
 H       0.712738    -2.886428    -1.612085      23.88
 C      -0.981192    -1.669816    -0.740859       5.09
 O      -1.859468    -2.786916    -0.731994     224.08
 C      -2.000269    -3.705664    -1.737231     133.48
 H      -2.923477    -3.498060    -2.327312      26.53
 H      -0.969869    -3.829190    -2.195232      23.58
 H      -1.876629    -4.702510    -1.422374      28.06
 C      -1.372171    -0.408482    -0.257362     -15.80
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 O      -2.603944    -0.331143     0.260095     134.55
 C      -0.302790     0.697810    -0.426229      49.78
 H      -0.480514     1.634721    -0.156679      30.59
 C       1.327850    -0.863123    -1.280698      20.30
 C       2.741707    -1.362382    -1.877563      76.03
 H       2.604158    -2.314847    -2.461169      25.52
 O       3.385315    -0.220251    -2.560686     210.66
 H       4.356680    -0.536997    -2.846078      26.96
 C       3.622168    -1.939713    -0.628428      73.53
 H       2.536746    -2.256355    -0.240336      26.20
 O       4.671645    -3.026100    -0.852382     194.83
 H       5.472308    -2.578165    -1.179676      27.84
 C       3.979143    -0.807885     0.504775      90.94
 O       5.022285     0.165629     0.167589     217.12
 H       4.685670     1.158822     0.037779      26.37
 H       4.500901    -1.519266     1.427005      24.63
 H       3.280364    -0.124803     1.042889      25.43
55
name = lig-Water-frame_285
 C      -0.885218     2.333155     2.559802      44.73
 H      -1.285436     3.153393     2.001177      25.48
 C      -0.518384    -0.019039     3.380154      61.66
 H      -0.905255    -0.927734     3.584757      25.53
 C       0.870639     0.177579     3.811382      -8.30
 O       1.840632    -0.542877     4.300918     126.05
 C       1.226925    -1.950869     4.476589      94.17
 H       2.051488    -2.442378     4.835291      27.08
 H       0.755596    -2.538615     3.617102      27.63
 H       0.288496    -1.840526     5.316886      21.68
 C       1.328084     1.574499     3.514301      -2.47
 O       2.619656     1.896055     3.755447     207.31
 H       2.799208     2.774258     3.338277      24.99
 C       0.468170     2.541328     3.071306      58.90
 H       0.748887     3.702686     3.174467      22.11
 C      -1.472046     0.994350     2.874964       8.35
 C      -2.854738     0.776991     2.421937     106.98
 H      -3.204845     1.817104     2.907416      26.11
 O      -3.258972    -0.309528     3.145989     217.92
 H      -4.240053    -0.448588     3.111357      25.79
 C      -3.161738     0.848151     0.899500      85.51
 H      -2.687597     1.867549     0.272643      24.53
 C      -4.780652     0.831488     0.682714     107.32
 O      -5.577727    -0.320107     1.072383     205.94
 H      -5.025489    -1.211179     0.853265      23.16
 H      -4.964481     1.014514    -0.408910      27.42
 H      -5.065697     1.512212     1.275869      32.00
 C       0.996527     0.422351    -0.880803      46.30
 H       1.699511     1.220557    -0.977427      23.92
 C       0.422861    -1.890294    -1.125224      39.67
 H       0.690711    -2.878955    -1.419608      25.28
 C      -0.967038    -1.617051    -0.784752     -27.28
 O      -1.907235    -2.846777    -0.675978     131.10
 C      -1.958205    -3.691452    -1.788358     106.48
 H      -2.814359    -3.353246    -2.565920      25.00
 H      -0.992061    -3.849756    -2.447329      23.79
 H      -2.128436    -4.869284    -1.433988      24.49
 C      -1.292040    -0.336043    -0.178233     -15.10
 O      -2.659537    -0.292974     0.221537     126.87
 C      -0.318124     0.723229    -0.391058      51.96
 H      -0.630172     1.913259    -0.359263      24.86
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 C       1.352024    -0.910298    -1.359154      52.11
 C       2.761032    -1.369854    -1.796449      83.91
 H       2.938578    -2.227348    -2.600924      24.20
 O       3.408124    -0.207312    -2.514165     246.63
 H       4.302732    -0.364012    -2.884609      30.82
 C       3.609415    -1.901627    -0.621991      77.70
 H       2.901579    -2.560963    -0.145910      30.30
 O       4.686757    -3.022280    -0.847974     188.48
 H       5.323602    -2.404437    -1.215015      28.36
 C       3.982260    -0.837007     0.517691     110.76
 O       5.044427     0.176889     0.115322     246.60
 H       4.675455     1.021215     0.104021      31.57
 H       4.315064    -1.330539     1.287837      30.03
 H       3.073319    -0.238275     0.756898      27.49
55
name = lig-Water-frame_286
 C      -0.826357     2.317782     2.644133      67.21
 H      -1.239334     3.184638     2.056043      28.10
 C      -0.595244     0.012055     3.378031      59.45
 H      -0.761345    -1.168523     3.592989      21.64
 C       0.800952     0.252901     3.741750     -36.68
 O       1.796787    -0.618266     4.333140     189.08
 C       1.272385    -1.928819     4.527112     114.12
 H       2.173675    -2.653987     4.726974      24.41
 H       1.046731    -2.171923     3.444541      28.03
 H       0.410544    -2.120549     5.046029      25.47
 C       1.333750     1.569510     3.573312     -13.92
 O       2.661740     1.907700     3.774247     122.68
 H       2.838017     2.801494     3.340703      26.92
 C       0.374233     2.588026     3.052046      57.80
 H       0.785598     3.525198     2.963476      26.77
 C      -1.400162     1.001951     2.858751      59.99
 C      -2.816292     0.843753     2.410015      95.91
 H      -3.273574     1.748279     3.027463      26.99
 O      -3.261848    -0.356821     3.186984     185.27
 H      -4.265631    -0.385433     3.036053      23.29
 C      -3.180316     0.906477     0.880569      99.25
 H      -2.856442     1.806007     0.503351      29.38
 C      -4.748369     0.865967     0.672358      71.09
 O      -5.611198    -0.408049     1.071381     159.89
 H      -5.111100    -1.212831     0.768407      24.99
 H      -4.925341     0.937854    -0.447664      25.60
 H      -5.083310     1.869321     1.466641      25.08
 C       0.968478     0.356370    -0.851326      43.48
 H       1.667616     1.184346    -1.078046      23.55
 C       0.370607    -1.926490    -1.150344      32.70
 H       0.618490    -3.021201    -1.253076      23.67
 C      -0.921606    -1.598661    -0.796885     -31.83
 O      -1.927655    -2.844932    -0.598881      42.70
 C      -1.929613    -3.739465    -1.891141     105.15
 H      -2.626200    -3.334405    -2.622944      26.45
 H      -1.058595    -3.630715    -2.640463      21.91
 H      -2.401704    -4.558876    -1.463878      26.80
 C      -1.228990    -0.295866    -0.148524     -25.59
 O      -2.684440    -0.263018     0.168824      99.37
 C      -0.338337     0.752682    -0.366086      64.87
 H      -0.661665     1.712711    -0.384184      28.61
 C       1.394825    -0.924592    -1.406709      33.75
 C       2.850520    -1.362034    -1.762304      94.12
 H       2.840751    -2.079117    -2.615049      25.46
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 O       3.406514    -0.182484    -2.461369     261.94
 H       4.292011    -0.418078    -2.750902      29.74
 C       3.582731    -1.892732    -0.548911      74.30
 H       3.149624    -2.782196     0.079284      26.39
 O       4.679951    -2.959659    -0.853103     129.86
 H       5.441519    -2.400311    -1.392826      25.79
 C       3.992413    -0.827998     0.468925      93.80
 O       5.075477     0.151284     0.066999     223.73
 H       4.327080     1.027410     0.145963      21.06
 H       4.304756    -1.336827     1.591915      23.63
 H       2.882399    -0.513108     0.472454      25.54
55
name = lig-Water-frame_287
 C      -0.850085     2.283686     2.702331      60.84
 H      -1.487520     3.027215     2.248502      26.41
 C      -0.601473    -0.008199     3.413970      61.06
 H      -0.959317    -1.045319     3.406784      27.73
 C       0.752864     0.374354     3.678945      -7.43
 O       1.726173    -0.666343     4.375159     157.49
 C       1.360187    -1.963201     4.491192     119.14
 H       2.109051    -2.687923     4.797707      26.45
 H       1.209418    -2.131620     3.410717      26.98
 H       0.372956    -2.265606     5.157629      25.69
 C       1.296008     1.599221     3.605451      15.80
 O       2.697520     1.905367     3.794940     129.90
 H       2.939842     2.844377     3.489381      27.75
 C       0.431465     2.620065     3.077947      57.56
 H       0.914108     3.611830     2.704830      23.29
 C      -1.307973     1.039034     2.802563      43.12
 C      -2.783199     0.898870     2.452784      78.21
 H      -3.582808     1.670466     2.865265      24.40
 O      -3.287711    -0.400590     3.206707     172.01
 H      -4.234364    -0.443109     3.043525      24.15
 C      -3.237591     0.895320     0.908835      73.05
 H      -2.885061     2.068382     0.541981      23.45
 C      -4.733464     0.902298     0.688454      99.52
 O      -5.624473    -0.441029     1.066292     154.20
 H      -5.042856    -1.255012     0.779464      22.50
 H      -4.933734     1.066659    -0.345966      26.87
 H      -5.173195     1.648282     1.107859      30.27
 C       0.964959     0.311733    -0.871034      47.70
 H       1.619409     1.185195    -1.111223      21.84
 C       0.345851    -1.973574    -1.205134       6.52
 H       0.524640    -3.075014    -1.156804      23.36
 C      -0.911984    -1.609885    -0.740385     -26.85
 O      -1.905719    -2.799021    -0.566060      -1.06
 C      -1.920761    -3.728440    -1.985268      58.96
 H      -2.740486    -3.109668    -2.641439      22.93
 H      -0.934599    -3.726922    -2.481432      20.50
 H      -2.598982    -4.660544    -1.496333      22.66
 C      -1.252064    -0.325011    -0.174811     -17.35
 O      -2.658109    -0.218926     0.110500      78.45
 C      -0.325682     0.721866    -0.358327      52.35
 H      -0.655650     1.853091    -0.228832      25.20
 C       1.386356    -0.942832    -1.385095      25.98
 C       2.898705    -1.329725    -1.764575      80.74
 H       2.657750    -2.213686    -2.517809      23.53
 O       3.407517    -0.153410    -2.396836     245.46
 H       4.398316    -0.499005    -2.575014      24.50
 C       3.626029    -1.957076    -0.445430      75.91
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 H       2.837811    -2.529993     0.151621      27.59
 O       4.689524    -2.855098    -0.886070     220.43
 H       5.383981    -2.632612    -1.460323      31.79
 C       4.007485    -0.843862     0.444111     125.99
 O       5.038268     0.135770     0.032273     320.26
 H       4.573310     0.930672     0.040023      30.38
 H       4.159668    -1.126676     1.367848      28.82
 H       3.031041    -0.361163     0.543991      26.76
55
name = lig-Water-frame_288
 C      -0.871056     2.326463     2.739075      53.46
 H      -1.721756     2.984750     2.447857      20.37
 C      -0.564379    -0.004747     3.424933      67.36
 H      -1.123600    -0.989132     3.372175      25.99
 C       0.735008     0.352948     3.696097       6.33
 O       1.660329    -0.612497     4.420638     166.99
 C       1.380181    -2.062742     4.411298     115.77
 H       2.282400    -2.567851     4.934905      25.82
 H       1.120302    -2.623055     3.430998      26.21
 H       0.584214    -2.179634     5.108164      28.02
 C       1.312259     1.725809     3.605188       2.35
 O       2.703297     1.874320     3.821386     200.27
 H       2.919252     2.835190     3.604702      25.99
 C       0.551208     2.673670     3.095893      58.10
 H       0.904221     3.588351     2.659459      27.43
 C      -1.303675     1.017090     2.761645      37.91
 C      -2.815623     0.880129     2.499027      78.26
 H      -3.480112     1.732569     2.775723      25.17
 O      -3.299686    -0.419673     3.206231     184.41
 H      -4.291323    -0.533729     3.065689      23.52
 C      -3.251799     0.889665     0.961564      82.00
 H      -2.989314     1.853238     0.613673      24.29
 C      -4.749980     0.852452     0.678783      79.22
 O      -5.606933    -0.419300     1.047485     184.86
 H      -4.959275    -1.231623     0.914686      23.41
 H      -4.918063     1.128836    -0.464866      24.06
 H      -5.508188     1.769762     1.205104      22.61
 C       0.968723     0.321376    -0.921258      50.62
 H       1.643547     1.132736    -1.047965      23.47
 C       0.354706    -1.996356    -1.249467      27.28
 H       0.548981    -3.050017    -1.281552      24.20
 C      -0.939446    -1.672953    -0.651320     -18.48
 O      -1.852394    -2.732788    -0.583274     129.77
 C      -1.992023    -3.664009    -2.021534      72.59
 H      -2.569063    -3.072639    -2.572322      25.83
 H      -0.857156    -4.060580    -2.141555      24.08
 H      -2.322895    -4.572413    -1.780882      29.08
 C      -1.323127    -0.366819    -0.239318      28.58
 O      -2.620352    -0.159404     0.060592      97.75
 C      -0.304189     0.664424    -0.368440      47.34
 H      -0.425530     1.692695     0.028673      21.62
 C       1.344939    -0.993186    -1.317997     -21.22
 C       2.844335    -1.314170    -1.756965      82.22
 H       2.734671    -2.272108    -2.334326      21.15
 O       3.444259    -0.150966    -2.332435     277.45
 H       4.374520    -0.284256    -2.467664      26.30
 C       3.677481    -1.992854    -0.422242      85.61
 H       2.673175    -2.397953     0.068668      24.60
 O       4.687818    -2.787875    -0.893346     239.99
 H       5.280281    -2.499020    -1.622312      28.98
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 C       4.009611    -0.805771     0.429645     100.71
 O       5.007753     0.091201    -0.004643     262.56
 H       4.667927     1.129212    -0.043986      23.07
 H       4.287449    -1.184284     1.626321      22.03
 H       3.210255    -0.031644     0.687065      19.96
55
name = lig-Water-frame_289
 C      -0.851683     2.394251     2.773537      54.68
 H      -1.613518     3.186275     2.641376      19.88
 C      -0.532258     0.014094     3.385334      62.33
 H      -1.057633    -1.045116     3.573101      23.18
 C       0.780402     0.278453     3.786024      21.24
 O       1.592993    -0.531881     4.431987     137.12
 C       1.398286    -2.168779     4.348442      95.57
 H       2.376485    -2.242604     4.880483      24.75
 H       1.104840    -2.775478     3.579692      27.66
 H       0.532809    -2.242850     5.148406      25.18
 C       1.386116     1.767113     3.613060       2.23
 O       2.686217     1.831283     3.852937     139.11
 H       2.967777     2.792495     3.618762      20.72
 C       0.551185     2.765852     3.053696      39.78
 H       0.974342     3.756171     2.799325      29.34
 C      -1.351840     1.004972     2.762272      34.25
 C      -2.881511     0.786932     2.518545      81.55
 H      -3.188628     1.905433     2.951878      22.25
 O      -3.306264    -0.412505     3.194283     225.61
 H      -4.301874    -0.512071     3.107281      24.37
 C      -3.246681     0.852903     1.026291      71.90
 H      -2.910765     1.946922     0.572459      20.61
 C      -4.850693     0.804903     0.659734     108.78
 O      -5.555783    -0.367641     1.019846     289.86
 H      -5.012057    -1.158561     0.942953      27.05
 H      -4.834324     0.960347    -0.362415      28.64
 H      -5.246713     1.498073     1.236457      29.35
 C       0.957191     0.341539    -0.967663      55.62
 H       1.806123     1.113411    -0.955822      20.19
 C       0.344734    -1.990851    -1.241954      50.17
 H       0.674479    -3.057862    -1.588328      22.31
 C      -0.935535    -1.753209    -0.603900      23.54
 O      -1.824963    -2.701421    -0.624764     182.33
 C      -1.993635    -3.592386    -1.963979      63.88
 H      -2.447976    -2.847417    -2.871325      22.24
 H      -1.061786    -3.927226    -2.144099      26.91
 H      -2.511985    -4.724704    -1.813139      23.72
 C      -1.347468    -0.381327    -0.317232      24.16
 O      -2.625772    -0.101639     0.030754     131.37
 C      -0.274895     0.572492    -0.380598      43.07
 H      -0.328335     1.529666     0.172914      19.79
 C       1.325698    -1.032039    -1.263722      -1.37
 C       2.762807    -1.325272    -1.698675      66.79
 H       2.882732    -2.240729    -2.477167      20.77
 O       3.462474    -0.153262    -2.278244     245.48
 H       4.450420    -0.204763    -2.362387      25.24
 C       3.645383    -1.918874    -0.468259      72.75
 H       2.885483    -2.669340     0.010104      24.20
 O       4.708579    -2.769294    -0.886625     198.67
 H       4.981860    -2.116580    -1.718144      24.16
 C       4.013487    -0.733454     0.529281     108.15
 O       5.027450     0.061507    -0.061516     320.92
 H       4.579682     1.003248     0.031743      22.96
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 H       4.425183    -1.187609     1.319545      24.97
 H       3.126767    -0.183764     0.736815      23.76
55
name = lig-Water-frame_290
 C      -0.826869     2.434791     2.804558      65.05
 H      -1.385631     3.373041     2.698336      21.14
 C      -0.509482     0.023325     3.336881      57.13
 H      -0.807044    -0.952698     3.662910      25.07
 C       0.804202     0.320456     3.844931      17.37
 O       1.559704    -0.518235     4.438824     114.49
 C       1.409932    -2.192554     4.381402      88.19
 H       2.401978    -2.328588     4.713090      26.77
 H       1.153610    -2.690491     3.330500      25.18
 H       0.615839    -2.427521     5.146481      26.00
 C       1.380855     1.708727     3.597200      20.97
 O       2.701935     1.802256     3.892176     134.06
 H       3.088873     2.671179     3.599102      19.08
 C       0.509812     2.822173     3.006853      56.17
 H       0.904553     3.892631     3.104532      27.22
 C      -1.378374     1.048282     2.803592      26.08
 C      -2.895729     0.729212     2.531347     110.06
 H      -3.250843     1.621706     3.061927      26.19
 O      -3.325142    -0.404134     3.188521     254.53
 H      -4.285433    -0.407580     3.167719      27.97
 C      -3.257989     0.842749     1.044630      75.43
 H      -2.912302     1.878092     0.781737      23.59
 C      -4.868327     0.747738     0.653297      84.65
 O      -5.524786    -0.335734     1.003576     231.22
 H      -4.968813    -1.238049     0.792639      23.40
 H      -4.855794     0.916076    -0.540518      25.25
 H      -5.218426     1.719610     1.393028      24.94
 C       0.983442     0.325695    -0.995251      67.75
 H       1.746294     1.022363    -0.905305      23.31
 C       0.336138    -2.014419    -1.210596      63.55
 H       0.615223    -2.858903    -1.726679      24.81
 C      -0.883350    -1.764101    -0.624214      20.83
 O      -1.872489    -2.752769    -0.671579     213.32
 C      -2.010815    -3.525189    -1.887588     117.28
 H      -2.331385    -2.949009    -2.611217      29.81
 H      -0.900947    -3.754495    -2.375867      23.69
 H      -2.751122    -4.176708    -1.705285      28.11
 C      -1.313596    -0.397481    -0.378170      15.08
 O      -2.660544    -0.067820     0.013959     129.53
 C      -0.263638     0.504411    -0.386132      29.88
 H      -0.438579     1.481369     0.251819      20.95
 C       1.333828    -1.009013    -1.248965       3.05
 C       2.740118    -1.372066    -1.644370      92.45
 H       2.826344    -1.971521    -2.555806      22.61
 O       3.442426    -0.146563    -2.234490     195.55
 H       4.464074    -0.383634    -2.165101      21.65
 C       3.549674    -1.832022    -0.495940      69.33
 H       3.028831    -2.768859     0.060263      24.33
 O       4.736212    -2.714890    -0.912433     182.40
 H       5.077631    -2.191445    -1.586257      29.89
 C       4.012936    -0.716193     0.594312      82.53
 O       5.061321     0.062860    -0.113465     252.19
 H       4.595611     0.953464    -0.008044      23.74
 H       4.616853    -1.322594     1.482967      23.17
 H       2.952345    -0.351350     0.892728      23.36
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name = lig-Water-frame_291
 C      -0.828812     2.464371     2.820312      52.52
 H      -1.447177     3.372173     2.591880      22.37
 C      -0.477732     0.080363     3.299754      30.09
 H      -0.761451    -1.076337     3.629014      23.97
 C       0.756816     0.469013     3.817914      23.64
 O       1.585748    -0.596779     4.479293      98.54
 C       1.411803    -2.153704     4.407331     123.31
 H       2.472653    -2.673189     4.595505      27.77
 H       1.237871    -2.211817     3.373030      28.18
 H       0.702603    -2.565559     5.171881      28.60
 C       1.318757     1.649902     3.548861      31.51
 O       2.737939     1.769108     3.935622     123.62
 H       3.084547     2.682387     3.589333      22.67
 C       0.516398     2.784825     3.028960      56.81
 H       0.681048     3.795283     3.270663      22.11
 C      -1.366934     1.105385     2.872300      15.39
 C      -2.850014     0.731360     2.530681      98.89
 H      -3.689387     1.472728     3.069942      23.89
 O      -3.350582    -0.440746     3.203153     177.54
 H      -4.368008    -0.318520     3.256899      25.09
 C      -3.287560     0.838114     1.031336      70.27
 H      -2.957599     1.989295     0.853626      22.88
 C      -4.785216     0.811113     0.645775     118.74
 O      -5.528225    -0.390078     1.007411     259.78
 H      -4.997428    -1.093538     0.679737      29.71
 H      -4.944860     1.021954    -0.337065      30.28
 H      -5.275404     1.612463     1.055141      30.42
 C       1.012312     0.285282    -0.978574      79.77
 H       1.764656     1.139040    -0.933100      26.51
 C       0.371099    -2.019250    -1.174704      72.02
 H       0.519568    -3.005674    -1.802013      25.57
 C      -0.889561    -1.750142    -0.688680      13.35
 O      -1.928463    -2.808348    -0.682915     191.94
 C      -1.979259    -3.454935    -1.832297     117.95
 H      -2.538733    -2.623199    -2.656283      24.06
 H      -1.196668    -3.899872    -2.297215      27.41
 H      -3.009186    -4.074470    -1.572626      23.53
 C      -1.290421    -0.425150    -0.389176      10.45
 O      -2.677530    -0.073537    -0.007464      88.74
 C      -0.271495     0.511983    -0.375188      26.73
 H      -0.533385     1.400277     0.061368      25.61
 C       1.343687    -0.982015    -1.269072       5.86
 C       2.742824    -1.362748    -1.640016      95.77
 H       2.637838    -2.123246    -2.524804      23.85
 O       3.410370    -0.147171    -2.187418     231.66
 H       4.292716    -0.430298    -2.108157      24.97
 C       3.498631    -1.813843    -0.459023      67.54
 H       2.921234    -2.631672     0.164560      27.12
 O       4.746998    -2.636176    -0.936827     112.38
 H       5.471800    -2.267123    -1.618868      25.10
 C       4.021691    -0.785365     0.621426     110.90
 O       5.072487     0.079170    -0.130537     174.03
 H       4.680436     1.130164    -0.192603      22.04
 H       4.497724    -1.224607     1.439452      29.19
 H       3.219245    -0.240158     1.104584      28.27
55
name = lig-Water-frame_292
 C      -0.867269     2.480102     2.815220      53.53
 H      -1.608715     3.184998     2.496359      23.79
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 C      -0.485280     0.129623     3.294523      45.71
 H      -0.829597    -0.799443     3.336659      26.71
 C       0.716609     0.481309     3.791905      -3.32
 O       1.631765    -0.670483     4.536115      17.83
 C       1.439992    -2.057603     4.411574     153.04
 H       2.268644    -2.671140     4.500561      33.21
 H       1.084091    -2.091292     3.326545      28.05
 H       0.670067    -2.642515     5.118412      30.32
 C       1.349334     1.689903     3.507913      31.75
 O       2.742008     1.740116     3.959591     119.81
 H       2.951877     2.693009     3.714700      24.59
 C       0.523652     2.682943     3.097600      67.73
 H       0.714756     3.810193     3.309431      21.86
 C      -1.365361     1.156639     2.934112      14.04
 C      -2.855427     0.774453     2.541893      88.13
 H      -3.527154     1.510674     2.778807      29.96
 O      -3.369339    -0.510347     3.227573     163.24
 H      -4.341359    -0.338379     3.335267      25.01
 C      -3.275617     0.863720     0.996456      75.86
 H      -3.022933     1.959628     0.756610      25.02
 C      -4.703908     0.867193     0.649523      91.16
 O      -5.538597    -0.440567     1.011735     172.23
 H      -4.928853    -1.200064     0.637927      25.59
 H      -4.866663     1.102572    -0.519056      25.60
 H      -5.437187     1.759490     1.110360      25.47
 C       1.012853     0.310039    -0.898775      71.51
 H       1.700080     1.119727    -1.067658      26.71
 C       0.414131    -2.039756    -1.170766      40.68
 H       0.512186    -2.998767    -1.538877      26.06
 C      -0.957619    -1.753050    -0.758120     -49.17
 O      -1.923634    -2.798492    -0.606595     191.60
 C      -2.105073    -3.402162    -1.883659     120.77
 H      -2.413442    -2.663569    -2.482938      29.54
 H      -1.262524    -4.250173    -2.229306      21.99
 H      -2.773991    -4.189485    -1.779144      27.29
 C      -1.308991    -0.437005    -0.344256     -41.68
 O      -2.668852    -0.111447    -0.037166      31.03
 C      -0.272541     0.541700    -0.385890      14.77
 H      -0.629700     1.697868    -0.141313      26.74
 C       1.354083    -1.008306    -1.306960      23.13
 C       2.737180    -1.314037    -1.693580      97.56
 H       2.612329    -2.331842    -2.185830      25.11
 O       3.356792    -0.164641    -2.149841     221.12
 H       4.392147    -0.330569    -2.214848      24.93
 C       3.533052    -1.834682    -0.393483      64.87
 H       2.782116    -2.540846     0.143790      29.85
 O       4.735971    -2.567787    -0.945377     116.60
 H       5.553785    -2.118646    -1.457913      24.51
 C       4.042874    -0.821419     0.587075     109.10
 O       5.070501     0.106666    -0.120458     218.79
 H       4.656534     0.897957    -0.179813      31.22
 H       4.610006    -1.373970     1.491738      27.23
 H       3.458785    -0.027459     1.150323      27.92
55
name = lig-Water-frame_293
 C      -0.910925     2.455786     2.813509      58.03
 H      -1.647291     3.240931     2.454320      26.05
 C      -0.530412     0.180466     3.309523      49.31
 H      -1.046599    -0.945214     3.066824      25.57
 C       0.760110     0.372384     3.792238     -13.27
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 O       1.681921    -0.671182     4.596754      94.56
 C       1.402697    -1.976403     4.351681     138.90
 H       2.431838    -2.575902     4.434838      28.41
 H       0.893586    -2.362492     3.441078      27.22
 H       0.617321    -2.394515     5.043803      29.04
 C       1.451203     1.691341     3.531577       1.59
 O       2.706705     1.734613     3.960131     169.06
 H       3.026910     2.718627     3.902598      22.45
 C       0.482761     2.671307     3.164789      58.98
 H       0.941810     3.614017     3.139695      23.47
 C      -1.409112     1.199159     2.957548      48.18
 C      -2.871112     0.785402     2.536182      57.81
 H      -3.421164     1.912742     2.803007      25.46
 O      -3.362459    -0.548262     3.242014     148.59
 H      -4.349308    -0.446535     3.373418      23.45
 C      -3.202451     0.878872     0.957326      64.89
 H      -2.876860     1.970910     0.577143      24.48
 C      -4.732451     0.900094     0.629952      90.56
 O      -5.518734    -0.458770     0.992513     193.46
 H      -4.912087    -1.272606     0.823562      25.01
 H      -4.637649     0.996499    -0.388355      28.58
 H      -5.205139     1.609799     1.285738      28.69
 C       0.989225     0.332157    -0.815979      34.73
 H       1.681897     1.131935    -1.122335      20.82
 C       0.389037    -2.043403    -1.165353      14.09
 H       0.703318    -3.172174    -1.314653      23.50
 C      -1.001626    -1.746801    -0.798107     -10.95
 O      -1.886658    -2.772696    -0.514273     115.26
 C      -2.220800    -3.445156    -1.950238      75.45
 H      -2.381350    -2.552505    -2.753030      25.68
 H      -1.327367    -3.960833    -2.110837      23.37
 H      -3.021403    -4.340545    -1.900604      24.37
 C      -1.334569    -0.425278    -0.281389     -30.16
 O      -2.654513    -0.160529    -0.060547      73.48
 C      -0.304932     0.622835    -0.405019      64.72
 H      -0.541637     1.569935    -0.354607      31.32
 C       1.337771    -1.021748    -1.321960      38.67
 C       2.743161    -1.316286    -1.681111      80.50
 H       2.855911    -2.312928    -2.252618      25.49
 O       3.322329    -0.173698    -2.156093     244.67
 H       4.295118    -0.201518    -2.409729      28.59
 C       3.597534    -1.839418    -0.374244      75.62
 H       2.746440    -2.607744     0.049451      29.06
 O       4.709515    -2.527868    -0.925306     202.17
 H       5.191250    -1.784131    -1.203930      28.83
 C       4.123352    -0.805263     0.578452     117.18
 O       5.083554     0.092239    -0.094194     222.03
 H       4.376998     1.011083    -0.083952      20.77
 H       4.705353    -1.441342     1.258576      28.23
 H       3.405704    -0.130020     1.070971      28.16
55
name = lig-Water-frame_294
 C      -0.926174     2.468992     2.824655      71.35
 H      -1.422785     3.369120     2.544881      31.31
 C      -0.584330     0.137649     3.335961      46.70
 H      -0.914903    -0.754032     3.164127      28.99
 C       0.873295     0.267520     3.803642       4.53
 O       1.705870    -0.586785     4.609167     125.03
 C       1.351388    -1.998078     4.288609     115.87
 H       2.271663    -2.425087     4.408465      30.50
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 H       0.875225    -2.349963     3.363417      26.28
 H       0.650259    -2.134231     5.236345      25.17
 C       1.435973     1.592805     3.594839       8.14
 O       2.702892     1.759457     3.964741     188.20
 H       3.108495     2.662872     3.939788      28.14
 C       0.453753     2.689655     3.211962      59.45
 H       0.989795     3.644386     2.884226      16.86
 C      -1.484879     1.184526     2.950519      57.20
 C      -2.892043     0.832424     2.518694      84.60
 H      -3.377274     1.610569     2.945474      29.67
 O      -3.333090    -0.526175     3.234463     178.78
 H      -4.364577    -0.511900     3.342642      22.22
 C      -3.130850     0.871462     0.926624      74.17
 H      -2.611909     1.825501     0.485812      24.52
 C      -4.742522     0.840732     0.643359      79.05
 O      -5.475252    -0.442467     0.961934     238.07
 H      -4.838395    -1.193438     0.953836      26.44
 H      -4.754064     1.015238    -0.533596      25.02
 H      -5.170332     1.653563     1.392421      26.03
 C       0.970347     0.313276    -0.785025      34.72
 H       1.662328     1.165226    -1.021636      19.53
 C       0.326405    -2.056560    -1.162771      38.01
 H       0.777860    -3.011927    -1.105118      26.20
 C      -0.989697    -1.711569    -0.781596      -4.37
 O      -1.870072    -2.773939    -0.471327      62.29
 C      -2.334043    -3.499389    -1.982509      56.42
 H      -2.438623    -2.641573    -2.715609      25.91
 H      -1.207119    -3.768867    -2.214653      19.52
 H      -3.266538    -4.008534    -1.885357      24.97
 C      -1.319334    -0.399991    -0.258837     -21.23
 O      -2.660610    -0.201781    -0.053010     112.52
 C      -0.357954     0.652203    -0.427139      43.42
 H      -0.623218     1.855816    -0.362454      23.82
 C       1.291721    -1.004501    -1.291462      38.20
 C       2.775878    -1.382691    -1.609591      84.77
 H       3.036603    -2.012702    -2.535746      23.25
 O       3.296385    -0.135720    -2.210214     267.71
 H       4.173036    -0.292721    -2.521682      30.79
 C       3.592081    -1.844348    -0.399965      96.97
 H       2.989378    -2.606658     0.096088      29.43
 O       4.695145    -2.503473    -0.897983     209.23
 H       5.099627    -1.508856    -1.120985      22.99
 C       4.212669    -0.789458     0.583423     109.10
 O       5.074112     0.107463    -0.061740     304.85
 H       4.632707     0.946842    -0.062377      28.33
 H       4.854149    -1.405395     1.315893      26.98
 H       3.257475    -0.423931     1.097264      28.22
55
name = lig-Water-frame_295
 C      -0.887046     2.502492     2.866751      86.61
 H      -1.359614     3.501091     2.607353      30.93
 C      -0.569980     0.099848     3.392679       8.76
 H      -0.963221    -1.094339     3.373485      27.30
 C       0.933265     0.236358     3.801378      29.08
 O       1.702806    -0.499665     4.558772     125.55
 C       1.284896    -2.022299     4.298943      95.73
 H       2.280774    -2.644573     4.426635      27.24
 H       0.884131    -2.030228     3.220047      26.29
 H       0.728459    -2.233621     5.152809      27.33
 C       1.312008     1.515151     3.657203      25.49
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 O       2.737117     1.770064     3.985271     111.64
 H       2.930270     2.780818     3.721818      31.98
 C       0.465054     2.669711     3.228382      57.66
 H       0.762095     3.617910     2.807115      11.88
 C      -1.502898     1.130731     2.941177      27.93
 C      -2.893785     0.828094     2.488708      93.12
 H      -3.788137     1.479827     3.120053      22.82
 O      -3.290419    -0.465685     3.199625     199.58
 H      -4.253747    -0.439295     3.273357      21.71
 C      -3.106926     0.831855     0.893806      92.58
 H      -2.570264     1.763290     0.566220      24.77
 C      -4.715644     0.767686     0.649805     103.44
 O      -5.417693    -0.401862     0.929712     284.32
 H      -4.676741    -1.165176     0.961991      24.14
 H      -5.100819     1.123528    -0.293656      26.43
 H      -5.196571     1.636621     1.212515      26.07
 C       0.944300     0.296036    -0.802841      36.34
 H       1.655582     1.081309    -0.822550      21.45
 C       0.285425    -2.021200    -1.152964      39.24
 H       0.659548    -3.084343    -1.072766      24.99
 C      -0.966433    -1.691744    -0.707726      -6.02
 O      -1.876950    -2.794107    -0.481086      97.12
 C      -2.384904    -3.491024    -1.963007      53.08
 H      -2.659898    -2.581689    -2.579077      25.73
 H      -1.474472    -4.017606    -2.427128      21.85
 H      -3.383426    -3.950449    -1.766166      23.67
 C      -1.296515    -0.367039    -0.290619     -22.82
 O      -2.677600    -0.236645    -0.004913     120.07
 C      -0.407255     0.685988    -0.446928      85.85
 H      -0.642945     1.645924    -0.197937      26.89
 C       1.256133    -0.998202    -1.227416      30.54
 C       2.786502    -1.399066    -1.574494      91.92
 H       2.851808    -2.035730    -2.453068      23.87
 O       3.270644    -0.075391    -2.266699     208.17
 H       4.193335    -0.433905    -2.642701      24.67
 C       3.561249    -1.843800    -0.417559      84.94
 H       3.061907    -2.639763     0.419360      26.37
 O       4.733921    -2.466189    -0.896879     217.24
 H       5.488269    -1.955030    -1.298642      28.51
 C       4.239337    -0.809637     0.619743      95.19
 O       5.090787     0.129025    -0.031386     288.21
 H       4.664964     1.139396    -0.062334      23.74
 H       4.901878    -1.314513     1.421624      26.07
 H       3.348697    -0.488709     1.215776      29.16
55
name = lig-Water-frame_296
 C      -0.856614     2.493046     2.926221      30.90
 H      -1.458230     3.335379     2.643952      21.39
 C      -0.541850     0.018375     3.451389      57.52
 H      -0.951731    -0.891329     3.678371      35.45
 C       0.832240     0.264348     3.767056      14.39
 O       1.710781    -0.508713     4.506455     134.76
 C       1.286610    -2.010281     4.315696     110.67
 H       2.083389    -2.708517     4.300571      28.85
 H       0.883066    -1.888262     3.376525      28.36
 H       0.421335    -2.482369     5.087320      25.54
 C       1.256823     1.575289     3.700741      17.91
 O       2.738305     1.786197     3.992544     113.48
 H       2.727038     2.682715     3.577351      21.27
 C       0.473750     2.601478     3.220850      54.58
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 H       0.852512     3.627938     3.016899      31.06
 C      -1.426947     1.102504     2.948931     -50.33
 C      -2.931158     0.792240     2.497634      99.83
 H      -3.628139     1.459131     2.708001      28.25
 O      -3.231330    -0.408558     3.142509     217.36
 H      -4.248025    -0.396891     3.245559      18.48
 C      -3.153121     0.779341     0.864700      89.21
 H      -2.728300     1.914552     0.632830      23.57
 C      -4.682890     0.777256     0.640175     100.81
 O      -5.344732    -0.401354     0.915620     294.52
 H      -4.790620    -1.163180     0.828946      28.81
 H      -5.108630     1.171209    -0.359992      25.33
 H      -5.168806     1.610561     1.333323      24.88
 C       0.892537     0.309818    -0.832587      45.58
 H       1.774738     1.020703    -0.654701      23.82
 C       0.288054    -1.991312    -1.127139      29.66
 H       0.378096    -3.099084    -1.284473      26.18
 C      -0.974826    -1.709729    -0.613810      -4.04
 O      -1.887341    -2.824046    -0.534383     147.11
 C      -2.424891    -3.435715    -1.907247      68.00
 H      -2.879893    -2.443822    -2.438005      22.87
 H      -1.849591    -4.247230    -2.489274      25.33
 H      -3.269041    -4.137271    -1.496286      24.96
 C      -1.331733    -0.354808    -0.345289      13.27
 O      -2.676591    -0.271898     0.068826     135.37
 C      -0.407783     0.675029    -0.463311      78.05
 H      -0.681827     1.722793     0.016861      24.16
 C       1.271429    -1.012458    -1.158027      -6.96
 C       2.715119    -1.324379    -1.582103      79.30
 H       2.540539    -2.362839    -2.183823      19.80
 O       3.260040    -0.053533    -2.313663     222.13
 H       4.151271    -0.306750    -2.636176      23.50
 C       3.617753    -1.823202    -0.364818      83.28
 H       3.018833    -2.404234     0.189062      29.54
 O       4.808223    -2.495026    -0.918130     229.34
 H       5.554293    -2.185825    -1.371321      28.89
 C       4.219547    -0.822857     0.666148     100.23
 O       5.122397     0.170847    -0.000438     246.46
 H       4.473560     1.014498     0.057769      22.31
 H       4.854364    -1.407939     1.359921      25.69
 H       3.508199    -0.215985     1.337262      25.37
55
name = lig-Water-frame_297
 C      -0.884974     2.388657     2.972426      76.92
 H      -1.589640     3.182913     2.651680      25.42
 C      -0.544007    -0.009162     3.492405      81.56
 H      -1.066768    -0.982389     3.909488      29.57
 C       0.699831     0.316398     3.768122      -3.48
 O       1.708006    -0.593722     4.457874     143.97
 C       1.266201    -1.978639     4.347544     135.57
 H       2.149928    -2.688014     4.250646      27.31
 H       0.739693    -2.055308     3.280839      28.64
 H       0.453194    -2.323117     4.860267      29.89
 C       1.306209     1.652233     3.735183      21.69
 O       2.669244     1.789252     3.981226     117.65
 H       2.969837     2.765018     3.626381      22.92
 C       0.497317     2.596466     3.205009      83.05
 H       1.022281     3.551709     3.400562      25.24
 C      -1.328881     1.099904     2.964809      -9.36
 C      -2.885385     0.758117     2.464995      75.95
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 H      -3.535106     1.886673     2.552372      24.60
 O      -3.201115    -0.388141     3.096868     215.44
 H      -4.178886    -0.497800     3.273408      21.47
 C      -3.220169     0.772518     0.866967      94.39
 H      -2.930295     1.794011     0.544637      27.78
 C      -4.674739     0.863942     0.611744     100.11
 O      -5.296929    -0.436813     0.917243     217.73
 H      -4.794317    -1.317945     0.589013      24.45
 H      -4.747737     1.154508    -0.454618      27.16
 H      -5.022075     1.465152     1.507932      25.00
 C       0.878289     0.342678    -0.841801      54.26
 H       1.676425     0.988700    -0.677712      25.60
 C       0.281415    -1.997990    -1.089243      25.05
 H       0.349881    -2.979045    -1.565530      27.68
 C      -0.995150    -1.744674    -0.556075       7.23
 O      -1.885372    -2.857948    -0.602587     189.91
 C      -2.497062    -3.370707    -1.800279     115.82
 H      -2.916238    -2.619680    -2.372061      27.64
 H      -2.012793    -4.146795    -2.542533      26.20
 H      -3.157199    -4.056497    -1.310209      27.29
 C      -1.415255    -0.380878    -0.383837      16.24
 O      -2.658731    -0.307774     0.140163     126.60
 C      -0.408534     0.674389    -0.458112      58.71
 H      -0.601114     1.641743     0.057583      27.63
 C       1.303818    -1.003271    -1.099298       3.76
 C       2.643041    -1.244904    -1.588717      86.81
 H       2.537986    -2.220422    -2.004563      24.60
 O       3.233413    -0.080864    -2.344785     216.51
 H       4.183657    -0.210147    -2.541614      25.15
 C       3.735257    -1.733434    -0.351581      57.47
 H       2.834364    -2.597643     0.000775      24.82
 O       4.852031    -2.588794    -0.914818     113.86
 H       5.477597    -1.824806    -1.475530      22.79
 C       4.207071    -0.802117     0.707372     102.49
 O       5.142720     0.200856     0.043635     181.44
 H       4.466010     1.038515     0.095205      21.82
 H       4.845448    -1.605489     1.312921      24.83
 H       3.634745    -0.105645     1.343909      25.19
55
name = lig-Water-frame_298
 C      -0.901944     2.305498     2.991362      71.74
 H      -1.609224     3.078524     2.678425      26.90
 C      -0.618523    -0.015563     3.516477      83.52
 H      -1.068241    -0.978546     3.923760      29.41
 C       0.722871     0.359687     3.857640       6.12
 O       1.664804    -0.674196     4.393963     162.31
 C       1.246944    -1.959295     4.286899     130.03
 H       2.183006    -2.562357     4.438972      27.31
 H       0.855470    -2.288305     3.369873      29.95
 H       0.362897    -2.158682     5.171395      26.03
 C       1.352539     1.651176     3.737029      32.79
 O       2.606786     1.799351     3.964429     134.60
 H       3.023936     2.628073     3.823197      27.83
 C       0.519510     2.665335     3.222718      71.80
 H       0.805463     3.664787     3.509377      23.12
 C      -1.318820     1.036587     2.961634      33.19
 C      -2.790078     0.840909     2.384293      93.56
 H      -3.182532     1.650128     2.830164      30.84
 O      -3.200104    -0.408228     3.082308     204.60
 H      -4.163094    -0.515588     3.206047      20.53
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 C      -3.228940     0.789088     0.912461      98.83
 H      -2.807258     1.779820     0.298804      25.73
 C      -4.673431     0.886656     0.600164     105.87
 O      -5.272372    -0.483908     0.911473     189.84
 H      -4.760353    -1.172072     0.395205      27.13
 H      -4.675083     1.247771    -0.460552      27.53
 H      -5.112122     1.577031     1.364856      27.20
 C       0.889798     0.353803    -0.824043      49.60
 H       1.633559     1.231932    -0.815387      25.42
 C       0.283733    -2.007307    -1.049610      24.38
 H       0.535276    -2.858125    -1.782512      27.51
 C      -1.003969    -1.777054    -0.570931      20.04
 O      -1.861333    -2.878410    -0.635088     206.04
 C      -2.573505    -3.343478    -1.702898     115.87
 H      -3.177884    -2.568085    -2.507847      23.79
 H      -1.828998    -3.841469    -2.428248      26.27
 H      -3.425946    -4.034948    -1.229726      26.59
 C      -1.459629    -0.413812    -0.387609      17.30
 O      -2.665612    -0.346528     0.203198     115.14
 C      -0.449014     0.643071    -0.436670      41.84
 H      -0.600953     1.654419    -0.027323      27.18
 C       1.279112    -0.955743    -1.050565      13.69
 C       2.678093    -1.172710    -1.564119      85.56
 H       2.767512    -2.142962    -2.300693      24.36
 O       3.182217    -0.128145    -2.371184     214.09
 H       4.229264    -0.264859    -2.347490      23.53
 C       3.751004    -1.707514    -0.390075      78.09
 H       3.256699    -2.450862    -0.021220      31.20
 O       4.887743    -2.628712    -0.914505     195.98
 H       5.136587    -1.879484    -1.357868      30.40
 C       4.261376    -0.782958     0.742705     112.45
 O       5.158606     0.216124     0.097150     216.04
 H       4.653684     1.174682     0.053216      23.64
 H       4.833886    -1.403742     1.367689      28.90
 H       3.453338    -0.330114     1.382438      28.43
55
name = lig-Water-frame_299
 C      -0.841339     2.310302     2.988875      43.65
 H      -1.563729     3.075004     2.692043      25.77
 C      -0.624336    -0.009408     3.563286      43.07
 H      -1.022494    -0.983359     3.762875      36.70
 C       0.787858     0.340496     3.974384      27.20
 O       1.613661    -0.674872     4.309918     141.38
 C       1.197578    -2.010993     4.281035     135.24
 H       2.082153    -2.541768     4.696758      29.51
 H       0.872532    -2.459041     3.252084      29.61
 H       0.644681    -2.104000     5.129844      30.66
 C       1.295809     1.631177     3.691611      29.32
 O       2.623267     1.773538     3.976965      89.62
 H       2.876964     2.821651     3.826778      20.71
 C       0.474433     2.730557     3.279328      52.26
 H       0.509076     3.860491     3.365741      19.18
 C      -1.387256     0.934858     2.913948      33.18
 C      -2.683309     0.888204     2.351081      75.30
 H      -3.244768     1.648599     3.172571      20.50
 O      -3.201097    -0.433296     3.069817     157.43
 H      -4.225532    -0.373780     3.037300      17.02
 C      -3.148801     0.856231     0.924247     114.36
 H      -2.676277     1.645909     0.394897      26.84
 C      -4.687476     0.849616     0.617381     103.17
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 O      -5.267883    -0.482295     0.884805     230.32
 H      -4.679492    -1.082072     0.422078      27.62
 H      -4.900533     1.232192    -0.442571      26.22
 H      -5.367575     1.742134     1.032189      24.54
 C       0.886724     0.395104    -0.775777      48.79
 H       1.460281     1.270823    -1.011678      22.44
 C       0.328847    -1.996470    -1.040014      73.21
 H       0.647282    -2.807370    -1.612614      31.18
 C      -0.999483    -1.793575    -0.654082      -6.20
 O      -1.835498    -2.878306    -0.591530     200.46
 C      -2.694808    -3.340103    -1.705109     128.34
 H      -3.198204    -2.583951    -2.181491      27.21
 H      -1.757907    -3.647747    -2.304095      26.61
 H      -3.395093    -4.026539    -1.470069      31.76
 C      -1.439897    -0.440077    -0.347167     -17.25
 O      -2.708051    -0.392168     0.264553     106.09
 C      -0.503062     0.583565    -0.411805      42.41
 H      -0.781139     1.728959    -0.209898      26.29
 C       1.254095    -0.917795    -1.026573     -13.38
 C       2.776920    -1.191984    -1.543519     116.13
 H       2.784969    -1.938059    -2.293816      25.40
 O       3.155021    -0.149740    -2.385613     304.26
 H       4.088701    -0.243779    -2.351519      28.44
 C       3.736706    -1.711214    -0.426163      59.35
 H       3.182181    -2.584520     0.364480      26.26
 O       4.891779    -2.622369    -0.908082     120.77
 H       5.436505    -1.978784    -1.653410      26.17
 C       4.316043    -0.750622     0.739994      89.86
 O       5.186621     0.233766     0.153711     248.00
 H       4.648047     1.050087     0.188129      27.92
 H       5.038416    -1.238564     1.603132      25.11
 H       3.294992    -0.602606     1.237372      27.78
55
name = lig-Water-frame_300
 C      -0.805219     2.315166     2.950088      49.49
 H      -1.508934     3.142488     2.695176      26.98
 C      -0.564018     0.006369     3.626634      23.57
 H      -0.907540    -1.172651     3.512444      32.37
 C       0.748955     0.314376     4.031823      31.37
 O       1.609258    -0.648311     4.227118      95.87
 C       1.172709    -2.106465     4.288110     112.37
 H       2.088886    -2.620879     4.745863      27.75
 H       0.849348    -2.470167     3.357745      29.56
 H       0.324125    -2.241583     5.210104      25.13
 C       1.242197     1.624220     3.665674       7.75
 O       2.674250     1.774310     3.990863     196.43
 H       2.709477     2.695253     3.762604      27.59
 C       0.375193     2.759889     3.352692      47.73
 H       0.574488     3.808127     3.199252      20.70
 C      -1.343706     0.931467     2.879096      41.33
 C      -2.700070     0.877392     2.431855      89.02
 H      -3.326767     1.596245     2.806044      30.47
 O      -3.213162    -0.446694     3.035900     199.41
 H      -4.167268    -0.308428     2.940515      22.04
 C      -3.080661     0.910878     0.911072      78.31
 H      -2.469417     1.869673     0.355091      25.51
 C      -4.729623     0.833839     0.618000     105.00
 O      -5.280249    -0.431121     0.852035     216.85
 H      -4.571767    -1.212401     0.638643      21.40
 H      -4.883404     0.962736    -0.463961      26.69
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 H      -5.363835     1.562406     1.064533      28.36
 C       0.821773     0.433698    -0.726235      49.23
 H       1.439395     1.282684    -1.072539      21.79
 C       0.384946    -1.959137    -1.043343      25.27
 H       0.748644    -3.059699    -1.304681      22.06
 C      -0.986702    -1.781494    -0.758759     -46.47
 O      -1.842987    -2.892118    -0.496201      95.35
 C      -2.732830    -3.324495    -1.752291      88.48
 H      -3.338980    -2.223410    -1.945265      24.90
 H      -2.089052    -3.700891    -2.531939      28.53
 H      -3.376866    -4.349583    -1.513715      23.78
 C      -1.420422    -0.500926    -0.270910     -29.69
 O      -2.740459    -0.431898     0.315184      49.35
 C      -0.537291     0.576407    -0.398244      98.84
 H      -0.949105     1.493226    -0.332379      34.30
 C       1.299561    -0.895286    -1.028583      -1.26
 C       2.823995    -1.260348    -1.498424      73.15
 H       2.583236    -2.243914    -2.192817      22.95
 O       3.156506    -0.124386    -2.386138     263.80
 H       4.159929    -0.102907    -2.579865      27.45
 C       3.765935    -1.780805    -0.377313      82.75
 H       3.119447    -2.268786     0.175005      31.26
 O       4.883556    -2.569495    -0.925006     232.42
 H       5.512889    -2.409100    -1.625450      31.85
 C       4.360926    -0.774024     0.722026     111.35
 O       5.217966     0.262289     0.209735     280.86
 H       4.483394     1.127001     0.377078      20.46
 H       4.899465    -1.211682     1.446770      28.02
 H       3.418574    -0.376611     1.136127      27.95
55
name = lig-Water-frame_301
 C      -0.884254     2.309849     2.871743      75.45
 H      -1.526320     3.118901     2.604540      28.54
 C      -0.550064    -0.013377     3.632805      83.86
 H      -0.694387    -0.955762     3.494705      30.39
 C       0.665021     0.345516     4.015917      19.40
 O       1.653113    -0.682685     4.172278      55.18
 C       1.142354    -2.177160     4.368335     117.46
 H       2.041601    -2.684516     4.585733      28.88
 H       0.790758    -2.529658     3.319853      27.65
 H       0.263819    -2.293667     4.845936      28.46
 C       1.248097     1.631343     3.708929      -0.62
 O       2.679132     1.776376     3.985612     153.53
 H       2.925120     2.796852     3.754461      26.59
 C       0.352736     2.732470     3.434404      25.13
 H       0.847738     3.702254     3.189021      16.18
 C      -1.210391     1.013841     2.902407      54.42
 C      -2.786476     0.794888     2.496282      75.23
 H      -3.496989     1.836848     2.695479      25.30
 O      -3.226227    -0.435344     2.983878     228.33
 H      -4.219765    -0.445271     2.992757      23.99
 C      -3.046934     0.941559     0.887261      83.50
 H      -2.657413     1.753885     0.466299      27.41
 C      -4.724534     0.837383     0.577214      89.26
 O      -5.300398    -0.409390     0.838451     248.27
 H      -4.747359    -1.173301     0.940761      26.67
 H      -4.653167     0.913758    -0.566587      24.71
 H      -5.330975     1.532718     1.375183      24.20
 C       0.763718     0.437583    -0.713530      45.60
 H       1.432848     1.310431    -0.919556      21.44
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 C       0.439749    -1.957083    -1.055302      -5.84
 H       0.720907    -2.948059    -0.925800      24.36
 C      -0.980915    -1.765421    -0.818724     -30.42
 O      -1.866321    -2.928891    -0.429143      68.82
 C      -2.758502    -3.289853    -1.773359      98.60
 H      -3.333102    -2.518611    -1.830588      28.84
 H      -2.391399    -3.539771    -2.887099      25.68
 H      -3.194188    -4.100246    -1.388313      28.17
 C      -1.426228    -0.592344    -0.192815     -15.15
 O      -2.726380    -0.446233     0.342504      53.35
 C      -0.559449     0.571649    -0.388175      56.53
 H      -1.160190     1.639457    -0.354107      24.64
 C       1.382027    -0.875816    -1.032014      13.22
 C       2.808809    -1.327967    -1.479698      71.56
 H       2.622365    -2.249087    -1.922209      23.78
 O       3.177200    -0.101539    -2.365782     250.05
 H       4.122551    -0.117117    -2.789832      26.85
 C       3.864615    -1.785470    -0.355130      75.41
 H       2.916008    -2.523516     0.189118      24.13
 O       4.853204    -2.572326    -0.900691     237.32
 H       5.327135    -2.256936    -1.672974      31.24
 C       4.359163    -0.798373     0.665397     103.60
 O       5.227782     0.321915     0.266817     231.45
 H       4.736271     1.125082     0.338238      26.52
 H       4.856565    -1.570146     1.524672      24.53
 H       3.637194    -0.087135     1.173609      22.99
55
name = lig-Water-frame_302
 C      -0.929836     2.379600     2.817645      69.14
 H      -1.690133     3.091086     2.367068      26.28
 C      -0.587432     0.011923     3.589102      57.93
 H      -0.787422    -1.228569     3.482987      24.92
 C       0.711254     0.364274     3.982501       5.90
 O       1.682185    -0.752333     4.148202      39.88
 C       1.125654    -2.193285     4.369820     104.48
 H       2.056071    -2.864467     4.650701      26.58
 H       0.913352    -2.516465     3.345155      28.70
 H       0.050469    -2.293370     4.973867      24.17
 C       1.288089     1.669799     3.812203      13.23
 O       2.645156     1.795187     3.960417     197.07
 H       3.062929     2.687990     3.905715      28.97
 C       0.392296     2.666456     3.478700      42.42
 H       0.924564     3.605773     3.326740      15.44
 C      -1.222369     1.049996     2.936520      43.11
 C      -2.851642     0.787500     2.493728     100.01
 H      -3.313543     1.576416     2.945850      31.09
 O      -3.254632    -0.433944     2.940755     264.83
 H      -4.239881    -0.564558     3.159299      21.92
 C      -3.104566     0.857922     0.926793      67.53
 H      -2.692170     1.952911     0.352370      22.63
 C      -4.648801     0.862568     0.549844     104.96
 O      -5.355008    -0.407280     0.844066     245.69
 H      -4.754498    -1.193283     1.023552      24.25
 H      -4.682076     1.210715    -0.474659      26.68
 H      -5.101033     1.569153     1.140959      29.63
 C       0.771045     0.417705    -0.738671      35.83
 H       1.331405     1.330774    -0.689085      22.85
 C       0.461940    -1.936887    -1.044144     -29.32
 H       0.807099    -3.018357    -0.782300      22.86
 C      -0.976339    -1.783536    -0.796063     -15.17
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 O      -1.874932    -2.959352    -0.442541      89.71
 C      -2.738753    -3.267412    -1.772047      80.55
 H      -3.732589    -2.406702    -1.782160      23.29
 H      -2.369850    -3.266399    -2.735485      26.20
 H      -3.283405    -4.188185    -1.233345      21.25
 C      -1.432209    -0.627339    -0.147482      -3.66
 O      -2.673133    -0.441876     0.346624      67.00
 C      -0.626047     0.569106    -0.372495      57.32
 H      -0.934556     1.503293    -0.295068      26.30
 C       1.414387    -0.876211    -1.022940      26.27
 C       2.802889    -1.308210    -1.448247      61.72
 H       2.752407    -2.373970    -2.088186      19.06
 O       3.195848    -0.105396    -2.337907     268.58
 H       4.010014    -0.343939    -2.729238      28.94
 C       3.854244    -1.769244    -0.343685      93.35
 H       3.422596    -2.502477     0.147939      28.59
 O       4.847638    -2.620160    -0.875737     185.97
 H       5.001594    -1.803358    -1.644255      22.33
 C       4.359213    -0.793370     0.674018     125.29
 O       5.282425     0.337825     0.305312     249.87
 H       4.706200     1.313709     0.331948      21.02
 H       4.789378    -1.426748     1.303643      27.60
 H       3.562435    -0.378223     1.267736      27.64
55
name = lig-Water-frame_303
 C      -0.893901     2.468464     2.820339      41.35
 H      -1.565803     3.081964     2.264758      21.78
 C      -0.587821     0.017678     3.532654      65.19
 H      -1.013087    -0.879857     3.529224      32.36
 C       0.822033     0.308034     3.937966     -10.21
 O       1.680861    -0.825832     4.150542     147.50
 C       1.109818    -2.185344     4.344452     128.98
 H       1.806264    -2.753969     4.866911      29.48
 H       0.922899    -2.556195     3.317241      28.83
 H       0.400858    -2.193608     5.062840      29.31
 C       1.310225     1.675665     3.934822      15.58
 O       2.627239     1.802297     3.944773     113.16
 H       2.869775     2.763055     3.987528      28.29
 C       0.404208     2.642380     3.453465      49.57
 H       0.777315     3.672238     3.487631      30.93
 C      -1.397078     1.051066     2.940271       3.63
 C      -2.840819     0.813850     2.450019      96.38
 H      -3.402048     1.589035     3.283183      22.79
 O      -3.299015    -0.488916     2.927061     263.48
 H      -4.203288    -0.379870     3.284870      20.42
 C      -3.184856     0.787712     0.958965     114.33
 H      -2.782222     1.552453     0.533137      28.23
 C      -4.545952     0.860699     0.537420      93.82
 O      -5.419073    -0.388469     0.847071     210.15
 H      -4.692009    -1.136476     0.857718      24.31
 H      -4.845175     1.343685    -0.486180      23.88
 H      -5.034996     1.867559     1.091992      24.18
 C       0.785187     0.384847    -0.763457      37.45
 H       1.325103     1.366405    -0.551528      24.80
 C       0.444256    -1.948327    -0.992070      35.87
 H       0.866044    -2.932517    -1.022608      26.48
 C      -0.961600    -1.839542    -0.698591     -22.60
 O      -1.865090    -2.965719    -0.530176     180.18
 C      -2.795587    -3.221341    -1.667096     109.96
 H      -3.530768    -2.616690    -1.749514      29.60
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 H      -2.028320    -3.129576    -2.586238      25.72
 H      -3.151289    -4.259792    -1.653110      26.73
 C      -1.412973    -0.575227    -0.156681       3.63
 O      -2.633126    -0.439572     0.352475      92.50
 C      -0.616639     0.504173    -0.373102      62.83
 H      -0.857057     1.661617    -0.088904      24.06
 C       1.371583    -0.888715    -1.004180      29.25
 C       2.814059    -1.268985    -1.443239      90.15
 H       2.796365    -2.015184    -2.149547      23.26
 O       3.209312    -0.141203    -2.293121     245.19
 H       4.109898    -0.545202    -2.659789      25.31
 C       3.788169    -1.736225    -0.332253      63.13
 H       3.354008    -2.575233     0.539512      25.29
 O       4.868565    -2.622031    -0.913371     182.32
 H       5.302075    -2.027954    -1.498487      31.11
 C       4.358188    -0.734064     0.702414      91.84
 O       5.324663     0.348937     0.334420     234.35
 H       4.682274     1.011528     0.422299      30.86
 H       5.153905    -1.384615     1.425045      22.93
 H       3.363214    -0.658082     1.318884      25.97
55
name = lig-Water-frame_304
 C      -0.839934     2.449020     2.870045      55.50
 H      -1.268647     3.358093     2.298309      24.42
 C      -0.556171     0.098754     3.469904      33.65
 H      -1.205918    -0.918219     3.625560      25.55
 C       0.871399     0.212113     3.876535       5.18
 O       1.675001    -0.874228     4.162505     164.99
 C       1.116505    -2.150202     4.308356     118.52
 H       1.906225    -2.689599     4.996364      24.01
 H       0.731578    -2.735885     3.378176      25.91
 H       0.259795    -2.008988     5.164727      24.38
 C       1.262288     1.597819     4.018653     -13.04
 O       2.658958     1.832510     3.950901      51.31
 H       2.659592     2.879090     3.971242      23.52
 C       0.385446     2.676582     3.396043      56.60
 H       0.625923     3.752486     3.590287      25.32
 C      -1.527097     1.093404     2.934392      18.27
 C      -2.849378     0.832086     2.479089     108.17
 H      -3.528474     1.498577     2.923307      27.41
 O      -3.348645    -0.557383     2.934454     230.72
 H      -4.225089    -0.224323     3.322669      22.07
 C      -3.204904     0.713504     0.989510      91.54
 H      -2.511087     1.685867     0.434518      22.33
 C      -4.591236     0.895020     0.535791     114.35
 O      -5.451803    -0.337271     0.839469     244.44
 H      -4.873518    -1.055103     0.697220      28.77
 H      -4.687382     1.024564    -0.507539      27.94
 H      -4.887584     1.644626     1.138636      29.89
 C       0.791739     0.369029    -0.759435      64.68
 H       1.426317     1.203833    -0.673825      26.13
 C       0.394184    -1.996584    -0.931813      50.48
 H       0.832209    -2.964520    -1.369335      24.47
 C      -0.946981    -1.891021    -0.566172      27.19
 O      -1.843048    -2.960806    -0.607098     227.54
 C      -2.756870    -3.208590    -1.610318     122.70
 H      -3.739077    -2.346896    -1.726286      24.39
 H      -2.087293    -3.037697    -2.384613      25.95
 H      -2.958511    -4.307623    -1.869292      27.89
 C      -1.385969    -0.533281    -0.208121     -15.24
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 O      -2.635040    -0.462249     0.373670      89.95
 C      -0.516502     0.508210    -0.383453      92.86
 H      -0.839457     1.388472     0.101105      26.99
 C       1.305244    -0.901936    -0.987361       3.35
 C       2.794172    -1.201123    -1.425024      71.54
 H       2.674100    -2.110202    -2.271097      20.33
 O       3.253844    -0.185509    -2.249103     248.83
 H       4.198380    -0.395163    -2.526193      24.54
 C       3.754357    -1.748382    -0.279911      67.62
 H       3.131391    -2.206774     0.364336      28.11
 O       4.876945    -2.612687    -0.947996     155.69
 H       5.688254    -2.226892    -1.473962      27.35
 C       4.403382    -0.736855     0.772423     109.43
 O       5.321769     0.341156     0.358622     209.96
 H       4.642361     1.222407     0.452363      24.05
 H       5.069740    -1.240856     1.308486      26.48
 H       3.548975    -0.413345     1.348712      25.95
55
name = lig-Water-frame_305
 C      -0.858369     2.405178     2.894509      70.26
 H      -1.069731     3.384110     2.538033      25.61
 C      -0.577873     0.160912     3.406246      58.10
 H      -0.978148    -0.821265     3.695082      28.51
 C       0.825209     0.164979     3.804298      -5.29
 O       1.679758    -0.879740     4.153249     166.09
 C       1.089086    -2.153081     4.359770     134.10
 H       1.912562    -2.668395     4.737481      26.51
 H       0.679145    -2.710300     3.549236      27.43
 H       0.198809    -1.990342     4.846693      26.61
 C       1.216456     1.510465     4.015201     -17.99
 O       2.677883     1.888581     3.983576      67.30
 H       2.784855     2.843003     3.872924      26.69
 C       0.409484     2.680750     3.398546      26.42
 H       0.674032     3.709720     3.541857      22.74
 C      -1.474582     1.171054     2.961496      49.52
 C      -2.923936     0.773365     2.494452      82.07
 H      -3.806384     1.684823     2.696491      22.18
 O      -3.398766    -0.590852     2.964238     248.43
 H      -4.357021    -0.426042     3.309426      22.89
 C      -3.105611     0.717462     0.962601     107.81
 H      -2.719390     1.502816     0.572084      28.23
 C      -4.684351     0.870499     0.537001      68.06
 O      -5.478198    -0.260069     0.833619     230.18
 H      -5.008528    -1.152562     0.589154      26.58
 H      -4.470583     0.875335    -0.607327      25.62
 H      -5.129517     1.747060     1.281699      24.73
 C       0.846871     0.356925    -0.751529      76.13
 H       1.636840     1.159333    -0.898391      25.24
 C       0.366888    -2.078054    -0.895793      -1.73
 H       0.587471    -2.915617    -1.579457      27.06
 C      -0.945119    -1.893870    -0.454262      26.81
 O      -1.801668    -2.969515    -0.597298     233.04
 C      -2.730847    -3.152033    -1.653817     124.72
 H      -3.525873    -2.604539    -1.556601      28.58
 H      -2.281827    -2.811664    -2.745356      23.86
 H      -2.892546    -4.285651    -1.675879      27.85
 C      -1.372323    -0.554174    -0.256811     -11.39
 O      -2.648991    -0.506906     0.393509     107.44
 C      -0.448362     0.539784    -0.361881      69.39
 H      -0.799051     1.459165     0.187021      27.03
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 C       1.263684    -0.937314    -0.980865     -11.96
 C       2.743311    -1.198370    -1.425985      93.28
 H       2.593804    -2.147438    -1.889810      25.86
 O       3.315364    -0.187788    -2.216741     265.10
 H       4.276905    -0.305500    -2.326826      26.03
 C       3.790125    -1.707616    -0.279580      54.72
 H       2.893614    -2.399961     0.282359      24.78
 O       4.838979    -2.628821    -0.945838     112.11
 H       5.750853    -2.052132    -1.239194      25.08
 C       4.443646    -0.740173     0.810657      97.31
 O       5.276307     0.360562     0.370325     178.47
 H       4.884632     1.231913     0.399395      29.67
 H       5.096203    -1.532351     1.527405      24.32
 H       3.778324    -0.057582     1.474252      24.21
55
name = lig-Water-frame_306
 C      -0.862582     2.441161     2.919049      65.65
 H      -1.467863     3.358535     2.578856      24.29
 C      -0.593991     0.155233     3.375298      66.51
 H      -0.991894    -0.876242     3.552561      26.92
 C       0.746779     0.192819     3.740912     -15.10
 O       1.670679    -0.848018     4.116368     147.21
 C       1.048564    -2.176064     4.407710     101.36
 H       1.888796    -2.877740     4.761940      23.08
 H       0.758780    -2.622725     3.316964      23.63
 H       0.037515    -2.090445     5.027896      21.88
 C       1.236069     1.524752     3.916541       4.94
 O       2.671018     1.913500     4.038451      92.33
 H       2.862878     2.893266     3.793419      25.78
 C       0.458797     2.589565     3.461316      54.38
 H       0.913001     3.626321     3.429825      25.50
 C      -1.411545     1.192758     2.996275      36.62
 C      -3.029975     0.714500     2.502207      95.35
 H      -3.640096     1.546030     2.695538      28.11
 O      -3.445426    -0.585814     3.009583     277.96
 H      -4.395511    -0.635821     3.240947      24.51
 C      -3.061034     0.711292     0.953743      72.94
 H      -2.643278     1.827976     0.406793      21.18
 C      -4.720106     0.841357     0.547339     105.68
 O      -5.518872    -0.212968     0.838370     273.54
 H      -5.108465    -1.095400     0.575782      28.87
 H      -4.588307     1.103329    -0.481652      29.02
 H      -5.264820     1.654703     0.839618      29.22
 C       0.941062     0.352508    -0.749561      49.62
 H       1.655787     1.111189    -1.026972      24.38
 C       0.362501    -2.123803    -0.890569      15.03
 H       0.435705    -3.010545    -1.522769      27.17
 C      -0.929128    -1.874475    -0.406511      15.19
 O      -1.757300    -2.992229    -0.544572     179.72
 C      -2.659709    -3.114445    -1.759641     104.34
 H      -3.810781    -2.580378    -1.373615      22.92
 H      -2.579103    -2.753938    -2.737989      25.57
 H      -2.928006    -4.145940    -1.570498      27.50
 C      -1.369552    -0.571981    -0.251414       7.34
 O      -2.644756    -0.553186     0.391425     129.69
 C      -0.454857     0.571534    -0.301022      25.64
 H      -0.690488     1.670555     0.027331      22.91
 C       1.267878    -1.003746    -0.986003       2.77
 C       2.711787    -1.228075    -1.395083      82.19
 H       2.670368    -2.366402    -1.813127      23.41
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 O       3.355523    -0.164273    -2.204566     182.55
 H       4.393383    -0.429658    -2.115725      20.91
 C       3.787762    -1.675823    -0.271697      78.85
 H       3.347230    -2.498967     0.155137      27.66
 O       4.783763    -2.624848    -0.907262     218.24
 H       5.360209    -1.978394    -1.008098      30.82
 C       4.471792    -0.740942     0.871032     111.73
 O       5.282611     0.360625     0.349915     227.94
 H       4.696230     1.191916     0.466340      26.25
 H       4.947319    -1.447776     1.456131      28.52
 H       3.783340    -0.254794     1.560290      27.71
55
name = lig-Water-frame_307
 C      -0.865566     2.533450     2.960490      56.30
 H      -1.697053     3.140953     2.673254      20.43
 C      -0.602054     0.064961     3.377777      58.13
 H      -1.182023    -0.967126     3.195523      24.08
 C       0.725871     0.253457     3.715857      16.13
 O       1.625638    -0.811263     4.079668     114.28
 C       0.995729    -2.206464     4.397913     119.32
 H       1.688377    -2.857648     4.908911      28.03
 H       0.818963    -2.480104     3.450991      27.18
 H       0.280632    -2.224615     5.184671      28.16
 C       1.329945     1.578234     3.772211      24.18
 O       2.647996     1.906962     4.102139     168.20
 H       2.735592     2.866490     3.790626      29.55
 C       0.470810     2.541583     3.502473      73.53
 H       1.063636     3.411152     3.348760      23.82
 C      -1.434838     1.155908     3.011969     -19.46
 C      -3.046371     0.666289     2.497503      79.91
 H      -3.759648     1.593180     2.988694      22.05
 O      -3.465474    -0.568154     3.056246     261.81
 H      -4.516715    -0.564734     3.190945      20.04
 C      -3.107612     0.751862     0.936415      89.97
 H      -2.642693     1.482591     0.536921      25.91
 C      -4.671922     0.852039     0.518075      96.15
 O      -5.584195    -0.222469     0.857369     284.03
 H      -5.120612    -1.010233     0.629722      30.55
 H      -4.767995     1.150711    -0.621417      24.67
 H      -5.305466     1.864099     0.759448      24.47
 C       0.949890     0.316580    -0.733749      30.68
 H       1.645124     1.139589    -0.988318      21.45
 C       0.373775    -2.118116    -0.900138      46.48
 H       0.515884    -3.205675    -1.272720      24.04
 C      -0.882112    -1.875648    -0.429496      13.10
 O      -1.733943    -3.005678    -0.508147     194.73
 C      -2.677796    -3.068369    -1.775828      96.16
 H      -3.532623    -2.633406    -1.521267      28.39
 H      -2.418882    -2.696271    -2.820958      25.03
 H      -2.961180    -4.249331    -1.773224      26.24
 C      -1.368307    -0.533489    -0.174029       2.52
 O      -2.627566    -0.572178     0.372125     151.64
 C      -0.431200     0.591958    -0.263585      52.15
 H      -0.697362     1.598433    -0.183182      20.42
 C       1.315140    -1.057646    -0.998023      20.50
 C       2.733370    -1.312429    -1.359527      83.33
 H       2.813849    -2.153401    -2.019025      22.19
 O       3.379629    -0.160340    -2.183450     238.84
 H       4.264557    -0.480748    -2.225781      24.06
 C       3.760336    -1.672745    -0.236049      75.37
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 H       3.350590    -2.551520     0.511043      23.18
 O       4.722072    -2.597000    -0.854807     132.29
 H       5.526654    -1.851662    -1.146756      24.13
 C       4.456646    -0.742152     0.887144      83.61
 O       5.299001     0.363230     0.324645     239.63
 H       4.483638     1.005495     0.519435      23.47
 H       5.207563    -1.468915     1.495319      24.11
 H       3.552541    -0.532511     1.602263      24.49
55
name = lig-Water-frame_308
 C      -0.909245     2.505201     3.032287      60.73
 H      -1.618599     3.368381     2.787061      26.35
 C      -0.646816    -0.021380     3.357755      44.44
 H      -0.974553    -0.899629     3.088339      26.99
 C       0.771221     0.281451     3.725577       9.84
 O       1.564186    -0.789408     4.061183      83.13
 C       0.978561    -2.189899     4.396200      97.50
 H       1.830843    -2.730847     4.882178      26.64
 H       0.552753    -2.708523     3.327143      23.36
 H       0.172069    -2.119155     5.205743      27.02
 C       1.419461     1.544366     3.643121      24.49
 O       2.623523     1.888057     4.157163     185.17
 H       2.738828     2.829239     3.929501      33.02
 C       0.427743     2.619949     3.471885      64.66
 H       0.994226     3.584851     3.348987      18.22
 C      -1.483997     1.112087     3.010929       8.25
 C      -3.008917     0.708602     2.516316      95.28
 H      -3.674756     1.339629     3.073853      25.50
 O      -3.479190    -0.558868     3.097633     248.06
 H      -4.430522    -0.361476     3.228554      23.37
 C      -3.248810     0.728920     0.948577      69.73
 H      -2.412084     1.610556     0.481514      18.73
 C      -4.642323     0.931767     0.436191     101.49
 O      -5.636093    -0.237731     0.883221     173.87
 H      -5.070069    -1.116084     0.736520      25.01
 H      -4.716339     0.835267    -0.616363      26.97
 H      -4.926562     1.749814     1.035924      28.19
 C       0.895245     0.249082    -0.709866      48.74
 H       1.595641     1.104709    -0.821722      23.49
 C       0.425864    -2.115052    -0.918822      52.48
 H       0.741871    -3.119446    -0.968779      26.01
 C      -0.865165    -1.865667    -0.483638      -2.91
 O      -1.743620    -2.999242    -0.507070     181.98
 C      -2.680282    -3.079816    -1.768999      83.06
 H      -3.716899    -2.344395    -1.537208      22.25
 H      -1.917796    -2.758266    -2.579613      24.44
 H      -2.840734    -4.068194    -2.026266      27.08
 C      -1.323491    -0.500554    -0.073010      -6.74
 O      -2.623881    -0.553205     0.356432     120.12
 C      -0.378659     0.555649    -0.259953      63.58
 H      -0.840799     1.683167    -0.341593      19.22
 C       1.370459    -1.065969    -1.002833      25.55
 C       2.806309    -1.374872    -1.341203      70.57
 H       2.901053    -2.071295    -2.292900      18.18
 O       3.366513    -0.171614    -2.145320     205.38
 H       4.333534    -0.487663    -2.498322      22.21
 C       3.731614    -1.748678    -0.140300      85.98
 H       3.108280    -2.134240     0.656741      26.27
 O       4.706855    -2.527839    -0.807303     225.28
 H       5.418489    -2.253206    -1.427033      28.79
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 C       4.440217    -0.790982     0.876817      94.38
 O       5.262121     0.363964     0.325095     238.06
 H       4.722700     1.166077     0.334257      27.59
 H       5.307945    -1.305756     1.302405      24.85
 H       3.603104    -0.556057     1.547197      25.46
55
name = lig-Water-frame_309
 C      -0.984312     2.413658     3.115299      47.36
 H      -1.296320     3.441565     2.966455      21.72
 C      -0.653192     0.013981     3.332158      35.90
 H      -0.740112    -1.214546     3.039911      23.55
 C       0.781905     0.260589     3.720211      13.81
 O       1.518745    -0.807870     4.060774     120.09
 C       0.956036    -2.149832     4.370330     125.10
 H       1.948558    -2.547333     4.651271      26.45
 H       0.512679    -2.746474     3.707085      27.60
 H       0.098106    -1.922371     5.009734      27.14
 C       1.390730     1.530124     3.540573      22.12
 O       2.623183     1.859131     4.204854     148.86
 H       2.862609     2.861128     4.100292      28.14
 C       0.409197     2.713751     3.390694      82.98
 H       0.618769     3.803585     3.470292      18.10
 C      -1.529709     1.057659     2.999343      39.53
 C      -2.941522     0.755711     2.545306      86.80
 H      -3.706173     1.612619     3.046544      24.27
 O      -3.468939    -0.550635     3.129156     187.13
 H      -4.476414    -0.369901     3.361275      21.45
 C      -3.291281     0.711235     0.948601      94.97
 H      -2.804993     1.519617     0.646466      27.01
 C      -4.636152     0.948037     0.394662      86.15
 O      -5.651079    -0.243729     0.901321     182.62
 H      -5.132327    -1.076620     0.959399      26.27
 H      -4.587050     0.840341    -0.714898      25.27
 H      -4.847815     1.843088     1.111233      25.42
 C       0.883557     0.191721    -0.696228      55.34
 H       1.554016     1.015599    -0.710056      23.12
 C       0.494583    -2.103367    -0.923430      14.17
 H       0.977484    -3.164477    -0.816454      23.41
 C      -0.883449    -1.840246    -0.533863     -28.35
 O      -1.781407    -2.977771    -0.518975     163.57
 C      -2.635749    -3.041355    -1.730776     102.06
 H      -3.445730    -2.348710    -1.814197      26.07
 H      -1.813244    -2.720456    -2.317841      26.02
 H      -2.884506    -4.163128    -2.120905      23.10
 C      -1.256004    -0.539232    -0.002096     -24.19
 O      -2.640716    -0.505037     0.353608     100.89
 C      -0.391043     0.527247    -0.269412      67.96
 H      -0.686608     1.463698    -0.297339      25.23
 C       1.411334    -1.052882    -0.999093      15.07
 C       2.888338    -1.373683    -1.373720      74.40
 H       2.857618    -2.225070    -2.003313      20.90
 O       3.353986    -0.192070    -2.100930     273.41
 H       4.204134    -0.397579    -2.591963      26.01
 C       3.728059    -1.785805    -0.082659      87.97
 H       2.915570    -2.306604     0.631459      25.52
 O       4.712250    -2.535495    -0.746400     214.83
 H       5.117951    -2.154759    -1.536628      28.52
 C       4.438417    -0.787972     0.820768     100.61
 O       5.210287     0.357980     0.331600     258.79
 H       4.878382     1.307615     0.191897      25.12
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 H       5.275046    -1.437247     1.303614      24.57
 H       3.779031    -0.338862     1.665249      24.24
55
name = lig-Water-frame_310
 C      -1.007080     2.333341     3.195060      57.78
 H      -1.566581     3.315360     3.079689      19.37
 C      -0.589210     0.035071     3.294329      70.41
 H      -0.727920    -0.925183     3.155110      28.39
 C       0.720701     0.248661     3.668930       9.52
 O       1.504673    -0.839888     4.054435     149.93
 C       0.952264    -2.064854     4.367521     118.72
 H       1.839537    -2.615007     4.707960      27.27
 H       0.449248    -2.853401     3.508470      24.99
 H       0.166502    -1.882996     5.153700      27.22
 C       1.310689     1.613674     3.505778       4.09
 O       2.624617     1.819476     4.233476     120.31
 H       2.839268     2.760160     4.130261      24.63
 C       0.380765     2.715877     3.297907      65.34
 H       0.452592     3.768812     3.573423      22.95
 C      -1.550838     1.020377     2.987232      25.50
 C      -2.959918     0.792147     2.585902      89.52
 H      -3.432076     1.767383     2.729059      27.35
 O      -3.451280    -0.518833     3.163157     194.18
 H      -4.417079    -0.515836     3.376594      24.59
 C      -3.247377     0.668277     0.978666      72.36
 H      -2.828253     1.878156     0.533982      21.80
 C      -4.664417     0.891664     0.428245      95.76
 O      -5.646155    -0.218378     0.902530     219.76
 H      -5.111814    -0.982059     1.140476      29.72
 H      -4.559511     1.153817    -0.664011      25.07
 H      -5.144899     1.877966     0.657121      26.60
 C       0.923808     0.190335    -0.688976      47.24
 H       1.635720     1.073819    -0.727548      21.68
 C       0.536521    -2.116872    -0.895049      23.39
 H       0.882680    -3.092518    -0.938389      23.72
 C      -0.876266    -1.845081    -0.563906     -26.64
 O      -1.826955    -2.939554    -0.503527     173.34
 C      -2.526152    -3.034937    -1.725977     100.87
 H      -3.494220    -2.213297    -1.886197      22.64
 H      -1.833189    -2.617114    -2.643730      25.50
 H      -2.910044    -3.963437    -1.827713      26.33
 C      -1.249759    -0.622279     0.023368     -14.26
 O      -2.652888    -0.449550     0.354030     103.48
 C      -0.415157     0.463550    -0.275021      50.12
 H      -0.626443     1.667063    -0.077180      21.75
 C       1.448261    -1.057301    -0.997611      50.54
 C       2.914137    -1.321935    -1.373585      82.12
 H       2.844188    -2.466237    -1.742585      21.52
 O       3.336483    -0.213107    -2.066862     283.05
 H       4.189317    -0.374394    -2.479815      27.53
 C       3.697651    -1.772227    -0.075318      89.87
 H       3.159212    -2.627382     0.341972      26.16
 O       4.760683    -2.605181    -0.680611     117.60
 H       4.702132    -1.860154    -1.477188      21.79
 C       4.437200    -0.729948     0.810435     120.97
 O       5.199710     0.342210     0.311373     283.72
 H       4.546884     1.153581     0.306968      25.06
 H       5.079378    -1.520059     1.319215      25.54
 H       3.961647    -0.284977     1.714498      25.58
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name = lig-Water-frame_311
 C      -1.040939     2.302712     3.231734      59.69
 H      -1.981970     2.894823     3.209715      20.92
 C      -0.547752     0.049372     3.241957      67.70
 H      -0.988006    -1.087738     3.208339      26.48
 C       0.701040     0.289561     3.598817      16.31
 O       1.521870    -0.824508     4.024925     166.71
 C       0.921637    -2.044288     4.372055     141.26
 H       1.629398    -2.757698     4.891500      27.59
 H       0.588176    -2.412693     3.507569      29.47
 H       0.290481    -2.023462     5.297290      27.99
 C       1.245215     1.693204     3.558758       7.22
 O       2.586432     1.772596     4.224058     112.28
 H       2.815842     2.737892     4.095203      24.83
 C       0.328445     2.650214     3.233803      60.19
 H       0.624926     3.683966     3.573872      25.67
 C      -1.519083     1.019328     2.995836      13.00
 C      -3.000758     0.787731     2.569438      80.44
 H      -3.529290     1.883330     2.764823      24.70
 O      -3.424066    -0.465226     3.205630     202.27
 H      -4.437001    -0.468150     3.307777      23.01
 C      -3.155308     0.734103     1.007238     100.65
 H      -2.838718     1.539221     0.612546      29.57
 C      -4.715963     0.825663     0.479103     102.77
 O      -5.627141    -0.171031     0.876567     247.15
 H      -5.029967    -0.927391     1.292927      26.14
 H      -4.598422     0.992590    -0.606864      26.00
 H      -5.344676     1.765380     0.569092      25.69
 C       0.972450     0.250714    -0.678867      43.14
 H       1.611331     1.081191    -0.806874      23.27
 C       0.517828    -2.125256    -0.854736      47.70
 H       0.719528    -3.233379    -1.213540      21.22
 C      -0.836416    -1.895743    -0.553734      -2.96
 O      -1.844419    -2.881141    -0.473895     186.11
 C      -2.440288    -2.974787    -1.789514     113.56
 H      -3.310221    -2.328949    -1.681437      26.34
 H      -1.969511    -2.938751    -2.695904      29.06
 H      -2.986521    -4.051317    -1.612046      23.31
 C      -1.301599    -0.664298     0.006162     -17.89
 O      -2.647912    -0.420902     0.346737     111.29
 C      -0.397731     0.440448    -0.264357      52.65
 H      -0.625789     1.338777     0.144016      28.02
 C       1.463420    -1.074497    -0.988707      43.71
 C       2.859703    -1.330073    -1.302994      97.45
 H       2.934001    -2.201587    -1.903929      25.43
 O       3.329045    -0.221780    -2.063144     257.71
 H       4.373958    -0.368787    -2.314258      25.00
 C       3.679856    -1.747864    -0.093323      83.88
 H       3.186402    -2.562941     0.398556      27.99
 O       4.818017    -2.647764    -0.644121     146.09
 H       5.105612    -2.160739    -1.468128      28.66
 C       4.422950    -0.711315     0.872835     113.14
 O       5.191213     0.344060     0.262601     303.22
 H       4.467805     0.934505     0.466327      28.24
 H       5.144677    -1.411874     1.348494      26.43
 H       3.769199    -0.351981     1.722594      26.76
55
name = lig-Water-frame_312
 C      -1.129902     2.302540     3.218400      70.46
 H      -2.050211     2.903396     3.371942      22.58
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 C      -0.595108    -0.012970     3.160942      54.99
 H      -1.042492    -1.011656     3.303057      28.44
 C       0.771211     0.331997     3.550258      20.20
 O       1.569435    -0.751406     3.997528      99.08
 C       0.899814    -2.051481     4.426784     116.19
 H       1.675745    -2.728351     4.761065      27.63
 H       0.390725    -2.317500     3.330386      26.07
 H       0.100106    -1.974697     5.191978      28.17
 C       1.218996     1.653606     3.664552      24.18
 O       2.503407     1.750960     4.175861     134.88
 H       2.888349     2.704067     4.106917      24.00
 C       0.272987     2.635813     3.228926      62.44
 H       0.709440     3.598540     3.365790      27.40
 C      -1.484855     1.024462     3.008194      16.50
 C      -3.000389     0.797817     2.539771     100.65
 H      -3.696780     1.513045     3.027462      26.19
 O      -3.413156    -0.398928     3.250269     219.48
 H      -4.424767    -0.311621     3.272252      22.38
 C      -3.133104     0.791038     1.045887      68.76
 H      -2.476869     1.815927     0.481858      22.67
 C      -4.735680     0.813282     0.500106      92.29
 O      -5.605015    -0.167509     0.864233     250.27
 H      -5.164718    -0.900022     1.293798      27.14
 H      -4.564672     0.490024    -0.586138      24.20
 H      -5.231006     1.771070     0.879885      25.94
 C       0.990821     0.283372    -0.670935      47.68
 H       1.639209     1.190856    -0.863273      21.60
 C       0.485809    -2.166361    -0.843838      78.73
 H       0.615852    -3.060285    -1.372456      25.08
 C      -0.825324    -1.924751    -0.476039       5.52
 O      -1.817993    -2.833029    -0.458489     185.16
 C      -2.442217    -2.994840    -1.806354      90.44
 H      -3.326875    -2.149853    -1.741686      23.79
 H      -1.749066    -3.272706    -2.812368      25.21
 H      -2.910106    -3.900615    -1.701507      28.16
 C      -1.317823    -0.636322    -0.060727       3.85
 O      -2.632438    -0.435273     0.336643      76.36
 C      -0.353265     0.388710    -0.226697      54.37
 H      -0.714356     1.382610     0.326816      27.75
 C       1.407257    -1.065176    -0.950432      11.06
 C       2.820516    -1.355763    -1.252051     106.03
 H       2.937299    -2.080824    -2.181374      22.04
 O       3.348459    -0.210490    -2.072779     276.82
 H       4.259740    -0.409836    -2.136528      28.91
 C       3.732555    -1.739749    -0.109508      63.11
 H       3.015378    -2.281503     0.705441      25.65
 O       4.878032    -2.676189    -0.618591     163.98
 H       5.524961    -2.501364    -1.389451      29.48
 C       4.402565    -0.757441     0.952190      87.78
 O       5.160721     0.348039     0.216083     183.17
 H       4.639166     1.292691     0.457553      23.34
 H       5.312141    -1.284086     1.475410      24.71
 H       3.511030    -0.391926     1.572687      25.67
55
name = lig-Water-frame_313
 C      -1.192534     2.369452     3.188691      58.12
 H      -1.809861     3.266858     3.359435      23.86
 C      -0.599927    -0.061381     3.103732      65.61
 H      -0.965022    -1.058203     3.234260      30.39
 C       0.785515     0.280787     3.515904      19.38
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 O       1.628175    -0.674469     3.991415      82.73
 C       0.867775    -2.035214     4.413701     105.38
 H       1.791496    -2.631141     4.569913      25.50
 H       0.344414    -2.480704     3.654189      29.61
 H      -0.023324    -1.762911     5.036451      26.57
 C       1.174362     1.586998     3.744175      29.13
 O       2.432895     1.758903     4.120670     155.31
 H       2.805553     2.624761     4.105190      28.62
 C       0.228407     2.640640     3.286073      49.22
 H       0.580820     3.726238     3.117710      25.99
 C      -1.522189     1.000974     2.997924      20.44
 C      -2.945909     0.795222     2.568728      97.71
 H      -3.718633     1.527452     3.087768      23.64
 O      -3.422591    -0.355018     3.285474     216.25
 H      -4.393945    -0.277905     3.396170      24.73
 C      -3.140342     0.866870     1.010959      78.87
 H      -2.600368     1.609093     0.722509      29.04
 C      -4.658341     0.842305     0.494455     101.63
 O      -5.621556    -0.219649     0.891653     249.11
 H      -5.255673    -1.025423     1.283085      26.39
 H      -4.477580     0.633043    -0.526357      26.33
 H      -4.963959     1.817416     0.859949      27.86
 C       0.982101     0.276793    -0.663351      79.02
 H       1.622592     1.127781    -0.805556      26.33
 C       0.453652    -2.171506    -0.853385      49.20
 H       0.729299    -3.115523    -1.438978      25.15
 C      -0.842829    -1.891180    -0.367187      26.90
 O      -1.802734    -2.843955    -0.467760     212.01
 C      -2.469641    -3.035799    -1.811835     108.67
 H      -2.986005    -2.094260    -2.235879      25.29
 H      -1.694651    -3.152884    -2.429142      28.60
 H      -3.113073    -4.021876    -1.761707      27.85
 C      -1.273643    -0.582267    -0.141722      33.51
 O      -2.616637    -0.460815     0.338124      49.35
 C      -0.327449     0.393265    -0.146439      53.06
 H      -0.627142     1.392430     0.178952      27.67
 C       1.335025    -1.044862    -0.896936      -3.56
 C       2.826877    -1.360009    -1.294798      85.86
 H       2.780483    -2.213433    -1.949267      25.06
 O       3.347458    -0.184681    -2.062802     266.73
 H       4.347893    -0.455719    -2.170892      24.50
 C       3.837736    -1.762622    -0.088121      78.29
 H       3.197511    -2.232688     0.586988      29.16
 O       4.900517    -2.716424    -0.562340     156.26
 H       5.752564    -2.525211    -1.281496      26.74
 C       4.391643    -0.777298     0.967626     101.45
 O       5.109252     0.375388     0.194771     213.04
 H       4.948327     1.260558     0.356916      28.88
 H       5.105855    -1.237487     1.606065      28.16
 H       3.553140    -0.366686     1.501911      27.88
55
name = lig-Water-frame_314
 C      -1.175640     2.440068     3.156945      39.64
 H      -1.667251     3.456113     3.080115      21.89
 C      -0.559985    -0.051347     3.080458      48.20
 H      -0.886120    -1.248018     2.937436      24.97
 C       0.712068     0.187125     3.494206      19.20
 O       1.669838    -0.653947     3.991218     148.74
 C       0.874233    -1.972325     4.375928      93.99
 H       1.722132    -2.561497     4.767450      25.97
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 H       0.327245    -2.677261     3.535418      25.23
 H       0.223441    -1.623917     5.169884      27.25
 C       1.062898     1.586668     3.748803       5.24
 O       2.409683     1.770140     4.082439     132.35
 H       2.609454     2.778113     4.065091      25.47
 C       0.198214     2.644175     3.375928      62.35
 H       0.406799     3.641308     3.111175      27.72
 C      -1.577421     1.008784     2.985698       1.40
 C      -2.933785     0.795144     2.630330      88.99
 H      -3.381098     1.853592     2.812212      24.25
 O      -3.437915    -0.353913     3.317753     212.16
 H      -4.455220    -0.265893     3.514881      22.03
 C      -3.184189     0.822515     0.995289      46.62
 H      -2.539495     1.939813     0.621082      23.15
 C      -4.531737     0.856676     0.499654      90.65
 O      -5.640236    -0.259619     0.924456     165.10
 H      -5.145901    -1.144845     1.238409      24.76
 H      -4.490364     1.089969    -0.664588      23.98
 H      -5.005700     1.935514     0.673866      24.23
 C       0.943319     0.248084    -0.633245      57.25
 H       1.690852     1.048285    -0.699326      24.60
 C       0.422226    -2.138110    -0.866705      46.89
 H       0.813972    -3.113803    -1.192642      24.69
 C      -0.850121    -1.871390    -0.317937      27.18
 O      -1.838559    -2.900909    -0.471397     158.18
 C      -2.477500    -3.083618    -1.804772     100.38
 H      -2.940651    -2.273815    -2.320313      25.93
 H      -1.398817    -3.183581    -2.399134      23.87
 H      -3.262412    -3.865446    -1.762386      27.21
 C      -1.261758    -0.533033    -0.166969      17.14
 O      -2.590916    -0.467108     0.344545      25.62
 C      -0.296739     0.481373    -0.081500      52.99
 H      -0.581478     1.547431     0.080961      25.21
 C       1.344282    -1.060544    -0.868204      15.09
 C       2.847038    -1.328251    -1.337694      61.39
 H       2.736584    -2.454161    -1.771096      22.79
 O       3.339471    -0.179309    -2.039012     240.02
 H       4.283835    -0.397486    -2.439863      25.80
 C       3.956048    -1.787209    -0.080353      75.24
 H       3.318173    -2.688697     0.463084      25.18
 O       4.919130    -2.771510    -0.495241     242.43
 H       5.445057    -2.239416    -0.979509      33.29
 C       4.388022    -0.722197     0.906896     101.21
 O       5.086306     0.362791     0.177547     198.65
 H       4.834158     1.298583     0.554641      24.67
 H       4.969588    -1.291635     1.818593      25.90
 H       3.520178    -0.230256     1.538994      25.58
55
name = lig-Water-frame_315
 C      -1.137894     2.442988     3.114660      60.91
 H      -1.777763     3.240151     2.747832      20.90
 C      -0.594416    -0.055785     3.045911      52.60
 H      -0.817289    -0.933011     2.684077      23.72
 C       0.663598     0.188339     3.517172      28.66
 O       1.670151    -0.698322     3.974071     207.73
 C       0.937208    -1.915617     4.349565     116.10
 H       1.583942    -2.533317     5.001726      26.43
 H       0.518164    -2.445922     3.534380      25.57
 H       0.390542    -1.606333     5.261477      26.61
 C       0.975039     1.588070     3.711656      25.44
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 O       2.388242     1.802066     4.047329     140.28
 H       2.429409     2.804328     4.056382      29.85
 C       0.168336     2.645057     3.468461      42.74
 H       0.580157     3.709819     3.359488      22.35
 C      -1.541484     1.072554     2.989697      31.54
 C      -2.976085     0.815267     2.630174      74.12
 H      -3.348476     1.912083     2.764361      26.62
 O      -3.469736    -0.360247     3.356624     226.23
 H      -4.459272    -0.218855     3.452254      21.95
 C      -3.135085     0.757724     1.000638      90.98
 H      -2.854795     1.616404     0.629821      27.95
 C      -4.506960     0.897285     0.459699      93.49
 O      -5.613430    -0.271962     0.935791     208.67
 H      -5.046809    -1.011790     1.084888      28.66
 H      -4.550133     1.092764    -0.561305      27.59
 H      -5.073759     1.716132     0.811733      27.60
 C       0.937729     0.227423    -0.580858      41.03
 H       1.757564     0.980560    -0.597729      21.16
 C       0.416115    -2.090396    -0.851690      50.99
 H       0.738699    -3.140836    -0.921615      23.74
 C      -0.870959    -1.885144    -0.353260       8.08
 O      -1.900973    -2.953959    -0.447229     157.96
 C      -2.394386    -3.129666    -1.810020     109.40
 H      -3.171605    -2.183563    -2.178359      22.39
 H      -1.710308    -3.495853    -2.491298      26.67
 H      -3.168988    -3.898967    -1.681618      27.18
 C      -1.288458    -0.487005    -0.112615       7.80
 O      -2.565321    -0.443296     0.352535      93.63
 C      -0.299922     0.599125    -0.051175      59.80
 H      -0.602630     1.736129     0.054287      20.11
 C       1.419416    -1.095842    -0.873792      24.61
 C       2.875208    -1.333413    -1.329125      81.38
 H       2.899237    -2.263929    -1.862893      23.78
 O       3.321097    -0.189603    -2.036414     304.72
 H       4.097958    -0.400158    -2.540558      29.75
 C       3.957417    -1.867715    -0.051935      80.53
 H       3.355071    -2.514602     0.412261      28.23
 O       4.957036    -2.805947    -0.441779     211.69
 H       5.512292    -2.018269    -0.947489      26.92
 C       4.379147    -0.655385     0.873973     119.34
 O       5.084440     0.356720     0.176016     301.17
 H       4.569115     1.046706     0.772444      23.39
 H       4.941967    -1.085824     1.636943      27.05
 H       3.521610    -0.247493     1.301859      27.21
55
name = lig-Water-frame_316
 C      -1.131198     2.402326     3.061866      59.86
 H      -1.927672     3.018540     2.561402      25.29
 C      -0.669697    -0.009216     3.025439      61.99
 H      -1.014858    -1.043883     2.371138      18.37
 C       0.660454     0.251025     3.572454      36.87
 O       1.641895    -0.747094     3.929407     216.46
 C       1.039836    -1.864759     4.402679     106.08
 H       1.709887    -2.608939     4.913150      26.29
 H       0.528093    -2.347268     3.454334      24.66
 H       0.134926    -1.618739     5.051714      28.13
 C       1.002836     1.559733     3.693829      25.74
 O       2.328993     1.842374     4.009430     186.19
 H       2.507467     2.780531     4.083573      29.44
 C       0.156260     2.709017     3.540687      13.61
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 H       0.719293     3.589637     3.770744       9.67
 C      -1.482981     1.115122     2.982741      38.89
 C      -2.999804     0.837596     2.576695      76.06
 H      -3.743962     1.679949     2.957846      24.09
 O      -3.496329    -0.343023     3.383701     232.69
 H      -4.536284    -0.255442     3.390205      23.56
 C      -3.104186     0.652067     1.038235      82.35
 H      -2.607896     1.779264     0.485405      19.30
 C      -4.586102     0.893566     0.449452      73.37
 O      -5.547202    -0.249298     0.913568     216.01
 H      -4.951615    -1.037029     0.975793      26.45
 H      -4.566491     0.843390    -0.722820      23.21
 H      -5.081845     1.676474     1.203118      23.90
 C       0.992386     0.221441    -0.514389      31.23
 H       1.729931     0.990048    -0.549436      20.36
 C       0.438023    -2.083445    -0.811716      10.56
 H       0.624359    -3.208694    -0.796241      19.97
 C      -0.918504    -1.857743    -0.425662     -23.31
 O      -1.934343    -2.972877    -0.416223     113.41
 C      -2.383262    -3.162987    -1.805307     102.94
 H      -2.919251    -2.335078    -1.987489      25.80
 H      -1.786416    -3.690971    -2.737838      23.40
 H      -3.059635    -4.106789    -1.553699      23.69
 C      -1.284282    -0.460992    -0.024225      -7.02
 O      -2.564750    -0.406264     0.370079     138.81
 C      -0.342554     0.670972    -0.068929      50.35
 H      -0.570315     1.658637     0.107797      18.93
 C       1.473024    -1.103505    -0.880696      11.88
 C       2.927586    -1.365293    -1.282596      83.25
 H       3.016868    -2.192932    -2.186109      18.47
 O       3.279565    -0.191281    -2.039889     221.87
 H       4.167391    -0.504187    -2.601243      22.37
 C       3.880201    -1.911452    -0.022555      62.90
 H       3.013028    -2.382379     0.752172      22.70
 O       5.022115    -2.790232    -0.418005     163.06
 H       5.824047    -2.353103    -0.979718      26.83
 C       4.357202    -0.666401     0.820395      85.05
 O       5.081374     0.382123     0.196157     273.08
 H       4.686198     1.156185     0.558470      28.95
 H       5.137796    -0.961604     1.719552      22.13
 H       3.276346    -0.267373     1.143824      21.76
55
name = lig-Water-frame_317
 C      -1.122156     2.430702     3.019264      82.59
 H      -1.873422     3.111577     2.681557      28.77
 C      -0.698241     0.006492     3.014769      61.33
 H      -1.054527    -0.827559     2.671650      22.80
 C       0.631551     0.253749     3.601471      44.06
 O       1.627362    -0.726017     3.863872     234.95
 C       1.065385    -1.895109     4.455385     117.24
 H       1.882480    -2.520162     4.757018      25.89
 H       0.637908    -2.475260     3.587309      26.22
 H       0.079540    -1.695953     4.863865      27.95
 C       1.073004     1.608552     3.704375      21.12
 O       2.286792     1.867368     3.983289     158.76
 H       2.608254     2.839039     4.069726      20.73
 C       0.155536     2.738657     3.593599      47.07
 H       0.584001     3.670543     4.061610      11.68
 C      -1.520905     1.080515     2.939034      29.72
 C      -3.015078     0.826305     2.551990      79.31
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 H      -3.818828     1.518264     2.910338      21.59
 O      -3.501431    -0.318722     3.387992     275.65
 H      -4.503900    -0.309663     3.426875      26.56
 C      -3.129742     0.690565     1.029347     106.39
 H      -2.536553     1.392501     0.746553      26.06
 C      -4.676848     0.840245     0.502493     108.70
 O      -5.462098    -0.224099     0.875119     281.17
 H      -4.962858    -1.138267     0.887794      26.03
 H      -4.626169     0.877892    -0.558938      26.32
 H      -4.921178     1.725576     0.969108      27.21
 C       1.045416     0.236189    -0.446995      50.24
 H       1.761827     1.112556    -0.534244      17.76
 C       0.444305    -2.121073    -0.750058      35.31
 H       0.654250    -3.148920    -0.916151      22.54
 C      -0.947292    -1.779561    -0.490605     -14.06
 O      -1.906951    -2.946262    -0.395282     142.40
 C      -2.406859    -3.293927    -1.785684      89.47
 H      -2.921578    -2.151644    -2.127594      21.95
 H      -1.665753    -3.441341    -2.552112      24.86
 H      -3.069541    -4.052870    -1.615062      25.21
 C      -1.238621    -0.463354     0.038982       4.53
 O      -2.586082    -0.404554     0.393226     174.45
 C      -0.350767     0.614102    -0.130323      38.63
 H      -0.558596     1.761577     0.276649      16.32
 C       1.464166    -1.091411    -0.860346      25.24
 C       2.979123    -1.438687    -1.264212      88.89
 H       2.956640    -2.137974    -2.062468      23.86
 O       3.262199    -0.192061    -2.053695     280.18
 H       4.134991    -0.383255    -2.362953      26.85
 C       3.803097    -1.897158    -0.005537      70.76
 H       3.261463    -2.363069     0.714334      27.33
 O       5.071611    -2.788780    -0.388857     214.70
 H       5.732486    -2.498035    -0.870806      33.31
 C       4.315678    -0.699070     0.805165     109.13
 O       5.091487     0.420266     0.199137     272.11
 H       4.818253     1.414358     0.298594      25.36
 H       4.826113    -0.975179     1.636951      25.81
 H       3.430603    -0.321314     1.160366      26.82
55
name = lig-Water-frame_318
 C      -1.102765     2.478638     3.014789      84.05
 H      -1.757561     3.427444     2.964009      21.86
 C      -0.648589     0.029911     3.066900      43.09
 H      -1.122296    -1.154151     3.007014      20.55
 C       0.595580     0.254611     3.588966      42.66
 O       1.610569    -0.669945     3.796016     208.74
 C       1.058252    -1.970231     4.444731      96.98
 H       2.001583    -2.388184     4.954118      24.32
 H       0.776240    -2.761856     3.611869      24.37
 H       0.210474    -1.761646     5.184523      26.83
 C       1.041757     1.686700     3.713763       6.77
 O       2.348890     1.893079     3.989216     201.57
 H       2.509463     2.879562     3.970472      27.44
 C       0.147258     2.729010     3.626217      44.32
 H       0.212380     3.735377     4.063701      15.92
 C      -1.627592     1.082735     2.870729      32.42
 C      -3.034489     0.769779     2.562500      69.16
 H      -3.661324     1.828822     2.736639      20.69
 O      -3.472182    -0.313357     3.379498     263.81
 H      -4.486785    -0.237771     3.489526      25.00
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 C      -3.223516     0.759363     1.021215      57.23
 H      -2.422084     1.752856     0.726035      17.16
 C      -4.662868     0.808183     0.553833     102.77
 O      -5.417326    -0.250097     0.856945     315.44
 H      -4.936756    -1.049436     0.812632      30.57
 H      -4.670424     1.073883    -0.592540      23.27
 H      -5.074106     1.937714     0.733280      23.07
 C       1.075336     0.266200    -0.405123      49.81
 H       1.755825     1.067189    -0.485124      18.38
 C       0.429894    -2.126835    -0.697017      39.04
 H       0.735007    -3.156404    -1.156514      21.14
 C      -0.925230    -1.737451    -0.528381       4.76
 O      -1.850626    -2.882506    -0.393611     144.81
 C      -2.435480    -3.326495    -1.746985      88.13
 H      -2.923262    -2.607641    -2.197167      27.27
 H      -1.414176    -3.394683    -2.343023      22.09
 H      -3.299802    -4.201607    -1.722787      21.88
 C      -1.235430    -0.494492     0.058476       1.54
 O      -2.600128    -0.452859     0.413658     128.52
 C      -0.294530     0.541926    -0.172394      61.00
 H      -0.493489     1.406151     0.225045      20.86
 C       1.427195    -1.087616    -0.803843       8.93
 C       2.955188    -1.476931    -1.248522      63.77
 H       2.898084    -2.481537    -1.943546      21.62
 O       3.257343    -0.204885    -2.045529     226.15
 H       4.279812    -0.225825    -2.269547      24.02
 C       3.835621    -1.830277    -0.054397      62.04
 H       3.364708    -2.690073     0.702980      22.47
 O       5.059517    -2.812059    -0.323929      85.66
 H       5.729640    -2.208400    -1.014978      25.11
 C       4.258474    -0.672634     0.792700      89.79
 O       5.130968     0.437905     0.180668     197.21
 H       4.606120     1.324011     0.286549      24.92
 H       4.741042    -1.219214     1.797755      23.00
 H       3.345347    -0.131363     1.345968      19.95
55
name = lig-Water-frame_319
 C      -1.138474     2.490843     3.038743      68.66
 H      -1.648123     3.411779     3.185716      23.74
 C      -0.673557     0.013200     3.130314      45.51
 H      -0.885254    -0.955423     3.401277      26.18
 C       0.605682     0.332221     3.555891      12.60
 O       1.572296    -0.644732     3.748521     165.72
 C       1.083507    -2.033934     4.428964     108.23
 H       1.888122    -2.201601     5.100958      26.50
 H       0.907998    -2.913391     3.725043      26.34
 H       0.503870    -1.846447     5.294948      28.32
 C       1.001736     1.704242     3.732917       4.64
 O       2.442544     1.925050     4.009680     208.78
 H       2.494716     2.914121     3.942683      26.96
 C       0.094179     2.729064     3.633375      63.07
 H       0.153241     3.765222     3.938307      19.26
 C      -1.651650     1.140663     2.824728      20.33
 C      -3.067346     0.767895     2.560335      85.30
 H      -3.491180     1.858734     2.752689      22.96
 O      -3.444745    -0.315955     3.367984     266.65
 H      -4.451957    -0.190225     3.532040      23.92
 C      -3.256416     0.846690     1.010954      79.66
 H      -2.967720     1.741262     0.672249      25.17
 C      -4.602715     0.904581     0.513563     105.16
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 O      -5.426146    -0.319452     0.863293     260.52
 H      -4.770200    -1.079326     0.764825      26.03
 H      -4.582803     0.987105    -0.568708      27.08
 H      -5.300787     1.611840     0.893478      26.63
 C       1.092287     0.247931    -0.404590      56.88
 H       1.849193     1.077514    -0.409654      20.09
 C       0.442812    -2.103115    -0.700601      64.08
 H       0.645252    -2.989285    -1.188614      26.24
 C      -0.890075    -1.775902    -0.524534      11.83
 O      -1.816279    -2.803308    -0.404419     185.83
 C      -2.422308    -3.359395    -1.694656      90.51
 H      -3.183454    -2.590068    -2.403700      22.00
 H      -1.481424    -3.727836    -2.184534      22.86
 H      -2.924772    -4.215838    -1.569985      25.74
 C      -1.276333    -0.538463     0.025163       2.08
 O      -2.606018    -0.491626     0.436410      86.33
 C      -0.229843     0.451640    -0.174378      48.86
 H      -0.546029     1.570473     0.262381      22.14
 C       1.416610    -1.100377    -0.725701      26.17
 C       2.868156    -1.494698    -1.263092      75.60
 H       2.858795    -2.487073    -1.692086      25.93
 O       3.259786    -0.250669    -2.022523     218.97
 H       4.278001    -0.229614    -2.244562      25.71
 C       3.898545    -1.808057    -0.085043      82.84
 H       3.315379    -2.528584     0.396537      27.42
 O       5.042875    -2.791112    -0.284655     209.32
 H       5.490607    -2.175712    -0.942088      27.54
 C       4.211165    -0.613075     0.858952     115.19
 O       5.156404     0.426625     0.167962     245.48
 H       4.492813     1.046164     0.396887      29.71
 H       4.759137    -1.096412     1.542468      27.08
 H       3.412023    -0.084315     1.242765      26.23
55
name = lig-Water-frame_320
 C      -1.216254     2.461399     3.084467      58.39
 H      -1.965575     3.319259     3.127918      26.81
 C      -0.738837     0.080304     3.203730      31.70
 H      -0.979769    -1.052970     3.544475      24.29
 C       0.632474     0.421231     3.515717       3.41
 O       1.525413    -0.660562     3.724731     136.98
 C       1.157132    -2.041808     4.431991      87.20
 H       2.138619    -2.199086     5.021661      23.59
 H       0.942227    -2.869298     3.753562      27.71
 H       0.256485    -1.844172     5.184110      24.42
 C       1.049746     1.699259     3.765456       4.24
 O       2.491291     1.955153     4.028297     132.35
 H       2.618213     3.006255     4.042789      25.29
 C       0.042264     2.744444     3.623285      62.47
 H       0.449205     3.783328     3.830306      23.84
 C      -1.579820     1.164761     2.828536      24.20
 C      -3.074555     0.843789     2.530304      91.81
 H      -3.679057     1.725887     3.059727      25.41
 O      -3.436251    -0.316241     3.355106     232.15
 H      -4.427402    -0.330073     3.474283      22.70
 C      -3.265422     0.861580     1.033566      57.27
 H      -2.919585     2.008788     0.493813      22.78
 C      -4.635632     0.948227     0.447171      86.36
 O      -5.426533    -0.397746     0.860774     171.64
 H      -4.695962    -1.133262     0.762852      23.07
 H      -4.507432     0.930180    -0.678271      25.82
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 H      -5.336130     1.558665     1.138261      24.07
 C       1.128219     0.195599    -0.425215      53.33
 H       1.841043     1.004695    -0.348967      25.61
 C       0.470198    -2.061955    -0.744846      64.75
 H       0.634855    -3.119096    -1.197049      25.23
 C      -0.875435    -1.830579    -0.475818      20.08
 O      -1.829622    -2.751940    -0.427722     251.60
 C      -2.382959    -3.362626    -1.660245     105.10
 H      -2.967812    -2.784828    -2.170227      27.98
 H      -1.592758    -3.906438    -2.342826      25.22
 H      -2.780450    -4.423108    -1.117609      22.76
 C      -1.296416    -0.566774    -0.052211     -11.77
 O      -2.610568    -0.485060     0.458281      45.83
 C      -0.257379     0.442246    -0.099064      52.25
 H      -0.482758     1.413182     0.058788      28.64
 C       1.472239    -1.123520    -0.663055      15.85
 C       2.805693    -1.462045    -1.244982      92.34
 H       2.735093    -2.487192    -1.901679      22.19
 O       3.247593    -0.318155    -2.004342     236.96
 H       4.133424    -0.509639    -2.255484      27.52
 C       3.907878    -1.793506    -0.093535      81.65
 H       3.014723    -2.404066     0.527570      25.08
 O       5.013429    -2.721671    -0.270997     235.71
 H       5.594375    -2.348578    -0.940360      29.27
 C       4.221868    -0.586234     0.876812      88.96
 O       5.156016     0.391116     0.171235     166.07
 H       4.565369     1.280419     0.415554      26.01
 H       5.007537    -0.973397     1.743384      24.46
 H       3.249142    -0.031658     1.222921      24.47
55
name = lig-Water-frame_321
 C      -1.287205     2.481096     3.154021      60.78
 H      -2.171658     3.055017     2.894895      27.02
 C      -0.759774     0.167179     3.296803      55.00
 H      -1.243578    -0.855765     3.279879      28.61
 C       0.631827     0.411046     3.496790      -1.13
 O       1.489304    -0.693281     3.711950     142.85
 C       1.229081    -1.980665     4.461320     105.98
 H       2.167537    -2.295512     4.812524      25.66
 H       0.969296    -2.763693     3.570130      25.58
 H       0.271935    -1.911014     4.849821      26.36
 C       1.128323     1.753989     3.786027      -1.05
 O       2.496359     1.988331     4.044149     170.74
 H       2.627361     2.948605     4.163760      27.77
 C       0.058917     2.766406     3.609261      54.35
 H       0.523624     3.707285     3.711394      25.44
 C      -1.552171     1.125477     2.866136       3.10
 C      -3.064588     0.936981     2.554632      77.01
 H      -3.837949     1.666508     3.085572      23.13
 O      -3.428789    -0.318392     3.328447     219.14
 H      -4.449391    -0.468414     3.303451      21.97
 C      -3.252714     0.888976     1.008168      83.86
 H      -2.592985     1.585210     0.679876      28.35
 C      -4.727079     0.891199     0.424465      87.40
 O      -5.404361    -0.459841     0.834339     232.68
 H      -4.797250    -1.162797     0.780575      28.16
 H      -4.662979     1.094860    -0.683294      27.82
 H      -5.152963     1.766668     0.957534      27.47
 C       1.107458     0.154900    -0.416142      42.13
 H       1.829986     0.970541    -0.366033      27.53
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 C       0.479020    -2.085833    -0.814474      31.50
 H       0.733934    -3.087994    -1.054310      26.23
 C      -0.847477    -1.841730    -0.416914      32.36
 O      -1.873099    -2.753660    -0.453420     205.26
 C      -2.298468    -3.472029    -1.573808     114.33
 H      -3.154016    -2.690698    -2.126927      23.94
 H      -1.699247    -3.779248    -2.509887      25.77
 H      -2.861825    -4.127580    -1.010410      27.57
 C      -1.287610    -0.541518    -0.116914      20.77
 O      -2.614651    -0.436679     0.476187      74.74
 C      -0.288724     0.432603    -0.030159      29.29
 H      -0.561706     1.598795     0.038405      25.97
 C       1.540177    -1.149282    -0.636282      26.32
 C       2.820548    -1.453859    -1.224051     102.40
 H       2.617313    -2.166899    -2.010512      23.66
 O       3.221473    -0.381537    -2.003315     220.52
 H       4.139526    -0.802752    -2.413474      24.05
 C       3.833774    -1.795405    -0.044513      89.97
 H       3.256043    -2.252934     0.729204      28.99
 O       4.966186    -2.635853    -0.264864     199.37
 H       5.801552    -2.590552    -1.000607      24.55
 C       4.288743    -0.580804     0.881135     128.38
 O       5.121874     0.383746     0.190339     211.65
 H       5.016954     1.320366     0.255105      28.12
 H       4.716790    -0.805351     1.780379      30.91
 H       3.345621    -0.177786     1.214783      29.13
55
name = lig-Water-frame_322
 C      -1.295757     2.496769     3.216221      46.28
 H      -2.071225     3.179961     2.804556      24.00
 C      -0.722207     0.190523     3.371993      55.29
 H      -1.249686    -0.780502     3.119809      27.70
 C       0.640608     0.360120     3.539103      10.29
 O       1.482661    -0.708908     3.701427     172.68
 C       1.265805    -1.911623     4.385928     120.07
 H       2.162664    -2.355863     4.938604      26.16
 H       1.117832    -2.579394     3.562317      27.70
 H       0.262070    -1.964895     5.023013      26.16
 C       1.138552     1.793043     3.766805       3.84
 O       2.477365     2.001337     4.059707     141.73
 H       2.575391     3.073601     4.213003      23.14
 C       0.111009     2.783618     3.585102      57.09
 H       0.358142     3.905006     3.653520      24.58
 C      -1.633975     1.171664     2.934850     -16.64
 C      -3.059920     0.956294     2.608528      77.61
 H      -3.832160     1.828153     2.882822      24.41
 O      -3.424907    -0.321681     3.286285     217.78
 H      -4.387094    -0.437052     3.150515      24.32
 C      -3.232650     0.853150     0.967770      73.30
 H      -2.297761     1.614931     0.621541      23.25
 C      -4.777267     0.801905     0.440961      96.08
 O      -5.388651    -0.467589     0.791035     239.04
 H      -4.698322    -1.246076     0.745832      25.32
 H      -4.896261     1.099897    -0.631568      27.08
 H      -5.248717     1.791803     0.760700      25.99
 C       1.042271     0.146213    -0.363806      52.48
 H       1.785624     0.981115    -0.426982      26.46
 C       0.485492    -2.132851    -0.852288      33.83
 H       0.827421    -3.195771    -1.015548      24.84
 C      -0.821990    -1.835209    -0.394504       7.95
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 O      -1.886514    -2.770450    -0.437337     186.67
 C      -2.301641    -3.529792    -1.552114     121.72
 H      -3.037059    -2.981292    -1.928781      28.11
 H      -1.561654    -3.749056    -2.350661      26.70
 H      -3.119977    -4.367775    -1.129945      24.70
 C      -1.292917    -0.482800    -0.117166      13.69
 O      -2.610650    -0.382972     0.482398     114.86
 C      -0.280068     0.466511    -0.002396      59.24
 H      -0.589718     1.500109     0.157374      27.51
 C       1.513913    -1.165487    -0.635772      17.69
 C       2.876335    -1.469570    -1.184385      94.72
 H       2.656991    -2.380000    -1.926574      23.03
 O       3.235512    -0.420766    -2.043450     272.05
 H       4.048805    -0.619725    -2.517946      28.97
 C       3.800108    -1.765495     0.027165      76.86
 H       3.347014    -2.469415     0.938901      26.33
 O       4.939015    -2.597733    -0.258862     221.63
 H       5.506147    -2.431967    -1.005445      30.31
 C       4.315666    -0.545560     0.849065     131.68
 O       5.122401     0.370174     0.194760     208.71
 H       5.069195     1.342245     0.326185      26.29
 H       4.669037    -0.962245     1.958351      27.06
 H       3.321885    -0.083982     1.200719      28.08
55
name = lig-Water-frame_323
 C      -1.243580     2.523773     3.253402      54.31
 H      -1.670887     3.529199     2.972244      22.70
 C      -0.712198     0.174832     3.400594      14.19
 H      -0.956202    -0.973440     3.081937      27.08
 C       0.652860     0.358427     3.630141       3.54
 O       1.523913    -0.678553     3.688437     197.34
 C       1.253831    -1.891990     4.319754     125.34
 H       2.031710    -2.094749     5.057627      26.82
 H       1.180294    -2.764375     3.471929      25.48
 H       0.551634    -1.898461     5.085449      27.77
 C       1.085219     1.780361     3.722409       8.20
 O       2.447702     2.021056     4.077714     128.52
 H       2.576592     3.008006     4.109282      25.10
 C       0.147994     2.823856     3.549972      63.67
 H       0.212181     3.873116     3.658731      24.75
 C      -1.715490     1.272587     3.068427     -24.85
 C      -3.082234     0.911112     2.613453      84.64
 H      -3.714341     1.918968     2.825132      25.17
 O      -3.425840    -0.311580     3.236151     225.15
 H      -4.421322    -0.375945     3.124111      22.10
 C      -3.171905     0.819382     0.926211      97.08
 H      -2.831820     1.776394     0.528039      26.68
 C      -4.767095     0.756997     0.455346      93.55
 O      -5.376906    -0.467301     0.750598     253.49
 H      -4.629363    -1.149710     0.705335      26.69
 H      -4.900300     0.822929    -0.690730      25.96
 H      -5.517185     1.483238     0.946828      25.82
 C       1.010429     0.155163    -0.304847      59.50
 H       1.691573     0.953321    -0.419886      25.71
 C       0.491384    -2.185181    -0.839171      58.79
 H       0.755815    -3.240273    -1.057491      25.70
 C      -0.841577    -1.825621    -0.421862     -19.23
 O      -1.876832    -2.796317    -0.366082     175.81
 C      -2.364180    -3.606582    -1.540233      93.64
 H      -3.189290    -2.908750    -2.195842      22.82
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 H      -1.315301    -3.871946    -2.041551      24.63
 H      -2.749274    -4.603434    -1.418043      26.89
 C      -1.303704    -0.456679    -0.060887       5.17
 O      -2.592920    -0.357146     0.469728     163.39
 C      -0.275073     0.511648     0.002174      62.43
 H      -0.520685     1.555651     0.333208      26.47
 C       1.421892    -1.164734    -0.674002      11.90
 C       2.911054    -1.524162    -1.145436      83.79
 H       2.967092    -2.603000    -1.429655      24.12
 O       3.252343    -0.429697    -2.100271     266.54
 H       4.189589    -0.475841    -2.523427      26.87
 C       3.816836    -1.740015     0.125839      90.83
 H       3.245859    -2.460768     0.731419      27.78
 O       4.922417    -2.590825    -0.252726     172.01
 H       5.212469    -2.097484    -1.116369      28.47
 C       4.263184    -0.511563     0.881899     136.48
 O       5.170364     0.362644     0.178313     193.31
 H       4.745896     1.255774     0.599231      24.60
 H       4.774399    -0.998212     1.640889      31.35
 H       3.391415     0.132146     1.139463      25.99
55
name = lig-Water-frame_324
 C      -1.148737     2.622057     3.275578      55.88
 H      -1.577043     3.601965     3.205519      22.99
 C      -0.735663     0.155090     3.383159       3.54
 H      -0.822494    -0.889810     3.218188      24.52
 C       0.621523     0.422590     3.721976     -43.85
 O       1.602985    -0.613077     3.667861     167.43
 C       1.251651    -1.931025     4.273698     116.91
 H       2.139325    -1.971906     4.943744      26.52
 H       1.157208    -2.748633     3.685227      29.54
 H       0.326908    -1.761877     5.003105      25.26
 C       1.055073     1.756183     3.696813      -4.24
 O       2.400625     2.011684     4.081484     105.04
 H       2.600822     3.064883     4.096944      19.71
 C       0.158750     2.828592     3.515474      50.56
 H       0.459864     3.904822     3.729486      18.92
 C      -1.732683     1.295386     3.233091     -18.72
 C      -3.093081     0.882403     2.561049      96.02
 H      -3.760278     1.805487     2.853063      27.28
 O      -3.454258    -0.301949     3.189917     246.66
 H      -4.463691    -0.382610     3.248191      24.73
 C      -3.192136     0.823755     0.928389      77.02
 H      -3.105989     1.897716     0.398514      23.64
 C      -4.736564     0.738315     0.459052     100.09
 O      -5.364421    -0.512569     0.729522     287.94
 H      -4.702438    -1.170713     0.720576      30.12
 H      -4.621343     0.840208    -0.614114      28.87
 H      -5.419803     1.325596     1.083306      27.88
 C       1.021633     0.153199    -0.272198      47.66
 H       1.794832     0.990745    -0.336983      24.90
 C       0.443018    -2.215808    -0.787472      46.09
 H       0.650625    -3.217103    -1.113652      22.32
 C      -0.902937    -1.812737    -0.475132      -0.80
 O      -1.889609    -2.849713    -0.271040     132.99
 C      -2.376102    -3.639704    -1.567728     100.71
 H      -2.889530    -3.128323    -2.291566      28.22
 H      -1.441454    -3.852688    -1.987343      26.99
 H      -2.571930    -4.760955    -1.278960      23.91
 C      -1.282023    -0.480940     0.009296       7.48
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 O      -2.562736    -0.357958     0.433168     164.00
 C      -0.314913     0.560782     0.010865      47.75
 H      -0.398217     1.620419     0.520889      22.82
 C       1.373714    -1.162004    -0.749495      28.91
 C       2.917774    -1.554494    -1.072308      69.88
 H       3.098265    -2.663602    -1.374769      23.97
 O       3.263761    -0.456609    -2.155296     223.99
 H       4.319088    -0.501468    -2.283694      24.67
 C       3.811321    -1.709651     0.185045      87.36
 H       2.993088    -2.353049     0.794365      26.35
 O       4.934164    -2.576874    -0.268752     102.03
 H       5.040602    -1.890280    -1.120566      26.13
 C       4.203360    -0.493419     0.920657     112.67
 O       5.209882     0.384451     0.180960     209.96
 H       4.771613     1.160412     0.440605      29.74
 H       4.967116    -0.912975     1.768572      26.54
 H       3.388594     0.148050     1.258066      25.39
55
name = lig-Water-frame_325
 C      -1.122238     2.705191     3.292554      44.95
 H      -1.916771     3.530509     3.319581      23.80
 C      -0.763639     0.209287     3.375973      35.91
 H      -1.093025    -1.017014     3.322921      20.40
 C       0.572591     0.471513     3.772192      -0.20
 O       1.672628    -0.538199     3.644323      52.69
 C       1.246668    -1.913280     4.299742     101.15
 H       2.166259    -2.224317     4.871052      25.02
 H       1.071030    -2.886061     3.533036      25.18
 H       0.277385    -1.753402     4.642588      27.28
 C       1.075031     1.757809     3.709398      18.70
 O       2.355378     1.993586     4.069241     173.37
 H       2.493832     2.955559     4.236168      23.39
 C       0.226094     2.843100     3.505436      44.46
 H       0.775695     3.731275     3.709419      21.09
 C      -1.690261     1.261727     3.353546       1.44
 C      -3.073753     0.907993     2.506418      81.96
 H      -3.968899     1.722857     2.837955      23.09
 O      -3.508400    -0.319144     3.158143     265.25
 H      -4.466534    -0.347321     3.343279      27.98
 C      -3.266797     0.854446     0.977557      63.09
 H      -2.813621     1.769942     0.375830      22.22
 C      -4.675444     0.694138     0.479848      82.75
 O      -5.360426    -0.587120     0.717075     247.95
 H      -4.695372    -1.417806     0.821881      24.22
 H      -4.505418     1.127134    -0.602043      25.22
 H      -5.181942     1.624508     1.041610      24.97
 C       1.043249     0.156896    -0.276642      29.91
 H       1.841820     0.848412    -0.191794      23.35
 C       0.349209    -2.193893    -0.732928      38.43
 H       0.588336    -3.245225    -1.152260      20.27
 C      -0.979984    -1.816118    -0.508001      12.89
 O      -1.925445    -2.914540    -0.200273     116.87
 C      -2.304018    -3.691895    -1.554863      66.39
 H      -2.994364    -3.144932    -2.384952      23.68
 H      -1.292874    -3.805708    -2.248471      22.29
 H      -2.754554    -4.589380    -0.940030      21.40
 C      -1.237405    -0.513763     0.062665       4.76
 O      -2.550624    -0.365819     0.387703     135.86
 C      -0.319451     0.586076     0.039159      49.62
 H      -0.472322     1.492835     0.503051      22.39
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 C       1.384748    -1.169007    -0.817862      29.53
 C       2.875056    -1.539409    -1.022140      82.19
 H       2.913315    -2.450582    -1.693220      23.63
 O       3.285639    -0.520351    -2.170583     262.00
 H       4.203844    -0.585000    -2.239044      28.62
 C       3.755878    -1.704283     0.218396      86.53
 H       3.041264    -2.155262     0.994411      26.72
 O       4.938854    -2.522402    -0.290489     179.90
 H       5.319371    -2.165516    -1.023257      32.06
 C       4.236171    -0.484011     0.992678     114.12
 O       5.219565     0.398223     0.199534     176.55
 H       4.959424     1.448365     0.113270      22.99
 H       4.738075    -0.644693     1.911264      28.30
 H       3.305418     0.038810     1.460328      25.22
55
name = lig-Water-frame_326
 C      -1.173245     2.713748     3.328934      34.22
 H      -1.998370     3.378486     3.301323      22.31
 C      -0.788917     0.225623     3.409530      57.89
 H      -1.285538    -0.623367     3.334774      26.07
 C       0.563375     0.459959     3.765575     -11.83
 O       1.700367    -0.485381     3.643838      44.65
 C       1.260625    -1.903229     4.264528     108.99
 H       1.918516    -2.373848     4.984205      28.16
 H       1.138192    -2.476730     3.443830      29.87
 H       0.199407    -1.770368     4.696847      28.05
 C       1.087090     1.765716     3.746682      19.92
 O       2.347540     1.961224     4.058507     117.08
 H       2.457868     2.961088     4.349126      22.29
 C       0.288268     2.874974     3.504594      48.26
 H       0.746228     3.851327     3.550415      24.30
 C      -1.655034     1.285974     3.371286      -2.77
 C      -3.069120     0.961396     2.533560      83.05
 H      -3.935059     1.647440     2.774084      24.87
 O      -3.560336    -0.354491     3.130975     236.55
 H      -4.558015    -0.218963     3.341022      26.30
 C      -3.253087     0.848441     1.021179      71.98
 H      -2.606140     1.714276     0.553133      23.13
 C      -4.617997     0.688117     0.497488     104.87
 O      -5.346123    -0.653720     0.707284     254.90
 H      -4.722335    -1.356977     0.989757      26.57
 H      -4.724560     1.001832    -0.504252      26.54
 H      -5.103172     1.569653     0.889244      26.91
 C       1.046389     0.144794    -0.307342      33.52
 H       1.920881     0.822144    -0.090035      24.81
 C       0.290166    -2.148414    -0.730913      45.45
 H       0.500802    -3.127123    -1.000782      24.40
 C      -1.048291    -1.838988    -0.479987       2.78
 O      -1.957930    -2.964643    -0.190204     132.15
 C      -2.210158    -3.718433    -1.531096     113.18
 H      -3.094145    -3.224944    -1.937796      26.51
 H      -1.420892    -3.928110    -2.111894      26.45
 H      -2.829251    -4.490029    -1.062212      25.48
 C      -1.227349    -0.519448     0.087597     -15.46
 O      -2.567544    -0.372488     0.356822     101.78
 C      -0.258011     0.524824     0.060045      63.07
 H      -0.680277     1.588985     0.524467      22.17
 C       1.371267    -1.164849    -0.824866      43.45
 C       2.790674    -1.486619    -1.058945      92.33
 H       2.722236    -2.378148    -1.690347      25.42
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 O       3.284747    -0.592997    -2.138773     231.18
 H       4.354772    -0.746857    -2.395656      23.15
 C       3.743112    -1.684263     0.214975      63.56
 H       3.222681    -2.324495     1.112599      26.72
 O       4.922390    -2.481602    -0.267399     160.29
 H       5.586515    -2.242229    -1.058267      26.14
 C       4.273764    -0.416837     1.055852     114.59
 O       5.202592     0.412561     0.240730     196.10
 H       5.042741     1.368666    -0.070441      26.37
 H       4.738575    -0.682958     2.115936      26.26
 H       3.349737     0.022279     1.356369      26.90
55
name = lig-Water-frame_327
 C      -1.195321     2.642447     3.385104      65.41
 H      -1.893524     3.524973     3.180661      26.58
 C      -0.775709     0.245949     3.477663      44.06
 H      -1.503813    -0.794233     3.270039      24.45
 C       0.600584     0.414300     3.713994      12.91
 O       1.683847    -0.465809     3.687451      89.89
 C       1.245053    -1.849724     4.208877     102.07
 H       1.807273    -2.311256     5.115862      25.31
 H       1.238717    -2.323395     3.098520      24.21
 H       0.319894    -1.776728     4.787363      26.22
 C       1.047638     1.779370     3.787373       7.33
 O       2.404428     1.939050     4.065686      67.67
 H       2.552357     2.901309     4.279058      26.67
 C       0.242879     2.926926     3.500719      74.04
 H       0.487603     4.009076     3.327747      24.03
 C      -1.666920     1.392815     3.295120       3.28
 C      -3.067725     0.967258     2.633890      63.01
 H      -3.881333     1.908716     2.876872      24.16
 O      -3.611957    -0.376403     3.109055     223.41
 H      -4.557542    -0.194937     3.304877      24.48
 C      -3.135564     0.802562     1.032002      80.78
 H      -2.629079     1.866832     0.712493      24.60
 C      -4.607186     0.684381     0.510920      79.49
 O      -5.320731    -0.674556     0.711760     213.14
 H      -4.674906    -1.285332     1.134417      25.76
 H      -4.792974     0.652446    -0.661192      22.06
 H      -5.409362     1.423529     1.037024      24.16
 C       1.063017     0.139933    -0.338477      77.05
 H       1.857888     0.846807    -0.154830      29.05
 C       0.271699    -2.089515    -0.771477      -2.68
 H       0.530884    -3.229239    -0.878256      22.90
 C      -1.075393    -1.860784    -0.391976     -29.12
 O      -1.961470    -2.995245    -0.223654     136.18
 C      -2.193247    -3.719503    -1.428947      96.59
 H      -3.034898    -3.071743    -1.840924      25.43
 H      -1.241640    -4.134463    -2.121048      21.58
 H      -2.749155    -4.842258    -1.323141      24.96
 C      -1.272633    -0.524776     0.078011     -42.45
 O      -2.600004    -0.366374     0.353838     117.22
 C      -0.220823     0.450228     0.099430      83.44
 H      -0.499521     1.348346     0.356805      34.14
 C       1.293003    -1.130419    -0.774273      34.19
 C       2.728072    -1.460375    -1.134496     100.06
 H       2.682469    -2.642665    -1.354486      22.98
 O       3.300751    -0.646254    -2.096815     282.36
 H       4.113700    -1.013094    -2.427602      27.88
 C       3.781027    -1.648105     0.197844      64.38
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 H       3.486634    -2.528663     0.854049      27.13
 O       4.905535    -2.469198    -0.222761     158.38
 H       5.457543    -1.956451    -0.978334      25.16
 C       4.298191    -0.342227     1.090863     113.58
 O       5.194035     0.403825     0.292184     245.66
 H       4.750679     1.231856     0.169360      31.24
 H       4.813968    -0.813426     1.937322      27.85
 H       3.330120     0.301509     1.216904      25.52
55
name = lig-Water-frame_328
 C      -1.192159     2.652608     3.423052      76.34
 H      -1.629212     3.567362     3.053526      26.13
 C      -0.805335     0.237680     3.526488      51.31
 H      -1.089562    -0.673996     3.401516      29.59
 C       0.627707     0.409473     3.648834       3.21
 O       1.647515    -0.471910     3.770339     172.18
 C       1.228360    -1.792377     4.129830     133.34
 H       1.986418    -2.101467     4.805867      28.09
 H       1.257738    -2.451237     3.324111      28.74
 H       0.222568    -1.726807     4.588424      27.08
 C       1.020239     1.834137     3.817281      -5.30
 O       2.473437     1.921311     4.072976     145.21
 H       2.651724     2.916037     4.164289      23.88
 C       0.136301     2.944592     3.507115      69.30
 H       0.404450     3.956538     3.289463      26.35
 C      -1.702956     1.386706     3.198475       9.09
 C      -3.083811     0.952898     2.740311      78.37
 H      -3.604759     1.924918     2.884000      27.25
 O      -3.646471    -0.363713     3.101188     221.39
 H      -4.620549    -0.292033     3.321462      24.70
 C      -3.048412     0.790659     1.044034      81.32
 H      -2.676107     1.834560     0.641235      27.40
 C      -4.665336     0.664566     0.519834      93.25
 O      -5.281564    -0.665930     0.736042     234.12
 H      -4.654762    -1.359786     1.245838      24.01
 H      -4.484324     0.726175    -0.508889      28.14
 H      -5.352678     1.236440     0.996921      28.32
 C       1.057166     0.171304    -0.345143      68.43
 H       1.822036     0.950966    -0.351440      26.61
 C       0.249421    -2.091097    -0.811950      51.35
 H       0.602257    -3.061663    -0.895959      26.45
 C      -1.036326    -1.882639    -0.297311      14.70
 O      -1.934413    -3.007359    -0.232288     168.44
 C      -2.214572    -3.767369    -1.387074     135.98
 H      -2.713160    -3.083388    -2.168731      24.89
 H      -1.351459    -3.891134    -1.877330      28.18
 H      -2.526095    -4.678484    -1.190927      31.71
 C      -1.332220    -0.554764     0.049520      52.02
 O      -2.632779    -0.339163     0.378463     148.42
 C      -0.228183     0.353390     0.132293      38.53
 H      -0.373138     1.560721     0.380459      27.19
 C       1.254925    -1.118260    -0.739254      14.66
 C       2.695548    -1.532891    -1.133249      86.08
 H       2.736055    -2.576700    -1.254164      25.74
 O       3.296002    -0.681001    -2.074991     269.96
 H       4.079694    -1.232222    -2.432771      24.91
 C       3.819365    -1.615203     0.180821      73.02
 H       3.249402    -2.447506     0.819904      27.12
 O       4.912977    -2.435722    -0.204077     247.85
 H       5.272487    -1.823594    -0.781066      30.09
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 C       4.267354    -0.328370     1.068665     114.92
 O       5.201129     0.410118     0.338108     224.54
 H       4.567567     1.271783     0.457524      24.47
 H       4.832269    -0.802944     1.935126      27.19
 H       3.522455     0.340390     1.376415      25.18
55
name = lig-Water-frame_329
 C      -1.238295     2.703055     3.401270      51.46
 H      -1.772331     3.577035     2.971567      23.82
 C      -0.794204     0.273890     3.545046      51.01
 H      -0.966827    -0.984080     3.487001      24.15
 C       0.608047     0.513447     3.606314      12.11
 O       1.606333    -0.468718     3.846065     139.95
 C       1.212422    -1.758191     4.075753     126.73
 H       2.157445    -2.085644     4.654053      23.89
 H       1.203468    -2.677787     3.301077      25.73
 H       0.137674    -1.818413     4.446281      25.48
 C       1.045713     1.873526     3.823058       6.89
 O       2.508600     1.925948     4.068421     159.00
 H       2.707766     2.940378     4.112014      23.52
 C       0.107796     2.910278     3.548969      66.87
 H       0.529980     3.933296     3.438778      26.86
 C      -1.707802     1.258277     3.164604      17.40
 C      -3.076149     0.922923     2.756187      77.06
 H      -3.814251     1.913857     2.936472      24.64
 O      -3.663558    -0.329669     3.123674     242.33
 H      -4.656249    -0.311745     3.353567      24.65
 C      -3.083134     0.831456     1.095135      72.24
 H      -2.626645     1.745157     0.415280      24.80
 C      -4.668733     0.612508     0.553342      76.78
 O      -5.240607    -0.653340     0.773825     278.11
 H      -4.697234    -1.355059     1.088843      27.21
 H      -4.352620     1.007587    -0.523904      24.83
 H      -5.398230     1.547515     0.969175      24.36
 C       1.022605     0.203896    -0.335195      48.35
 H       1.744183     1.041516    -0.546431      24.83
 C       0.247226    -2.107742    -0.823402      51.81
 H       0.663154    -3.148396    -1.095179      23.36
 C      -0.983708    -1.925378    -0.240596      28.54
 O      -1.907930    -2.988881    -0.187368     158.60
 C      -2.207636    -3.757383    -1.424416     104.15
 H      -2.694895    -3.339647    -2.301428      24.95
 H      -1.044458    -3.826716    -1.840256      24.64
 H      -2.681547    -4.827612    -0.818171      22.72
 C      -1.363773    -0.589810     0.039961      39.57
 O      -2.646277    -0.324955     0.413538     129.10
 C      -0.280836     0.359085     0.164003      52.01
 H      -0.461942     1.306461     0.463437      28.70
 C       1.301022    -1.147651    -0.749668      17.76
 C       2.697202    -1.603114    -1.042657      69.01
 H       2.756584    -2.734135    -1.554697      23.27
 O       3.278532    -0.717011    -2.084932     221.09
 H       4.148906    -1.198069    -2.469134      23.92
 C       3.767669    -1.614983     0.208395      89.02
 H       2.947245    -1.964402     0.930231      27.55
 O       4.930152    -2.388593    -0.195507     156.15
 H       5.496512    -1.688213    -0.867275      24.01
 C       4.232787    -0.414831     1.041571     113.94
 O       5.200420     0.468073     0.376494     201.96
 H       5.047710     1.440432     0.436325      27.01
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 H       4.732450    -0.765304     2.017218      26.69
 H       3.433863     0.191195     1.670897      24.72
55
name = lig-Water-frame_330
 C      -1.324801     2.683881     3.318618      27.47
 H      -2.070700     3.459121     3.007919      20.84
 C      -0.744797     0.242649     3.524624      69.87
 H      -1.079852    -0.703774     3.554586      27.30
 C       0.589760     0.643271     3.614977      26.93
 O       1.556295    -0.414546     3.887569     127.06
 C       1.206408    -1.824454     4.043711     131.41
 H       1.876763    -2.274910     4.738716      27.24
 H       1.156732    -2.347521     3.090934      28.53
 H       0.294064    -1.960740     4.611413      28.19
 C       1.111748     1.868119     3.804116      24.26
 O       2.503083     1.964626     4.051308     162.42
 H       2.701163     2.906824     4.180677      26.45
 C       0.147566     2.894878     3.611917      63.65
 H       0.573289     3.895333     3.704058      27.95
 C      -1.684669     1.186215     3.205981       2.09
 C      -3.101961     0.920337     2.686145     102.97
 H      -3.936780     1.592823     3.021450      24.87
 O      -3.664667    -0.307588     3.177944     262.51
 H      -4.611191    -0.149868     3.341399      26.20
 C      -3.202954     0.883706     1.131266      85.29
 H      -2.672950     1.745354     0.543737      23.47
 C      -4.625650     0.659652     0.594558     106.22
 O      -5.229334    -0.625729     0.801462     286.35
 H      -4.530624    -1.396650     0.906238      24.45
 H      -4.649230     0.898075    -0.447324      27.60
 H      -5.212836     1.408484     0.876055      28.67
 C       0.973005     0.185994    -0.339862      47.98
 H       1.604061     1.018704    -0.515154      25.88
 C       0.324371    -2.151585    -0.814339      51.04
 H       0.503762    -3.114960    -1.292345      26.14
 C      -0.961955    -1.958774    -0.226578      22.13
 O      -1.906475    -2.955218    -0.132444     190.03
 C      -2.125932    -3.785890    -1.440415     111.68
 H      -2.978084    -3.470044    -2.195543      25.71
 H      -1.236691    -4.132240    -1.776872      27.97
 H      -2.607156    -4.485711    -1.053684      31.72
 C      -1.348655    -0.610276     0.075192      20.08
 O      -2.640835    -0.347343     0.458163     112.52
 C      -0.346207     0.384354     0.167787      43.76
 H      -0.756382     1.405859     0.662909      23.48
 C       1.352255    -1.170410    -0.766630      28.55
 C       2.762094    -1.665995    -0.990603      98.58
 H       2.696996    -2.554909    -1.476818      27.18
 O       3.255835    -0.757420    -2.111291     258.93
 H       4.123909    -0.988267    -2.380022      28.71
 C       3.666630    -1.604186     0.233788      80.65
 H       3.031411    -2.018197     1.161929      27.14
 O       4.947541    -2.333910    -0.190668     173.06
 H       5.507162    -1.818190    -0.762812      28.48
 C       4.193416    -0.458207     1.055193     110.24
 O       5.214690     0.525442     0.406742     171.74
 H       5.237474     1.474403     0.558954      26.57
 H       4.741012    -0.951586     1.890380      27.35
 H       3.340192    -0.045066     1.494557      27.02
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name = lig-Water-frame_331
 C      -1.338466     2.576380     3.235781      55.15
 H      -2.125522     3.301410     3.128353      22.65
 C      -0.705064     0.239228     3.480641      55.69
 H      -1.166564    -0.873942     3.588652      23.94
 C       0.598370     0.627941     3.672949      23.58
 O       1.518347    -0.355387     3.925299     102.87
 C       1.179795    -1.880009     4.022615     104.08
 H       1.875971    -2.449925     4.747177      25.91
 H       1.111551    -2.069057     2.892009      27.95
 H       0.252620    -2.033317     4.722463      27.64
 C       1.168057     1.908774     3.766845       8.64
 O       2.480378     2.017022     4.030889     154.65
 H       2.649241     3.030277     4.287467      25.27
 C       0.141212     2.913404     3.669095      83.37
 H       0.429212     3.939739     3.921874      19.75
 C      -1.695418     1.243995     3.253175      20.51
 C      -3.131067     0.893463     2.616698      83.92
 H      -3.903796     1.770010     3.048682      22.90
 O      -3.648305    -0.310169     3.252557     262.04
 H      -4.640597    -0.122965     3.333440      26.31
 C      -3.314369     0.896866     1.129115      67.63
 H      -2.740400     1.955411     0.844286      22.22
 C      -4.593553     0.723157     0.602907      87.85
 O      -5.229426    -0.602897     0.835820     227.17
 H      -4.455061    -1.269024     0.752119      24.82
 H      -4.762904     0.727391    -0.540320      23.61
 H      -5.412146     1.500863     1.161330      23.90
 C       0.904781     0.129444    -0.345035      44.05
 H       1.621777     1.025489    -0.335870      25.67
 C       0.396158    -2.197731    -0.785685      41.26
 H       0.477162    -3.131478    -1.356213      25.45
 C      -0.929998    -1.946655    -0.249106      12.38
 O      -1.916885    -2.941448    -0.114661     169.87
 C      -2.078862    -3.785699    -1.429980      90.72
 H      -2.822690    -3.273222    -1.962947      27.06
 H      -1.169177    -4.417444    -1.937260      22.78
 H      -2.787608    -4.826435    -0.987861      22.50
 C      -1.313086    -0.623523     0.151054       5.88
 O      -2.629905    -0.393041     0.513820      66.31
 C      -0.404260     0.430222     0.152822      57.04
 H      -0.779752     1.336005     0.624641      24.17
 C       1.365147    -1.170816    -0.761271       5.90
 C       2.822765    -1.636338    -0.990476     101.08
 H       2.709612    -2.861511    -1.306322      22.77
 O       3.221350    -0.795370    -2.129448     214.79
 H       4.294727    -0.882254    -2.286862      23.74
 C       3.614099    -1.613410     0.251930      86.34
 H       3.482971    -2.432371     1.028324      27.07
 O       4.940289    -2.314402    -0.159516     117.88
 H       5.414178    -1.715471    -0.762410      27.73
 C       4.170293    -0.436374     1.069884      97.92
 O       5.229452     0.539377     0.430022     135.51
 H       4.926397     1.460799     0.964511      24.86
 H       4.837160    -1.142316     1.715788      25.84
 H       3.198726     0.113678     1.387171      25.65
55
name = lig-Water-frame_332
 C      -1.249955     2.498919     3.203915      75.34
 H      -2.026530     3.327704     3.229000      23.30
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 C      -0.731850     0.243894     3.432587      60.65
 H      -0.950350    -0.844669     3.549027      26.26
 C       0.613175     0.531801     3.745392       2.55
 O       1.527809    -0.351704     3.988895     126.12
 C       1.133830    -1.887238     4.026998     111.18
 H       2.077883    -2.333233     4.307498      28.06
 H       0.995809    -2.081149     2.915335      30.10
 H       0.184507    -1.997050     4.429354      28.10
 C       1.125962     1.982635     3.716672      -4.34
 O       2.476869     2.100599     4.023145     207.51
 H       2.605549     3.041774     4.264726      23.86
 C       0.088153     2.932315     3.703042      60.64
 H       0.170325     3.997299     4.016600      22.91
 C      -1.737090     1.274297     3.245367      37.20
 C      -3.173974     0.877904     2.640282      91.41
 H      -3.544389     1.908957     2.860649      27.09
 O      -3.628895    -0.311219     3.334683     254.77
 H      -4.639064    -0.359943     3.364214      25.03
 C      -3.300255     0.894711     1.132966      62.63
 H      -2.884195     1.945837     0.887028      25.44
 C      -4.720669     0.785230     0.577745     106.66
 O      -5.227233    -0.575408     0.871948     246.87
 H      -4.526870    -1.187226     0.808500      27.57
 H      -4.617361     0.951479    -0.525377      27.22
 H      -5.265814     1.386000     1.128661      30.86
 C       0.864527     0.104155    -0.333678      54.59
 H       1.606771     0.830413    -0.169967      27.72
 C       0.408622    -2.230215    -0.741504      55.55
 H       0.654587    -3.216125    -1.278797      24.04
 C      -0.884400    -1.916824    -0.282458       5.77
 O      -1.904094    -2.957721    -0.140772     146.56
 C      -2.082561    -3.852248    -1.356722     113.31
 H      -2.515854    -2.959964    -2.015924      25.67
 H      -1.244315    -4.187859    -1.940198      25.29
 H      -2.606454    -4.606630    -1.070532      29.21
 C      -1.297942    -0.632783     0.237623       1.10
 O      -2.624627    -0.442983     0.574584      56.24
 C      -0.420439     0.439048     0.111544      60.38
 H      -0.641063     1.478997     0.496675      26.09
 C       1.350636    -1.174014    -0.735929      16.12
 C       2.802443    -1.609784    -1.038998     112.65
 H       2.858260    -2.627494    -1.110523      28.10
 O       3.223178    -0.837194    -2.134422     298.68
 H       4.169674    -0.925991    -2.286155      28.98
 C       3.683618    -1.658209     0.260884      87.96
 H       3.365746    -2.556324     0.788048      28.37
 O       4.939620    -2.307753    -0.128059     110.32
 H       5.302867    -1.564581    -0.873139      25.98
 C       4.150704    -0.409882     1.071779     128.69
 O       5.200690     0.550714     0.486040     211.74
 H       4.700008     1.166321     0.949656      31.59
 H       4.718657    -0.892201     1.821870      29.81
 H       3.456126     0.305512     1.506416      26.59
55
name = lig-Water-frame_333
 C      -1.153477     2.543410     3.228975      62.18
 H      -1.806041     3.373796     3.182221      24.12
 C      -0.751018     0.247363     3.407289      56.59
 H      -0.979624    -0.840733     3.412096      25.68
 C       0.585564     0.530384     3.781746      -0.74
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 O       1.579219    -0.421676     4.075331     139.52
 C       1.121727    -1.829851     3.977005     109.58
 H       2.118568    -2.293167     4.073682      27.03
 H       0.885132    -2.184543     2.926570      30.61
 H       0.065281    -2.074796     4.463084      25.33
 C       1.037328     1.993105     3.693819      -9.04
 O       2.463827     2.189365     4.015710     171.94
 H       2.669696     3.212084     4.215324      21.68
 C       0.020680     2.942928     3.709843      59.09
 H       0.044857     3.983170     3.960398      22.85
 C      -1.766608     1.181728     3.183480      40.42
 C      -3.169756     0.881388     2.711134      85.36
 H      -3.732035     1.986507     2.894883      24.50
 O      -3.613522    -0.302069     3.420488     226.88
 H      -4.576014    -0.476674     3.349573      25.70
 C      -3.247741     0.840743     1.146225      56.21
 H      -2.821030     1.882366     0.619652      24.55
 C      -4.813118     0.787311     0.545821      84.93
 O      -5.253111    -0.528132     0.894180     185.93
 H      -4.457295    -1.249399     0.949454      21.50
 H      -4.684502     1.224000    -0.511411      25.80
 H      -5.488166     1.664556     1.162625      25.41
 C       0.879551     0.087783    -0.314066      48.58
 H       1.706307     0.837342    -0.124265      26.19
 C       0.404078    -2.250111    -0.706660      71.34
 H       0.745212    -3.193573    -0.993327      26.68
 C      -0.882063    -1.917478    -0.292380       1.37
 O      -1.852642    -2.985176    -0.172405     182.65
 C      -2.083346    -3.799369    -1.311568     102.84
 H      -2.370167    -3.194620    -2.137125      27.00
 H      -1.015056    -4.046700    -1.798449      21.37
 H      -2.866491    -4.751898    -1.007394      21.88
 C      -1.307813    -0.631161     0.294822      -6.62
 O      -2.631813    -0.479461     0.638932      97.88
 C      -0.411858     0.430559     0.074033      57.51
 H      -0.470744     1.590336     0.260803      25.02
 C       1.321712    -1.197010    -0.700878      44.01
 C       2.745724    -1.551879    -1.044061      82.86
 H       2.860610    -2.781606    -1.344375      24.33
 O       3.233713    -0.863433    -2.148501     239.08
 H       4.211777    -1.102626    -2.421365      24.40
 C       3.785472    -1.688791     0.255309      90.07
 H       2.865477    -2.291742     0.789299      26.59
 O       4.962870    -2.282265    -0.125338     207.72
 H       5.323408    -1.827495    -0.827924      30.49
 C       4.151863    -0.406162     1.093045     116.96
 O       5.148474     0.533337     0.539816     172.44
 H       4.692807     1.531389     0.744529      24.75
 H       4.574853    -0.635448     2.223000      26.67
 H       3.428951     0.273250     1.609988      25.85
55
name = lig-Water-frame_334
 C      -1.214658     2.563633     3.255540      48.42
 H      -1.861777     3.477894     3.016917      24.01
 C      -0.754341     0.207750     3.409058      46.32
 H      -1.162037    -0.912727     3.200146      23.93
 C       0.576291     0.607131     3.786889       6.86
 O       1.601773    -0.490837     4.152398     133.75
 C       1.120293    -1.774919     3.897565     118.55
 H       1.935478    -2.492610     4.218559      26.61
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 H       0.735327    -2.049706     2.846982      29.97
 H       0.476373    -2.097698     4.688695      29.32
 C       1.011380     1.928025     3.738169       7.22
 O       2.414209     2.274323     3.997643     154.66
 H       2.592893     3.256277     4.156451      26.07
 C       0.019701     2.959605     3.709038      41.25
 H       0.212144     4.055956     3.855322      16.27
 C      -1.717788     1.149565     3.111489      40.07
 C      -3.155111     0.928647     2.776985      93.17
 H      -4.019408     1.553199     3.045397      25.28
 O      -3.594215    -0.289261     3.505478     175.06
 H      -4.590513    -0.347755     3.266605      24.25
 C      -3.229151     0.772570     1.132212      79.47
 H      -2.635013     1.569156     0.558896      25.20
 C      -4.834246     0.813846     0.576721     106.43
 O      -5.303737    -0.491702     0.894681     235.06
 H      -4.555735    -1.085267     1.035581      26.11
 H      -4.951473     1.131320    -0.521675      26.25
 H      -5.449345     1.499335     0.988939      29.46
 C       0.953518     0.082115    -0.292640      50.39
 H       1.677127     0.881650    -0.277837      24.85
 C       0.386689    -2.239409    -0.668717      42.87
 H       0.749814    -3.366656    -0.716450      22.65
 C      -0.932259    -1.937058    -0.262429       0.82
 O      -1.800057    -2.997227    -0.172075     233.61
 C      -2.045338    -3.754611    -1.321436     108.80
 H      -2.572798    -3.364569    -2.304993      24.91
 H      -1.077488    -4.264459    -1.391428      22.55
 H      -2.806333    -4.528568    -1.112655      26.44
 C      -1.320298    -0.627468     0.290973      -9.27
 O      -2.651717    -0.499473     0.709425     141.17
 C      -0.379966     0.431574     0.043411      62.46
 H      -0.574692     1.438179     0.164813      26.25
 C       1.309283    -1.214632    -0.666315      59.38
 C       2.742588    -1.563840    -1.032147      91.73
 H       2.624396    -2.515093    -1.447716      25.61
 O       3.252998    -0.854857    -2.185977     256.78
 H       4.128881    -1.339920    -2.466266      25.62
 C       3.791327    -1.644834     0.251183      82.64
 H       3.113538    -2.042131     0.945023      28.31
 O       5.003176    -2.302215    -0.109800     191.58
 H       5.432524    -1.939909    -1.017350      26.39
 C       4.155397    -0.379858     1.200618     113.71
 O       5.082998     0.541225     0.587603     226.25
 H       4.917054     1.455199     0.430018      29.60
 H       4.480161    -0.680592     2.132326      28.85
 H       3.062486     0.020187     1.334281      26.10
55
name = lig-Water-frame_335
 C      -1.361103     2.580805     3.271869      77.64
 H      -2.026025     3.324644     2.903365      23.88
 C      -0.757869     0.143605     3.407418      57.00
 H      -1.047649    -0.802588     3.256620      22.85
 C       0.594456     0.598150     3.787163       5.88
 O       1.592381    -0.487146     4.201757     164.39
 C       1.131720    -1.786748     3.850969     104.09
 H       1.865708    -2.537189     4.086766      25.46
 H       0.665713    -1.815917     2.885880      28.69
 H       0.536240    -2.044946     4.836638      26.56
 C       1.045016     1.914241     3.836017       9.50
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 O       2.332966     2.315155     3.965272      74.26
 H       2.399526     3.324474     4.215024      27.71
 C       0.047898     2.961141     3.685241      79.18
 H       0.458742     3.964490     3.704219      11.86
 C      -1.633545     1.232877     3.071006      38.54
 C      -3.151474     0.927514     2.803453      81.87
 H      -4.030305     1.617427     3.188848      25.69
 O      -3.582587    -0.283574     3.573042     168.64
 H      -4.535381    -0.231431     3.353978      27.12
 C      -3.260421     0.722906     1.115275      75.81
 H      -2.384206     1.431604     0.616690      19.49
 C      -4.778823     0.813197     0.603170      90.81
 O      -5.385966    -0.466167     0.888329     230.97
 H      -4.629612    -1.083998     1.030968      26.76
 H      -4.970619     0.857346    -0.528346      24.68
 H      -5.498231     1.616525     1.231313      23.99
 C       1.009441     0.101083    -0.281083      55.17
 H       1.696069     0.943148    -0.496713      19.72
 C       0.352735    -2.241032    -0.607514      36.54
 H       0.595324    -3.226916    -0.592000      23.07
 C      -0.969456    -1.928715    -0.206507      15.93
 O      -1.791941    -2.995931    -0.134747     247.20
 C      -1.997088    -3.750287    -1.374692     104.06
 H      -2.452599    -3.274123    -2.216402      25.94
 H      -1.179721    -4.567790    -1.484059      22.91
 H      -2.872222    -4.535417    -1.007118      23.36
 C      -1.330187    -0.632023     0.228411      11.86
 O      -2.669909    -0.528501     0.779288     166.42
 C      -0.341361     0.395873     0.026697      43.77
 H      -0.839705     1.508949     0.214518      17.25
 C       1.345173    -1.212577    -0.634666      29.48
 C       2.777083    -1.578946    -1.001093      79.41
 H       2.489303    -2.710123    -1.419423      18.93
 O       3.263559    -0.833015    -2.224704     251.38
 H       4.051431    -1.293996    -2.429993      27.26
 C       3.784370    -1.545391     0.238160      52.24
 H       3.517604    -2.318443     1.196044      21.15
 O       5.052765    -2.346518    -0.093760     145.71
 H       5.304202    -2.006549    -1.071804      25.10
 C       4.084214    -0.330465     1.240550      94.75
 O       5.053713     0.528755     0.622027     228.61
 H       4.694513     1.449939     0.480315      25.96
 H       4.561550    -0.895657     2.218792      23.10
 H       3.065051    -0.071192     1.179873      22.62
55
name = lig-Water-frame_336
 C      -1.408671     2.629160     3.300225      31.03
 H      -2.241686     3.286110     2.915469      12.59
 C      -0.711867     0.184267     3.409408      64.38
 H      -0.999936    -1.047446     3.405378      17.04
 C       0.617980     0.474318     3.800738      46.39
 O       1.569647    -0.417931     4.220474     215.25
 C       1.135094    -1.828113     3.889549      75.30
 H       2.085956    -2.465422     3.635459      23.38
 H       0.530968    -1.700780     2.878686      23.63
 H       0.295886    -2.052933     4.507519      26.73
 C       1.011459     1.960838     3.928289       8.52
 O       2.277858     2.333073     3.936931     126.04
 H       2.332787     3.273041     4.325172      21.23
 C       0.032235     2.915920     3.627382      94.34
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 H       0.501671     3.919822     3.546690      28.78
 C      -1.608672     1.292563     3.072020      62.22
 C      -3.149054     0.898160     2.796210      67.23
 H      -3.548874     1.950061     3.109715      27.37
 O      -3.572491    -0.273445     3.616503     194.27
 H      -4.591115    -0.300759     3.559152      26.77
 C      -3.282208     0.713890     1.132919      86.23
 H      -2.671394     1.562813     0.766754      21.83
 C      -4.725489     0.806922     0.638634      97.87
 O      -5.476765    -0.458682     0.892281     222.88
 H      -4.788150    -1.274105     0.985009      25.49
 H      -4.723189     0.891779    -0.506602      25.23
 H      -5.108049     1.581314     1.211307      27.93
 C       1.026835     0.145725    -0.293103      51.91
 H       1.706603     0.953393    -0.651895      16.21
 C       0.330753    -2.187457    -0.524473      47.73
 H       0.563898    -3.346002    -0.645732      21.15
 C      -0.958716    -1.905061    -0.152671      21.01
 O      -1.819993    -3.015731    -0.094337     167.86
 C      -1.968796    -3.817156    -1.389496      97.14
 H      -2.153127    -3.005162    -2.200336      23.42
 H      -1.258221    -4.595077    -1.868155      23.76
 H      -2.957138    -4.295452    -0.987754      23.10
 C      -1.354325    -0.628640     0.155102      10.82
 O      -2.666362    -0.582174     0.831136     164.56
 C      -0.351118     0.380322     0.037145      40.64
 H      -0.660940     1.291458     0.207646      19.43
 C       1.391774    -1.212361    -0.601662      19.69
 C       2.801615    -1.628464    -0.977226      83.49
 H       2.845034    -2.649991    -1.153285      22.80
 O       3.242893    -0.815857    -2.229884     204.96
 H       4.281014    -1.128192    -2.448319      23.13
 C       3.819219    -1.538496     0.276420      83.95
 H       3.506595    -2.308628     0.816889      25.66
 O       5.083303    -2.369037    -0.094943     172.50
 H       5.347451    -2.059542    -0.936744      29.21
 C       4.028296    -0.339792     1.215714     114.92
 O       5.032155     0.535401     0.652383     246.16
 H       4.416072     1.384703     0.818609      20.54
 H       4.382901    -0.724409     2.066854      26.36
 H       3.002217     0.291526     1.494940      19.08
55
name = lig-Water-frame_337
 C      -1.368072     2.674937     3.321060      26.14
 H      -2.163269     3.403587     3.142142      18.65
 C      -0.653467     0.229537     3.413482      64.77
 H      -1.063565    -0.636525     3.470343      26.12
 C       0.627993     0.434760     3.834870      36.53
 O       1.550030    -0.374366     4.228486     194.09
 C       1.143027    -1.840959     3.879724      95.24
 H       2.009796    -2.272617     3.538636      27.58
 H       0.680747    -1.750215     2.952115      29.03
 H       0.255734    -2.324009     4.419594      25.62
 C       0.880009     1.942835     3.970764      19.80
 O       2.272799     2.340006     3.926898     226.14
 H       2.485793     3.235980     4.312361      21.77
 C      -0.025413     2.893427     3.559236      73.03
 H       0.308379     3.920805     3.422018      32.79
 C      -1.647513     1.258668     3.110603      22.94
 C      -3.092888     0.882187     2.760559      79.24
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 H      -3.467011     1.912607     2.969631      25.81
 O      -3.575948    -0.241344     3.634976     171.95
 H      -4.576276    -0.348820     3.643006      26.07
 C      -3.287506     0.691809     1.220191      69.40
 H      -3.036100     1.844456     0.800714      20.00
 C      -4.648262     0.739216     0.650919      86.98
 O      -5.560360    -0.459819     0.898148     208.99
 H      -5.010512    -1.202464     0.919090      32.36
 H      -4.531278     1.112961    -0.422435      25.84
 H      -5.063699     1.766714     1.211803      25.80
 C       1.010014     0.160986    -0.340980      33.63
 H       1.653320     0.976114    -0.594867      20.95
 C       0.382023    -2.154118    -0.447654      61.03
 H       0.562594    -3.133652    -0.754708      25.19
 C      -0.944043    -1.924042    -0.114667       7.35
 O      -1.837352    -3.055130    -0.060727     132.05
 C      -1.986072    -3.839067    -1.412339      96.13
 H      -1.857196    -2.940523    -2.050316      25.40
 H      -1.182317    -4.500207    -1.857051      25.06
 H      -3.063637    -4.252124    -1.272380      24.30
 C      -1.409126    -0.604824     0.124880       9.37
 O      -2.630380    -0.618062     0.849036     123.27
 C      -0.357339     0.358211     0.047249      52.12
 H      -0.536287     1.566148     0.295964      20.58
 C       1.416844    -1.211858    -0.566254      19.90
 C       2.854003    -1.633400    -0.955795      75.18
 H       3.215565    -2.802448    -1.098442      19.66
 O       3.231468    -0.827734    -2.205081     256.01
 H       4.170181    -0.816799    -2.280332      26.27
 C       3.856623    -1.583367     0.282829      64.33
 H       3.021605    -2.430109     0.803478      21.54
 O       5.092241    -2.366447    -0.074950      74.09
 H       5.604370    -1.944853    -1.016309      22.05
 C       3.956885    -0.349139     1.164781     117.52
 O       4.984764     0.576605     0.691042     203.64
 H       4.722449     1.460247     0.936932      26.09
 H       4.325397    -0.686418     2.325229      24.14
 H       3.273796     0.279882     1.611140      23.15
55
name = lig-Water-frame_338
 C      -1.355446     2.633631     3.317585      37.40
 H      -1.952330     3.564161     3.341030      20.81
 C      -0.660156     0.299479     3.403857      52.54
 H      -1.293440    -0.783954     3.448681      23.24
 C       0.606674     0.570229     3.883926      34.52
 O       1.552972    -0.412373     4.248089     154.80
 C       1.138148    -1.813147     3.841013     103.74
 H       2.190787    -2.368523     3.792596      25.20
 H       0.711595    -1.736237     2.739576      25.39
 H       0.665053    -2.480644     4.596368      27.49
 C       0.810647     1.891821     3.962417      30.21
 O       2.269986     2.318033     3.927103     205.22
 H       2.522916     3.275908     4.259838      16.20
 C      -0.071750     2.923535     3.509109      67.77
 H       0.223674     3.961917     3.429866      31.09
 C      -1.676654     1.232298     3.184233      23.68
 C      -3.026811     0.869266     2.736657     100.89
 H      -3.902807     1.711469     2.909672      23.60
 O      -3.579838    -0.198639     3.632471     144.81
 H      -4.557288    -0.223981     3.460935      26.42
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 C      -3.276737     0.669835     1.328634      85.58
 H      -2.923143     1.599593     0.842479      24.12
 C      -4.626474     0.678582     0.681728     108.48
 O      -5.630634    -0.423238     0.885532     205.29
 H      -4.973243    -1.245552     0.881788      28.58
 H      -4.485613     1.077364    -0.398064      26.58
 H      -5.192926     1.511582     1.051283      27.81
 C       0.965716     0.127662    -0.401595      35.55
 H       1.627014     1.066474    -0.415422      23.41
 C       0.449508    -2.146318    -0.390425      52.70
 H       0.712296    -3.179614    -0.813392      23.49
 C      -0.943985    -1.962101    -0.094068      -0.93
 O      -1.835218    -3.109316    -0.036703     157.46
 C      -1.999016    -3.791844    -1.417942      90.32
 H      -1.866844    -2.989767    -2.133855      27.31
 H      -1.091567    -4.541271    -1.393884      23.77
 H      -3.056931    -4.253472    -1.855662      25.05
 C      -1.440344    -0.603855     0.141724       1.91
 O      -2.582423    -0.605017     0.840121     136.16
 C      -0.364196     0.413883     0.055994      58.14
 H      -0.520497     1.365951     0.326035      26.41
 C       1.442952    -1.192811    -0.539664      23.32
 C       2.946353    -1.633399    -0.957311      98.94
 H       2.995097    -2.608737    -1.325202      25.21
 O       3.199892    -0.847256    -2.148501     304.61
 H       4.193622    -0.684976    -2.122274      26.17
 C       3.821259    -1.676356     0.276552      92.65
 H       3.206277    -2.137123     0.902831      28.68
 O       5.098428    -2.335608    -0.044825     199.01
 H       5.418828    -1.912402    -0.768744      32.53
 C       3.972850    -0.366772     1.193742     107.12
 O       4.952742     0.614893     0.717621     159.96
 H       4.963355     1.608757     0.943719      22.40
 H       4.282086    -0.736547     2.075178      29.40
 H       2.880396     0.228528     1.454987      22.48
55
name = lig-Water-frame_339
 C      -1.399867     2.579061     3.300908      65.63
 H      -2.012432     3.500404     3.338666      22.76
 C      -0.761979     0.292338     3.406059      40.54
 H      -0.960488    -0.716789     3.355569      24.64
 C       0.565513     0.646511     3.941044       1.63
 O       1.540487    -0.460572     4.265181     101.89
 C       1.207108    -1.790589     3.783383     129.89
 H       2.115536    -2.267171     3.959692      28.71
 H       0.730830    -1.874145     2.877305      30.24
 H       0.806761    -2.271408     4.709248      27.61
 C       0.881051     1.973957     3.907911      19.07
 O       2.254568     2.279012     3.939845     174.07
 H       2.279366     3.213509     4.198739      19.46
 C      -0.052081     2.955012     3.503045      44.51
 H       0.306386     4.005550     3.573059      22.77
 C      -1.698070     1.264844     3.262002      56.16
 C      -3.059737     0.863577     2.792906     105.53
 H      -3.844278     1.598195     2.932048      26.75
 O      -3.585376    -0.168233     3.609103     235.58
 H      -4.544428    -0.136802     3.299722      27.68
 C      -3.239870     0.615860     1.361528      77.19
 H      -2.471138     1.367110     0.777704      23.26
 C      -4.670244     0.633238     0.699903      97.95
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 O      -5.650174    -0.394922     0.857494     196.78
 H      -5.081292    -1.246638     0.876127      30.67
 H      -4.493539     0.693194    -0.407281      27.73
 H      -5.358110     1.502980     1.109198      25.03
 C       0.919944     0.124386    -0.435139      46.49
 H       1.560853     0.942274    -0.330595      25.54
 C       0.481644    -2.200951    -0.364661      41.54
 H       0.856074    -3.209401    -0.626580      24.24
 C      -0.930646    -1.990833    -0.093563      -0.56
 O      -1.835883    -3.152446    -0.029583     178.35
 C      -1.973899    -3.732923    -1.423055     102.65
 H      -1.756671    -3.031661    -2.327615      26.28
 H      -1.298840    -4.529682    -1.195289      25.14
 H      -2.929988    -4.207757    -1.823975      27.06
 C      -1.376808    -0.633382     0.177985       8.26
 O      -2.565875    -0.567205     0.834368     167.93
 C      -0.390724     0.422862     0.042871      63.25
 H      -0.662800     1.541854     0.422649      23.03
 C       1.480151    -1.169230    -0.526026       8.38
 C       2.952626    -1.621552    -0.970551      94.44
 H       2.575186    -2.646636    -1.510969      21.25
 O       3.192123    -0.846818    -2.080806     286.06
 H       4.212132    -0.620046    -2.145896      25.14
 C       3.812609    -1.700941     0.263568      61.51
 H       3.335990    -2.353250     1.251648      24.58
 O       5.080330    -2.314447     0.034984     133.47
 H       5.388712    -1.794926    -0.930734      23.42
 C       3.961459    -0.339206     1.206575     111.67
 O       4.949278     0.630170     0.723796     148.75
 H       4.739189     1.632262     1.011226      22.15
 H       4.412070    -0.895441     2.214725      25.64
 H       2.949972    -0.138266     1.123861      24.91
55
name = lig-Water-frame_340
 C      -1.401408     2.619677     3.305205      58.37
 H      -2.296968     3.242017     3.152343      23.55
 C      -0.776707     0.264905     3.465696      47.88
 H      -0.850093    -0.894558     3.241892      23.01
 C       0.488559     0.603927     3.968777     -11.70
 O       1.507305    -0.439415     4.261582     114.44
 C       1.295147    -1.777203     3.808689     110.87
 H       2.348791    -2.294511     3.742430      27.08
 H       0.683144    -2.064350     2.832198      27.13
 H       0.499933    -2.072961     4.589012      26.47
 C       0.998139     2.084604     3.821389       4.64
 O       2.245575     2.252353     3.966503     112.65
 H       2.290269     3.268696     4.189876      22.41
 C      -0.023147     2.985152     3.529949      56.84
 H       0.293618     4.005586     3.680478      24.21
 C      -1.771713     1.278835     3.308552      45.92
 C      -3.129620     0.872056     2.881472      78.09
 H      -3.666342     2.002362     3.005074      26.04
 O      -3.607525    -0.174775     3.581897     252.00
 H      -4.594795    -0.289343     3.469741      26.05
 C      -3.155635     0.578222     1.293089      90.19
 H      -2.625504     1.386932     0.881992      28.86
 C      -4.725710     0.638286     0.701071      92.52
 O      -5.652291    -0.414059     0.842715     184.03
 H      -5.192624    -1.233381     0.875728      34.02
 H      -4.447701     0.432029    -0.399665      26.50
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 H      -5.172757     1.642956     0.999029      27.22
 C       0.886041     0.144138    -0.429552      40.39
 H       1.649050     1.009778    -0.437067      24.20
 C       0.497240    -2.261414    -0.352751      51.15
 H       0.852649    -3.306380    -0.364521      24.34
 C      -0.882338    -2.021002    -0.097986       1.82
 O      -1.837989    -3.148151    -0.040375     178.45
 C      -1.918866    -3.681199    -1.440438      93.74
 H      -1.514252    -3.107188    -2.197853      26.89
 H      -1.341882    -4.773546    -1.425422      24.00
 H      -3.107424    -4.078408    -1.365038      23.03
 C      -1.273345    -0.673108     0.231420       7.81
 O      -2.571521    -0.569041     0.834148     157.59
 C      -0.438229     0.415659     0.025459      69.30
 H      -0.700230     1.415519     0.332084      25.42
 C       1.458375    -1.170369    -0.513462      16.19
 C       2.820421    -1.655173    -0.972040      94.02
 H       2.608586    -2.615158    -1.264572      26.41
 O       3.229978    -0.798380    -2.039483     332.51
 H       4.129990    -0.707209    -2.207322      29.93
 C       3.832566    -1.713996     0.327899      85.55
 H       3.415716    -2.419875     0.898333      29.78
 O       5.079639    -2.280022     0.083119     211.72
 H       5.443358    -2.111983    -0.814112      29.16
 C       3.996377    -0.369274     1.202078     124.56
 O       4.935517     0.644758     0.730907     206.60
 H       4.423236     1.426709     0.929659      27.95
 H       4.257802    -0.660120     2.150267      31.28
 H       2.795000    -0.106097     1.089054      24.44
55
name = lig-Water-frame_341
 C      -1.389346     2.662199     3.329345      42.02
 H      -2.294053     3.196700     2.958458      22.81
 C      -0.758228     0.218025     3.555885      52.37
 H      -1.057366    -0.811737     3.192862      24.72
 C       0.464185     0.579120     3.957212      13.34
 O       1.472696    -0.356424     4.233074     144.67
 C       1.337161    -1.797091     3.849257     132.54
 H       2.260585    -2.263655     3.663258      29.71
 H       0.929183    -1.900661     2.870002      30.69
 H       0.529391    -2.252664     4.404227      28.97
 C       0.968369     2.043703     3.734457       8.38
 O       2.312997     2.283205     4.012440     175.11
 H       2.657532     3.196400     4.199589      27.72
 C      -0.011429     3.041268     3.567049      44.58
 H       0.196156     4.131486     3.685355      19.00
 C      -1.809599     1.258075     3.342779      10.08
 C      -3.193225     0.951844     2.905732      86.31
 H      -3.672776     1.882155     3.015689      28.95
 O      -3.657548    -0.226718     3.585613     205.73
 H      -4.638909    -0.367910     3.665201      24.35
 C      -3.133995     0.593508     1.243876      65.79
 H      -2.937042     1.752496     0.842888      23.64
 C      -4.694031     0.647050     0.649563      93.74
 O      -5.673745    -0.451570     0.856497     146.23
 H      -5.031658    -1.334048     0.903244      26.83
 H      -4.443400     0.678471    -0.419335      27.62
 H      -5.060953     1.694524     0.828479      27.80
 C       0.899112     0.172969    -0.404053      51.72
 H       1.522378     0.986168    -0.686989      23.17
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 C       0.504584    -2.302032    -0.340107      55.59
 H       0.796864    -3.396370    -0.147837      22.46
 C      -0.822244    -2.055944    -0.080344       6.22
 O      -1.806196    -3.099585    -0.066149     192.59
 C      -1.899255    -3.722353    -1.405082     102.02
 H      -1.375570    -2.960459    -2.171613      25.50
 H      -1.416449    -4.620021    -1.661264      27.64
 H      -3.008466    -3.769979    -1.342137      24.04
 C      -1.226720    -0.730595     0.301186      16.18
 O      -2.554566    -0.627160     0.821072     136.90
 C      -0.448462     0.386578    -0.003920      55.55
 H      -0.779186     1.437460     0.238614      23.80
 C       1.356666    -1.194931    -0.508781      40.03
 C       2.710309    -1.648906    -0.925757      64.17
 H       2.832249    -2.858004    -1.175659      22.80
 O       3.257307    -0.735098    -2.013414     222.00
 H       4.291092    -0.979980    -2.139453      24.37
 C       3.851953    -1.686291     0.363851      66.01
 H       3.124369    -2.604440     0.899376      24.26
 O       5.117352    -2.278263     0.123426     199.06
 H       5.467068    -2.163872    -0.812423      28.58
 C       3.970540    -0.420596     1.153128     121.99
 O       4.904260     0.643284     0.739871     189.47
 H       4.252743     1.503151     0.704018      23.39
 H       4.154757    -0.538006     2.390831      25.77
 H       3.107491     0.146070     1.331183      25.20
55
name = lig-Water-frame_342
 C      -1.390820     2.637665     3.355918      50.30
 H      -1.969355     3.490807     2.930972      21.30
 C      -0.840233     0.202894     3.620495      53.42
 H      -1.194964    -0.794310     3.409778      25.35
 C       0.527448     0.603283     3.910411      18.07
 O       1.463080    -0.282933     4.205684     111.37
 C       1.333017    -1.779334     3.858282      99.46
 H       2.391067    -2.254120     3.935071      26.24
 H       1.084887    -1.616014     2.736099      25.47
 H       0.727253    -2.571382     4.479147      25.54
 C       0.903739     1.966797     3.700968      31.50
 O       2.398279     2.301798     4.052819     215.45
 H       2.679256     3.252020     4.226236      28.45
 C      -0.034259     3.092909     3.595596      36.04
 H       0.206778     4.143389     3.660346      14.06
 C      -1.763195     1.258325     3.382740      30.81
 C      -3.214782     0.968902     2.866282      61.62
 H      -4.158886     1.821644     3.027198      23.86
 O      -3.708360    -0.289806     3.605748     165.47
 H      -4.749066    -0.218565     3.622491      23.15
 C      -3.220961     0.686977     1.229323      66.91
 H      -2.893580     1.522986     0.728475      25.66
 C      -4.607957     0.639685     0.568599      86.74
 O      -5.658196    -0.489665     0.874077     176.26
 H      -5.039076    -1.202472     0.945950      30.97
 H      -4.528444     0.910976    -0.574680      25.33
 H      -5.198589     1.648666     0.894184      25.30
 C       0.907156     0.162443    -0.390721      57.75
 H       1.466215     0.996000    -0.898881      20.47
 C       0.499801    -2.348915    -0.304783      60.04
 H       0.853965    -3.320665    -0.232262      23.99
 C      -0.804096    -2.076425    -0.024570      29.86
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 O      -1.743663    -3.049775    -0.079910     192.86
 C      -1.888435    -3.717068    -1.378433     108.68
 H      -1.587676    -2.975423    -2.021309      27.58
 H      -1.355335    -4.775979    -1.669596      24.26
 H      -3.059972    -3.524377    -1.821227      23.23
 C      -1.229303    -0.787429     0.359683      21.00
 O      -2.522387    -0.684668     0.804338      94.78
 C      -0.422616     0.359369    -0.016526      43.93
 H      -0.927833     1.421470     0.055120      21.42
 C       1.270595    -1.222734    -0.522982      43.12
 C       2.715905    -1.629889    -0.880368      82.70
 H       2.851628    -2.575309    -1.234640      25.24
 O       3.290696    -0.693671    -1.975427     269.82
 H       4.146382    -1.203513    -2.010741      25.48
 C       3.793074    -1.695623     0.382709      79.74
 H       3.249459    -2.266683     1.003042      28.26
 O       5.164548    -2.296071     0.161633     134.84
 H       5.402365    -1.927627    -0.871116      25.04
 C       3.941021    -0.428928     1.191406     115.54
 O       4.863091     0.636322     0.735059     217.31
 H       4.504010     1.498731     0.544787      27.67
 H       4.221756    -0.665485     2.166151      27.42
 H       3.036647     0.321822     1.423299      20.49
55
name = lig-Water-frame_343
 C      -1.362304     2.642541     3.377626      54.04
 H      -1.831496     3.576470     3.067224      23.98
 C      -0.919152     0.241562     3.671532      54.20
 H      -1.255529    -0.921188     3.876397      22.21
 C       0.535937     0.634725     3.823424      23.89
 O       1.498231    -0.262498     4.210149     157.22
 C       1.357003    -1.743280     3.836819     112.32
 H       2.346883    -1.956897     4.199995      27.75
 H       1.172448    -1.702407     2.760479      26.92
 H       0.797856    -2.349213     4.459724      29.08
 C       0.912296     1.982593     3.734437      32.86
 O       2.442762     2.291841     4.075496     187.62
 H       2.288931     3.304331     4.207378      29.15
 C      -0.065362     3.046749     3.615493      61.85
 H       0.310774     4.083828     3.693251      11.35
 C      -1.752897     1.288915     3.394359      49.77
 C      -3.254746     0.929848     2.817473      97.57
 H      -3.991377     1.547148     2.977517      29.04
 O      -3.756457    -0.326140     3.605362     219.09
 H      -4.723246    -0.204813     3.480809      25.07
 C      -3.329943     0.741733     1.238115      47.25
 H      -2.490168     1.378694     0.571699      20.36
 C      -4.589854     0.656232     0.482625     105.91
 O      -5.592844    -0.488429     0.874202     120.82
 H      -5.030764    -1.337681     1.008134      26.55
 H      -4.571786     0.752883    -0.551938      28.71
 H      -5.183040     1.425475     0.998044      25.59
 C       0.894601     0.121336    -0.411575      59.00
 H       1.485945     0.888934    -0.931832      21.08
 C       0.498620    -2.367873    -0.263273      43.60
 H       1.011147    -3.413565    -0.506218      21.52
 C      -0.814820    -2.079612     0.054607      26.98
 O      -1.719065    -3.059347    -0.073646     236.24
 C      -1.907717    -3.678638    -1.404142     107.05
 H      -1.420073    -2.922946    -2.185661      26.03
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 H      -1.492507    -4.616150    -1.363176      27.10
 H      -2.939484    -3.701051    -1.863568      25.64
 C      -1.232056    -0.786979     0.388926      17.98
 O      -2.519500    -0.714757     0.805749      58.39
 C      -0.422984     0.326823    -0.002600      51.44
 H      -0.887012     1.251055    -0.093202      22.34
 C       1.292735    -1.242447    -0.548175      43.89
 C       2.784060    -1.553197    -0.842722      76.99
 H       2.683776    -2.631621    -1.469033      21.07
 O       3.311175    -0.683694    -1.908318     278.08
 H       4.153714    -1.073791    -2.164213      29.03
 C       3.723832    -1.670894     0.379039      45.53
 H       3.255699    -2.351503     1.365637      24.54
 O       5.178651    -2.293844     0.164890     147.13
 H       5.462185    -1.850693    -0.581917      32.42
 C       3.894896    -0.338811     1.245463      89.52
 O       4.860656     0.596567     0.716590     189.24
 H       4.490555     1.503762     0.595742      26.40
 H       4.476605    -0.899013     2.232937      23.73
 H       2.897190    -0.031768     1.341892      25.53
55
name = lig-Water-frame_344
 C      -1.339894     2.684108     3.388191      35.90
 H      -2.136252     3.444186     3.197641      23.35
 C      -0.910526     0.274246     3.740543      41.06
 H      -1.209503    -0.596215     4.123004      24.01
 C       0.479290     0.639766     3.743447      16.56
 O       1.533658    -0.260443     4.220981     155.20
 C       1.422968    -1.655392     3.831108     108.47
 H       2.453722    -1.929291     4.177984      25.58
 H       1.229467    -2.007487     2.754088      25.75
 H       0.470986    -2.055836     4.489181      25.05
 C       0.990447     2.027024     3.804184     -10.82
 O       2.401481     2.287079     4.081228     163.23
 H       2.242300     3.243722     4.218561      29.25
 C      -0.020524     2.951119     3.643506      41.08
 H       0.293079     3.992231     3.769177      28.51
 C      -1.842075     1.321798     3.356874      30.03
 C      -3.250198     0.824461     2.782463      84.57
 H      -4.030338     1.857208     3.100409      22.65
 O      -3.773759    -0.333182     3.566766     227.85
 H      -4.834556    -0.428530     3.457803      21.44
 C      -3.318048     0.739980     1.216495      66.92
 H      -2.603726     1.305675     0.849791      27.09
 C      -4.640281     0.652808     0.446231      84.00
 O      -5.490266    -0.477940     0.860322     128.56
 H      -5.032337    -1.408765     1.024676      25.34
 H      -4.514760     0.564329    -0.734793      24.49
 H      -5.292522     1.559320     0.965214      23.59
 C       0.872775     0.048179    -0.460374      32.31
 H       1.526982     0.834105    -0.817335      21.75
 C       0.538639    -2.366659    -0.246418      60.17
 H       0.823460    -3.267713    -0.646089      24.21
 C      -0.799545    -2.093135     0.127518       3.40
 O      -1.760714    -3.115439    -0.052141     250.11
 C      -1.899346    -3.577335    -1.465584     103.40
 H      -1.193041    -3.229262    -2.176947      27.04
 H      -1.480942    -4.679087    -1.144084      22.88
 H      -3.081990    -3.972596    -1.592586      22.93
 C      -1.242361    -0.747402     0.401704      20.80
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 O      -2.560432    -0.727144     0.829795      68.77
 C      -0.428621     0.277516     0.026047      64.36
 H      -0.882629     1.397156    -0.217198      20.32
 C       1.391435    -1.248680    -0.553738      31.27
 C       2.853754    -1.538675    -0.865837     102.49
 H       2.656682    -2.440421    -1.301018      25.52
 O       3.327686    -0.666935    -1.831493     290.10
 H       4.221981    -0.817452    -2.335495      28.16
 C       3.689009    -1.649149     0.430041      65.91
 H       3.346323    -2.363261     1.078914      28.89
 O       5.134384    -2.284003     0.181411      81.29
 H       5.672237    -1.707093    -0.615344      25.48
 C       3.894846    -0.302969     1.303995     125.94
 O       4.857133     0.556680     0.690857     177.78
 H       4.345420     1.474583     0.869846      23.53
 H       4.394609    -0.736398     2.099134      29.64
 H       2.757129    -0.148914     1.481960      24.76
55
name = lig-Water-frame_345
 C      -1.396522     2.672445     3.377785      31.33
 H      -2.222085     3.370908     3.327651      22.58
 C      -0.860870     0.373387     3.774427      41.95
 H      -1.280757    -0.671216     4.319015      20.41
 C       0.469331     0.644132     3.725221      25.93
 O       1.546425    -0.237284     4.198687     183.10
 C       1.468845    -1.583015     3.866164     142.60
 H       2.343983    -2.234907     4.135315      27.52
 H       1.331978    -2.048460     2.855995      27.89
 H       0.602304    -1.863807     4.306102      28.30
 C       1.062467     1.988676     3.861832      -5.17
 O       2.302348     2.289749     4.080565     191.24
 H       2.603185     3.282830     4.257125      27.18
 C       0.059480     2.921082     3.680060      43.68
 H       0.227140     3.983621     3.864286      29.04
 C      -1.919812     1.321920     3.309659      30.64
 C      -3.286499     0.790142     2.798355     116.90
 H      -3.758042     1.628317     2.957971      28.94
 O      -3.770884    -0.334648     3.504519     285.35
 H      -4.746589    -0.485400     3.501734      25.41
 C      -3.268493     0.649387     1.205769      61.46
 H      -2.604039     1.701954     0.902097      21.12
 C      -4.700279     0.650217     0.434448     108.53
 O      -5.399539    -0.484575     0.847037     232.63
 H      -4.816684    -1.195780     0.960026      29.05
 H      -4.453286     0.619936    -0.569714      29.01
 H      -5.254457     1.589239     0.551583      27.52
 C       0.863254    -0.024447    -0.511177      38.58
 H       1.514238     0.903760    -0.654696      22.92
 C       0.566183    -2.318416    -0.246427      55.97
 H       0.668928    -3.407056    -0.694897      23.13
 C      -0.764014    -2.114471     0.180837       0.68
 O      -1.815526    -3.149524    -0.019418     174.08
 C      -1.891458    -3.598228    -1.455208     114.90
 H      -1.137773    -3.248221    -2.269956      25.40
 H      -1.520807    -4.552680    -1.435054      28.23
 H      -2.932874    -3.745310    -1.561448      27.65
 C      -1.290709    -0.754484     0.417107      -0.65
 O      -2.623009    -0.711183     0.864703     101.36
 C      -0.430092     0.299431     0.021277      70.41
 H      -0.747889     1.216817    -0.080830      24.59
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 C       1.483721    -1.253557    -0.527587      43.86
 C       2.912828    -1.554232    -0.879092      80.44
 H       2.923194    -2.765275    -1.255304      22.65
 O       3.347257    -0.603061    -1.790850     259.39
 H       4.253780    -0.792819    -2.141095      27.53
 C       3.740534    -1.610517     0.455739      73.46
 H       3.153381    -2.587766     1.022655      24.58
 O       5.069974    -2.248247     0.194147     131.62
 H       5.489023    -1.847597    -0.579552      29.28
 C       3.871853    -0.363940     1.321347     117.30
 O       4.815424     0.563043     0.676771     122.67
 H       4.506297     1.392953     1.007685      27.06
 H       4.359560    -0.666603     2.481464      26.05
 H       3.005332     0.222137     1.681051      24.76
55
name = lig-Water-frame_346
 C      -1.447714     2.604464     3.372296      37.51
 H      -2.029131     3.568419     3.363605      23.16
 C      -0.876642     0.437831     3.785443      40.72
 H      -1.117473    -0.467786     4.067068      21.90
 C       0.555808     0.653266     3.773832      39.79
 O       1.566656    -0.190148     4.157005     219.40
 C       1.501170    -1.584769     3.893001     116.45
 H       2.221427    -2.254856     4.351158      26.48
 H       1.410860    -1.653652     2.750374      26.46
 H       0.503548    -2.098350     4.395558      25.44
 C       1.009415     1.947678     3.869224      10.86
 O       2.273355     2.293255     4.100331     216.11
 H       2.678603     3.196272     4.125809      25.62
 C       0.046097     2.952361     3.707945      41.69
 H       0.280760     4.013118     3.961500      24.91
 C      -1.901835     1.290490     3.293717      54.03
 C      -3.293637     0.777557     2.796335      89.75
 H      -4.126384     1.818045     2.845987      23.31
 O      -3.736344    -0.355775     3.455753     254.90
 H      -4.809265    -0.307589     3.457346      23.02
 C      -3.207519     0.595428     1.198503     106.58
 H      -2.898330     1.486647     0.888880      24.16
 C      -4.679911     0.655723     0.449571      78.32
 O      -5.352423    -0.507114     0.835257     234.75
 H      -4.496764    -1.120332     0.927518      22.07
 H      -4.300765     0.613591    -0.713330      23.89
 H      -5.308554     1.692154     0.260994      23.56
 C       0.875933    -0.025334    -0.529353      36.22
 H       1.424210     0.851435    -0.637724      20.97
 C       0.561240    -2.308659    -0.265909      59.24
 H       0.729477    -3.324782    -0.503441      22.02
 C      -0.758830    -2.112538     0.213415       6.87
 O      -1.832007    -3.157329     0.010724     121.18
 C      -1.855392    -3.663322    -1.422718      79.81
 H      -1.434030    -2.868433    -2.118246      24.08
 H      -1.537203    -4.792286    -1.694290      22.87
 H      -3.020921    -3.280789    -1.871861      23.09
 C      -1.329949    -0.799207     0.423544      -0.05
 O      -2.677808    -0.663975     0.894399     137.72
 C      -0.427588     0.270475     0.004012      61.52
 H      -0.748423     1.481469     0.123965      17.18
 C       1.525663    -1.295763    -0.496841      39.85
 C       2.961731    -1.618719    -0.873372      87.19
 H       3.297221    -2.535202    -1.183647      24.14
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 O       3.377253    -0.524831    -1.780109     296.34
 H       4.299430    -0.815482    -1.885561      25.67
 C       3.788264    -1.637413     0.485230     104.57
 H       3.092282    -2.305237     0.925878      25.98
 O       4.996936    -2.212113     0.223443     161.10
 H       5.352114    -1.885306    -0.727952      26.06
 C       3.880501    -0.428837     1.395593     127.47
 O       4.769695     0.572783     0.674264     133.84
 H       4.630194     1.514489     1.066887      24.11
 H       4.173458    -0.585146     2.366908      28.16
 H       3.161219     0.401068     1.624420      21.69
55
name = lig-Water-frame_347
 C      -1.421387     2.606644     3.387824      58.64
 H      -1.873407     3.580052     3.229133      25.52
 C      -0.853137     0.453050     3.752515      47.48
 H      -1.115824    -0.762349     3.825986      21.92
 C       0.600958     0.655221     3.854983      23.34
 O       1.609765    -0.163100     4.139378     214.78
 C       1.459251    -1.633165     3.904876     113.36
 H       2.364853    -1.965438     4.528279      26.13
 H       1.560229    -1.440020     2.824989      26.46
 H       0.631889    -2.114137     4.232228      29.04
 C       0.902363     2.008738     3.843510       5.16
 O       2.313518     2.269823     4.132398     200.15
 H       2.355376     3.268706     3.996081      23.76
 C      -0.074634     2.982126     3.721984      59.08
 H       0.306179     3.962125     3.955395      21.46
 C      -1.860196     1.265664     3.300355      51.22
 C      -3.302485     0.857645     2.760427     106.06
 H      -4.051254     1.456330     2.833906      28.60
 O      -3.716349    -0.389084     3.427243     272.43
 H      -4.682504    -0.316874     3.434316      25.66
 C      -3.237566     0.592771     1.226206      94.81
 H      -2.630288     1.528163     0.610583      22.01
 C      -4.588241     0.680517     0.402387     101.61
 O      -5.322547    -0.542833     0.818924     238.56
 H      -4.617233    -1.251902     0.949249      24.43
 H      -4.274346     0.480691    -0.552743      29.36
 H      -5.236828     1.479369     0.502755      27.16
 C       0.892539     0.000432    -0.502572      28.59
 H       1.523686     0.931885    -0.811783      19.62
 C       0.537698    -2.327513    -0.267070      54.43
 H       0.930802    -3.404749    -0.345220      20.47
 C      -0.809273    -2.103604     0.210984      21.17
 O      -1.807007    -3.172447     0.033200     161.20
 C      -1.873961    -3.663049    -1.424299      98.08
 H      -1.409674    -2.751100    -1.833798      24.18
 H      -1.675904    -4.649039    -1.680083      26.90
 H      -2.802512    -3.379668    -1.833047      27.98
 C      -1.330526    -0.823807     0.412131       5.82
 O      -2.686230    -0.636200     0.901971     139.91
 C      -0.449488     0.242312    -0.001557      53.38
 H      -0.624935     1.181806     0.243592      22.18
 C       1.501331    -1.349849    -0.490135      29.85
 C       3.000323    -1.592674    -0.835367      62.49
 H       3.389535    -2.625393    -1.412925      19.05
 O       3.414899    -0.472270    -1.770881     240.52
 H       4.466980    -0.626338    -1.838273      23.11
 C       3.762760    -1.636798     0.504451      72.30
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 H       3.019600    -2.407524     1.223802      22.27
 O       4.979167    -2.195794     0.249119     131.44
 H       5.327493    -1.956847    -0.738601      26.03
 C       3.890409    -0.395830     1.437151      86.00
 O       4.750216     0.581352     0.684221     179.98
 H       4.526404     1.489875     1.091440      23.40
 H       4.349676    -0.774498     2.560011      23.60
 H       2.824954     0.059491     1.421273      22.64
55
name = lig-Water-frame_348
 C      -1.389807     2.670788     3.397861      53.28
 H      -2.107797     3.443925     2.998348      25.97
 C      -0.784969     0.316191     3.700418      45.57
 H      -1.094910    -0.643782     3.546952      28.23
 C       0.546024     0.687777     3.934361       4.24
 O       1.646850    -0.156692     4.153298     170.00
 C       1.473655    -1.632219     3.908584     101.44
 H       2.387469    -1.823239     4.397700      27.15
 H       1.698896    -1.866361     2.825214      28.42
 H       0.402527    -2.144887     4.169353      24.92
 C       0.868535     2.076236     3.837573       7.50
 O       2.323924     2.268901     4.150464     189.39
 H       2.211502     3.287119     4.058674      27.37
 C      -0.185645     3.004150     3.737082      58.89
 H       0.127827     4.072235     3.856219      20.68
 C      -1.834817     1.296040     3.312356      14.09
 C      -3.243622     0.888973     2.719908      71.53
 H      -4.248499     1.690402     3.051991      21.67
 O      -3.677743    -0.414254     3.404449     205.69
 H      -4.736425    -0.533452     3.442062      20.55
 C      -3.257583     0.707702     1.202241     107.93
 H      -2.488416     1.185060     0.763146      26.82
 C      -4.474729     0.635376     0.390131      72.69
 O      -5.314978    -0.577524     0.795204     209.44
 H      -4.859236    -1.429564     0.964841      25.65
 H      -4.237606     0.490898    -0.776360      23.89
 H      -5.233675     1.486110     0.883352      22.33
 C       0.915916     0.018369    -0.457805      38.77
 H       1.480503     0.775822    -0.890524      20.57
 C       0.512889    -2.387595    -0.241191      53.38
 H       0.947946    -3.405245    -0.174510      21.77
 C      -0.876221    -2.135524     0.160895       6.10
 O      -1.766572    -3.205863     0.065556     206.71
 C      -1.895120    -3.568746    -1.407905      60.98
 H      -0.968715    -2.966441    -1.878423      22.31
 H      -1.544760    -4.671233    -1.553857      24.26
 H      -3.167617    -3.646428    -1.716067      22.62
 C      -1.325126    -0.805744     0.397115      20.84
 O      -2.643927    -0.658981     0.891674     115.85
 C      -0.432448     0.175191    -0.001586      56.97
 H      -0.695680     1.327956     0.323626      21.62
 C       1.437018    -1.345792    -0.520729      18.46
 C       3.018166    -1.540290    -0.818484      89.29
 H       3.006022    -2.396005    -1.399074      23.40
 O       3.465020    -0.442933    -1.744791     314.39
 H       4.381714    -0.377059    -1.902414      29.72
 C       3.678505    -1.642099     0.557378      75.14
 H       3.354553    -2.349024     1.246512      26.52
 O       5.021469    -2.212416     0.273316     139.70
 H       5.380723    -1.950942    -0.538378      32.50
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 C       3.878247    -0.350225     1.441166     114.88
 O       4.724584     0.589785     0.727914     266.39
 H       4.346891     1.420671     1.054016      25.23
 H       4.382042    -0.758329     2.276045      27.90
 H       2.777034    -0.315921     1.528833      25.88
55
name = lig-Water-frame_349
 C      -1.506696     2.690226     3.360848      55.25
 H      -2.300586     3.271255     2.892868      24.41
 C      -0.766333     0.208730     3.608939      38.39
 H      -1.066910    -0.895967     3.386705      24.26
 C       0.488452     0.721978     3.992587      12.36
 O       1.641305    -0.158652     4.161114     183.16
 C       1.499178    -1.608764     3.886772     111.94
 H       2.343450    -2.137430     4.498362      26.17
 H       1.666937    -2.229172     2.957533      27.40
 H       0.570535    -1.943011     4.235233      28.21
 C       0.891047     2.086953     3.880452      34.03
 O       2.264402     2.310289     4.146094     203.32
 H       2.597222     3.250947     4.341743      30.61
 C      -0.153292     3.086527     3.771544      59.98
 H      -0.120504     4.166157     3.753363      16.03
 C      -1.777889     1.322498     3.334042      12.11
 C      -3.230059     0.912163     2.739753      87.79
 H      -3.735187     1.665186     3.059115      30.27
 O      -3.630476    -0.425745     3.382766     215.67
 H      -4.609659    -0.571251     3.335909      23.80
 C      -3.205391     0.775135     1.170826      69.63
 H      -2.327956     1.488937     0.789787      21.54
 C      -4.440217     0.562136     0.398796     110.83
 O      -5.321256    -0.593957     0.759113     234.88
 H      -4.848447    -1.552894     0.933887      22.94
 H      -4.340282     0.784105    -0.611633      28.12
 H      -4.979575     1.347685     0.693746      28.39
 C       0.911843    -0.024959    -0.415058      54.30
 H       1.514116     0.833651    -0.875775      19.05
 C       0.490144    -2.429901    -0.191064      55.57
 H       0.806016    -3.473491    -0.117166      22.49
 C      -0.894307    -2.171748     0.091469     -10.12
 O      -1.735492    -3.245271     0.094713     239.33
 C      -1.915716    -3.523296    -1.390110     108.99
 H      -1.143386    -3.175844    -2.074442      26.67
 H      -1.476688    -4.513852    -1.290396      25.32
 H      -2.905680    -3.580757    -1.580921      27.84
 C      -1.328498    -0.812085     0.378526      16.07
 O      -2.579330    -0.704859     0.883291      86.66
 C      -0.389374     0.192168     0.023441      62.72
 H      -0.758717     1.177698     0.126836      24.30
 C       1.372062    -1.291865    -0.560630      28.85
 C       2.954319    -1.456333    -0.807420      82.92
 H       2.861510    -2.501032    -1.392287      21.63
 O       3.478261    -0.415996    -1.703487     294.38
 H       4.477055    -0.418504    -1.855606      26.23
 C       3.694920    -1.635350     0.573396      59.43
 H       3.234843    -2.516019     1.300946      23.47
 O       5.070056    -2.252091     0.325847      45.48
 H       5.554217    -1.713028    -0.572524      24.37
 C       3.845933    -0.366099     1.371429     104.64
 O       4.672193     0.610614     0.793923     224.40
 H       4.223851     1.574824     0.938933      21.90
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 H       4.472385    -0.708555     2.371535      24.43
 H       2.825552    -0.055931     1.943376      23.64
55
name = lig-Water-frame_350
 C      -1.589607     2.658654     3.337909      89.20
 H      -2.321806     3.353897     2.935195      24.88
 C      -0.796716     0.197079     3.509104      55.13
 H      -0.887811    -0.925329     3.377760      21.45
 C       0.470296     0.687089     4.007238      18.40
 O       1.616178    -0.165589     4.149884     169.50
 C       1.555931    -1.610480     3.908074     120.06
 H       2.066809    -2.198959     4.622809      28.18
 H       1.561767    -1.987985     2.869921      28.66
 H       0.504668    -1.867033     4.443712      25.50
 C       0.895793     2.141013     3.964476      31.36
 O       2.203438     2.365411     4.134328     208.11
 H       2.661182     3.106445     4.598731      29.51
 C      -0.133194     3.160112     3.773698      36.05
 H      -0.027024     4.266375     3.783604      13.94
 C      -1.731461     1.259284     3.333403      28.07
 C      -3.157314     0.864879     2.770333      60.64
 H      -3.764253     1.963341     3.141931      24.67
 O      -3.571615    -0.408300     3.359499     208.39
 H      -4.555807    -0.442621     3.196798      25.30
 C      -3.069696     0.772930     1.157156      54.49
 H      -2.729431     1.759902     0.789586      21.87
 C      -4.456269     0.499304     0.423168      91.87
 O      -5.316308    -0.611023     0.712911     278.94
 H      -4.687886    -1.302727     0.816904      27.73
 H      -4.328348     0.833922    -0.721096      24.07
 H      -5.143987     1.551012     0.599513      25.35
 C       0.889938    -0.027662    -0.403203      51.97
 H       1.500902     0.827225    -0.633768      21.84
 C       0.482413    -2.414848    -0.152158      57.55
 H       0.737906    -3.544371    -0.207962      22.70
 C      -0.841792    -2.159222     0.047868      11.43
 O      -1.725876    -3.268455     0.108861     176.55
 C      -1.887191    -3.564506    -1.329894      91.66
 H      -1.480710    -2.938046    -2.316649      24.87
 H      -1.622153    -4.640173    -1.312315      24.19
 H      -3.174223    -3.385193    -1.658580      22.13
 C      -1.291322    -0.855794     0.334655      15.66
 O      -2.518026    -0.724041     0.886190      66.65
 C      -0.388758     0.225433     0.061845      55.73
 H      -0.782480     1.309044    -0.028113      21.07
 C       1.350917    -1.299713    -0.574554      42.95
 C       2.844440    -1.428819    -0.817554      89.37
 H       3.092412    -2.399032    -1.230499      24.87
 O       3.470919    -0.385490    -1.655738     261.05
 H       4.451796    -0.776978    -1.695727      23.95
 C       3.749909    -1.660828     0.561884      82.58
 H       3.019454    -2.337609     1.004155      27.10
 O       5.113209    -2.267810     0.360499     160.90
 H       5.501605    -1.755436    -0.269822      32.46
 C       3.813516    -0.406936     1.401609     125.32
 O       4.612732     0.676502     0.841018     227.01
 H       4.201328     1.524858     0.872764      27.55
 H       4.408237    -0.650495     2.280016      27.89
 H       3.107557     0.245241     1.919731      24.72
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name = lig-Water-frame_351
 C      -1.525140     2.620257     3.364710      62.63
 H      -2.253295     3.437350     3.092330      25.19
 C      -0.764297     0.251391     3.455426      59.02
 H      -0.904392    -0.786309     3.349669      23.65
 C       0.482431     0.643479     3.970304      20.59
 O       1.598365    -0.165301     4.137650     166.69
 C       1.519520    -1.610765     3.973511     120.69
 H       2.275524    -2.104248     4.696725      26.89
 H       1.523308    -1.590801     2.856049      26.84
 H       0.530807    -1.889218     4.288749      28.23
 C       0.812122     2.200746     4.056636      53.65
 O       2.188066     2.401011     4.121717     209.19
 H       2.289611     3.206208     4.766974      16.16
 C      -0.181982     3.171632     3.741804      50.08
 H       0.213231     4.189458     3.903942      23.18
 C      -1.757611     1.182932     3.289964      50.52
 C      -3.059388     0.846576     2.797325     104.68
 H      -3.803038     1.476926     2.927297      29.19
 O      -3.525999    -0.370997     3.338826     226.01
 H      -4.548868    -0.400259     3.137695      26.45
 C      -3.024641     0.708046     1.174693      57.11
 H      -2.834728     1.719078     0.661511      23.33
 C      -4.506472     0.562052     0.423365      99.89
 O      -5.292755    -0.613105     0.659194     262.08
 H      -4.554627    -1.346088     0.764449      24.03
 H      -4.216321     0.425632    -0.604585      27.45
 H      -5.102399     1.304486     0.667296      30.07
 C       0.856162     0.010162    -0.397859      32.23
 H       1.573560     0.852311    -0.464143      21.93
 C       0.535696    -2.391711    -0.166162      59.06
 H       0.816996    -3.366451    -0.332006      25.34
 C      -0.791367    -2.137920     0.052203      31.38
 O      -1.717049    -3.259346     0.100871     175.48
 C      -1.950336    -3.631349    -1.314460     126.37
 H      -1.595115    -2.868967    -1.925354      28.91
 H      -1.828817    -4.704787    -1.661404      26.57
 H      -2.944346    -3.438919    -1.478843      27.80
 C      -1.231953    -0.865822     0.283184      14.08
 O      -2.460886    -0.699070     0.891096     104.89
 C      -0.432717     0.262834     0.091559      53.42
 H      -0.772079     1.351292    -0.022812      19.23
 C       1.363335    -1.357045    -0.552359      36.29
 C       2.803348    -1.441449    -0.822104      87.70
 H       3.175215    -2.430037    -1.326934      22.31
 O       3.459520    -0.377422    -1.603250     273.56
 H       4.245455    -0.843134    -1.733616      27.76
 C       3.753567    -1.657748     0.513539      70.61
 H       3.018256    -2.422621     0.994574      25.17
 O       5.106898    -2.282639     0.417142     123.41
 H       5.657558    -1.686506    -0.305409      25.14
 C       3.828376    -0.408335     1.477492      90.29
 O       4.594147     0.733383     0.850793     150.47
 H       4.024738     1.635735     0.955997      21.97
 H       4.454720    -0.810095     2.413662      25.30
 H       2.823281     0.219804     1.744886      22.09
55
name = lig-Water-frame_352
 C      -1.406143     2.595067     3.415511      32.02
 H      -2.186684     3.279975     3.270871      20.60
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 C      -0.683784     0.297161     3.442107      52.38
 H      -1.087178    -0.833909     3.247455      22.52
 C       0.521254     0.686150     3.913067      33.81
 O       1.587457    -0.140705     4.152167     184.71
 C       1.460162    -1.585575     4.030715     155.54
 H       2.442649    -1.890674     4.372077      28.23
 H       1.670629    -1.699848     2.952554      26.60
 H       0.417095    -2.079479     4.212608      25.75
 C       0.701436     2.155069     4.106719      60.78
 O       2.168623     2.447432     4.137889     193.06
 H       2.102988     3.284667     4.613327      14.46
 C      -0.230208     3.112651     3.722891      49.81
 H       0.128535     4.117991     3.911984      31.48
 C      -1.763593     1.224970     3.252085      53.54
 C      -3.006797     0.793266     2.736684      98.27
 H      -4.030619     1.519877     2.846056      22.36
 O      -3.502237    -0.367889     3.336558     267.49
 H      -4.418895    -0.479244     3.196195      30.43
 C      -3.070968     0.616425     1.192355      82.12
 H      -2.470893     1.367791     0.562761      21.40
 C      -4.500173     0.591901     0.425915      74.92
 O      -5.260001    -0.628813     0.617896     260.46
 H      -4.723553    -1.473686     0.778323      26.42
 H      -4.088492     0.352723    -0.613066      26.18
 H      -5.251562     1.537930     0.731301      23.77
 C       0.845592     0.033334    -0.386699      40.03
 H       1.617944     0.844290    -0.440667      22.21
 C       0.607179    -2.388047    -0.222450      52.44
 H       1.031509    -3.477676    -0.438345      21.14
 C      -0.765307    -2.161242     0.083934      13.45
 O      -1.694920    -3.241928     0.090586     138.95
 C      -2.041000    -3.701575    -1.313161      82.08
 H      -1.336486    -2.773272    -1.741263      21.28
 H      -1.734284    -4.603271    -1.803358      26.81
 H      -3.348080    -3.521861    -1.275769      22.77
 C      -1.221258    -0.817843     0.264441      12.67
 O      -2.418253    -0.649713     0.888012     161.69
 C      -0.437856     0.305361     0.074401      63.81
 H      -0.839705     1.284431     0.206405      18.17
 C       1.387895    -1.321356    -0.507985      21.93
 C       2.879583    -1.502376    -0.827361     100.08
 H       2.907916    -2.402373    -1.500881      23.20
 O       3.417386    -0.373776    -1.555886     240.70
 H       4.344965    -0.719299    -1.974820      25.22
 C       3.700886    -1.643021     0.495766      75.02
 H       3.374276    -2.522942     1.165577      24.53
 O       5.076618    -2.272981     0.454959     134.11
 H       5.703400    -1.863680    -0.296000      25.34
 C       3.845475    -0.375864     1.530690     117.16
 O       4.585036     0.771495     0.854927     171.06
 H       4.088983     1.616553     1.126527      21.59
 H       4.298169    -0.839967     2.461724      27.93
 H       2.756760    -0.289914     1.666372      25.03
55
name = lig-Water-frame_353
 C      -1.414797     2.569748     3.439558      46.83
 H      -2.307822     3.253964     3.351127      19.01
 C      -0.687221     0.297373     3.419075      42.98
 H      -0.906821    -0.637034     3.234351      24.45
 C       0.566231     0.776468     3.864687      42.18
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 O       1.581689    -0.107181     4.192599     142.94
 C       1.419890    -1.544368     4.021371     151.86
 H       2.405416    -1.912819     4.372589      25.74
 H       1.614965    -2.010195     2.993649      24.95
 H       0.580433    -2.209685     4.389291      26.57
 C       0.703040     2.046357     4.104849      39.43
 O       2.099559     2.480424     4.172864      52.16
 H       2.317593     3.518768     4.377452      20.85
 C      -0.184395     3.045015     3.759607     106.14
 H      -0.182961     4.160511     3.804679      29.71
 C      -1.670364     1.297790     3.240147      41.34
 C      -3.100072     0.780900     2.625215     108.73
 H      -3.602734     1.652267     2.854456      26.69
 O      -3.470723    -0.417638     3.365322     262.65
 H      -4.478544    -0.554091     3.234372      28.53
 C      -3.109866     0.537609     1.164895     106.25
 H      -2.388848     1.198684     0.739680      23.02
 C      -4.453520     0.583088     0.431402     101.24
 O      -5.256008    -0.648300     0.590736     308.46
 H      -4.754339    -1.431260     0.827528      29.48
 H      -4.168796     0.827338    -0.624942      27.00
 H      -5.004365     1.434430     0.519044      27.70
 C       0.892602     0.051550    -0.370458      54.36
 H       1.558535     0.853454    -0.536575      22.80
 C       0.643002    -2.434811    -0.295591      47.20
 H       1.061629    -3.361981    -0.393700      23.59
 C      -0.731035    -2.194317     0.107691       1.24
 O      -1.670840    -3.245884     0.099525     178.16
 C      -2.148655    -3.674250    -1.311051     108.29
 H      -1.642695    -3.063494    -1.967092      24.92
 H      -1.547824    -4.633942    -1.614252      24.46
 H      -3.139149    -3.703982    -1.346082      28.63
 C      -1.237573    -0.775391     0.274855       6.68
 O      -2.413459    -0.637095     0.886503     181.07
 C      -0.403572     0.332019     0.019254      62.55
 H      -0.822467     1.340051     0.542556      15.73
 C       1.441292    -1.202917    -0.464576      24.01
 C       2.966362    -1.557895    -0.828050      93.69
 H       2.826873    -2.454106    -1.514216      22.45
 O       3.384338    -0.375939    -1.534975     272.02
 H       4.246616    -0.415763    -2.016611      27.88
 C       3.710017    -1.655180     0.539552      79.10
 H       3.311331    -2.408663     1.235266      25.77
 O       5.054495    -2.260456     0.464871     183.01
 H       5.525811    -1.982617    -0.300670      29.48
 C       3.839814    -0.365958     1.497669     116.61
 O       4.566403     0.765497     0.886336     190.89
 H       4.201050     1.694702     1.159810      19.20
 H       4.302767    -0.709484     2.449949      27.60
 H       2.675231    -0.450686     1.775498      23.96
55
name = lig-Water-frame_354
 C      -1.505756     2.618373     3.455788      29.29
 H      -2.287079     3.322657     3.335364      19.41
 C      -0.688399     0.333542     3.403887      57.94
 H      -0.735960    -0.871799     3.172687      21.26
 C       0.560309     0.732370     3.813769      39.26
 O       1.585485    -0.095094     4.236167     161.75
 C       1.440705    -1.540797     3.987762     143.35
 H       2.225674    -1.977310     4.656164      24.77
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 H       1.282830    -1.947769     2.982428      24.26
 H       0.627263    -2.006273     4.694031      25.85
 C       0.841349     2.100023     4.079047      23.34
 O       2.044317     2.504792     4.225469     116.99
 H       2.297830     3.426246     4.177527      27.07
 C      -0.159864     3.011756     3.822780     102.56
 H      -0.133100     4.080820     3.804447      27.40
 C      -1.633160     1.235161     3.181204      41.45
 C      -3.146264     0.790412     2.588962      74.80
 H      -3.626780     1.838551     2.880438      24.81
 O      -3.460455    -0.474073     3.398784     223.77
 H      -4.472290    -0.606243     3.327942      28.41
 C      -3.123033     0.505584     1.110659      97.06
 H      -2.589383     1.580554     0.847420      19.77
 C      -4.382828     0.540509     0.387778      94.33
 O      -5.266474    -0.643642     0.556941     259.70
 H      -4.573454    -1.376270     0.896390      24.57
 H      -4.280104     0.965845    -0.659871      24.96
 H      -5.033843     1.526406     0.727939      25.10
 C       0.977527     0.102917    -0.359418      42.78
 H       1.594422     1.032245    -0.664645      21.08
 C       0.632854    -2.392889    -0.344504      42.42
 H       1.108273    -3.478952    -0.380754      21.09
 C      -0.685025    -2.192818     0.093107       5.73
 O      -1.663235    -3.259015     0.103549     146.90
 C      -2.152926    -3.652737    -1.291431      77.92
 H      -2.087319    -3.044105    -2.407137      22.31
 H      -1.698651    -4.600962    -1.208524      23.47
 H      -3.446984    -3.987175    -1.434363      22.66
 C      -1.210187    -0.769154     0.282289       3.83
 O      -2.441969    -0.702746     0.887745     142.50
 C      -0.397972     0.345050     0.001774      61.45
 H      -0.498156     1.241832     0.436140      22.30
 C       1.508540    -1.178994    -0.437807      22.15
 C       3.001801    -1.552799    -0.801949      84.31
 H       3.049542    -2.568541    -1.377190      22.53
 O       3.353098    -0.362599    -1.541380     293.64
 H       4.227488    -0.381860    -1.875171      28.78
 C       3.785082    -1.683078     0.609833      85.39
 H       2.891278    -2.246564     1.218439      23.11
 O       5.039582    -2.260144     0.473111     157.34
 H       5.375160    -1.968837    -0.588150      21.77
 C       3.785873    -0.388656     1.428117     116.57
 O       4.542707     0.732583     0.926312     190.72
 H       4.160447     1.692516     1.085054      22.34
 H       4.488632    -0.589441     2.390765      25.05
 H       2.836684     0.010275     1.819707      24.16
55
name = lig-Water-frame_355
 C      -1.537991     2.635935     3.476533      41.11
 H      -2.245539     3.452880     3.252027      26.56
 C      -0.641649     0.278167     3.380624      76.23
 H      -0.777859    -0.716404     3.189548      29.12
 C       0.574389     0.688416     3.802598      10.26
 O       1.604479    -0.114369     4.263470     152.64
 C       1.442311    -1.564162     4.028373     132.09
 H       2.264475    -2.032938     4.567940      28.36
 H       1.092574    -1.733473     2.991384      27.15
 H       0.553692    -1.531826     4.731632      27.62
 C       0.888677     2.170617     3.996575       5.44
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 O       2.106249     2.507515     4.296332      84.70
 H       2.103278     3.595830     4.299867      24.04
 C      -0.225944     3.012898     3.877139      67.75
 H       0.225192     4.075625     3.970731      20.74
 C      -1.740924     1.194976     3.084538       9.60
 C      -3.122180     0.798025     2.646150      88.22
 H      -3.966014     1.505081     2.783864      26.25
 O      -3.474990    -0.505361     3.420822     214.27
 H      -4.409954    -0.636179     3.417363      29.23
 C      -3.104334     0.561973     1.077532      84.93
 H      -2.792245     1.510372     0.722436      26.06
 C      -4.409683     0.553970     0.324600     104.54
 O      -5.249095    -0.631839     0.521126     295.49
 H      -4.681208    -1.348736     0.809231      28.81
 H      -4.327860     0.687891    -0.789729      26.32
 H      -4.860403     1.179091     1.056408      25.67
 C       1.058539     0.163021    -0.365480      23.96
 H       1.602925     1.003866    -0.625764      24.22
 C       0.638308    -2.311949    -0.358595      67.70
 H       0.977107    -3.304353    -0.451771      24.89
 C      -0.673338    -2.143794     0.045849      12.98
 O      -1.660954    -3.240192     0.092317     152.67
 C      -2.210215    -3.669218    -1.297600     112.63
 H      -2.228239    -3.103553    -2.094875      28.20
 H      -1.789117    -4.716197    -1.293188      25.56
 H      -3.170681    -3.927916    -1.128297      29.65
 C      -1.157608    -0.806050     0.289492       3.41
 O      -2.460762    -0.795921     0.873892      82.48
 C      -0.355204     0.311965    -0.003135      48.45
 H      -0.451009     1.509200     0.272855      22.12
 C       1.566475    -1.244626    -0.439471       9.92
 C       3.005461    -1.503048    -0.734326     100.59
 H       3.278724    -2.486173    -1.234779      23.59
 O       3.332345    -0.349341    -1.571945     225.64
 H       4.400068    -0.471506    -1.668622      23.79
 C       3.770675    -1.683465     0.655471     102.69
 H       3.030115    -2.272085     1.129566      27.51
 O       5.046080    -2.268629     0.449994     179.89
 H       5.341622    -2.027631    -0.359406      31.36
 C       3.760551    -0.387498     1.412728     133.02
 O       4.546556     0.708580     0.928449     165.46
 H       3.979152     1.489259     1.051389      26.42
 H       4.315907    -0.737262     2.271789      30.86
 H       2.947070     0.341222     1.796023      24.57
55
name = lig-Water-frame_356
 C      -1.541446     2.588970     3.471275      53.34
 H      -2.178548     3.446681     3.179816      26.26
 C      -0.651894     0.240067     3.332483      30.96
 H      -0.939386    -0.878540     3.180526      27.29
 C       0.639974     0.729379     3.830156      11.16
 O       1.655138    -0.130105     4.270552     137.70
 C       1.390819    -1.544965     4.119465     134.00
 H       2.352202    -2.154532     4.212268      28.82
 H       1.118746    -1.700879     3.046021      30.67
 H       0.417850    -1.696911     4.635082      30.26
 C       0.813265     2.128109     3.886527       1.85
 O       2.224133     2.537073     4.372901     188.36
 H       2.226904     3.474531     4.639875      23.72
 C      -0.262545     3.050374     3.922826      56.24
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 H       0.128815     4.003604     4.169633      18.42
 C      -1.829376     1.243867     3.049827       9.21
 C      -3.122646     0.737750     2.692809      88.47
 H      -4.101563     1.289596     2.849730      24.99
 O      -3.483192    -0.516907     3.432619     155.43
 H      -4.534812    -0.618179     3.409237      22.83
 C      -3.091370     0.579240     1.064859      60.36
 H      -2.468896     1.418097     0.396196      23.60
 C      -4.470327     0.531408     0.300734      94.47
 O      -5.236182    -0.629080     0.481088     275.98
 H      -4.772192    -1.502246     0.685637      24.96
 H      -4.358156     0.658145    -0.780023      26.94
 H      -5.026245     1.334560     0.966804      24.32
 C       1.089375     0.130161    -0.365839      28.55
 H       1.763282     1.050296    -0.559366      25.67
 C       0.654311    -2.237537    -0.355240      74.65
 H       0.957769    -3.311514    -0.599017      25.12
 C      -0.709431    -2.084860    -0.018988      16.80
 O      -1.637130    -3.192474     0.063629     137.74
 C      -2.246851    -3.748990    -1.234203      83.32
 H      -2.089298    -2.798528    -2.062490      27.29
 H      -1.749209    -4.610262    -1.800370      26.19
 H      -3.387666    -3.821278    -0.630223      20.92
 C      -1.133864    -0.849978     0.309440     -15.05
 O      -2.449342    -0.851302     0.837687      71.44
 C      -0.246746     0.322065     0.003367      60.67
 H      -0.743446     1.219311    -0.012992      27.88
 C       1.580557    -1.263986    -0.460472      16.81
 C       3.003105    -1.449895    -0.665081     116.67
 H       3.343129    -2.392625    -1.257758      23.31
 O       3.364014    -0.351808    -1.603981     245.81
 H       4.320988    -0.402843    -1.572421      27.76
 C       3.692911    -1.634533     0.626627      60.85
 H       3.282672    -2.639450     1.265235      25.18
 O       5.050025    -2.291146     0.465624      27.24
 H       5.589591    -1.915101    -0.495426      21.37
 C       3.762474    -0.349704     1.468377     151.90
 O       4.588001     0.687484     0.893544     168.63
 H       3.920714     1.514922     0.995514      22.73
 H       4.088767    -0.905438     2.507070      29.73
 H       2.745738    -0.075574     1.727226      31.05
55
name = lig-Water-frame_357
 C      -1.538024     2.562036     3.444698      57.93
 H      -2.249851     3.310006     3.211310      25.79
 C      -0.702420     0.261967     3.281477      25.50
 H      -0.971645    -0.846791     3.263959      26.27
 C       0.649565     0.735094     3.831301      -2.59
 O       1.711782    -0.129468     4.273736     108.84
 C       1.323019    -1.521578     4.171023     140.62
 H       2.197226    -2.127757     4.138391      30.71
 H       1.126193    -1.736102     3.103189      32.08
 H       0.512017    -2.212575     4.670350      28.74
 C       0.803452     2.109696     3.847403      18.69
 O       2.289787     2.514495     4.431204     163.94
 H       2.402167     3.471078     4.776532      26.53
 C      -0.267131     3.041203     3.939857      69.46
 H      -0.270004     4.137438     4.317521      18.07
 C      -1.785257     1.281865     3.107534      24.39
 C      -3.187353     0.649406     2.679020      83.58
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 H      -3.975587     1.454862     2.994888      27.09
 O      -3.499391    -0.530274     3.437347     214.32
 H      -4.469301    -0.596286     3.332996      25.05
 C      -3.074503     0.542673     1.021125      80.17
 H      -2.360212     1.090038     0.583442      28.10
 C      -4.517345     0.526111     0.337372     104.50
 O      -5.253018    -0.658487     0.449135     280.73
 H      -4.730907    -1.565484     0.519640      24.87
 H      -4.311982     0.864714    -0.762523      25.25
 H      -5.177592     1.433529     0.344089      24.73
 C       1.111296     0.079084    -0.359588      71.18
 H       1.791647     0.871021    -0.490660      29.87
 C       0.651903    -2.250557    -0.361712      53.53
 H       0.976700    -3.256185    -0.707101      26.42
 C      -0.731251    -2.083014    -0.101522       9.57
 O      -1.582457    -3.157311     0.030498     188.01
 C      -2.284215    -3.750950    -1.168907     133.75
 H      -2.258872    -2.912009    -1.691323      31.73
 H      -1.799776    -4.413785    -1.887073      28.25
 H      -3.215950    -3.927740    -1.003033      29.92
 C      -1.133895    -0.827486     0.330391     -12.19
 O      -2.427523    -0.849362     0.791032     113.65
 C      -0.178217     0.289810     0.019063      62.02
 H      -0.914741     1.162415    -0.226646      25.70
 C       1.555902    -1.200396    -0.483271      55.66
 C       3.008547    -1.431523    -0.678663     112.98
 H       3.142573    -2.357996    -1.253326      27.42
 O       3.416565    -0.357542    -1.615517     262.22
 H       4.381358    -0.272598    -1.659085      28.75
 C       3.673675    -1.620294     0.626771      80.47
 H       3.301133    -2.377916     1.138996      30.97
 O       5.069928    -2.293629     0.455373      87.05
 H       5.549288    -1.844836    -0.222559      30.62
 C       3.753339    -0.375611     1.574658     144.54
 O       4.604363     0.671137     0.863202      89.88
 H       4.278850     1.571455     0.989401      23.17
 H       4.064431    -0.603783     2.506224      35.54
 H       2.594730    -0.382978     1.566944      31.10
55
name = lig-Water-frame_358
 C      -1.514473     2.592197     3.425573      45.60
 H      -2.433236     3.242915     3.350955      21.83
 C      -0.712194     0.333567     3.279383      68.19
 H      -0.917132    -0.680578     3.280873      26.60
 C       0.588312     0.692855     3.792801      -4.28
 O       1.714606    -0.123556     4.278300     103.46
 C       1.276866    -1.559007     4.160133     115.89
 H       2.279623    -2.071380     4.405420      26.31
 H       0.913038    -1.683823     3.110709      28.18
 H       0.698646    -2.120802     4.879272      28.88
 C       0.889038     2.169858     3.910278     -13.91
 O       2.301304     2.446484     4.469014     182.44
 H       2.335842     3.485406     4.536883      27.30
 C      -0.281527     3.018645     3.925018      68.75
 H      -0.471191     3.989872     4.331508      19.23
 C      -1.716181     1.196831     3.176565      25.85
 C      -3.207603     0.633777     2.645901      82.24
 H      -3.820421     1.514616     2.909430      26.26
 O      -3.519282    -0.545063     3.431532     250.22
 H      -4.491317    -0.742253     3.330067      25.13
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 C      -3.118730     0.435090     1.034213      82.11
 H      -2.250909     1.313844     0.776454      21.50
 C      -4.514837     0.560601     0.308506      96.72
 O      -5.289468    -0.709658     0.420578     282.58
 H      -4.655633    -1.392632     0.453669      28.90
 H      -4.141952     0.692796    -0.755738      26.30
 H      -5.267868     1.342953     0.311781      24.59
 C       1.118020     0.076581    -0.343359      56.54
 H       1.847631     0.893274    -0.535134      25.33
 C       0.642333    -2.303559    -0.400762      47.41
 H       1.013834    -3.272672    -0.700102      25.77
 C      -0.706267    -2.097036    -0.175857       3.22
 O      -1.537614    -3.178656     0.015253     183.72
 C      -2.274104    -3.684954    -1.125648      91.72
 H      -2.617095    -2.659201    -1.802609      24.26
 H      -1.629284    -4.480241    -1.706289      23.88
 H      -3.490687    -4.256496    -1.150837      21.48
 C      -1.112618    -0.784967     0.316690       0.02
 O      -2.424652    -0.807238     0.745216     169.42
 C      -0.246252     0.251526     0.043624      70.05
 H      -0.528989     1.280927    -0.246688      24.86
 C       1.533579    -1.176935    -0.501079      40.72
 C       3.014606    -1.418696    -0.761442      83.41
 H       2.946787    -2.510921    -1.244525      25.13
 O       3.471246    -0.364056    -1.614898     218.14
 H       4.518943    -0.253375    -1.754460      25.06
 C       3.777942    -1.601091     0.653864      72.00
 H       2.861845    -2.381649     1.219341      25.91
 O       5.066508    -2.293119     0.472955      60.08
 H       5.556131    -1.707827    -0.316535      24.81
 C       3.708485    -0.424508     1.597509     112.01
 O       4.603013     0.642683     0.845743      44.88
 H       4.430080     1.611937     1.173760      22.35
 H       4.256015    -0.367324     2.636399      28.55
 H       2.698623    -0.045777     1.583412      28.62
55
name = lig-Water-frame_359
 C      -1.515284     2.574498     3.405778      53.03
 H      -2.354300     3.197374     3.559318      27.32
 C      -0.627651     0.348986     3.330252      61.19
 H      -0.910133    -0.838090     3.192275      21.01
 C       0.574723     0.737746     3.766543      17.75
 O       1.634587    -0.126342     4.265394     137.96
 C       1.301156    -1.616950     4.143649     107.23
 H       2.258511    -2.002091     4.410559      26.52
 H       0.760800    -1.794943     3.235858      25.66
 H       0.626466    -1.625424     5.150365      25.87
 C       0.986434     2.181934     4.025752     -21.16
 O       2.248178     2.390570     4.479226     227.62
 H       2.337007     3.339773     4.291472      27.54
 C      -0.272829     3.002577     3.900059     103.52
 H      -0.227061     4.025009     4.378102      23.31
 C      -1.746076     1.150117     3.204037      29.66
 C      -3.149934     0.636720     2.624447      76.88
 H      -3.917836     1.561526     2.719566      23.09
 O      -3.548248    -0.553540     3.421821     236.63
 H      -4.533508    -0.914014     3.359505      24.06
 C      -3.147737     0.398546     1.110652     111.72
 H      -2.771891     1.310149     0.890277      25.39
 C      -4.479785     0.554469     0.222089      81.67
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 O      -5.326855    -0.737426     0.388444     215.22
 H      -4.572697    -1.450322     0.512527      23.08
 H      -4.053664     0.388360    -0.800544      25.48
 H      -5.190036     1.330330     0.729699      23.64
 C       1.079827     0.115106    -0.314791      44.59
 H       1.733331     0.986320    -0.571154      21.31
 C       0.656748    -2.339323    -0.471473      51.14
 H       1.055168    -3.425477    -0.638313      22.39
 C      -0.666475    -2.092390    -0.203139       2.71
 O      -1.525707    -3.234911     0.019813     208.00
 C      -2.309752    -3.596795    -1.161883     131.08
 H      -2.711263    -2.927409    -1.789481      28.49
 H      -1.575092    -4.263825    -1.520392      24.83
 H      -2.990423    -4.201035    -0.789027      28.58
 C      -1.111046    -0.793005     0.257006      15.53
 O      -2.439931    -0.757196     0.695644     174.18
 C      -0.297264     0.289275     0.041316      50.38
 H      -0.395231     1.401120     0.080693      20.52
 C       1.548926    -1.227817    -0.524579      25.06
 C       3.021231    -1.437748    -0.829507      86.58
 H       3.108381    -2.424923    -1.263521      25.00
 O       3.529946    -0.366577    -1.628174     280.32
 H       4.468401    -0.491911    -1.690441      28.43
 C       3.820287    -1.640468     0.691641     105.52
 H       3.122195    -2.208645     1.057939      29.04
 O       5.056301    -2.270283     0.501719     129.19
 H       5.422498    -1.890217    -0.409948      26.63
 C       3.703590    -0.403853     1.561151     117.98
 O       4.602429     0.624867     0.836547     102.09
 H       4.281667     1.418036     1.375364      25.40
 H       4.264922    -0.613379     2.469107      29.38
 H       2.835874     0.285588     1.763734      23.82
55
name = lig-Water-frame_360
 C      -1.518959     2.501636     3.413894      90.09
 H      -2.287467     3.273265     3.649928      31.73
 C      -0.589432     0.272951     3.374400      41.69
 H      -0.684435    -0.666682     3.157473      23.89
 C       0.675461     0.837025     3.798194      11.98
 O       1.529698    -0.133956     4.215028     165.29
 C       1.311045    -1.606076     4.203130     111.02
 H       2.289997    -2.177050     4.241038      26.32
 H       0.714597    -2.111918     3.347871      25.99
 H       0.640984    -1.501078     4.948234      28.90
 C       0.942164     2.114467     4.105939      12.59
 O       2.188796     2.364972     4.482319     174.74
 H       2.574853     3.326682     4.280192      16.86
 C      -0.185842     3.007810     3.898132     127.54
 H       0.084744     4.021040     4.265982      21.07
 C      -1.812586     1.165288     3.192978      42.23
 C      -3.107886     0.634127     2.640387     123.82
 H      -3.885743     1.392049     2.682087      25.89
 O      -3.574368    -0.560648     3.421054     229.44
 H      -4.493215    -0.762066     3.273189      28.30
 C      -3.194082     0.409729     1.177868      68.97
 H      -2.914187     1.545987     0.681973      18.81
 C      -4.447467     0.460759     0.199672      90.25
 O      -5.343794    -0.750634     0.351016     232.29
 H      -4.822236    -1.563439     0.676772      26.11
 H      -4.164450     0.548386    -0.860068      25.15
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 H      -4.860647     1.288548     0.695459      27.25
 C       1.024369     0.109685    -0.303258      58.22
 H       1.586021     0.993740    -0.491961      21.63
 C       0.707384    -2.367272    -0.550759      51.36
 H       0.978520    -3.357733    -0.596345      23.36
 C      -0.657782    -2.102906    -0.178482       9.04
 O      -1.517647    -3.244819     0.039400     178.53
 C      -2.298606    -3.562522    -1.174958      87.05
 H      -2.818292    -2.745025    -1.959193      22.07
 H      -1.500356    -4.154098    -1.906478      22.99
 H      -2.912015    -4.296704    -0.389493      20.15
 C      -1.150367    -0.820501     0.172562      12.37
 O      -2.449834    -0.724637     0.638326     133.39
 C      -0.282955     0.390273     0.019406      33.55
 H      -0.688816     1.317572     0.657528      14.98
 C       1.577491    -1.259511    -0.562477      32.24
 C       3.035087    -1.463192    -0.836434      75.88
 H       3.439370    -2.426279    -1.447101      21.18
 O       3.581861    -0.374825    -1.647410     226.07
 H       4.531268    -0.693148    -1.675497      25.37
 C       3.772786    -1.644785     0.655573      56.69
 H       3.122811    -2.676008     1.236277      22.45
 O       5.061941    -2.250181     0.535522      86.69
 H       5.464919    -2.032321    -0.378380      27.33
 C       3.767033    -0.344022     1.488803     117.15
 O       4.592900     0.619635     0.853080     196.37
 H       4.228746     1.412225     1.269297      23.40
 H       4.216766    -0.904224     2.471437      25.04
 H       2.836242     0.103046     1.929314      22.55
55
name = lig-Water-frame_361
 C      -1.483205     2.488398     3.483643      55.13
 H      -2.242304     3.293734     3.471388      18.45
 C      -0.610260     0.292625     3.409747      43.96
 H      -0.475416    -0.900422     3.058241      18.92
 C       0.681132     0.787921     3.819340      44.23
 O       1.506807    -0.158923     4.149414     192.18
 C       1.292670    -1.578819     4.240555     112.38
 H       2.231653    -2.145936     4.263504      28.18
 H       0.833123    -2.138935     3.456007      28.78
 H       0.532189    -1.922327     5.161813      27.28
 C       0.833282     2.114239     4.149572      26.45
 O       2.181345     2.369708     4.497074     230.94
 H       2.523317     3.268442     4.475842      21.49
 C      -0.099049     2.991117     3.889979      52.76
 H       0.090520     4.043972     4.062809      32.26
 C      -1.783922     1.140174     3.178944      50.52
 C      -3.115865     0.610085     2.686417     102.94
 H      -3.969179     1.451911     2.915211      24.54
 O      -3.577724    -0.558333     3.423536     233.64
 H      -4.590033    -0.554583     3.200512      25.38
 C      -3.200767     0.473969     1.114003      82.42
 H      -2.751388     1.280294     0.730944      23.58
 C      -4.421205     0.316625     0.253073     106.02
 O      -5.360901    -0.757005     0.320210     243.21
 H      -5.006124    -1.533891     0.790361      29.49
 H      -4.239824     0.805313    -0.780771      22.41
 H      -4.981600     1.379297     0.443852      23.87
 C       1.001952     0.078334    -0.320576      40.93
 H       1.732830     0.983530    -0.330468      20.32
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 C       0.721783    -2.347397    -0.602051      40.24
 H       1.029385    -3.500724    -0.664039      21.42
 C      -0.649156    -2.124392    -0.138893      13.81
 O      -1.498023    -3.201325     0.048477     221.03
 C      -2.260281    -3.580343    -1.198339     118.32
 H      -2.791878    -2.725198    -1.490504      26.49
 H      -1.798330    -3.966403    -2.054042      28.00
 H      -3.016812    -4.323091    -0.868206      27.86
 C      -1.175307    -0.794546     0.085064       3.94
 O      -2.450133    -0.716801     0.581952     110.76
 C      -0.323873     0.427645     0.052136      37.62
 H      -0.736477     1.079737     0.715279      16.38
 C       1.580383    -1.254880    -0.623150      35.89
 C       3.088123    -1.507570    -0.823648      92.11
 H       3.329067    -2.350048    -1.395029      24.72
 O       3.638634    -0.388708    -1.655105     235.89
 H       4.642662    -0.703830    -1.823190      24.80
 C       3.647639    -1.688229     0.587156      78.48
 H       3.272258    -2.387209     1.137578      28.89
 O       5.081481    -2.234353     0.576133      32.10
 H       5.638521    -2.020324    -0.365877      25.11
 C       3.838004    -0.358678     1.464589     116.78
 O       4.580728     0.638591     0.879874     237.47
 H       4.260199     1.623480     1.031947      20.42
 H       4.248073    -0.833206     2.351364      26.77
 H       2.810828    -0.198503     1.810007      25.47
55
name = lig-Water-frame_362
 C      -1.421536     2.517947     3.562414      52.62
 H      -2.176752     3.220043     3.227368      17.83
 C      -0.638966     0.296869     3.408510      65.17
 H      -0.622990    -0.663132     3.093764      26.42
 C       0.534973     0.665846     3.828753      30.90
 O       1.578565    -0.224511     4.103175     192.83
 C       1.234422    -1.589893     4.303852     124.47
 H       2.300080    -1.904509     4.493229      26.64
 H       0.823354    -1.952069     3.279213      26.83
 H       0.823671    -2.107121     5.072600      30.05
 C       0.857458     2.109760     4.193613      -0.58
 O       2.179558     2.372573     4.523825     154.09
 H       2.255985     3.377554     4.648131      23.49
 C      -0.148039     3.009412     3.855127      70.99
 H      -0.040698     4.143410     3.875152      32.51
 C      -1.688684     1.110078     3.187082      47.53
 C      -3.166592     0.619841     2.734438      93.61
 H      -3.791232     1.421721     3.038714      28.63
 O      -3.583757    -0.553340     3.413439     246.01
 H      -4.608693    -0.564347     3.388168      24.95
 C      -3.166383     0.487719     1.027304      72.13
 H      -2.433433     1.419103     0.685216      19.75
 C      -4.456799     0.304387     0.307227     117.37
 O      -5.380722    -0.773650     0.306417     213.79
 H      -4.948682    -1.553457     0.904560      26.68
 H      -4.124157     0.463369    -0.710989      26.26
 H      -5.192900     1.023638     0.453161      26.02
 C       1.029191     0.075066    -0.339805      35.56
 H       1.805348     0.743526    -0.171210      23.86
 C       0.684559    -2.342715    -0.616462      53.89
 H       1.063106    -3.273890    -0.798529      24.45
 C      -0.616251    -2.113542    -0.129895      11.59
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 O      -1.486366    -3.179455     0.041864     186.20
 C      -2.244010    -3.585339    -1.190762     101.67
 H      -2.885383    -2.545025    -1.178817      22.68
 H      -1.732975    -3.852607    -2.290467      24.30
 H      -3.156996    -4.413785    -1.199146      25.58
 C      -1.174336    -0.742215     0.019068      21.04
 O      -2.449651    -0.738693     0.535770     133.54
 C      -0.362821     0.328558     0.070589      58.61
 H      -0.626663     1.374295     0.705539      17.92
 C       1.558720    -1.212990    -0.696298      13.69
 C       3.117323    -1.516626    -0.823593      92.43
 H       3.047050    -2.593650    -1.411265      22.72
 O       3.707867    -0.415383    -1.653264     270.03
 H       4.558722    -0.610432    -1.919086      29.61
 C       3.633918    -1.662157     0.501712      62.92
 H       2.897249    -2.436909     1.322781      23.05
 O       5.111826    -2.230381     0.597836      73.87
 H       5.512072    -1.919236    -0.165147      31.28
 C       3.840499    -0.442044     1.453494     103.76
 O       4.584221     0.693089     0.883862     187.40
 H       4.135724     1.562971     1.029264      26.15
 H       4.481296    -0.692651     2.416253      24.82
 H       2.740669    -0.143205     1.620202      24.06
55
name = lig-Water-frame_363
 C      -1.416027     2.509831     3.580129      62.60
 H      -2.147355     3.210144     3.069717      18.89
 C      -0.706711     0.230008     3.371857      41.11
 H      -0.933758    -0.881216     3.034450      24.92
 C       0.503559     0.642413     3.919335      15.12
 O       1.641494    -0.263140     4.077355     176.42
 C       1.249940    -1.644246     4.301742     114.53
 H       2.298973    -1.912934     4.539642      26.23
 H       0.908760    -1.917930     3.352167      28.84
 H       0.644291    -2.012624     5.292396      26.02
 C       0.900799     2.028098     4.196002      -8.43
 O       2.170493     2.395161     4.555223      83.46
 H       2.020846     3.388214     4.809117      23.03
 C      -0.205592     3.059006     3.833431      76.94
 H      -0.109791     4.102962     3.837808      33.33
 C      -1.667238     1.162387     3.218502      46.08
 C      -3.152020     0.647764     2.739004      74.06
 H      -3.810597     1.640687     3.047942      27.15
 O      -3.596839    -0.558611     3.404105     222.74
 H      -4.578511    -0.683424     3.543180      23.75
 C      -3.084031     0.487561     0.998815      80.95
 H      -2.687351     1.356718     0.651755      27.24
 C      -4.516776     0.374327     0.299884      78.53
 O      -5.388517    -0.851661     0.348538     215.30
 H      -4.893166    -1.552410     0.757663      30.06
 H      -4.079514     0.089009    -0.745983      24.05
 H      -5.329462     1.163079     0.637130      24.48
 C       1.054847     0.059425    -0.348245      44.48
 H       1.870628     0.828663    -0.048387      25.17
 C       0.644760    -2.295297    -0.620076      63.32
 H       1.085651    -3.329857    -0.944512      24.41
 C      -0.600955    -2.076361    -0.163876      17.57
 O      -1.480343    -3.209813     0.036702     182.81
 C      -2.272978    -3.524846    -1.216080     127.58
 H      -2.915512    -2.657822    -1.309818      26.43
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 H      -1.595514    -3.551612    -1.973442      28.01
 H      -2.940608    -4.457640    -1.140024      29.01
 C      -1.188599    -0.754867    -0.002836      24.27
 O      -2.460851    -0.769208     0.503643     121.36
 C      -0.301802     0.280648     0.084802      69.68
 H      -0.417669     1.230545     0.275930      26.47
 C       1.526192    -1.160465    -0.756985      17.61
 C       3.072550    -1.522184    -0.906917      94.52
 H       3.048513    -2.459024    -1.296794      28.10
 O       3.748354    -0.450555    -1.642267     257.64
 H       4.690284    -0.729578    -1.980587      26.44
 C       3.703042    -1.660195     0.552418     103.92
 H       2.974566    -2.207828     0.912451      28.18
 O       5.107424    -2.244906     0.621586      40.46
 H       5.548059    -1.763705    -0.307583      23.33
 C       3.792636    -0.493547     1.431666     118.46
 O       4.587806     0.743947     0.866342     132.98
 H       3.980031     1.447404     1.245102      27.37
 H       4.373739    -0.677857     2.391305      28.59
 H       2.907695    -0.002111     1.684716      25.89
55
name = lig-Water-frame_364
 C      -1.479448     2.517136     3.520570      36.73
 H      -2.182405     3.232786     3.186915      21.09
 C      -0.756824     0.129753     3.341009      23.25
 H      -1.091862    -0.921119     3.062973      25.01
 C       0.582533     0.634066     4.027430      31.84
 O       1.659564    -0.264227     4.067117     136.05
 C       1.317748    -1.710777     4.320359      98.15
 H       2.224657    -2.315531     4.496312      27.13
 H       0.874210    -2.267487     3.378340      29.52
 H       0.471355    -1.595141     4.958090      28.22
 C       0.855685     1.972896     4.151042      26.73
 O       2.147162     2.428435     4.594438     168.90
 H       2.096723     3.316461     4.882908      27.53
 C      -0.174188     3.036665     3.855819      82.99
 H      -0.020611     4.188834     3.930517      25.93
 C      -1.739639     1.199167     3.253644      23.90
 C      -3.104680     0.719937     2.710210      88.84
 H      -3.803254     1.469257     2.812555      30.20
 O      -3.587927    -0.561791     3.393386     185.99
 H      -4.666987    -0.636991     3.424396      22.21
 C      -3.080047     0.448352     1.036913      63.59
 H      -2.740439     1.489101     0.479560      24.82
 C      -4.570359     0.425571     0.271087      80.15
 O      -5.397647    -0.930743     0.422242     145.43
 H      -4.719601    -1.734949     0.719522      21.49
 H      -4.313425     0.376546    -0.762875      25.94
 H      -5.033527     1.332578     0.505685      28.66
 C       1.099350     0.074221    -0.328745      55.40
 H       1.677825     0.934116    -0.177973      27.73
 C       0.668488    -2.245443    -0.657870      59.64
 H       0.887548    -3.255707    -0.925745      26.13
 C      -0.663419    -2.063517    -0.208978       9.37
 O      -1.479276    -3.250717     0.033049     164.57
 C      -2.290514    -3.441397    -1.215720      92.12
 H      -3.101307    -2.609367    -1.585508      24.58
 H      -1.295502    -3.340808    -1.969110      23.85
 H      -2.706862    -4.495416    -0.972289      26.13
 C      -1.190331    -0.811299     0.020214      26.60
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 O      -2.482581    -0.780458     0.484858     104.06
 C      -0.178543     0.251010     0.056131      55.42
 H      -0.524962     1.460729     0.031054      22.68
 C       1.530536    -1.156727    -0.802966      46.14
 C       3.016869    -1.469406    -0.970500      76.80
 H       3.257606    -2.590960    -1.464606      23.75
 O       3.781472    -0.488597    -1.650725     227.97
 H       4.651297    -0.995490    -1.899568      26.23
 C       3.803076    -1.655979     0.585187      79.83
 H       2.904293    -2.556541     0.888472      25.59
 O       5.087500    -2.246918     0.603362     117.18
 H       5.575678    -2.008635    -0.161451      30.84
 C       3.763805    -0.455124     1.419521     114.77
 O       4.574279     0.772605     0.846141      70.26
 H       4.105265     1.502110     1.449756      24.12
 H       4.191055    -0.854126     2.403863      30.48
 H       2.788815     0.023781     1.860232      26.02
55
name = lig-Water-frame_365
 C      -1.507299     2.580395     3.448454      46.38
 H      -2.360986     3.354079     3.394030      28.97
 C      -0.757640     0.142842     3.379176      18.72
 H      -0.910388    -0.809551     3.063621      23.48
 C       0.604087     0.537160     4.050289      17.86
 O       1.682680    -0.274697     4.062420     132.34
 C       1.360698    -1.762155     4.287784      90.35
 H       2.097706    -2.504594     4.729256      26.53
 H       0.946946    -2.337860     3.498081      30.41
 H       0.414373    -1.516448     4.857677      25.40
 C       0.801912     2.024090     4.118532      26.76
 O       2.110232     2.432784     4.624718     216.05
 H       2.153535     3.420728     4.897602      27.32
 C      -0.148314     2.950129     3.887562      38.28
 H       0.136766     3.937073     4.074737      18.61
 C      -1.811739     1.134724     3.275317      49.03
 C      -3.057845     0.743844     2.639330      81.90
 H      -4.054346     1.477115     2.615747      23.15
 O      -3.574240    -0.543618     3.370399     212.36
 H      -4.518714    -0.498001     3.177774      26.58
 C      -3.143274     0.442474     1.052245      85.24
 H      -2.640903     1.213914     0.553238      25.23
 C      -4.577691     0.408847     0.267892      67.67
 O      -5.400439    -0.967830     0.495776     175.01
 H      -4.697469    -1.613836     0.778912      24.87
 H      -4.480462     0.767366    -0.881347      22.60
 H      -5.078512     1.434689     0.508827      23.90
 C       1.165698     0.107349    -0.318747      36.50
 H       1.739628     1.091177    -0.449361      25.54
 C       0.660582    -2.207391    -0.704122      50.12
 H       0.882652    -3.282251    -0.920057      24.93
 C      -0.719506    -2.096470    -0.245973      12.03
 O      -1.487821    -3.252350     0.023258     221.33
 C      -2.251355    -3.354614    -1.235043     119.64
 H      -3.136255    -2.796180    -1.572613      27.28
 H      -1.645249    -3.409462    -2.015920      29.99
 H      -2.493263    -4.513972    -1.071310      25.52
 C      -1.146552    -0.827832     0.077438      10.87
 O      -2.505027    -0.766989     0.481059      68.28
 C      -0.164905     0.276834     0.008551      56.38
 H      -0.609732     1.161189     0.050059      26.45
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 C       1.591591    -1.188604    -0.827486      35.03
 C       3.022315    -1.466568    -1.001817     101.14
 H       3.203286    -2.311617    -1.493721      29.01
 O       3.814555    -0.522324    -1.687472     284.61
 H       4.563126    -1.025417    -1.817934      32.27
 C       3.779131    -1.702634     0.556545      78.24
 H       3.368148    -2.447575     1.074079      30.31
 O       5.078677    -2.262726     0.586508      95.48
 H       5.667722    -2.158105    -0.281109      27.56
 C       3.743031    -0.354743     1.460343     134.31
 O       4.543235     0.772584     0.858715      96.92
 H       4.391227     1.607611     1.322643      24.88
 H       4.174855    -0.879682     2.408033      31.84
 H       2.730196    -0.192911     1.684208      30.12
55
name = lig-Water-frame_366
 C      -1.511823     2.607652     3.400166      57.11
 H      -2.281976     3.307529     3.552278      29.42
 C      -0.701531     0.236039     3.482067      35.84
 H      -0.647264    -0.894426     2.943030      21.17
 C       0.541069     0.483889     3.987024      19.24
 O       1.726502    -0.318545     4.058754     161.88
 C       1.351238    -1.790738     4.273414     101.70
 H       2.073051    -2.168112     4.994793      26.41
 H       1.103535    -2.236924     3.232430      26.45
 H       0.475426    -1.863396     5.005558      26.56
 C       0.827712     2.008889     4.133446       7.71
 O       2.057527     2.424821     4.646596     180.06
 H       2.101698     3.444799     4.731759      29.49
 C      -0.213139     2.872323     3.895486      61.86
 H       0.199159     3.904721     4.203585      19.16
 C      -1.819098     1.119591     3.282485      39.92
 C      -3.117074     0.708130     2.541958     100.07
 H      -3.793062     1.453890     2.690006      27.21
 O      -3.533770    -0.494981     3.326327     235.03
 H      -4.586545    -0.573737     3.064149      22.87
 C      -3.212007     0.427357     1.019662      91.54
 H      -2.507240     1.294649     0.589250      22.73
 C      -4.583123     0.400654     0.286132      95.00
 O      -5.403653    -0.913679     0.537718     197.12
 H      -4.703522    -1.634330     0.944649      20.95
 H      -4.489840     0.677045    -0.727432      26.78
 H      -5.337640     1.010696     0.825200      24.54
 C       1.227522     0.147229    -0.350992      37.67
 H       1.854656     0.969647    -0.683894      23.75
 C       0.611739    -2.223220    -0.749869      45.14
 H       1.058337    -3.250652    -0.939719      23.71
 C      -0.694854    -2.119458    -0.261266      19.88
 O      -1.502268    -3.213617    -0.010665     227.36
 C      -2.224029    -3.375721    -1.249587     108.12
 H      -3.233926    -2.717575    -1.275523      24.17
 H      -1.665513    -3.408973    -2.380896      23.90
 H      -2.586509    -4.442274    -1.319919      26.41
 C      -1.094935    -0.806874     0.150028       8.09
 O      -2.507485    -0.750421     0.489226      97.94
 C      -0.216298     0.265069    -0.038990      47.95
 H      -0.727877     1.357560     0.216525      20.96
 C       1.636344    -1.179387    -0.804558      19.15
 C       3.082990    -1.498223    -0.966136      82.57
 H       3.054523    -2.564918    -1.645087      23.61
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 O       3.834563    -0.526810    -1.739957     198.62
 H       4.808083    -0.967028    -1.866095      24.39
 C       3.722139    -1.691742     0.496818      55.14
 H       3.278291    -2.424303     1.438468      24.40
 O       5.116528    -2.286745     0.549998      78.32
 H       5.590063    -2.182426    -0.419348      25.93
 C       3.744567    -0.297625     1.482240     104.95
 O       4.517487     0.739084     0.882770     170.96
 H       4.354115     1.710834     1.241475      20.98
 H       4.249400    -0.555617     2.429886      29.23
 H       2.589883    -0.152702     1.478333      26.67
55
name = lig-Water-frame_367
 C      -1.511272     2.534946     3.389578      34.19
 H      -2.274759     3.368467     3.519200      26.09
 C      -0.678946     0.255607     3.536902      45.51
 H      -0.699670    -0.611894     3.108334      27.38
 C       0.565033     0.559606     3.925999      25.49
 O       1.721649    -0.377421     4.062400     168.50
 C       1.329651    -1.799272     4.277246     112.55
 H       2.262568    -1.913457     4.909261      24.60
 H       1.487213    -2.192100     3.275091      27.11
 H       0.457340    -2.094525     4.855055      28.24
 C       0.859820     1.895666     4.165287      -2.41
 O       2.005244     2.416539     4.658827      97.62
 H       2.014424     3.358288     4.588500      31.50
 C      -0.269078     2.859150     3.909203      98.49
 H      -0.107603     3.882445     4.198316      19.10
 C      -1.781072     1.177992     3.244715      15.84
 C      -3.170599     0.627448     2.487252      90.70
 H      -3.730430     1.684703     2.839181      22.41
 O      -3.515971    -0.444107     3.261909     197.24
 H      -4.419855    -0.769767     3.279160      24.00
 C      -3.216408     0.445043     0.944470      97.94
 H      -2.785316     1.402012     0.644284      26.63
 C      -4.629900     0.370530     0.381601      97.62
 O      -5.385805    -0.840030     0.558689     245.97
 H      -4.931312    -1.639966     0.939971      25.53
 H      -4.474662     0.499484    -0.779480      24.20
 H      -5.375337     0.858420     1.013652      23.48
 C       1.219226     0.144392    -0.429649      43.13
 H       1.931456     0.954514    -0.673339      22.79
 C       0.626987    -2.257430    -0.792762      53.54
 H       1.048222    -3.199624    -0.996664      24.30
 C      -0.622742    -2.091741    -0.243246      13.76
 O      -1.510101    -3.180284    -0.070533     216.56
 C      -2.249235    -3.437609    -1.329807     114.45
 H      -2.970915    -2.678009    -0.967201      24.09
 H      -1.704504    -3.103599    -2.111068      27.95
 H      -2.837804    -4.490715    -1.430168      25.21
 C      -1.073526    -0.789744     0.206328       3.50
 O      -2.480515    -0.742681     0.501988     124.68
 C      -0.252323     0.306463    -0.070958      57.78
 H      -0.498061     1.268012     0.301237      23.49
 C       1.615723    -1.138073    -0.743488      14.69
 C       3.155887    -1.599404    -0.930829      88.73
 H       3.070838    -2.476699    -1.376781      27.48
 O       3.858969    -0.539608    -1.796232     245.64
 H       4.833619    -0.714974    -1.872374      27.24
 C       3.704726    -1.669789     0.526252      86.04
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 H       2.988509    -2.160182     1.049911      28.23
 O       5.149944    -2.304570     0.483537     150.27
 H       5.507216    -2.138316    -0.328832      31.25
 C       3.723359    -0.291207     1.443362     103.92
 O       4.516164     0.725139     0.891572     248.91
 H       3.999429     1.513403     1.226561      26.04
 H       4.122460    -0.327029     2.565718      26.35
 H       2.735771     0.098740     1.517025      24.76
55
name = lig-Water-frame_368
 C      -1.522393     2.476618     3.419289      43.80
 H      -2.228600     3.275790     3.206666      22.21
 C      -0.736528     0.272584     3.538557      30.62
 H      -0.984297    -0.905873     3.167697      22.00
 C       0.690422     0.618269     3.892984      29.47
 O       1.648307    -0.395997     4.068590     190.26
 C       1.390021    -1.787012     4.285090     123.98
 H       2.288599    -2.131571     4.780022      26.97
 H       1.680348    -2.394577     3.382128      27.81
 H       0.306936    -2.168639     4.569062      26.63
 C       0.813125     1.885329     4.187516      31.55
 O       1.985335     2.395750     4.672516     165.83
 H       1.935626     3.437614     4.547148      22.59
 C      -0.262698     2.837599     3.939967      56.54
 H      -0.312919     3.921432     4.215774      28.26
 C      -1.735530     1.173841     3.154104       4.29
 C      -3.177184     0.648672     2.490870      94.96
 H      -3.795536     1.438000     2.628288      27.63
 O      -3.495967    -0.445039     3.231600     199.53
 H      -4.482788    -0.769415     3.287383      21.63
 C      -3.201944     0.476392     0.910040      76.13
 H      -2.943649     1.523817     0.443378      23.75
 C      -4.680586     0.331398     0.472180      97.33
 O      -5.398267    -0.810701     0.566007     316.22
 H      -4.876428    -1.592491     0.872890      25.85
 H      -4.648957     0.535385    -0.601218      24.36
 H      -5.140817     1.347171     0.908556      24.53
 C       1.134135     0.138171    -0.519025      46.97
 H       1.852728     1.004033    -0.449279      23.15
 C       0.704187    -2.247424    -0.806609      42.33
 H       0.951186    -3.361068    -1.145330      22.79
 C      -0.574976    -2.062322    -0.208034       1.16
 O      -1.482927    -3.174105    -0.121755     195.63
 C      -2.324742    -3.468692    -1.369166      89.62
 H      -3.118715    -2.649591    -1.264482      24.55
 H      -1.604936    -2.868503    -2.183853      23.06
 H      -2.744434    -4.421363    -1.401503      26.28
 C      -1.070300    -0.769433     0.220369       7.23
 O      -2.431675    -0.733024     0.512897     120.74
 C      -0.211212     0.354513    -0.084337      58.51
 H      -0.437819     1.416314     0.319725      22.52
 C       1.602252    -1.155879    -0.706274      11.46
 C       3.198775    -1.602856    -0.874837      63.80
 H       3.281468    -2.800198    -1.303762      21.95
 O       3.859126    -0.569928    -1.844140     230.55
 H       4.792747    -0.644121    -1.811946      27.29
 C       3.748740    -1.614201     0.565145      72.84
 H       2.750651    -2.367926     0.829127      22.56
 O       5.131517    -2.319328     0.449262      32.61
 H       5.594855    -1.937655    -0.526870      21.71
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 C       3.705070    -0.320446     1.401710     115.04
 O       4.527931     0.741601     0.880284     261.17
 H       3.945568     1.495988     1.138997      26.73
 H       3.856472    -0.563067     2.451968      27.25
 H       2.687054     0.177223     1.586750      23.49
55
name = lig-Water-frame_369
 C      -1.510860     2.477460     3.449767      50.66
 H      -2.202258     3.180468     2.933207      21.63
 C      -0.758898     0.216228     3.490168      49.18
 H      -1.056110    -0.741604     3.486656      24.43
 C       0.687288     0.535656     3.837354      14.77
 O       1.581543    -0.380107     4.081765     197.45
 C       1.465595    -1.815744     4.253572     125.75
 H       2.108768    -2.342780     5.074931      27.04
 H       1.604490    -2.400808     3.318650      28.38
 H       0.482484    -1.986947     4.468776      29.62
 C       0.762622     2.012816     4.218232      18.17
 O       1.995416     2.397770     4.683482     211.95
 H       2.000177     3.380670     4.722122      26.06
 C      -0.274332     2.827749     3.974173      52.16
 H      -0.147811     3.892819     4.298476      28.90
 C      -1.734096     1.095772     3.036027      18.01
 C      -3.100453     0.725504     2.486811      63.35
 H      -4.114244     1.477553     2.530738      21.65
 O      -3.491440    -0.505100     3.238086     157.65
 H      -4.500318    -0.508496     3.039002      22.23
 C      -3.182791     0.503626     0.922976      79.13
 H      -2.909472     1.334336     0.212144      22.01
 C      -4.693970     0.385938     0.519114      96.01
 O      -5.450699    -0.833546     0.586942     313.44
 H      -4.703811    -1.535157     0.869288      22.45
 H      -4.764866     0.728680    -0.610911      22.52
 H      -4.965947     1.370333     0.779097      25.15
 C       1.046608     0.146196    -0.575171      45.36
 H       1.678548     0.965893    -0.366896      24.22
 C       0.755531    -2.251080    -0.783210      47.08
 H       0.891760    -3.172283    -1.176350      25.41
 C      -0.560574    -2.046832    -0.190231       3.72
 O      -1.447945    -3.181128    -0.165573     192.61
 C      -2.367639    -3.364843    -1.397487      89.30
 H      -3.399834    -2.915112    -1.724262      24.40
 H      -1.778295    -3.269084    -2.293164      27.32
 H      -2.488427    -4.608783    -1.384547      23.45
 C      -1.047754    -0.735330     0.181458       6.38
 O      -2.384243    -0.709991     0.523747     119.92
 C      -0.170466     0.395252    -0.065395      60.11
 H      -0.497376     1.477937     0.172597      21.33
 C       1.654514    -1.224857    -0.728616       6.94
 C       3.208804    -1.559254    -0.857003      91.23
 H       3.450512    -2.481679    -1.123551      26.66
 O       3.824458    -0.627376    -1.877478     217.92
 H       4.889100    -0.676065    -1.677590      24.55
 C       3.769390    -1.601914     0.559254      87.42
 H       3.305463    -2.407785     0.975794      28.09
 O       5.091374    -2.307409     0.409009     124.74
 H       5.581407    -1.869564    -0.252331      30.91
 C       3.668397    -0.354688     1.376181     121.86
 O       4.544401     0.754941     0.866626     204.47
 H       4.186162     1.730198     1.080844      22.52
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 H       3.890658    -0.912637     2.422655      26.19
 H       2.599636    -0.085165     1.407778      25.22
55
name = lig-Water-frame_370
 C      -1.519545     2.447421     3.416110      44.72
 H      -2.126940     3.235082     2.899212      22.47
 C      -0.716293     0.138777     3.431738      60.60
 H      -1.025307    -0.967743     3.664225      21.98
 C       0.516177     0.510970     3.787371      16.96
 O       1.589565    -0.370724     4.114698     180.20
 C       1.517947    -1.865784     4.214850     122.69
 H       1.846588    -2.125536     5.208426      27.88
 H       1.639350    -2.220964     3.201469      28.43
 H       0.357915    -1.930499     4.559904      24.92
 C       0.768704     2.026804     4.226073      -7.85
 O       2.022845     2.416964     4.696848     187.98
 H       2.133611     3.364571     4.947863      26.23
 C      -0.314090     2.889705     4.019543      33.45
 H       0.013718     3.865288     4.322340      26.16
 C      -1.733315     1.096719     2.965364      36.60
 C      -3.044112     0.797156     2.471752      74.05
 H      -3.768042     1.445278     2.721162      26.00
 O      -3.497503    -0.546430     3.225701     152.94
 H      -4.460269    -0.581706     3.032071      22.42
 C      -3.156031     0.490825     0.930997      86.64
 H      -2.703258     1.275284     0.246830      22.76
 C      -4.668285     0.464056     0.468528      79.22
 O      -5.487469    -0.860849     0.624706     279.94
 H      -4.871503    -1.524570     0.894512      26.48
 H      -4.724748     0.714432    -0.590540      24.94
 H      -5.311984     1.304307     1.164976      22.75
 C       1.060983     0.115893    -0.603087      24.09
 H       1.754922     1.044663    -0.563379      25.19
 C       0.739299    -2.254754    -0.717431      36.31
 H       1.014982    -3.307732    -1.223440      23.00
 C      -0.561331    -2.028940    -0.202868      19.78
 O      -1.432429    -3.167397    -0.222320     180.20
 C      -2.389384    -3.337781    -1.443073      99.97
 H      -3.423378    -3.054798    -1.628744      26.15
 H      -1.752886    -3.478611    -2.496610      25.11
 H      -2.368667    -4.322152    -1.307955      27.71
 C      -1.018454    -0.707973     0.112837       7.69
 O      -2.355839    -0.682104     0.542212     122.86
 C      -0.208492     0.412300    -0.033897      66.57
 H      -0.534886     1.420255     0.054519      23.10
 C       1.725501    -1.239297    -0.786205       1.55
 C       3.173067    -1.456449    -0.865386      93.55
 H       3.427626    -2.626618    -1.277695      23.04
 O       3.799509    -0.695313    -1.884547     269.41
 H       4.737318    -0.681149    -1.701816      28.19
 C       3.822393    -1.604776     0.503450      74.58
 H       3.472154    -2.476479     1.362178      24.78
 O       5.055560    -2.282188     0.393022      63.41
 H       5.756011    -1.739306    -0.198403      24.58
 C       3.653848    -0.392637     1.382572     122.53
 O       4.558227     0.752082     0.859672     190.95
 H       4.288201     1.591849     1.238099      25.74
 H       4.056132    -0.673133     2.332445      30.72
 H       2.564787    -0.248797     1.272558      26.33
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name = lig-Water-frame_371
 C      -1.519679     2.428141     3.339725      56.51
 H      -2.138854     3.273318     3.065324      28.43
 C      -0.743337     0.048966     3.343459      53.25
 H      -0.891944    -1.068783     3.563072      19.84
 C       0.424043     0.559160     3.810557      18.85
 O       1.619682    -0.340895     4.154442     138.94
 C       1.452545    -1.851556     4.201122     114.21
 H       2.049681    -2.029560     5.139861      25.26
 H       1.873901    -2.263966     3.210027      26.80
 H       0.488505    -2.160264     4.358989      28.46
 C       0.766937     1.964851     4.196691       4.89
 O       2.054104     2.415734     4.702089     174.49
 H       2.083204     3.401877     5.072839      32.20
 C      -0.319332     2.937379     4.068997      55.20
 H      -0.107863     4.068510     4.277408      13.05
 C      -1.667752     1.136498     2.978519      46.26
 C      -3.014698     0.765987     2.444943      58.74
 H      -3.627481     1.746133     2.950697      21.79
 O      -3.485493    -0.551628     3.193552     159.26
 H      -4.529402    -0.819390     3.179826      23.10
 C      -3.121384     0.486752     0.921131      86.98
 H      -2.547276     1.421401     0.529159      21.45
 C      -4.676941     0.512347     0.447483      86.37
 O      -5.503725    -0.851768     0.648348     255.15
 H      -4.959574    -1.671229     0.984984      23.03
 H      -4.713502     0.746744    -0.659706      24.56
 H      -5.289118     0.911042     1.153442      25.60
 C       1.160114     0.094681    -0.600670      39.39
 H       1.761593     0.903513    -0.920248      23.91
 C       0.736821    -2.284584    -0.664716      50.46
 H       1.028699    -3.231345    -0.942204      24.76
 C      -0.566562    -2.023204    -0.250335      16.08
 O      -1.435953    -3.120383    -0.289851     244.80
 C      -2.346981    -3.367000    -1.509585      73.02
 H      -3.378016    -2.821757    -1.222072      22.70
 H      -1.818707    -3.243318    -2.476984      25.10
 H      -2.571729    -4.565901    -1.153723      22.49
 C      -1.036843    -0.697066     0.059805       7.02
 O      -2.348587    -0.674746     0.566525     146.94
 C      -0.218149     0.386958    -0.044243      62.66
 H      -0.622758     1.544731     0.005863      18.44
 C       1.690708    -1.175397    -0.830306       7.52
 C       3.141074    -1.475016    -0.916531     114.13
 H       3.039338    -2.418590    -1.270965      25.43
 O       3.779427    -0.731258    -1.892245     317.50
 H       4.735265    -0.667801    -1.797601      29.80
 C       3.861284    -1.637930     0.503573     120.47
 H       3.178949    -2.148477     1.098171      27.43
 O       5.078968    -2.249658     0.368281     147.02
 H       5.860596    -1.698902    -0.111970      24.77
 C       3.697422    -0.400228     1.369228     110.67
 O       4.562713     0.722367     0.854502     173.71
 H       4.138878     1.475366     1.450538      24.74
 H       4.104357    -0.289894     2.492248      26.65
 H       2.574946    -0.152495     1.376063      24.13
55
name = lig-Water-frame_372
 C      -1.441982     2.490277     3.306196      60.97
 H      -2.363158     3.193165     3.211308      24.97
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 C      -0.779519     0.020598     3.258792      44.76
 H      -0.922967    -1.004003     3.178434      23.41
 C       0.475538     0.597836     3.896587       6.70
 O       1.613956    -0.295368     4.187329     132.02
 C       1.419525    -1.791286     4.191041     115.22
 H       2.229782    -2.137267     4.859675      26.29
 H       2.010317    -2.255073     3.432242      29.62
 H       0.398745    -2.424049     4.181292      26.10
 C       0.732563     1.952289     4.167378      15.34
 O       2.068524     2.383478     4.698116     183.28
 H       1.857073     3.283183     4.892701      32.90
 C      -0.301816     2.929733     4.076085      64.60
 H      -0.330995     3.947869     4.209194      17.85
 C      -1.617929     1.091416     3.007415      32.09
 C      -3.045935     0.701610     2.465895      87.81
 H      -3.565198     1.555809     2.671896      26.57
 O      -3.462243    -0.542164     3.158787     267.48
 H      -4.429528    -0.642467     3.211384      27.14
 C      -3.094577     0.534713     0.926793      83.66
 H      -2.647522     1.476462     0.612326      23.85
 C      -4.652498     0.458147     0.428280      71.46
 O      -5.497077    -0.834561     0.645983     249.69
 H      -4.937481    -1.616280     0.989692      24.82
 H      -4.832569     0.877905    -0.634580      23.78
 H      -5.315357     1.151967     1.249179      22.94
 C       1.211919     0.125082    -0.581510      60.48
 H       1.815123     0.917206    -1.143897      22.23
 C       0.761405    -2.261950    -0.613770      35.93
 H       1.060545    -3.400182    -0.681268      21.48
 C      -0.582024    -2.027859    -0.328790      12.93
 O      -1.448201    -3.077763    -0.352500     246.45
 C      -2.332509    -3.430375    -1.475649     101.70
 H      -3.020299    -2.668304    -1.224262      25.59
 H      -1.859616    -3.032589    -2.545947      25.29
 H      -2.727994    -4.342271    -1.440776      28.09
 C      -1.089331    -0.700775     0.030656      -3.34
 O      -2.358063    -0.687829     0.585299     135.25
 C      -0.154968     0.382224    -0.115642      55.77
 H      -0.510150     1.288251     0.024426      24.51
 C       1.586802    -1.125965    -0.832512      31.03
 C       3.103216    -1.541061    -0.953204      71.15
 H       2.904176    -2.696783    -1.337520      22.87
 O       3.768726    -0.727698    -1.926700     218.49
 H       4.847735    -0.711106    -1.863630      24.64
 C       3.834488    -1.620639     0.501623      88.54
 H       2.864914    -2.360232     0.838957      24.86
 O       5.154424    -2.239312     0.356956     166.96
 H       5.689225    -1.687210    -0.117847      30.27
 C       3.783461    -0.351788     1.377964     137.35
 O       4.550606     0.702425     0.857752     230.43
 H       4.092559     1.495213     1.305523      24.97
 H       3.900688    -0.454518     2.431164      30.33
 H       2.770934    -0.014319     1.470982      26.84
55
name = lig-Water-frame_373
 C      -1.372824     2.533472     3.308933      65.18
 H      -2.296056     2.991293     3.281523      26.41
 C      -0.710001     0.087354     3.241978      43.59
 H      -0.992837    -0.982774     2.634105      24.91
 C       0.543425     0.549381     3.963560      14.73
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 O       1.574469    -0.253435     4.218444     162.11
 C       1.437062    -1.744076     4.173955     116.12
 H       2.047129    -2.186832     4.988469      28.87
 H       1.986664    -2.032586     3.181147      30.18
 H       0.493670    -2.224435     4.196572      29.67
 C       0.732586     1.969989     4.172165      16.84
 O       2.039098     2.325770     4.675273     204.00
 H       1.865781     3.330375     4.713167      30.01
 C      -0.308317     2.877852     4.016950      71.08
 H      -0.274953     4.014547     4.340327      22.03
 C      -1.647616     1.041087     3.013846      23.79
 C      -3.045183     0.614514     2.490681      77.90
 H      -3.935678     1.541265     2.563985      22.40
 O      -3.431136    -0.523610     3.126084     245.78
 H      -4.469645    -0.403083     3.167957      23.71
 C      -3.108125     0.565566     0.950001      67.97
 H      -2.743594     1.552369     0.370629      23.04
 C      -4.653577     0.406807     0.462981     103.49
 O      -5.461793    -0.804512     0.619405     282.81
 H      -4.858256    -1.456511     0.927132      29.44
 H      -4.855770     0.821808    -0.528330      26.22
 H      -4.986623     1.291671     0.931223      28.12
 C       1.194006     0.229671    -0.585393      57.65
 H       1.821118     1.000546    -0.969728      25.68
 C       0.766562    -2.238249    -0.570265      39.63
 H       1.107360    -3.256335    -0.470944      24.74
 C      -0.618495    -2.006197    -0.415688      10.51
 O      -1.455854    -3.092809    -0.379812     196.61
 C      -2.306960    -3.401090    -1.448434     118.81
 H      -3.143064    -2.497912    -1.498963      25.55
 H      -1.880937    -3.095817    -2.481188      27.08
 H      -2.847762    -4.470977    -1.689538      24.04
 C      -1.093761    -0.713134    -0.005656      -5.48
 O      -2.373271    -0.697204     0.588480      64.14
 C      -0.087066     0.341615    -0.205923      51.14
 H      -0.462383     1.489178     0.138798      23.51
 C       1.563901    -1.172593    -0.812319      39.28
 C       3.058926    -1.625538    -0.998357      81.93
 H       3.216543    -2.604093    -1.304744      28.67
 O       3.767439    -0.712272    -1.974095     268.14
 H       4.681793    -0.855885    -1.854946      30.10
 C       3.735160    -1.616796     0.471657      62.85
 H       3.322886    -2.516613     0.832033      28.07
 O       5.209820    -2.242744     0.374936      65.06
 H       5.667324    -1.553345    -0.363338      24.77
 C       3.828869    -0.329756     1.394859     138.79
 O       4.560052     0.714744     0.857902     196.18
 H       4.159481     1.598895     1.053300      26.94
 H       3.988455    -0.902869     2.461671      27.79
 H       2.730854     0.087625     1.399714      26.34
55
name = lig-Water-frame_374
 C      -1.406692     2.444583     3.287767      60.09
 H      -2.344706     3.185682     3.298592      27.40
 C      -0.590749     0.147927     3.231408      64.66
 H      -0.704835    -0.642467     2.689825      28.54
 C       0.537653     0.513238     3.968774      28.87
 O       1.561714    -0.249059     4.271313     196.46
 C       1.508036    -1.691354     4.128856     124.17
 H       1.814247    -2.070109     5.130520      26.91
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 H       1.767260    -1.813078     3.123110      30.63
 H       0.328714    -1.901934     4.216869      26.17
 C       0.771391     1.930742     4.201108      10.99
 O       1.977365     2.289054     4.644252     191.44
 H       2.265959     3.294338     4.607715      22.16
 C      -0.268619     2.888622     3.969988      64.93
 H      -0.023627     3.780895     4.425048      16.53
 C      -1.701673     1.084875     3.016864      43.79
 C      -3.034837     0.648050     2.486064     107.50
 H      -3.822328     1.224989     2.738332      26.09
 O      -3.435819    -0.536531     3.108084     270.58
 H      -4.448904    -0.544121     3.243507      26.86
 C      -3.150598     0.552366     0.935735      74.34
 H      -2.820290     1.335478     0.360323      26.18
 C      -4.635181     0.391275     0.487013      91.38
 O      -5.413846    -0.763176     0.591340     238.07
 H      -4.751733    -1.508593     0.938120      25.13
 H      -4.623715     0.565781    -0.714445      24.54
 H      -5.001821     1.477043     0.928368      25.50
 C       1.198457     0.255505    -0.635224      21.15
 H       1.861629     1.184340    -0.654260      24.43
 C       0.719802    -2.219982    -0.533717      38.32
 H       1.178731    -3.227876    -0.438899      24.21
 C      -0.667844    -1.966330    -0.483264      12.04
 O      -1.464005    -3.158380    -0.368278     185.72
 C      -2.351330    -3.314261    -1.491482     111.74
 H      -3.225716    -2.762245    -1.605949      28.23
 H      -1.637249    -3.245926    -2.553813      25.90
 H      -2.606191    -4.329437    -1.492799      28.77
 C      -1.061545    -0.725831    -0.059499      -5.60
 O      -2.370222    -0.694855     0.565439      58.98
 C      -0.135019     0.375626    -0.238141      59.51
 H      -0.329135     1.280876     0.067384      26.44
 C       1.644051    -1.203311    -0.793278      11.62
 C       3.050144    -1.639283    -1.021309      86.80
 H       3.394168    -2.717745    -1.413045      24.20
 O       3.739275    -0.706171    -2.008509     222.54
 H       4.680391    -0.967984    -1.878202      27.19
 C       3.700155    -1.626899     0.411599      47.79
 H       3.486534    -2.590128     1.159486      24.42
 O       5.240759    -2.205101     0.377939      65.62
 H       5.762878    -1.809344    -0.373892      24.33
 C       3.774761    -0.375304     1.414647     119.09
 O       4.616438     0.735928     0.850113     219.16
 H       4.093230     1.651082     1.025717      26.02
 H       4.290757    -0.814222     2.210628      30.06
 H       2.814260    -0.022794     1.518166      27.71
55
name = lig-Water-frame_375
 C      -1.519830     2.391037     3.297970      86.78
 H      -2.108535     3.208853     3.191968      31.92
 C      -0.529303     0.247847     3.219432      65.99
 H      -0.378873    -0.920295     2.711854      23.10
 C       0.514637     0.547695     3.945940      26.67
 O       1.607579    -0.259305     4.347308     210.72
 C       1.485875    -1.619738     4.108458     129.79
 H       1.949838    -2.105909     4.977629      27.61
 H       1.824249    -2.017401     3.054377      28.25
 H       0.411354    -1.689389     4.120605      26.15
 C       0.754251     1.894870     4.214409      20.53
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 O       1.974127     2.267219     4.631342     175.38
 H       2.283514     3.137587     4.572757      22.33
 C      -0.183846     2.855023     3.925434     140.49
 H       0.081620     3.886843     4.391605      15.81
 C      -1.697938     1.136484     3.021542      49.67
 C      -3.019082     0.708511     2.461543      89.80
 H      -3.807956     1.538835     2.989684      24.30
 O      -3.449150    -0.605861     3.110332     243.10
 H      -4.409541    -0.725550     3.276959      29.97
 C      -3.189484     0.475322     0.927139      74.23
 H      -2.707946     1.433918     0.323570      23.45
 C      -4.587053     0.454900     0.436337     113.19
 O      -5.362998    -0.755705     0.587607     230.93
 H      -4.871379    -1.509531     0.952119      29.67
 H      -4.360431     0.469300    -0.623808      27.85
 H      -5.219876     1.159913     0.878568      29.06
 C       1.220751     0.196364    -0.694528      37.71
 H       1.800977     1.067440    -0.386399      24.99
 C       0.686848    -2.198303    -0.531162      37.01
 H       1.065461    -3.289550    -0.541053      23.76
 C      -0.692472    -1.988150    -0.512211      14.00
 O      -1.480118    -3.202546    -0.344683     142.63
 C      -2.351655    -3.252065    -1.584864     100.41
 H      -3.455662    -2.755664    -1.591532      24.53
 H      -1.588212    -3.401617    -2.368386      25.96
 H      -2.520829    -4.420814    -1.302419      23.66
 C      -1.075666    -0.684008    -0.105919       3.93
 O      -2.347733    -0.692531     0.518108      85.68
 C      -0.195813     0.398516    -0.259220      48.83
 H      -0.516431     1.527180     0.129137      20.61
 C       1.707565    -1.178100    -0.776734       8.01
 C       3.109350    -1.640404    -1.029463     105.28
 H       3.108594    -2.633685    -1.462514      26.57
 O       3.699076    -0.712664    -2.016534     210.76
 H       4.747075    -0.966350    -2.022254      24.52
 C       3.760679    -1.666088     0.388384      81.78
 H       3.224136    -2.275185     1.136417      26.90
 O       5.247202    -2.157784     0.376274     105.97
 H       5.880771    -1.969494    -0.376671      25.20
 C       3.742733    -0.430647     1.362661      93.32
 O       4.660017     0.753997     0.841690     210.70
 H       4.151311     1.451684     1.228251      29.47
 H       4.551579    -0.619551     2.210938      25.78
 H       2.699283    -0.086904     1.897967      24.56
55
name = lig-Water-frame_376
 C      -1.524010     2.470417     3.389254      69.43
 H      -2.237960     3.349219     2.972065      14.52
 C      -0.549912     0.250027     3.146329      63.12
 H      -0.469489    -0.687130     2.940038      25.33
 C       0.575998     0.596492     3.952960      18.77
 O       1.669455    -0.231917     4.412951     175.91
 C       1.441949    -1.592155     4.077784     133.54
 H       2.114670    -2.234812     4.723835      27.24
 H       1.920736    -2.070941     3.259842      28.59
 H       0.333293    -1.948248     4.101503      25.39
 C       0.730056     1.918860     4.223124      16.08
 O       2.025824     2.224187     4.643973     173.11
 H       2.026027     3.316529     4.591663      19.75
 C      -0.168183     2.823492     3.870321     102.62
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 H      -0.061740     3.882508     4.018901      36.77
 C      -1.665492     1.085431     2.993953      24.47
 C      -3.064016     0.742224     2.472069      78.06
 H      -3.535400     1.615777     2.753426      28.40
 O      -3.437546    -0.678400     3.120897     188.08
 H      -4.526758    -0.691781     3.161475      24.26
 C      -3.147134     0.463506     0.938337     100.65
 H      -2.757558     1.300829     0.558536      26.27
 C      -4.537865     0.478219     0.354143      82.31
 O      -5.333272    -0.779413     0.585359     246.90
 H      -4.830278    -1.488180     1.001292      29.80
 H      -4.316243     0.662269    -0.835622      25.09
 H      -5.421479     1.162109     0.757748      23.83
 C       1.192674     0.114580    -0.697821      69.85
 H       1.902738     0.911339    -0.452312      27.31
 C       0.700182    -2.188112    -0.581793      40.93
 H       0.883050    -3.225838    -0.669573      25.11
 C      -0.677724    -2.037074    -0.483222     -17.68
 O      -1.503171    -3.182437    -0.331949     155.70
 C      -2.363250    -3.301344    -1.613090      91.38
 H      -3.160076    -2.638363    -1.619350      26.71
 H      -1.621601    -3.284654    -2.617237      24.86
 H      -2.757787    -4.304775    -1.485875      27.10
 C      -1.136745    -0.622587    -0.151722     -19.23
 O      -2.342758    -0.693168     0.465377     116.96
 C      -0.218292     0.440607    -0.282316      64.47
 H      -0.614983     1.366094     0.008961      22.72
 C       1.688500    -1.141343    -0.754552       5.19
 C       3.170475    -1.611573    -1.020643     110.32
 H       2.896987    -2.675203    -1.478178      23.42
 O       3.678408    -0.732506    -2.011513     285.53
 H       4.573858    -0.807430    -2.184272      28.73
 C       3.880794    -1.671160     0.379708      87.34
 H       2.997517    -2.403746     0.936525      25.34
 O       5.227015    -2.116053     0.395307     130.55
 H       5.815584    -2.027707    -0.550751      21.87
 C       3.786013    -0.450282     1.318875     117.60
 O       4.662312     0.753543     0.834795     186.50
 H       4.296119     1.523496     1.505941      23.90
 H       4.347268    -0.731968     2.152561      31.17
 H       2.966210    -0.233426     1.863087      28.68
55
name = lig-Water-frame_377
 C      -1.477144     2.554101     3.462373      36.26
 H      -2.171064     3.141222     3.017126      16.40
 C      -0.553754     0.231504     3.120195      39.20
 H      -0.822898    -0.993644     2.848646      22.31
 C       0.635379     0.607193     3.943733      18.15
 O       1.696909    -0.197141     4.447651     169.83
 C       1.419792    -1.635361     4.071960     114.16
 H       2.042368    -2.205670     4.762771      28.27
 H       1.911823    -1.766613     3.001984      27.28
 H       0.463428    -2.209592     4.205346      26.45
 C       0.786036     1.944996     4.248205      -0.23
 O       2.080359     2.235956     4.662663     165.83
 H       1.953047     3.189807     4.800052      21.42
 C      -0.269412     2.868618     3.793588      95.82
 H      -0.052544     3.958612     3.715145      32.79
 C      -1.649925     1.072331     2.968656       2.44
 C      -3.058946     0.669539     2.477187      66.00
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 H      -3.782402     1.699375     2.579601      25.85
 O      -3.447587    -0.703946     3.132181     169.26
 H      -4.379219    -0.667108     3.063405      27.91
 C      -3.088841     0.489850     0.972342      83.99
 H      -2.581183     1.541206     0.563334      20.58
 C      -4.536749     0.466231     0.247591      90.95
 O      -5.307004    -0.811889     0.565309     233.83
 H      -4.586510    -1.432944     1.022871      25.33
 H      -4.504354     0.737791    -0.802422      26.35
 H      -5.053114     1.333639     0.539219      28.03
 C       1.125850     0.113926    -0.640739      55.02
 H       1.977844     0.849989    -0.809116      24.32
 C       0.709362    -2.200526    -0.664370      44.77
 H       0.979855    -3.348415    -0.849502      22.99
 C      -0.647811    -2.017874    -0.412989     -12.03
 O      -1.535152    -3.137220    -0.348227     142.42
 C      -2.335958    -3.387249    -1.626558     104.13
 H      -2.931591    -2.306287    -1.638191      23.43
 H      -1.909980    -3.063389    -2.638117      23.66
 H      -3.014919    -4.332132    -1.726276      25.16
 C      -1.168410    -0.619387    -0.210474     -19.21
 O      -2.380088    -0.684592     0.424403     108.08
 C      -0.218566     0.426407    -0.328781      67.50
 H      -0.557583     1.513646    -0.078273      21.46
 C       1.644064    -1.170844    -0.736118       2.23
 C       3.183958    -1.578188    -1.001409     102.51
 H       3.057558    -2.618343    -1.362786      22.44
 O       3.650758    -0.737664    -2.018547     271.00
 H       4.614977    -0.729659    -2.269874      27.44
 C       3.940368    -1.665869     0.373288     106.69
 H       3.348739    -2.517634     0.588711      27.34
 O       5.233489    -2.096641     0.400258     258.30
 H       5.468937    -2.008251    -0.444057      31.99
 C       3.911306    -0.452712     1.275860     106.21
 O       4.621360     0.747025     0.853521     174.11
 H       4.552887     1.469451     1.509165      24.52
 H       4.350171    -1.052112     2.255685      26.69
 H       2.750687    -0.151551     1.583143      24.74
55
name = lig-Water-frame_378
 C      -1.509114     2.485270     3.449310      13.67
 H      -2.302362     3.290363     3.088890      18.84
 C      -0.550477     0.145902     3.136427      46.95
 H      -0.951778    -0.736067     2.844998      25.60
 C       0.652920     0.593701     3.911134      15.94
 O       1.669530    -0.196331     4.455963     143.47
 C       1.472672    -1.694801     4.056576     110.74
 H       2.105007    -2.152722     4.834857      26.47
 H       1.595670    -1.497824     3.022884      28.02
 H       0.428274    -2.094974     4.234137      27.03
 C       0.831819     1.970948     4.232496       7.00
 O       2.111608     2.280716     4.694969      84.61
 H       2.251994     3.243457     4.999601      22.88
 C      -0.248531     2.984997     3.773849     121.81
 H       0.104575     4.028028     3.596366      26.42
 C      -1.646817     1.131928     2.992722      -2.11
 C      -3.031047     0.579564     2.485355      91.62
 H      -3.897408     1.152795     2.598128      27.40
 O      -3.447182    -0.677518     3.137507     166.47
 H      -4.532756    -0.771752     3.039981      23.51
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 C      -3.043657     0.563446     0.923773      86.68
 H      -2.576907     1.389414     0.615307      26.23
 C      -4.524268     0.442497     0.188693      66.77
 O      -5.255354    -0.826943     0.536209     264.00
 H      -4.529343    -1.349191     0.866722      28.11
 H      -4.546915     0.533482    -1.038764      23.87
 H      -4.854176     1.512379     0.604357      24.31
 C       1.103420     0.151480    -0.589582      26.77
 H       1.711531     0.907663    -1.041849      22.00
 C       0.703227    -2.281632    -0.756241      51.60
 H       1.103223    -3.186175    -0.961194      27.12
 C      -0.637163    -1.958960    -0.358014      19.00
 O      -1.560726    -3.111307    -0.376999     149.91
 C      -2.338218    -3.366457    -1.630437     114.56
 H      -2.888399    -2.537284    -1.595466      27.60
 H      -1.707139    -3.229156    -2.621105      24.79
 H      -3.094003    -4.228113    -1.734246      26.62
 C      -1.159248    -0.679806    -0.245471       8.71
 O      -2.431208    -0.660560     0.389386     126.72
 C      -0.238312     0.414133    -0.373630      56.43
 H      -0.345371     1.549976    -0.243071      21.58
 C       1.620695    -1.227721    -0.727009     -16.19
 C       3.163887    -1.538289    -0.971609      92.35
 H       3.313960    -2.679140    -1.342666      23.11
 O       3.622269    -0.713422    -2.053448     224.99
 H       4.687084    -0.768270    -2.183345      24.91
 C       3.936604    -1.627172     0.337635      72.82
 H       3.418909    -2.672847     0.858850      23.81
 O       5.293520    -2.103950     0.391778     169.71
 H       5.599808    -2.037381    -0.649003      24.26
 C       3.975853    -0.453763     1.310717     140.45
 O       4.598034     0.711556     0.862484     237.10
 H       4.480416     1.400536     1.566312      24.74
 H       4.296092    -0.884937     2.187185      30.88
 H       3.008871    -0.174520     1.174473      27.04
55
name = lig-Water-frame_379
 C      -1.570665     2.429827     3.374454      98.79
 H      -2.270491     3.203850     3.343360      29.99
 C      -0.555599     0.155414     3.201578      58.42
 H      -0.855555    -0.986139     2.840691      21.69
 C       0.629408     0.572844     3.871971      17.64
 O       1.613481    -0.228433     4.451681     138.35
 C       1.516996    -1.700939     4.068319     104.10
 H       2.344840    -2.245689     4.600071      25.83
 H       1.525484    -1.709502     2.919209      27.37
 H       0.403224    -1.807590     4.318997      24.53
 C       0.829306     2.050942     4.165157       1.56
 O       2.127952     2.317881     4.738770     145.01
 H       2.451518     3.334096     4.885884      21.32
 C      -0.125053     3.051496     3.794885     124.33
 H       0.120905     4.095795     3.718386      21.02
 C      -1.644682     1.152471     3.047905      32.67
 C      -3.004748     0.489192     2.478159      79.58
 H      -4.000386     1.126757     2.835639      23.36
 O      -3.450962    -0.657521     3.141033     230.36
 H      -4.398128    -0.799147     3.050395      29.11
 C      -3.043369     0.568775     0.823690      75.53
 H      -2.454956     1.573884     0.470420      22.11
 C      -4.486389     0.457937     0.155148      95.00
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 O      -5.190687    -0.808190     0.500638     255.48
 H      -4.493911    -1.490160     0.715627      26.69
 H      -4.361980     0.375527    -0.873742      27.91
 H      -5.083267     1.228472     0.571623      27.53
 C       1.121183     0.136603    -0.581367      22.95
 H       1.560763     1.092439    -1.021986      19.38
 C       0.685009    -2.316826    -0.816408      30.87
 H       1.132009    -3.404440    -1.093766      21.73
 C      -0.640238    -1.988483    -0.371959      18.92
 O      -1.570782    -3.105147    -0.385324     170.14
 C      -2.326917    -3.288979    -1.651965      93.26
 H      -3.238202    -2.447887    -1.760188      23.02
 H      -1.426794    -3.688482    -2.326821      23.14
 H      -2.895065    -4.238810    -1.458230      26.54
 C      -1.161422    -0.707758    -0.214587      14.03
 O      -2.451739    -0.639811     0.338340     159.27
 C      -0.256490     0.406189    -0.414615      51.09
 H      -0.470951     1.446569    -0.354221      22.60
 C       1.621630    -1.252593    -0.732789     -11.01
 C       3.124166    -1.540402    -0.964218     100.64
 H       3.383249    -2.534136    -1.339631      23.89
 O       3.609359    -0.672503    -2.089675     268.49
 H       4.508979    -0.789788    -2.058613      28.79
 C       3.931959    -1.625152     0.356224      82.16
 H       3.425382    -2.166504     1.095389      26.75
 O       5.383039    -2.121368     0.321261     157.73
 H       6.026071    -2.167114    -0.497959      23.67
 C       3.966848    -0.465924     1.318089      97.87
 O       4.628611     0.691473     0.861063     195.40
 H       4.183630     1.406050     1.548452      20.86
 H       4.308993    -0.664376     2.484251      23.67
 H       2.773470    -0.178289     1.296535      22.14
55
name = lig-Water-frame_380
 C      -1.513778     2.477625     3.331592      78.49
 H      -2.455657     3.133979     3.460875      23.18
 C      -0.573423     0.180045     3.276701      66.43
 H      -0.480865    -0.879348     3.039667      22.34
 C       0.590429     0.587177     3.852576      15.18
 O       1.568002    -0.270415     4.428845     168.57
 C       1.527624    -1.653159     4.062700     121.99
 H       2.367028    -2.277465     4.357620      27.49
 H       1.618678    -2.047807     3.036841      28.86
 H       0.577391    -1.977659     4.491874      26.63
 C       0.849254     2.133454     4.093203       5.75
 O       2.127876     2.331989     4.772372     136.11
 H       2.216188     3.368748     4.564049      24.88
 C      -0.058142     3.029088     3.800947      95.53
 H       0.009299     4.155204     4.015391      30.77
 C      -1.671818     1.055420     3.078864      21.50
 C      -3.032967     0.506262     2.464316      79.88
 H      -3.555834     1.386885     2.773226      25.94
 O      -3.421248    -0.689848     3.151371     215.68
 H      -4.451003    -0.717963     2.997983      23.08
 C      -3.058073     0.569939     0.745469      97.32
 H      -2.596184     1.454711     0.449129      26.09
 C      -4.440992     0.460867     0.174726      84.72
 O      -5.117540    -0.791896     0.469701     162.39
 H      -4.521772    -1.653991     0.491868      25.04
 H      -4.096988     0.477055    -1.048794      23.93
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 H      -5.399818     1.091726     0.380801      23.41
 C       1.128800     0.101723    -0.617826      40.41
 H       1.746265     0.980341    -0.728801      23.58
 C       0.683250    -2.326937    -0.845051      51.76
 H       0.838287    -3.308783    -1.075461      23.36
 C      -0.653161    -2.088729    -0.439165     -15.37
 O      -1.577455    -3.087673    -0.370202     229.81
 C      -2.324645    -3.244559    -1.643751     110.53
 H      -2.981467    -2.606833    -2.132889      26.49
 H      -1.561710    -3.675227    -2.309403      26.67
 H      -2.684179    -4.229862    -1.144004      22.59
 C      -1.156317    -0.695204    -0.147584       0.78
 O      -2.440856    -0.636956     0.264540     151.58
 C      -0.263147     0.355253    -0.439414      64.60
 H      -0.832754     1.434642    -0.410251      22.56
 C       1.631182    -1.246707    -0.758849      26.63
 C       3.093199    -1.543613    -0.977005      88.85
 H       3.171902    -2.632796    -1.419054      21.82
 O       3.583808    -0.631040    -2.098892     207.08
 H       4.594724    -0.752630    -2.051561      25.45
 C       3.991290    -1.591530     0.400565      60.97
 H       3.270492    -2.292920     1.182349      24.76
 O       5.466867    -2.155584     0.259103     151.79
 H       6.033912    -2.081197    -0.496344      26.25
 C       3.893127    -0.442659     1.341766     126.33
 O       4.660235     0.705298     0.876115     262.25
 H       4.213366     1.470564     1.226554      28.78
 H       4.205492    -0.573664     2.321376      29.17
 H       2.912521    -0.301988     1.670265      27.84
55
name = lig-Water-frame_381
 C      -1.394144     2.515311     3.316792      54.42
 H      -2.356558     3.003838     3.428631      20.78
 C      -0.575266     0.192267     3.351550      46.77
 H      -0.495044    -0.924387     3.134454      24.47
 C       0.593115     0.682103     3.877709      11.53
 O       1.540474    -0.288156     4.380167     169.95
 C       1.510814    -1.644695     4.056354     126.38
 H       2.479047    -2.076368     4.537700      25.90
 H       1.496574    -1.971169     2.982874      28.83
 H       0.840629    -2.441799     4.651937      26.30
 C       0.940856     2.066660     4.059559      18.49
 O       2.089230     2.347592     4.769510      86.11
 H       2.161115     3.367049     4.595841      25.03
 C      -0.143188     3.028460     3.775040      82.92
 H      -0.088512     3.962616     4.260230      20.60
 C      -1.700942     0.985691     3.081279      19.15
 C      -3.008499     0.589527     2.440582      68.18
 H      -3.581170     1.635665     2.623180      23.49
 O      -3.407259    -0.723869     3.146871     163.28
 H      -4.451876    -0.695725     3.041282      21.76
 C      -3.085539     0.547084     0.768224      86.24
 H      -2.612942     1.545065     0.400353      24.83
 C      -4.425192     0.445592     0.135103     119.68
 O      -5.051112    -0.811322     0.436572     195.02
 H      -4.473608    -1.530098     0.318978      29.06
 H      -4.191146     0.631667    -0.884737      27.83
 H      -5.206821     1.195624     0.162861      26.64
 C       1.125405     0.060098    -0.661010      46.48
 H       2.000584     0.754032    -0.442237      24.66
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 C       0.655601    -2.297289    -0.838751      57.16
 H       0.820953    -3.435643    -1.119662      22.99
 C      -0.655014    -2.100132    -0.495190       5.55
 O      -1.589973    -3.059206    -0.349853     211.24
 C      -2.299791    -3.315081    -1.594112     101.62
 H      -2.846890    -2.444984    -2.270696      24.01
 H      -1.624135    -3.549407    -2.622537      24.43
 H      -2.956882    -4.129354    -1.370604      25.62
 C      -1.097214    -0.737967    -0.108464       1.73
 O      -2.431122    -0.641595     0.185835     127.75
 C      -0.289333     0.312225    -0.445572      73.32
 H      -0.705071     1.183027    -0.369571      27.11
 C       1.623477    -1.225740    -0.794750      28.56
 C       3.099850    -1.556425    -1.007796      81.98
 H       2.945585    -2.599566    -1.392324      24.32
 O       3.564400    -0.606251    -2.074360     203.58
 H       4.619678    -0.633638    -2.175338      24.53
 C       4.035868    -1.601598     0.442404      67.27
 H       3.605191    -2.522584     0.686016      26.18
 O       5.502358    -2.191594     0.237447      80.99
 H       5.797270    -1.756358    -0.783613      20.55
 C       3.854652    -0.385026     1.367011     105.00
 O       4.682599     0.721957     0.881054     179.65
 H       4.299865     1.687728     1.087028      24.22
 H       4.426064    -0.812562     2.407295      26.17
 H       2.757638    -0.204294     1.733430      25.16
55
name = lig-Water-frame_382
 C      -1.311581     2.461104     3.300853      62.30
 H      -2.168242     3.172562     3.312989      26.59
 C      -0.602430     0.184360     3.401963      33.77
 H      -0.791111    -0.976676     3.268912      23.17
 C       0.638428     0.745891     3.923675      26.09
 O       1.518516    -0.267111     4.333138     162.14
 C       1.522225    -1.719396     4.077550     123.43
 H       2.519418    -1.749841     4.495781      26.34
 H       1.338910    -1.708122     2.979046      27.05
 H       0.948295    -2.418306     4.611547      29.12
 C       0.981442     1.980271     4.034301      34.88
 O       2.043421     2.353443     4.747647     126.46
 H       2.347408     3.482516     4.885736      22.28
 C      -0.226868     2.983153     3.765912     119.05
 H      -0.166845     3.922845     4.387123      21.24
 C      -1.664341     1.014700     3.071755      40.77
 C      -2.972145     0.681090     2.413742      86.89
 H      -3.837708     1.343906     2.514893      25.99
 O      -3.413834    -0.712077     3.119952     176.69
 H      -4.381913    -0.792684     3.137404      25.79
 C      -3.072993     0.539055     0.843914      85.99
 H      -2.632888     1.482065     0.441680      25.74
 C      -4.429883     0.429604     0.082828      97.50
 O      -5.013977    -0.839363     0.394866     146.79
 H      -4.220790    -1.466161     0.228636      25.04
 H      -4.256473     0.597138    -1.137082      24.45
 H      -5.009318     1.427461     0.356719      26.34
 C       1.130475     0.038904    -0.675726      50.05
 H       1.910940     0.716212    -0.365975      22.88
 C       0.644831    -2.305302    -0.838832      64.25
 H       1.031928    -3.258778    -1.105701      25.38
 C      -0.651595    -2.023107    -0.509543      31.30
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 O      -1.621501    -3.065100    -0.346230     166.13
 C      -2.291878    -3.389169    -1.624134     118.34
 H      -2.648627    -2.375488    -1.709721      25.79
 H      -1.603894    -3.636450    -2.400352      27.93
 H      -3.304494    -4.004901    -1.737856      24.56
 C      -1.047031    -0.819112    -0.113515      21.76
 O      -2.427650    -0.647312     0.121183     108.36
 C      -0.252888     0.265860    -0.437533      54.49
 H      -0.572563     1.453435    -0.252800      20.35
 C       1.600589    -1.237097    -0.835662      24.09
 C       3.123211    -1.547534    -1.032118      81.40
 H       3.123060    -2.626793    -1.432216      24.56
 O       3.555604    -0.592929    -2.038312     266.93
 H       4.435779    -0.586525    -2.225359      29.71
 C       4.063424    -1.648754     0.399374      53.04
 H       3.740947    -2.760333     0.646554      23.95
 O       5.494003    -2.179166     0.195756     173.53
 H       5.724604    -1.752856    -0.573811      27.41
 C       3.875238    -0.358391     1.445059     105.08
 O       4.694910     0.741983     0.871568     199.20
 H       4.308384     1.570049     1.294842      25.33
 H       4.388493    -0.818401     2.178509      29.73
 H       2.866709    -0.027219     1.514173      24.36
55
name = lig-Water-frame_383
 C      -1.372127     2.381267     3.256101      69.20
 H      -1.993475     3.294030     3.050518      22.73
 C      -0.652449     0.175249     3.443801      65.76
 H      -0.912137    -0.837377     3.453320      27.36
 C       0.627175     0.617071     3.932957      20.57
 O       1.521996    -0.226594     4.324935     139.72
 C       1.555673    -1.743870     4.076183     107.65
 H       2.703081    -1.856554     4.179198      27.15
 H       1.332293    -1.799376     3.013082      28.10
 H       0.723177    -2.318753     4.713240      26.55
 C       0.933000     2.063069     4.016375      26.27
 O       2.052866     2.364102     4.745445     261.61
 H       2.135873     3.292751     4.797446      32.59
 C      -0.155353     2.901971     3.824679     101.12
 H      -0.228890     3.915934     4.223065      19.04
 C      -1.594668     1.111444     3.047002      50.79
 C      -2.981457     0.676637     2.394702      88.86
 H      -3.949046     1.237319     2.654164      24.77
 O      -3.398464    -0.667533     3.082498     178.65
 H      -4.483588    -0.769739     3.120923      22.44
 C      -3.026172     0.526168     0.869368      89.64
 H      -2.546066     1.457182     0.485913      26.44
 C      -4.427609     0.462856     0.031720     104.43
 O      -4.991684    -0.872970     0.339467     176.01
 H      -4.112047    -1.401045     0.322296      24.55
 H      -4.275872     0.475238    -0.974783      28.57
 H      -4.918406     1.222220     0.638247      28.71
 C       1.135556     0.043819    -0.657133      45.56
 H       1.747387     0.979006    -0.555276      24.52
 C       0.691491    -2.310130    -0.854011      64.34
 H       1.135351    -3.309345    -1.086439      24.47
 C      -0.661740    -2.050849    -0.513040       3.20
 O      -1.642173    -3.120396    -0.326121     143.70
 C      -2.331237    -3.399807    -1.665241      92.02
 H      -2.606658    -2.297009    -1.676213      23.87
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 H      -1.353378    -3.897645    -2.290050      23.63
 H      -3.202734    -3.945821    -1.679624      28.45
 C      -1.073383    -0.789858    -0.136189      10.68
 O      -2.418427    -0.653096     0.085822     108.08
 C      -0.176901     0.291866    -0.398980      54.52
 H      -0.392394     1.251857    -0.158485      24.09
 C       1.601634    -1.297464    -0.876417      37.64
 C       3.151823    -1.552152    -1.040425      98.42
 H       3.492574    -2.544276    -1.512497      24.07
 O       3.531456    -0.572996    -2.001715     250.06
 H       4.535802    -0.638796    -2.220495      25.51
 C       4.051069    -1.728976     0.314578      62.18
 H       3.555445    -2.487478     0.989043      27.03
 O       5.446573    -2.139519     0.176125     132.83
 H       6.076372    -1.702456    -0.690073      20.32
 C       3.945421    -0.375671     1.429195      82.39
 O       4.700944     0.750578     0.875467     136.93
 H       4.320746     1.501545     1.536422      22.73
 H       4.377203    -0.756751     2.570758      27.92
 H       2.883958     0.023011     1.476289      24.45
55
name = lig-Water-frame_384
 C      -1.413160     2.451966     3.225057      74.84
 H      -2.050492     3.156011     2.735836      20.54
 C      -0.665338     0.172059     3.490288      68.80
 H      -1.066280    -0.994543     3.646358      23.07
 C       0.535735     0.505777     3.892838      29.94
 O       1.592551    -0.233224     4.355205     171.26
 C       1.584150    -1.715407     4.056061     117.60
 H       2.536528    -2.221892     4.057093      28.97
 H       1.279885    -2.054373     3.014352      28.40
 H       0.905597    -2.099236     4.709095      30.07
 C       0.874057     2.086708     4.036326      10.21
 O       2.076702     2.334794     4.737464     167.84
 H       2.087027     3.492642     4.711220      28.88
 C      -0.114695     2.845518     3.874549      76.24
 H      -0.111804     3.923910     3.986484      26.29
 C      -1.608555     1.134958     2.979905      36.19
 C      -3.019422     0.591042     2.410853      90.51
 H      -3.701973     1.435062     2.782749      26.84
 O      -3.383801    -0.615777     3.045618     283.07
 H      -4.322500    -0.599362     2.946420      26.72
 C      -2.981681     0.523562     0.804130     100.97
 H      -2.385473     1.464217     0.481194      22.89
 C      -4.396004     0.477876     0.098794      84.29
 O      -4.968304    -0.902098     0.280815     201.30
 H      -4.266683    -1.482852     0.466273      29.22
 H      -4.232068     0.665669    -1.158658      23.40
 H      -5.181970     1.116605     0.590414      26.31
 C       1.188285     0.054499    -0.636130      42.33
 H       1.683561     1.003537    -0.949590      23.13
 C       0.729225    -2.353070    -0.872407      50.22
 H       1.009226    -3.447186    -1.007532      21.73
 C      -0.676221    -2.147698    -0.502015     -33.72
 O      -1.642083    -3.195476    -0.297041     139.00
 C      -2.308288    -3.363453    -1.688219      92.43
 H      -2.623692    -2.438247    -2.357948      24.78
 H      -1.652135    -3.857282    -2.247197      28.30
 H      -3.175807    -4.148226    -1.409649      23.91
 C      -1.105819    -0.719971    -0.191025       6.07
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 O      -2.412999    -0.646791     0.090410     146.21
 C      -0.129563     0.300627    -0.325128      50.53
 H      -0.440386     1.414966    -0.027859      19.94
 C       1.665264    -1.323076    -0.902073      30.22
 C       3.191974    -1.588070    -1.044232     104.85
 H       3.496284    -2.536474    -1.571396      24.15
 O       3.529955    -0.528916    -1.972210     240.55
 H       4.552757    -0.699502    -2.138601      26.12
 C       4.023021    -1.729199     0.282230      83.17
 H       3.398845    -2.307321     1.052388      26.69
 O       5.394275    -2.090117     0.140494     216.63
 H       6.096295    -1.849328    -0.488008      26.95
 C       4.033662    -0.434194     1.379160     125.67
 O       4.704687     0.753414     0.910925     212.39
 H       4.455168     1.564560     1.496555      23.24
 H       4.139954    -0.496577     2.396174      31.51
 H       2.963022    -0.199096     1.552698      29.85
55
name = lig-Water-frame_385
 C      -1.405419     2.553451     3.193939      57.29
 H      -2.131832     3.159733     2.555060      17.81
 C      -0.752746     0.100363     3.517431      51.74
 H      -1.037946    -0.815435     3.645271      24.52
 C       0.530360     0.516321     3.881007      16.57
 O       1.691280    -0.284196     4.375483     148.62
 C       1.601586    -1.674379     4.006027     120.56
 H       2.495869    -2.383267     4.242298      26.13
 H       1.094082    -1.990487     3.090703      27.06
 H       0.961085    -2.140320     4.921821      25.43
 C       0.899026     1.916480     4.107614      -5.16
 O       2.084421     2.332140     4.705706     225.63
 H       2.387030     3.242845     4.786734      31.23
 C      -0.230293     2.913348     3.860931      31.79
 H       0.162276     4.003074     3.853299      19.89
 C      -1.668345     1.088278     2.921458      29.62
 C      -2.994090     0.547381     2.420639      90.89
 H      -3.550602     1.515327     2.639852      27.24
 O      -3.367660    -0.578562     3.016495     275.60
 H      -4.438300    -0.650614     2.841731      23.36
 C      -2.965250     0.551246     0.717123      95.18
 H      -2.414005     1.396235     0.440801      23.04
 C      -4.364393     0.482414     0.161403     100.31
 O      -4.951425    -0.915421     0.223187     218.66
 H      -4.371830    -1.672495     0.611970      26.08
 H      -4.283182     0.850858    -0.775186      27.12
 H      -5.293717     1.072260     0.350723      25.07
 C       1.264256     0.038617    -0.653625      33.70
 H       1.874567     0.797997    -1.121888      21.17
 C       0.707992    -2.428094    -0.864457      45.93
 H       0.949299    -3.458820    -0.959044      21.82
 C      -0.658861    -2.173293    -0.470101     -14.48
 O      -1.627748    -3.240683    -0.313066     142.07
 C      -2.322617    -3.354252    -1.684904      88.33
 H      -2.629194    -2.715612    -2.488625      23.51
 H      -1.630864    -4.091244    -2.501846      22.80
 H      -3.025994    -4.042869    -1.327006      25.79
 C      -1.081194    -0.737723    -0.269517       5.28
 O      -2.417179    -0.630099     0.125978     164.32
 C      -0.128363     0.323757    -0.225753      51.75
 H      -0.453666     1.375360    -0.067875      17.59
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 C       1.733130    -1.314262    -0.899586       6.32
 C       3.212688    -1.616277    -1.060828      89.11
 H       3.247706    -2.646899    -1.608648      22.22
 O       3.570051    -0.483712    -1.941811     291.24
 H       4.454629    -0.537282    -2.110498      29.10
 C       4.007142    -1.625127     0.310689      78.19
 H       3.434397    -2.529866     0.805167      24.60
 O       5.337159    -2.092118     0.143923     175.85
 H       5.871319    -1.670933    -0.688548      23.79
 C       4.053954    -0.470866     1.281851     125.47
 O       4.733797     0.750203     0.937975     232.29
 H       4.365269     1.586827     1.429347      20.16
 H       4.345938    -0.691326     2.468355      25.90
 H       2.926372    -0.362226     1.374682      25.00
55
name = lig-Water-frame_386
 C      -1.410758     2.568321     3.118218      36.03
 H      -2.025883     3.343681     2.693587      26.92
 C      -0.847355     0.093663     3.509808      32.54
 H      -1.121099    -1.151257     3.580420      20.46
 C       0.620014     0.556916     3.930506      19.49
 O       1.769861    -0.335281     4.361815     163.61
 C       1.583118    -1.695222     4.034754     127.75
 H       2.559903    -2.084666     4.210887      28.68
 H       1.010326    -1.746492     3.074751      26.86
 H       1.001471    -2.158210     4.748540      30.29
 C       0.850067     1.800957     4.178677      12.34
 O       2.096727     2.278068     4.670108     142.08
 H       2.321957     3.302549     4.751196      24.82
 C      -0.281247     2.979703     3.817951      16.18
 H       0.157604     3.911813     3.848264      19.66
 C      -1.674312     1.044631     2.937836      43.18
 C      -2.918690     0.617578     2.357978      91.32
 H      -3.777793     1.407831     2.379443      23.70
 O      -3.396364    -0.590430     3.005693     255.24
 H      -4.340425    -0.793779     2.911427      29.15
 C      -2.969828     0.570396     0.700870      81.02
 H      -2.466508     1.591995     0.292854      19.43
 C      -4.382713     0.462541     0.211604      86.04
 O      -4.936470    -0.922439     0.171578     225.42
 H      -4.426520    -1.629035     0.689099      26.26
 H      -4.244792     0.883132    -0.990295      22.49
 H      -5.144940     1.148731     0.627469      25.27
 C       1.295413    -0.007827    -0.686119      33.56
 H       2.143099     0.717232    -0.955993      22.62
 C       0.681897    -2.450230    -0.822784      42.66
 H       1.048435    -3.558950    -0.982735      21.83
 C      -0.607777    -2.139517    -0.442914      20.26
 O      -1.596122    -3.232533    -0.381136     148.84
 C      -2.296283    -3.463913    -1.695403      95.63
 H      -2.736411    -2.425989    -2.256331      22.59
 H      -1.725463    -4.037021    -2.232599      27.95
 H      -3.266475    -4.041551    -1.425496      25.31
 C      -1.038754    -0.792489    -0.309352       1.99
 O      -2.398336    -0.629589     0.158122     146.17
 C      -0.093135     0.305602    -0.175390      41.97
 H      -0.442144     1.363799    -0.079416      18.72
 C       1.716674    -1.331859    -0.866759      -3.29
 C       3.201197    -1.603048    -1.094196      80.64
 H       3.235092    -2.603234    -1.529949      23.62
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 O       3.618707    -0.450121    -1.914558     245.83
 H       4.649462    -0.301973    -2.130717      23.61
 C       4.004888    -1.566755     0.318626      78.94
 H       3.547443    -2.526934     0.693911      25.58
 O       5.321409    -2.114606     0.129762     144.64
 H       5.454170    -1.523101    -0.700530      23.00
 C       4.006736    -0.474078     1.253404     146.29
 O       4.779747     0.737400     0.945091     232.52
 H       4.139399     1.432458     1.423667      22.42
 H       4.511054    -1.057994     1.970596      31.23
 H       2.921227    -0.230923     1.314181      24.29
55
name = lig-Water-frame_387
 C      -1.392317     2.529693     3.049910      42.00
 H      -2.018836     3.427177     2.796604      24.44
 C      -0.843455     0.072470     3.515254      44.01
 H      -1.106889    -0.855900     3.407331      24.92
 C       0.666627     0.471091     3.995487     -13.91
 O       1.802991    -0.338237     4.334784     140.98
 C       1.557549    -1.725952     4.063505     117.94
 H       2.680641    -1.982035     3.891821      26.35
 H       1.215514    -1.696014     3.002600      28.20
 H       0.814606    -2.327908     4.767377      26.11
 C       0.766780     1.895322     4.246115      -8.80
 O       2.111446     2.214090     4.638030     115.59
 H       1.866256     3.224248     4.625164      24.67
 C      -0.258697     2.931477     3.765739      46.12
 H       0.011652     4.081517     3.917760      21.93
 C      -1.644203     1.066183     2.999860      44.01
 C      -2.929566     0.697858     2.239699      88.59
 H      -3.810365     1.337467     2.381705      24.37
 O      -3.398422    -0.618067     3.000115     195.98
 H      -4.452057    -0.683488     2.869698      23.66
 C      -2.946989     0.595612     0.721436     102.53
 H      -2.667992     1.476440     0.292554      25.63
 C      -4.428358     0.452298     0.188149     103.48
 O      -4.923546    -0.915213     0.138458     248.15
 H      -4.390949    -1.450834     0.680243      28.81
 H      -4.395509     0.629206    -0.775182      28.19
 H      -4.868531     1.122919     1.021009      25.91
 C       1.285059    -0.040031    -0.692678      57.93
 H       2.058217     0.679502    -0.568876      27.68
 C       0.732704    -2.438995    -0.773218      70.30
 H       1.015787    -3.390878    -0.973908      26.18
 C      -0.586917    -2.131615    -0.448249      26.89
 O      -1.555173    -3.195024    -0.456594     156.03
 C      -2.326654    -3.536280    -1.667645      92.61
 H      -2.531573    -2.526245    -1.846262      25.25
 H      -1.481859    -4.228561    -2.372184      23.15
 H      -3.339598    -3.968050    -1.577643      26.59
 C      -1.011241    -0.789040    -0.268069       8.63
 O      -2.339323    -0.650864     0.169898     155.54
 C      -0.015154     0.236067    -0.202888      37.16
 H      -0.407498     1.350326    -0.025967      20.08
 C       1.645635    -1.392468    -0.833008       7.53
 C       3.188427    -1.538581    -1.106400      94.84
 H       3.500947    -2.593117    -1.576851      23.79
 O       3.677649    -0.422140    -1.910276     256.64
 H       4.678242    -0.203834    -1.943456      23.04
 C       3.969964    -1.617175     0.239283      69.04
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 H       3.371746    -2.382869     0.973299      27.99
 O       5.311522    -2.119478     0.092437     113.14
 H       5.779338    -1.650392    -0.621177      22.95
 C       3.943763    -0.448318     1.240463     124.32
 O       4.805720     0.709438     0.949479     187.03
 H       4.365954     1.414437     1.417160      26.31
 H       4.560357    -1.152140     1.985710      28.71
 H       2.980524    -0.059956     1.614411      26.33
55
name = lig-Water-frame_388
 C      -1.344435     2.471754     3.025592      62.92
 H      -2.116732     3.200060     2.733220      23.87
 C      -0.705882     0.095596     3.541235      42.03
 H      -1.170068    -1.041350     3.239791      22.86
 C       0.605183     0.408889     4.058786     -12.23
 O       1.778773    -0.307262     4.313441     148.15
 C       1.568290    -1.764947     4.042818     124.80
 H       2.488808    -2.255680     3.848551      29.47
 H       1.250877    -1.874656     2.998820      30.40
 H       0.957180    -2.316031     4.693110      29.68
 C       0.698165     1.968985     4.273669     -18.47
 O       2.069549     2.189146     4.605198     156.28
 H       2.063179     3.129431     4.705534      28.33
 C      -0.173240     2.857343     3.730172      72.91
 H      -0.237629     3.860857     3.966537      27.21
 C      -1.645144     1.151860     3.031239      14.36
 C      -2.962429     0.718716     2.179062      74.45
 H      -3.716952     1.536908     2.611528      24.10
 O      -3.395460    -0.627925     2.968156     191.88
 H      -4.396205    -0.455027     2.890917      22.94
 C      -2.937606     0.560399     0.715670      94.02
 H      -2.591251     1.595711     0.175947      22.64
 C      -4.445678     0.431594     0.221338      92.24
 O      -4.915751    -0.902735     0.132220     214.77
 H      -4.289435    -1.477531     0.730697      23.99
 H      -4.677747     0.860073    -0.984393      22.78
 H      -4.966796     1.008257     0.947795      27.87
 C       1.257462    -0.072204    -0.651384      65.55
 H       1.961122     0.748821    -0.312111      26.65
 C       0.782730    -2.417970    -0.724688      58.56
 H       1.050818    -3.534869    -0.999039      23.15
 C      -0.606421    -2.144447    -0.492328       4.25
 O      -1.505350    -3.178253    -0.476905     203.17
 C      -2.303320    -3.596322    -1.667724     102.10
 H      -2.410389    -2.421859    -2.096991      24.09
 H      -1.798878    -4.038853    -2.361337      30.27
 H      -3.262261    -4.094931    -1.444263      25.89
 C      -0.985762    -0.769979    -0.175775      11.94
 O      -2.265113    -0.663947     0.177092     169.16
 C       0.022812     0.184387    -0.264105      75.53
 H      -0.225542     1.136468     0.029910      26.70
 C       1.649184    -1.418878    -0.834764      28.27
 C       3.202377    -1.502161    -1.114873     114.75
 H       3.538589    -2.355438    -1.666818      26.98
 O       3.720788    -0.390602    -1.916867     293.72
 H       4.616701    -0.270662    -1.672724      28.00
 C       3.894133    -1.671489     0.170884      79.56
 H       3.302104    -2.302211     0.898555      28.89
 O       5.301463    -2.129110     0.058728     123.92
 H       6.149146    -1.816034    -0.501552      23.01
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 C       3.932537    -0.434618     1.256940     130.02
 O       4.829173     0.666881     0.942536     148.88
 H       4.665141     1.587638     1.518306      20.08
 H       4.345040    -0.751222     2.211293      31.47
 H       3.066214    -0.072588     1.908404      28.35
55
name = lig-Water-frame_389
 C      -1.301024     2.428979     3.034536      62.48
 H      -2.075165     3.050176     2.596164      24.96
 C      -0.589359     0.091572     3.533261      60.57
 H      -0.901126    -0.859783     3.287646      27.62
 C       0.492506     0.452195     4.114637      19.15
 O       1.715729    -0.298456     4.291048     154.76
 C       1.601279    -1.794306     3.970564     107.95
 H       2.551979    -2.460784     4.131632      26.63
 H       0.992569    -1.995531     3.027197      29.24
 H       0.979781    -2.271083     4.829040      26.64
 C       0.714139     1.907121     4.273695       9.87
 O       2.000098     2.198179     4.589399      86.96
 H       2.509848     3.104845     4.848012      28.51
 C      -0.119944     2.819336     3.697040      78.35
 H      -0.165289     3.910770     4.058888      24.69
 C      -1.650634     1.148736     3.019535       8.09
 C      -2.953097     0.711074     2.263843      75.39
 H      -3.568320     1.541009     2.481538      27.74
 O      -3.383832    -0.589378     2.904882     233.05
 H      -4.419798    -0.573186     2.986435      23.42
 C      -2.943739     0.542043     0.637182      99.55
 H      -2.460513     1.352737     0.268496      29.19
 C      -4.456437     0.435676     0.199824     115.20
 O      -4.900768    -0.910644     0.153857     257.98
 H      -4.366735    -1.602835     0.638166      25.55
 H      -4.680617     1.031065    -0.561898      28.56
 H      -5.284259     0.990178     0.833632      26.05
 C       1.299414    -0.105578    -0.584301      47.63
 H       1.959669     0.705718    -0.425490      27.36
 C       0.775342    -2.467383    -0.704120      45.39
 H       1.071503    -3.443863    -0.916838      25.33
 C      -0.598875    -2.129768    -0.546847      15.56
 O      -1.469551    -3.203924    -0.461873     180.45
 C      -2.286464    -3.539079    -1.679527      92.04
 H      -2.607829    -2.812580    -2.380469      26.89
 H      -1.730444    -4.232501    -2.634781      23.86
 H      -3.096228    -4.184253    -1.133456      22.22
 C      -0.939963    -0.821308    -0.103397      24.45
 O      -2.234797    -0.651771     0.205231     184.34
 C      -0.032874     0.171362    -0.306794      66.57
 H      -0.121244     1.290009     0.228884      25.47
 C       1.758200    -1.368616    -0.869761      40.60
 C       3.204581    -1.479121    -1.147796      91.82
 H       3.385294    -2.413617    -1.883613      24.84
 O       3.741619    -0.356863    -1.924443     239.88
 H       4.683039    -0.246566    -1.419578      23.93
 C       3.877284    -1.647825     0.180610      67.59
 H       3.312680    -2.644950     0.643030      25.99
 O       5.287323    -2.177556     0.063430     105.46
 H       5.885544    -1.650471    -0.592165      25.22
 C       3.936368    -0.409999     1.324673     117.07
 O       4.867871     0.647640     0.923397     152.98
 H       4.660344     1.378278     1.532375      26.01
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 H       4.333710    -0.774329     2.352259      29.64
 H       2.920202    -0.065317     1.607936      28.13
55
name = lig-Water-frame_390
 C      -1.277452     2.421225     3.054717      42.91
 H      -1.878755     3.201101     2.481651      24.45
 C      -0.638768     0.107970     3.454293      20.65
 H      -0.710453    -1.085794     3.295203      24.05
 C       0.503907     0.542279     4.193277      26.73
 O       1.641351    -0.321820     4.262821      91.78
 C       1.596729    -1.834015     3.941398     123.38
 H       2.583216    -2.168141     4.223074      28.76
 H       1.011973    -2.035871     3.095424      31.29
 H       0.987807    -2.068502     4.816086      28.89
 C       0.770355     1.838258     4.253021      15.66
 O       1.980141     2.203000     4.606176     180.36
 H       2.388522     3.107057     4.867532      22.06
 C      -0.112070     2.847544     3.687689      49.84
 H       0.227087     3.843156     3.960371      23.65
 C      -1.619168     1.013476     2.994301      35.10
 C      -2.906614     0.662121     2.371494      71.08
 H      -3.711239     1.575339     2.285205      25.80
 O      -3.370922    -0.526184     2.842287     249.96
 H      -4.364299    -0.732281     2.918969      25.91
 C      -2.950133     0.525558     0.609505      75.58
 H      -2.294832     1.432110     0.185050      25.80
 C      -4.471784     0.446032     0.228822     101.00
 O      -4.902279    -0.940427     0.159299     246.90
 H      -4.353158    -1.608535     0.546845      27.50
 H      -4.583288     1.154161    -0.850596      24.29
 H      -5.141152     0.884167     0.933405      28.61
 C       1.344193    -0.108250    -0.519656      37.54
 H       2.090821     0.737592    -0.705482      23.85
 C       0.794119    -2.458893    -0.726198      46.19
 H       1.100136    -3.554801    -0.874696      23.15
 C      -0.535638    -2.133685    -0.580455      19.31
 O      -1.459959    -3.231754    -0.465485     162.34
 C      -2.246820    -3.545694    -1.710427     113.69
 H      -3.014999    -2.879956    -2.419433      25.04
 H      -1.711760    -4.229680    -2.175192      29.87
 H      -2.917994    -4.128081    -1.210056      27.55
 C      -0.923334    -0.877615    -0.071361       8.49
 O      -2.258772    -0.652930     0.247503     157.37
 C      -0.065876     0.236996    -0.288683      64.51
 H      -0.232245     1.096004     0.131122      28.38
 C       1.811807    -1.344246    -0.899539      33.51
 C       3.222225    -1.484844    -1.224825      90.28
 H       3.272911    -2.387298    -1.753471      26.76
 O       3.766117    -0.328363    -1.912920     292.91
 H       4.624237     0.007740    -1.563369      27.66
 C       3.924341    -1.649566     0.248264      69.17
 H       3.426947    -2.616966     0.505429      26.45
 O       5.257120    -2.219283     0.078334     160.19
 H       5.556034    -1.650860    -0.678618      26.74
 C       3.928408    -0.418209     1.388542     111.67
 O       4.903969     0.621093     0.902248     190.43
 H       4.539713     1.362868     1.542681      23.52
 H       4.270603    -0.993822     2.230372      28.71
 H       2.907109    -0.003756     1.104760      24.24
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name = lig-Water-frame_391
 C      -1.261658     2.427748     3.067176      52.46
 H      -1.715097     3.216166     2.536190      26.09
 C      -0.715063     0.080152     3.390436      33.49
 H      -0.612305    -1.019784     3.343245      25.55
 C       0.525207     0.518469     4.208360       7.56
 O       1.584052    -0.351687     4.234963      51.06
 C       1.552237    -1.805822     3.988892     113.03
 H       2.676732    -1.944478     4.016785      28.30
 H       1.230648    -2.151570     2.883762      28.59
 H       0.900806    -2.215928     4.786765      28.57
 C       0.795354     1.890939     4.215355      20.01
 O       2.036431     2.207077     4.657363     204.12
 H       1.920987     3.176711     4.780317      25.63
 C      -0.093851     2.849021     3.706932      39.79
 H       0.449886     3.841327     3.661502      19.81
 C      -1.570541     0.923598     2.960961      59.21
 C      -2.899602     0.657432     2.373554      90.03
 H      -3.597746     1.397643     2.486624      29.75
 O      -3.358612    -0.516708     2.819878     273.50
 H      -4.353171    -0.551515     2.673105      25.64
 C      -2.904886     0.549374     0.640415      94.91
 H      -2.529975     1.404946     0.153197      28.22
 C      -4.451665     0.459073     0.215450     104.04
 O      -4.925598    -0.966493     0.145239     222.55
 H      -4.141863    -1.570784     0.504492      23.98
 H      -4.535899     0.724077    -0.728577      28.92
 H      -4.927382     0.978505     1.138522      27.42
 C       1.352800    -0.041656    -0.489719      52.55
 H       2.019355     0.698790    -0.892753      25.02
 C       0.887617    -2.419857    -0.796985      58.07
 H       1.088295    -3.500604    -0.876429      23.37
 C      -0.483558    -2.172950    -0.569291       1.18
 O      -1.460351    -3.224641    -0.487002     148.57
 C      -2.246785    -3.572961    -1.713779     102.50
 H      -2.827573    -2.807260    -2.078858      26.42
 H      -1.387846    -4.370213    -2.183659      23.06
 H      -3.119245    -4.325784    -1.295561      24.20
 C      -0.940560    -0.855934    -0.080405       1.86
 O      -2.298677    -0.701790     0.282659     167.64
 C      -0.027347     0.238815    -0.242143      43.57
 H      -0.506606     1.364590     0.104939      23.40
 C       1.766113    -1.354490    -0.903636      30.14
 C       3.283881    -1.471771    -1.241955      65.26
 H       3.481144    -2.557543    -1.764099      23.00
 O       3.775197    -0.301176    -1.922372     313.83
 H       4.579345     0.146090    -1.688425      28.69
 C       3.992028    -1.673489     0.301285      58.43
 H       3.209644    -2.535199     0.778592      26.08
 O       5.227409    -2.242284     0.097961     142.36
 H       5.685084    -1.889343    -0.877377      22.86
 C       3.916262    -0.471693     1.326922     111.92
 O       4.923100     0.588552     0.915578     190.49
 H       4.599695     1.500369     1.359390      23.94
 H       4.067355    -0.970646     2.333372      28.83
 H       2.981098     0.024348     1.169594      26.23
55
name = lig-Water-frame_392
 C      -1.230406     2.399758     3.082937      51.15
 H      -1.869976     3.183461     2.520494      24.65
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 C      -0.644687    -0.004784     3.436918      41.45
 H      -0.847620    -1.097635     3.242985      24.47
 C       0.468280     0.455429     4.116332      24.35
 O       1.551503    -0.377663     4.222670     137.40
 C       1.508955    -1.756232     4.022121     145.29
 H       2.590089    -1.992174     3.934735      29.60
 H       1.422020    -2.038149     3.022719      31.41
 H       0.983318    -2.565294     4.636628      29.76
 C       0.811606     1.898775     4.193131      31.66
 O       2.117757     2.252358     4.725328      45.90
 H       1.711827     3.234331     4.754570      27.88
 C      -0.060883     2.848102     3.719456      61.17
 H       0.300038     3.812439     3.273569      15.07
 C      -1.578598     1.013795     2.896877      21.00
 C      -2.877385     0.680025     2.270741      87.09
 H      -3.567558     1.559963     2.851586      22.50
 O      -3.372737    -0.571057     2.830260     242.59
 H      -4.345019    -0.466567     2.588473      23.57
 C      -2.885742     0.562968     0.712233      94.47
 H      -2.580879     1.500332     0.101925      22.57
 C      -4.391838     0.416510     0.251217      86.61
 O      -4.935184    -0.984198     0.145931     213.43
 H      -4.158666    -1.507718     0.413258      26.84
 H      -4.668018     0.699845    -0.944805      22.69
 H      -4.893740     1.141221     0.904927      27.04
 C       1.322087     0.022682    -0.518425      48.37
 H       1.966006     0.852180    -0.862216      23.10
 C       0.941200    -2.406038    -0.878305      48.37
 H       1.267831    -3.427369    -1.033505      21.66
 C      -0.474508    -2.179962    -0.517517     -16.65
 O      -1.461117    -3.208154    -0.496194     201.10
 C      -2.221617    -3.692097    -1.673236     110.69
 H      -2.466030    -2.522258    -2.022572      22.82
 H      -1.617741    -3.972061    -2.489723      29.21
 H      -2.992273    -4.300552    -1.480489      28.78
 C      -0.950541    -0.827701    -0.128483      -1.17
 O      -2.318488    -0.765741     0.303591     146.54
 C      -0.003083     0.251965    -0.150349      49.83
 H      -0.393344     1.159259    -0.169016      23.34
 C       1.752038    -1.318907    -0.900098      27.04
 C       3.352155    -1.477534    -1.183020      90.03
 H       3.711925    -2.273249    -1.731173      25.68
 O       3.755484    -0.285704    -1.958516     257.05
 H       4.708123     0.138651    -1.620390      25.08
 C       3.992254    -1.691962     0.311590      88.65
 H       3.228056    -2.347647     0.966358      26.32
 O       5.247027    -2.273043     0.100861     203.23
 H       5.784589    -2.210645    -0.629228      31.93
 C       3.928121    -0.524215     1.224281     124.67
 O       4.935185     0.555843     0.940988     210.70
 H       4.701165     1.383588     1.298531      28.31
 H       3.916871    -0.630737     2.344960      28.38
 H       2.897885    -0.033252     1.414563      25.38
55
name = lig-Water-frame_393
 C      -1.233461     2.363128     3.070027      57.34
 H      -1.946900     3.013723     2.662077      25.39
 C      -0.627377    -0.064536     3.467056      54.37
 H      -1.142442    -1.033647     3.145150      24.59
 C       0.440543     0.427299     3.992249      30.16
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 O       1.540567    -0.386434     4.253835     159.20
 C       1.515147    -1.765507     4.020736     130.99
 H       2.564703    -2.140075     4.208760      26.72
 H       1.183801    -1.865151     2.866225      25.94
 H       1.031752    -2.518964     4.603991      28.94
 C       0.851362     1.830880     4.193758       8.16
 O       2.137313     2.320459     4.774195      68.37
 H       2.242126     3.281850     4.961302      34.03
 C      -0.029625     2.851842     3.683726      51.35
 H       0.172059     3.817811     3.266302      21.86
 C      -1.538073     1.115213     2.871655      26.85
 C      -2.869281     0.721934     2.206000     108.83
 H      -3.425565     1.442567     2.580460      28.29
 O      -3.388098    -0.621902     2.837298     196.31
 H      -4.413369    -0.685401     2.802910      24.71
 C      -2.919034     0.556320     0.756776      90.47
 H      -2.416782     1.399978     0.222794      24.20
 C      -4.355090     0.372693     0.212923     111.46
 O      -4.931771    -0.978657     0.169886     225.05
 H      -4.266620    -1.661560     0.387672      28.76
 H      -4.454075     0.860794    -0.655063      28.79
 H      -5.101974     1.129480     0.693490      26.58
 C       1.292281     0.056403    -0.592385      37.90
 H       1.902628     0.988700    -0.636217      23.28
 C       0.904393    -2.406014    -0.938372      35.59
 H       1.477704    -3.364419    -1.287895      22.16
 C      -0.475330    -2.156594    -0.474685      16.02
 O      -1.446983    -3.225537    -0.467976     146.60
 C      -2.158557    -3.676026    -1.675801     112.49
 H      -2.463434    -2.803290    -2.078913      25.89
 H      -1.656120    -3.875573    -2.790690      23.64
 H      -3.080461    -4.436151    -1.454357      24.58
 C      -0.948992    -0.848974    -0.176428       5.63
 O      -2.299201    -0.803192     0.313439     129.61
 C       0.000448     0.226511    -0.076252      56.40
 H      -0.360748     1.399753    -0.255385      20.57
 C       1.819181    -1.234638    -0.904007       8.35
 C       3.371179    -1.442177    -1.077236      83.31
 H       3.805597    -2.291342    -1.828869      22.07
 O       3.747718    -0.267837    -1.981206     277.32
 H       4.585711    -0.030690    -1.643284      29.05
 C       3.965433    -1.686508     0.255284      82.28
 H       3.350395    -2.441246     0.936781      25.55
 O       5.284369    -2.335558     0.159744      94.57
 H       5.904352    -2.246802    -0.783214      24.02
 C       3.936953    -0.480166     1.187732     133.68
 O       4.953086     0.505410     0.942064     185.23
 H       4.607510     1.396749     1.543976      20.11
 H       4.163117    -0.685216     2.260060      28.84
 H       2.885577    -0.187899     1.162231      26.18
55
name = lig-Water-frame_394
 C      -1.228662     2.401088     3.059941      56.21
 H      -2.028972     3.153168     2.754242      24.63
 C      -0.778685    -0.042291     3.394486      68.99
 H      -1.076021    -1.034151     3.252974      30.48
 C       0.550734     0.420366     3.924145      16.58
 O       1.554234    -0.384711     4.328993     188.43
 C       1.543019    -1.815409     3.957491     123.53
 H       2.522564    -2.190333     4.330200      27.08
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 H       1.093888    -1.868344     3.044564      30.74
 H       0.718326    -2.224922     4.738312      24.99
 C       0.882282     1.859486     4.185302      10.40
 O       2.129350     2.345565     4.804852     142.96
 H       2.442591     3.243464     4.970321      27.82
 C       0.006352     2.806086     3.626364      46.79
 H       0.282688     3.952738     3.660447      27.92
 C      -1.488761     1.037440     2.880695      25.75
 C      -2.849512     0.701867     2.217971      73.20
 H      -3.752351     1.649980     2.252633      25.10
 O      -3.391066    -0.651545     2.847873     136.01
 H      -4.371886    -0.705533     2.972360      23.45
 C      -2.952744     0.501977     0.744450      89.90
 H      -2.322741     1.296413     0.312083      26.79
 C      -4.354495     0.355292     0.181976     101.73
 O      -4.924329    -0.957501     0.193532     167.41
 H      -4.344713    -1.807748     0.411918      26.38
 H      -4.113432     0.926296    -0.936831      25.06
 H      -5.184920     0.815606     0.724712      26.30
 C       1.279502     0.076937    -0.652881      48.29
 H       1.873141     0.957786    -0.496909      30.13
 C       0.879469    -2.341850    -0.979339      52.62
 H       1.261193    -3.219080    -1.369866      28.12
 C      -0.453991    -2.164712    -0.486167      22.21
 O      -1.416899    -3.268722    -0.426562     135.65
 C      -2.107499    -3.629455    -1.740598     102.83
 H      -2.955388    -2.760848    -2.149330      23.57
 H      -1.468085    -4.138019    -2.433130      27.67
 H      -2.748560    -4.364306    -1.373279      28.86
 C      -0.959591    -0.865003    -0.174515      10.66
 O      -2.251484    -0.815388     0.314205     102.98
 C      -0.030259     0.227102    -0.070328      49.62
 H      -0.311222     1.247951     0.029029      28.26
 C       1.865136    -1.193338    -0.915545     -10.38
 C       3.340341    -1.407644    -1.071596     108.97
 H       3.458116    -2.291115    -1.589832      28.28
 O       3.740581    -0.261757    -1.974900     247.72
 H       4.675027     0.043171    -1.749770      27.28
 C       3.997280    -1.679940     0.220287      68.37
 H       3.309343    -2.570839     0.650186      27.00
 O       5.344282    -2.401245     0.202830     120.37
 H       5.654559    -2.081590    -0.624437      28.18
 C       3.956595    -0.440005     1.200008     164.31
 O       4.961280     0.508501     0.941474     157.81
 H       4.740338     1.177188     1.532116      31.07
 H       4.269205    -1.051741     2.098430      32.86
 H       2.923615    -0.103692     0.918332      28.24
55
name = lig-Water-frame_395
 C      -1.211198     2.461294     3.046542      65.82
 H      -1.919393     3.244003     2.831986      28.07
 C      -0.827878     0.015400     3.342758      46.63
 H      -0.938273    -1.124477     3.401813      29.21
 C       0.654545     0.446360     3.880617     -13.59
 O       1.599299    -0.394640     4.409199     127.36
 C       1.513126    -1.848278     3.980638     105.03
 H       2.472065    -2.302727     4.160059      29.98
 H       1.179868    -2.079453     2.835009      31.98
 H       0.703214    -2.013304     4.575581      26.44
 C       0.915970     1.913839     4.155876      18.12
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 O       2.107061     2.304110     4.819415      90.62
 H       2.109805     3.399114     4.705160      23.46
 C       0.035890     2.797583     3.581492      64.41
 H       0.297094     3.705276     4.067239      25.87
 C      -1.544525     0.962792     2.869547      36.20
 C      -2.902103     0.667108     2.271231     100.98
 H      -3.548245     1.388031     2.220544      33.35
 O      -3.376223    -0.653641     2.870003     175.25
 H      -4.397931    -0.473874     2.907421      21.63
 C      -2.928843     0.408127     0.720294      92.41
 H      -2.381455     1.332284     0.239570      29.00
 C      -4.348827     0.360811     0.105110     122.17
 O      -4.921244    -0.965723     0.198546     190.19
 H      -4.286352    -1.633834     0.422060      31.61
 H      -4.195279     0.517243    -0.872788      31.41
 H      -5.088049     0.890720     0.752841      27.64
 C       1.262815     0.085252    -0.660661      67.38
 H       1.967342     0.960556    -0.537232      31.57
 C       0.878032    -2.218042    -0.996120      63.41
 H       1.008657    -3.331746    -1.419512      26.39
 C      -0.435103    -2.183705    -0.532555       2.12
 O      -1.373535    -3.294856    -0.409494     112.45
 C      -2.087458    -3.563050    -1.776199     112.68
 H      -2.858208    -3.002071    -2.067300      27.14
 H      -1.189928    -4.191835    -2.244545      25.30
 H      -2.630911    -4.528207    -1.291152      25.90
 C      -0.959536    -0.858998    -0.126425      25.48
 O      -2.213379    -0.820955     0.312901     123.02
 C      -0.052062     0.202199    -0.126001      58.27
 H      -0.415949     1.240651     0.385567      30.69
 C       1.819779    -1.179294    -0.927140      -2.61
 C       3.295395    -1.360511    -1.152345      97.80
 H       3.187878    -2.496987    -1.630672      23.31
 O       3.743465    -0.269238    -1.949270     212.05
 H       4.728049     0.158491    -1.960243      23.73
 C       4.061340    -1.682180     0.234862      79.02
 H       3.220504    -2.480543     0.366015      29.59
 O       5.373359    -2.431041     0.222005     105.99
 H       5.834951    -2.031603    -0.620303      22.83
 C       3.979695    -0.493747     1.201665     135.61
 O       4.986688     0.526188     0.928758      75.68
 H       4.832645     1.408066     1.582609      23.27
 H       4.004168    -1.046059     2.143707      33.97
 H       3.021424     0.104328     1.146381      30.22
55
name = lig-Water-frame_396
 C      -1.191910     2.454032     3.023184      48.05
 H      -1.872996     3.297008     2.803020      28.10
 C      -0.660462     0.012458     3.376878      11.06
 H      -0.967851    -1.008347     3.413389      33.78
 C       0.692240     0.521856     3.850266       3.59
 O       1.656544    -0.420871     4.460211     120.60
 C       1.459088    -1.848947     3.982131     124.80
 H       2.410580    -2.472893     4.140770      29.76
 H       1.451011    -2.021494     2.954889      34.33
 H       0.566512    -2.364107     4.610063      27.28
 C       0.964964     1.846860     4.096649      27.74
 O       2.057262     2.291354     4.808286      98.82
 H       1.866938     3.156922     4.595034      26.67
 C       0.044217     2.821088     3.573853      65.19
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 H       0.092168     3.800037     4.212029      22.26
 C      -1.680081     1.056822     2.830060     -32.98
 C      -2.935840     0.551439     2.290429      86.23
 H      -3.732920     1.571655     2.572464      25.17
 O      -3.386107    -0.619059     2.900567     210.59
 H      -4.356141    -0.496932     2.808166      21.41
 C      -2.868172     0.345660     0.690273     107.77
 H      -2.530107     1.222049     0.201323      31.22
 C      -4.333916     0.326489     0.068684      92.54
 O      -4.929527    -0.988469     0.193268     163.33
 H      -4.145783    -1.552814     0.462448      27.92
 H      -4.431825     0.434131    -1.166168      25.53
 H      -4.836198     1.295407     0.508175      27.71
 C       1.250867     0.108686    -0.619463      53.84
 H       1.933484     0.913354    -0.683903      32.47
 C       0.857914    -2.187566    -1.019664      52.34
 H       1.087542    -3.126503    -1.344338      29.68
 C      -0.461233    -2.139638    -0.560283      -8.01
 O      -1.318276    -3.281207    -0.420279     147.99
 C      -2.028899    -3.626973    -1.714480     102.45
 H      -2.780209    -2.787748    -2.221004      25.19
 H      -1.145147    -3.770591    -2.482591      27.24
 H      -2.575204    -4.539964    -1.522657      29.40
 C      -0.912339    -0.888852    -0.087625       5.69
 O      -2.216601    -0.829071     0.323654     139.07
 C      -0.073772     0.222335    -0.195036      72.04
 H      -0.363725     0.960796     0.593194      34.62
 C       1.745516    -1.137783    -0.947439      15.40
 C       3.280123    -1.368125    -1.253287     114.97
 H       3.341574    -2.234105    -1.799988      27.66
 O       3.745980    -0.263907    -1.951122     298.38
 H       4.629853    -0.044560    -1.892958      30.73
 C       4.088987    -1.683086     0.197209      87.46
 H       3.298461    -2.453719     0.623050      29.93
 O       5.375561    -2.416348     0.200312      97.06
 H       6.172078    -2.182301    -0.455697      23.06
 C       3.992339    -0.546971     1.222173     141.32
 O       5.029345     0.556881     0.936486     137.10
 H       4.757635     1.416069     1.373923      26.02
 H       3.906904    -0.736543     2.374898      33.27
 H       3.069510     0.008116     1.341805      33.24
55
name = lig-Water-frame_397
 C      -1.212120     2.415172     2.982995      53.65
 H      -1.866535     3.286114     2.715582      24.10
 C      -0.483095     0.101201     3.396335       5.18
 H      -0.889959    -0.926542     3.392393      30.11
 C       0.683553     0.492396     3.838204      34.44
 O       1.681317    -0.463254     4.472949      74.89
 C       1.421363    -1.862430     4.027406     128.10
 H       2.265070    -2.399144     4.409085      31.05
 H       1.417722    -1.767705     2.847996      32.10
 H       0.712793    -2.535835     4.378677      31.16
 C       0.983047     1.802141     4.006318      31.00
 O       2.000581     2.278772     4.785542       8.93
 H       1.976901     3.353392     4.730712      25.94
 C       0.039964     2.837552     3.619567      52.14
 H      -0.085895     3.842475     3.926021      19.80
 C      -1.670750     1.141240     2.858789     -40.18
 C      -3.001360     0.526795     2.273820     113.77
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 H      -3.624406     1.187458     2.607430      31.14
 O      -3.413874    -0.599006     2.942983     210.68
 H      -4.420750    -0.771110     2.825466      21.74
 C      -2.867164     0.332048     0.661513      87.03
 H      -2.384013     1.314595     0.145531      27.76
 C      -4.305309     0.302790    -0.015249     114.34
 O      -4.938070    -1.001267     0.198515     201.76
 H      -4.197021    -1.670123     0.500132      25.04
 H      -4.360500     0.568804    -1.002830      29.38
 H      -4.712646     1.263016     0.287011      29.74
 C       1.245325     0.147697    -0.572011      -1.96
 H       1.897972     1.054551    -0.737002      26.12
 C       0.818271    -2.214045    -1.035400      22.49
 H       1.410510    -3.190599    -1.379681      27.57
 C      -0.500563    -2.087363    -0.579132      40.43
 O      -1.268607    -3.254810    -0.450414     163.72
 C      -1.959271    -3.662256    -1.680936     120.08
 H      -2.393040    -2.771246    -2.022620      28.03
 H      -1.228575    -3.536908    -2.689563      24.80
 H      -2.587501    -4.627027    -1.679808      25.62
 C      -0.872470    -0.918370    -0.071233      26.93
 O      -2.226168    -0.863641     0.342589     113.23
 C      -0.098140     0.252158    -0.218425      46.81
 H      -0.317837     1.058406     0.515289      30.61
 C       1.719349    -1.102744    -0.993413       5.83
 C       3.270707    -1.384442    -1.297475      85.78
 H       3.598823    -2.255193    -2.111793      24.80
 O       3.735686    -0.234680    -1.978048     229.08
 H       4.761971    -0.242597    -1.720365      24.83
 C       4.067847    -1.695216     0.140482      72.00
 H       3.602795    -2.411132     0.920939      28.95
 O       5.373177    -2.396983     0.176759     127.69
 H       6.020486    -2.083233    -0.413522      28.50
 C       4.019973    -0.530525     1.279405     123.39
 O       5.065358     0.559975     0.939273     183.83
 H       4.642599     1.410986     1.373249      25.35
 H       4.273007    -0.687164     2.321620      31.74
 H       2.899517    -0.175678     1.100885      30.24
55
name = lig-Water-frame_398
 C      -1.236486     2.433963     2.949164      61.41
 H      -1.889143     3.198396     2.608836      29.03
 C      -0.484809     0.203008     3.341326      63.10
 H      -0.678501    -0.912696     3.369621      27.44
 C       0.752889     0.393597     3.883420       1.59
 O       1.643852    -0.502070     4.466272     124.68
 C       1.440225    -1.865253     4.040670     122.46
 H       2.341474    -2.305023     4.572265      26.76
 H       1.369078    -1.726779     2.979854      30.57
 H       0.418768    -2.462552     4.308226      24.95
 C       0.965601     1.909629     3.926046      17.28
 O       1.973552     2.283739     4.766076     178.51
 H       2.162661     3.252509     4.946235      29.85
 C      -0.012485     2.790670     3.636463      76.80
 H       0.119393     3.938305     3.697200      19.00
 C      -1.555169     1.103699     2.924175      44.05
 C      -3.005311     0.552752     2.225767      65.12
 H      -3.984504     1.410966     2.421854      23.99
 O      -3.440676    -0.640084     2.997551     197.62
 H      -4.409550    -0.872169     2.865393      24.13
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 C      -2.907612     0.383902     0.631201      98.80
 H      -2.296067     1.132098     0.307716      28.82
 C      -4.241201     0.279264    -0.078991      92.20
 O      -4.939206    -0.993701     0.202321     178.02
 H      -4.417586    -1.755127     0.421121      26.99
 H      -4.047377     0.551302    -1.281807      24.85
 H      -4.980259     1.054333     0.458943      25.62
 C       1.256586     0.194935    -0.561857      11.60
 H       1.796847     1.123592    -0.609208      23.04
 C       0.840728    -2.246054    -1.058791      67.00
 H       1.334822    -3.144490    -1.319130      28.86
 C      -0.483826    -2.121720    -0.625240       2.40
 O      -1.230750    -3.256226    -0.474743     184.42
 C      -1.854078    -3.654043    -1.695678     116.71
 H      -2.595148    -2.667541    -1.798281      24.49
 H      -1.246557    -3.702848    -2.622947      26.75
 H      -2.525024    -4.594177    -1.666630      25.50
 C      -0.906729    -0.865264    -0.051278      -7.03
 O      -2.217057    -0.921598     0.363807     124.87
 C      -0.108395     0.282578    -0.182335      55.81
 H      -0.416609     1.412092     0.164825      24.64
 C       1.726149    -1.118925    -1.055711      19.51
 C       3.259792    -1.423884    -1.323743      92.05
 H       3.473018    -2.218432    -1.921906      27.27
 O       3.752374    -0.190886    -1.997398     268.34
 H       4.761451    -0.182263    -1.753612      25.02
 C       4.053366    -1.704504     0.154156      64.08
 H       3.419053    -2.445432     0.685741      27.43
 O       5.353642    -2.379702     0.154141     122.14
 H       5.883754    -1.796290    -0.658717      21.48
 C       4.061432    -0.474533     1.263958     113.72
 O       5.069835     0.549261     0.934399     225.56
 H       4.729418     1.402221     1.530043      22.29
 H       4.504067    -0.971121     2.200172      27.89
 H       3.070658    -0.249457     1.085465      28.46
55
name = lig-Water-frame_399
 C      -1.246766     2.470188     2.941100      69.89
 H      -2.008862     3.199112     2.483322      28.77
 C      -0.539202     0.192422     3.279263      61.36
 H      -0.736781    -0.834908     3.226350      27.85
 C       0.820938     0.433295     3.925439       3.65
 O       1.574064    -0.520721     4.464752     137.89
 C       1.452025    -1.890720     4.063856     125.99
 H       2.297998    -2.422395     4.448016      30.71
 H       1.532096    -2.001585     2.898035      27.70
 H       0.472209    -2.048467     4.368307      27.35
 C       0.968281     1.960151     3.909598      24.55
 O       1.996378     2.289886     4.765968     216.45
 H       2.095992     3.211518     4.907222      29.37
 C      -0.110762     2.809321     3.589339      88.67
 H       0.439960     3.739249     3.602402      19.12
 C      -1.479545     1.023507     2.947671      37.35
 C      -3.019756     0.617340     2.214511      75.44
 H      -3.671071     1.338391     2.144532      28.54
 O      -3.442005    -0.691860     3.025989     213.91
 H      -4.415325    -0.700040     2.890903      26.02
 C      -2.946164     0.391711     0.658034      73.89
 H      -2.157332     1.241966     0.302434      21.41
 C      -4.202837     0.269225    -0.138841     113.53
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 O      -4.938152    -0.967366     0.184005     136.86
 H      -4.390784    -1.870367     0.283503      23.15
 H      -3.911382     0.298252    -1.131444      28.74
 H      -4.996638     0.774028     0.284293      25.99
 C       1.254103     0.188889    -0.588996      15.55
 H       1.854092     1.119816    -0.491063      23.66
 C       0.891614    -2.235893    -1.078943      59.04
 H       1.173530    -3.334102    -1.345669      22.27
 C      -0.415562    -2.132411    -0.648106     -28.29
 O      -1.191640    -3.297984    -0.480076     192.10
 C      -1.824786    -3.589167    -1.729830     117.35
 H      -2.746487    -3.069296    -1.816344      25.63
 H      -0.999097    -3.822807    -2.638940      23.98
 H      -2.346660    -4.550293    -1.477482      25.09
 C      -0.960476    -0.822579    -0.068433     -31.16
 O      -2.215261    -0.963752     0.392495     102.88
 C      -0.099042     0.349475    -0.134062      60.85
 H      -0.505485     1.319812    -0.160363      23.46
 C       1.755276    -1.126742    -1.097323      12.88
 C       3.249212    -1.397465    -1.297040      71.16
 H       3.291062    -2.499629    -1.890495      21.42
 O       3.777630    -0.165278    -2.007981     272.28
 H       4.683389     0.053150    -1.937842      28.06
 C       4.026018    -1.703920     0.198529      62.78
 H       3.090256    -2.426896     0.292672      24.88
 O       5.325324    -2.335421     0.098454     187.97
 H       5.821522    -1.955477    -0.621799      27.70
 C       4.148577    -0.478432     1.192933     118.32
 O       5.056606     0.541891     0.930601     188.74
 H       4.906744     1.388982     1.649439      20.83
 H       4.330782    -1.160703     2.035644      29.17
 H       3.037991     0.018206     1.464453      25.48
55
name = lig-Water-frame_400
 C      -1.302728     2.462830     2.928216      46.35
 H      -1.974084     3.138890     2.513467      32.41
 C      -0.485291     0.074687     3.279058      21.25
 H      -0.948201    -0.993960     3.004980      24.15
 C       0.748965     0.580984     3.883403      27.30
 O       1.547518    -0.511723     4.478435     115.53
 C       1.453060    -1.907972     4.039582     133.02
 H       2.206551    -2.611768     4.536662      30.67
 H       1.658156    -2.265241     3.010669      28.86
 H       0.413396    -2.142768     4.505677      28.38
 C       0.972807     1.876176     3.961011      28.79
 O       2.046094     2.312580     4.770650     135.94
 H       1.972866     3.395442     4.766010      30.59
 C      -0.118801     2.876947     3.526650      88.15
 H       0.357643     3.880354     3.539443      11.95
 C      -1.540377     1.047417     2.882933       6.52
 C      -2.947620     0.600406     2.237012      65.12
 H      -3.682036     1.696108     2.312340      22.95
 O      -3.437057    -0.706261     3.004744     168.81
 H      -4.477850    -0.518918     3.029598      22.64
 C      -2.909963     0.371032     0.723437      92.27
 H      -2.472102     1.171776     0.285967      26.12
 C      -4.182516     0.213493    -0.155734      85.54
 O      -4.925776    -0.971524     0.149931     187.06
 H      -4.294472    -1.734277     0.148446      26.02
 H      -3.901780     0.187283    -1.328332      25.59
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 H      -5.040383     1.158855    -0.108906      24.30
 C       1.242459     0.141068    -0.630604      38.10
 H       1.995643     0.938660    -0.519051      26.40
 C       0.941801    -2.236393    -1.101983      50.67
 H       1.090903    -3.293387    -1.417644      24.62
 C      -0.361789    -2.070103    -0.604234      -3.79
 O      -1.138842    -3.325544    -0.481614     145.05
 C      -1.834533    -3.597814    -1.766504     108.93
 H      -2.805482    -3.069759    -2.137749      24.74
 H      -0.981927    -3.712875    -2.524223      25.71
 H      -2.009852    -4.701967    -1.406621      24.08
 C      -0.952693    -0.834236    -0.138581      -3.78
 O      -2.230630    -0.968364     0.427054      90.78
 C      -0.081292     0.357562    -0.114983      50.69
 H      -0.652345     1.444916    -0.325077      19.70
 C       1.795726    -1.087534    -1.097617      11.78
 C       3.281648    -1.345321    -1.272490      97.05
 H       3.280275    -2.235185    -1.761234      24.14
 O       3.770908    -0.168370    -2.024742     274.09
 H       4.805938     0.161494    -2.017994      23.19
 C       3.955607    -1.668001     0.156114      74.18
 H       3.249291    -2.379815     0.517502      27.35
 O       5.255921    -2.312438     0.074553     133.96
 H       5.964892    -1.942550    -0.783769      21.56
 C       4.136297    -0.524989     1.154124     132.97
 O       5.069884     0.544122     0.921317     200.83
 H       4.904799     1.217358     1.667586      25.29
 H       4.355634    -1.066799     2.140955      29.07
 H       3.406116     0.007727     1.625306      27.10
55
name = lig-Water-frame_401
 C      -1.336770     2.424096     2.931799      48.51
 H      -2.067707     3.233328     2.540265      18.20
 C      -0.502423     0.001012     3.253814      57.39
 H      -0.704828    -0.965434     3.054101      31.58
 C       0.601467     0.553999     3.802547      16.07
 O       1.559799    -0.470257     4.482979      51.05
 C       1.420888    -1.944986     4.053158     136.43
 H       2.089128    -2.390660     4.793107      28.81
 H       1.574090    -2.181894     2.969834      29.76
 H       0.526963    -2.526888     4.317319      29.35
 C       0.947973     1.900599     4.046661      17.63
 O       2.084842     2.367387     4.759273      82.97
 H       2.031876     3.322897     4.662811      29.00
 C      -0.030855     2.918917     3.470281      72.37
 H      -0.050675     4.057626     3.497004      25.70
 C      -1.598850     1.050894     2.800609     -11.83
 C      -2.878688     0.593979     2.295830     115.30
 H      -3.441465     1.308041     2.613319      29.41
 O      -3.444802    -0.667806     2.950866     168.26
 H      -4.386006    -0.532516     3.160078      23.47
 C      -2.891121     0.311956     0.773936      86.88
 H      -2.497353     1.295309     0.184994      25.14
 C      -4.207270     0.190315    -0.191402     113.29
 O      -4.914624    -0.976267     0.102235     226.33
 H      -4.253816    -1.689665     0.164182      26.68
 H      -3.810808     0.126320    -1.191185      27.98
 H      -4.616023     1.142728    -0.357286      28.21
 C       1.241012     0.105138    -0.659393      52.10
 H       2.012426     0.861177    -0.650363      26.69
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 C       0.962906    -2.210810    -1.115534      35.81
 H       1.280222    -3.187772    -1.509349      25.60
 C      -0.329811    -2.027064    -0.537534      12.51
 O      -1.087435    -3.298109    -0.492455     138.30
 C      -1.839231    -3.682923    -1.763640     103.39
 H      -2.554861    -2.989240    -2.278635      24.51
 H      -0.975869    -3.555555    -2.695585      25.44
 H      -2.005766    -4.725318    -1.721436      28.55
 C      -0.912031    -0.847290    -0.200322      11.79
 O      -2.225848    -0.938926     0.454561     117.55
 C      -0.095010     0.334278    -0.166031      61.11
 H      -0.442580     1.254979    -0.107217      26.46
 C       1.815989    -1.069591    -1.067923       2.04
 C       3.326960    -1.243108    -1.233774     101.33
 H       3.526473    -2.237065    -1.956623      22.01
 O       3.768658    -0.170781    -2.051417     273.75
 H       4.712911    -0.075575    -1.874365      26.41
 C       3.898722    -1.601355     0.076334      74.19
 H       3.462347    -2.361795     0.911489      25.67
 O       5.192127    -2.301416     0.038146     168.61
 H       5.736049    -1.855387    -0.573996      28.01
 C       4.109425    -0.582227     1.193368     103.10
 O       5.112871     0.522768     0.890762     208.13
 H       4.791551     1.310848     1.603908      20.59
 H       4.659228    -0.969823     2.070831      28.59
 H       3.089023     0.022364     1.569306      25.78
55
name = lig-Water-frame_402
 C      -1.311141     2.395781     2.946605      52.39
 H      -2.042118     3.126193     2.692260      24.00
 C      -0.621509     0.035478     3.179741      81.69
 H      -0.489839    -1.173125     3.144314      26.63
 C       0.531896     0.439844     3.785882     -22.41
 O       1.545553    -0.428759     4.453692      24.36
 C       1.390207    -1.969912     4.099848     127.95
 H       2.193812    -2.172871     4.827032      26.58
 H       1.657051    -1.911980     2.975084      28.41
 H       0.441733    -2.599499     4.160484      25.36
 C       0.876783     2.037293     4.102488     -20.76
 O       2.099455     2.402222     4.728234      95.75
 H       2.211799     3.411039     4.657316      26.44
 C       0.026153     2.907063     3.420169      63.05
 H      -0.147846     3.946856     3.582999      27.18
 C      -1.554589     1.000619     2.763739      44.02
 C      -2.862133     0.525463     2.332368      87.54
 H      -3.734257     1.358743     2.812199      23.47
 O      -3.431296    -0.625017     2.903198     188.36
 H      -4.429814    -0.501097     3.073397      24.01
 C      -2.902712     0.304339     0.749812      99.23
 H      -2.345570     1.086288     0.364400      28.28
 C      -4.162617     0.163122    -0.200965      97.04
 O      -4.936397    -0.976811     0.045855     194.42
 H      -4.295270    -1.795976     0.311455      22.78
 H      -3.517465    -0.023766    -1.221380      25.25
 H      -4.674684     1.279305    -0.300853      24.92
 C       1.246585     0.126345    -0.666450      43.74
 H       1.866956     1.064703    -0.751085      24.89
 C       0.969814    -2.160302    -1.107737      52.54
 H       1.499286    -3.102853    -1.549897      23.91
 C      -0.295963    -2.091737    -0.527193      19.77
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 O      -1.062419    -3.257584    -0.512673     201.47
 C      -1.752802    -3.741876    -1.790294     110.24
 H      -2.542169    -2.955522    -1.996331      25.67
 H      -1.114693    -3.485746    -2.642613      27.27
 H      -2.251621    -4.834958    -2.006786      26.30
 C      -0.910267    -0.816562    -0.195728      10.85
 O      -2.174902    -0.901914     0.466645     138.07
 C      -0.079471     0.258895    -0.270662      58.30
 H      -0.318656     1.369145     0.320873      23.94
 C       1.820211    -1.111589    -1.039278      23.52
 C       3.317289    -1.208002    -1.264092     106.48
 H       3.641047    -2.011269    -1.809195      26.41
 O       3.781665    -0.157707    -2.067501     296.96
 H       4.736197    -0.098527    -1.830109      26.67
 C       3.909389    -1.555083     0.112717      81.95
 H       3.256015    -2.226919     0.602276      29.14
 O       5.111144    -2.307540     0.013869     153.37
 H       5.823250    -1.742348    -0.598285      22.18
 C       4.079076    -0.552451     1.260530     128.76
 O       5.139705     0.500237     0.873493     193.58
 H       4.854679     1.412433     1.231480      23.63
 H       4.656600    -1.148592     1.978565      30.71
 H       3.098639    -0.291397     1.348160      27.25
55
name = lig-Water-frame_403
 C      -1.229504     2.337357     2.961363      76.58
 H      -2.074194     3.048831     2.789525      23.64
 C      -0.674121     0.024488     3.128822      73.56
 H      -0.795911    -1.000499     3.062864      26.60
 C       0.559080     0.422779     3.850713     -21.20
 O       1.471508    -0.394776     4.396833     102.21
 C       1.398835    -1.936267     4.132271     125.89
 H       2.279660    -2.327322     4.686183      27.93
 H       1.813911    -1.906026     3.168012      26.99
 H       0.379295    -2.356247     4.244821      24.78
 C       0.815487     2.098940     4.114964     -13.54
 O       2.083609     2.428127     4.683964     139.51
 H       2.394697     3.447971     4.695324      23.37
 C      -0.005928     2.875699     3.383904      68.06
 H       0.131183     3.977832     3.696664      27.84
 C      -1.508879     0.979677     2.754850      47.59
 C      -2.966766     0.516354     2.328193     102.46
 H      -3.555725     1.298337     2.421069      30.38
 O      -3.422144    -0.633522     2.896677     256.49
 H      -4.417573    -0.488859     2.788875      24.97
 C      -2.915302     0.325930     0.723366      82.10
 H      -2.173685     1.167403     0.384318      24.65
 C      -4.057081     0.170020    -0.220091     115.36
 O      -4.973740    -0.989615    -0.003223     195.16
 H      -4.536158    -1.745666     0.351913      29.80
 H      -3.529854    -0.026080    -1.134033      27.97
 H      -4.788438     0.895068    -0.174871      27.47
 C       1.282458     0.178338    -0.686363      51.32
 H       1.697157     1.152387    -0.761720      23.38
 C       0.988103    -2.167273    -1.097932      65.39
 H       1.385289    -3.052016    -1.440821      24.39
 C      -0.301336    -2.162877    -0.566895      16.17
 O      -1.063267    -3.267009    -0.523707     247.74
 C      -1.694885    -3.743035    -1.837939     100.99
 H      -2.617295    -3.124116    -1.571850      23.70
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 H      -0.915519    -3.542334    -2.759400      25.17
 H      -2.149818    -4.661323    -1.823273      29.11
 C      -0.922826    -0.843998    -0.158607      12.70
 O      -2.094710    -0.884517     0.472251     153.05
 C      -0.058924     0.269105    -0.331601      64.99
 H      -0.218011     0.968060     0.315048      26.62
 C       1.837080    -1.084797    -1.025156      38.07
 C       3.281031    -1.200776    -1.291676      66.18
 H       3.570160    -2.294098    -1.802569      22.08
 O       3.807717    -0.115087    -2.081036     229.02
 H       4.839239     0.155881    -1.907783      23.94
 C       3.946655    -1.512360     0.176368      68.51
 H       2.913566    -2.235734     0.249189      22.66
 O       5.052540    -2.319654    -0.016906     183.89
 H       5.863807    -1.963852    -0.536389      25.71
 C       4.105302    -0.509095     1.280292     119.61
 O       5.142011     0.466741     0.858373     204.97
 H       4.918278     1.358504     1.159531      22.94
 H       4.346151    -1.243356     2.115680      27.31
 H       2.942903    -0.195527     1.500689      24.51
55
name = lig-Water-frame_404
 C      -1.197682     2.299323     2.942245      62.30
 H      -2.050239     2.993527     2.807447      23.46
 C      -0.582710    -0.013643     3.158422      41.36
 H      -1.171826    -1.080853     2.896646      23.15
 C       0.544949     0.511326     3.904012      13.56
 O       1.412750    -0.395905     4.360836     180.37
 C       1.438426    -1.841876     4.154246     132.76
 H       2.114640    -2.482149     4.755586      28.15
 H       1.813223    -2.151445     3.032244      24.85
 H       0.431687    -2.148119     4.402060      28.08
 C       0.827658     2.017783     4.105004       6.87
 O       2.052338     2.446344     4.638441     140.71
 H       2.216695     3.359563     4.611931      24.42
 C      -0.052602     2.896242     3.397585      58.67
 H       0.279844     3.889806     3.502828      29.51
 C      -1.559646     1.000098     2.744314       6.26
 C      -3.007650     0.557437     2.229208      77.02
 H      -3.707453     1.635006     2.193337      24.52
 O      -3.444423    -0.675554     2.921409     185.31
 H      -4.396997    -0.726849     2.708393      24.71
 C      -2.853202     0.366266     0.719503      86.32
 H      -2.391723     1.285526     0.341370      27.62
 C      -3.979251     0.146430    -0.231497      92.90
 O      -5.013906    -0.997951    -0.045506     130.39
 H      -4.562870    -1.881956     0.318434      25.06
 H      -3.617542     0.106097    -1.360184      25.50
 H      -4.939980     0.905567    -0.178587      23.51
 C       1.310840     0.222873    -0.725850      51.17
 H       1.868254     1.204585    -0.737937      22.59
 C       0.996938    -2.194485    -1.072568      43.08
 H       1.317159    -3.314586    -1.398531      21.53
 C      -0.338020    -2.149574    -0.617299      14.99
 O      -1.073179    -3.341293    -0.523387     231.83
 C      -1.663917    -3.682200    -1.847490     106.84
 H      -2.607272    -3.206622    -1.857573      26.70
 H      -0.952995    -3.632535    -2.768425      24.88
 H      -1.814888    -4.858232    -1.513318      23.83
 C      -0.850841    -0.924824    -0.157579      37.62
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 O      -2.039501    -0.887350     0.493696     121.28
 C      -0.060808     0.250972    -0.357752      58.22
 H      -0.366677     1.217362     0.397428      22.66
 C       1.850627    -0.986205    -1.045570      31.52
 C       3.312922    -1.214930    -1.316153      84.06
 H       3.314162    -2.168290    -1.715582      26.33
 O       3.837130    -0.063375    -2.103684     293.98
 H       4.666863     0.257484    -1.878160      30.17
 C       3.917364    -1.496774     0.165284      91.07
 H       3.184740    -2.163012     0.450963      28.88
 O       5.024261    -2.373198    -0.022154     212.91
 H       5.735342    -2.030916    -0.596816      29.00
 C       4.084128    -0.481125     1.292601     128.47
 O       5.131132     0.413803     0.860174     222.69
 H       4.917985     1.359684     1.418943      19.13
 H       4.238317    -0.923477     2.295021      27.93
 H       3.316739     0.154381     1.604746      25.73
55
name = lig-Water-frame_405
 C      -1.257123     2.331352     2.891695      55.08
 H      -2.017383     3.066812     2.664117      30.89
 C      -0.539315    -0.005278     3.191293      32.46
 H      -0.928348    -0.982569     2.990410      23.10
 C       0.482557     0.594793     3.914963      35.98
 O       1.438936    -0.406171     4.370860     118.94
 C       1.459862    -1.763504     4.130015     155.63
 H       1.992222    -2.236042     5.009418      28.53
 H       1.529083    -2.177673     3.195243      29.90
 H       0.399519    -2.146828     4.431366      29.84
 C       0.849313     1.898362     4.045624      33.99
 O       2.013102     2.428119     4.597842      70.79
 H       1.906656     3.498726     4.448198      28.11
 C      -0.037114     2.874741     3.471718      67.29
 H       0.166802     3.993846     3.204448      14.23
 C      -1.611562     0.967730     2.762492      -8.98
 C      -3.011295     0.648678     2.117374      88.14
 H      -3.707889     1.345589     2.282863      28.50
 O      -3.468322    -0.693288     2.941424     134.48
 H      -4.437709    -0.974424     2.774310      23.32
 C      -2.776709     0.371150     0.691048      81.95
 H      -2.454492     1.389685     0.251251      25.96
 C      -4.014714     0.120979    -0.269677     106.31
 O      -5.020969    -1.017848    -0.071454     159.78
 H      -4.498910    -1.870738     0.050194      26.46
 H      -3.760539     0.269077    -1.343033      27.03
 H      -4.516692     1.030706    -0.209541      29.25
 C       1.299225     0.296791    -0.760918      40.84
 H       2.049772     1.069586    -0.714116      21.74
 C       1.013927    -2.215737    -1.044376      40.94
 H       1.338976    -3.136005    -1.285458      25.97
 C      -0.344288    -2.132515    -0.667620       9.50
 O      -1.078997    -3.403906    -0.528125     200.86
 C      -1.655484    -3.704463    -1.796155     118.36
 H      -2.614134    -3.219413    -2.399165      24.89
 H      -0.944923    -3.581707    -2.755399      25.30
 H      -1.578151    -4.707677    -1.685219      26.58
 C      -0.753934    -0.948657    -0.172853      30.35
 O      -2.004903    -0.896666     0.529320      89.10
 C      -0.064930     0.262867    -0.312947      68.09
 H      -0.499768     1.164705    -0.079599      26.44
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 C       1.847097    -0.956323    -1.101871       7.37
 C       3.349396    -1.165339    -1.298061      78.77
 H       3.391820    -2.191849    -1.945950      23.19
 O       3.839953    -0.039495    -2.132917     245.46
 H       4.737009     0.316277    -1.694422      25.60
 C       3.876927    -1.501615     0.126172      69.90
 H       3.169041    -2.310523     0.866572      24.79
 O       5.019223    -2.444841    -0.001578     116.74
 H       5.636163    -1.978528    -0.801240      25.19
 C       4.057396    -0.438140     1.303846     119.02
 O       5.136752     0.399562     0.897287     201.29
 H       5.088901     1.129415     1.451274      30.64
 H       4.372220    -0.760762     2.338119      28.32
 H       3.300038     0.478297     1.452983      23.05
55
name = lig-Water-frame_406
 C      -1.324282     2.388549     2.858657      61.01
 H      -1.987415     3.204777     2.380907      25.85
 C      -0.606465     0.093725     3.198908      52.44
 H      -0.529991    -1.156763     3.179107      23.04
 C       0.465333     0.536498     3.915602      25.19
 O       1.508761    -0.349618     4.400637     121.28
 C       1.398297    -1.737426     4.168933     127.85
 H       2.096813    -1.972997     4.950861      27.11
 H       1.532349    -2.160120     3.019215      27.73
 H       0.432035    -2.175653     4.385116      27.60
 C       0.859401     1.892092     3.964128      12.67
 O       1.973711     2.407634     4.560095     191.12
 H       1.833908     3.365129     4.375950      28.08
 C      -0.060526     2.813240     3.510559      75.09
 H       0.080918     3.800966     3.205065      15.30
 C      -1.632110     0.942753     2.800067      34.03
 C      -2.971123     0.646817     2.084184      73.08
 H      -3.910572     1.356167     2.428150      24.44
 O      -3.468400    -0.688609     2.944796     157.57
 H      -4.431062    -0.853934     2.799602      26.56
 C      -2.744789     0.326077     0.590462      78.75
 H      -2.279764     1.243652     0.133621      25.29
 C      -4.081772     0.110604    -0.295368      99.16
 O      -4.993939    -1.013112    -0.101741     171.17
 H      -4.426336    -1.814284    -0.115687      27.69
 H      -3.709668     0.128675    -1.394795      26.75
 H      -4.433623     1.247149    -0.082817      26.52
 C       1.273325     0.323545    -0.791519      42.04
 H       2.013921     1.142507    -0.733947      22.63
 C       1.041257    -2.161882    -1.026549      53.57
 H       1.609609    -3.195110    -1.279148      23.25
 C      -0.299744    -2.176213    -0.703444       7.76
 O      -1.085588    -3.402251    -0.532096     196.01
 C      -1.646016    -3.761301    -1.826381     115.27
 H      -2.472238    -3.333797    -2.255051      28.27
 H      -0.737855    -3.384447    -2.490833      25.33
 H      -1.747703    -4.963049    -2.043771      25.15
 C      -0.740074    -0.891664    -0.155435       5.36
 O      -1.956011    -0.901362     0.557850     111.32
 C      -0.019441     0.290283    -0.290015      67.88
 H      -0.703515     1.287385    -0.339929      22.17
 C       1.812591    -0.994662    -1.157276      19.67
 C       3.336228    -1.134378    -1.294574      87.00
 H       3.684494    -1.876087    -1.966671      25.14
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 O       3.856917    -0.028807    -2.136001     266.73
 H       4.690450     0.370548    -1.677089      26.60
 C       3.836421    -1.567268     0.160411      71.20
 H       3.123408    -2.096628     0.670259      30.35
 O       5.026971    -2.482321     0.006141     187.72
 H       5.585614    -2.235105    -0.666032      32.07
 C       4.023751    -0.347380     1.295259     108.64
 O       5.193381     0.397035     0.921149     175.06
 H       5.232332     1.332941     1.528925      21.31
 H       4.251270    -0.911848     2.202630      29.17
 H       3.069574     0.127159     1.230313      29.30
55
name = lig-Water-frame_407
 C      -1.359564     2.411713     2.852819      64.95
 H      -1.871511     3.108377     2.269460      28.65
 C      -0.700421     0.121399     3.219605      50.43
 H      -0.424589    -0.923368     3.235952      26.75
 C       0.530534     0.476933     3.921545      -6.49
 O       1.555281    -0.259074     4.420398     109.22
 C       1.346319    -1.744450     4.195622     124.56
 H       2.290632    -2.175191     4.693107      28.04
 H       1.713966    -1.887545     3.249625      30.49
 H       0.328822    -2.193206     4.533520      24.10
 C       0.845210     1.912720     3.902896       6.38
 O       1.947292     2.376664     4.526244     229.41
 H       2.082393     3.369813     4.397503      26.00
 C      -0.180842     2.746376     3.466778      61.03
 H       0.232597     3.850932     3.455634      20.09
 C      -1.677070     1.012145     2.808235      68.58
 C      -2.948271     0.569849     2.128694      83.60
 H      -3.697864     1.342491     2.249696      29.82
 O      -3.443156    -0.665007     2.924900     192.81
 H      -4.437129    -0.516755     2.809555      25.40
 C      -2.766082     0.244763     0.495473      83.33
 H      -2.150368     1.017335     0.016363      28.30
 C      -4.106131     0.154761    -0.321031     114.27
 O      -4.960451    -0.978800    -0.130477     157.82
 H      -4.366693    -1.860611    -0.070184      25.56
 H      -3.708314    -0.063765    -1.361939      28.04
 H      -4.724399     0.960842    -0.106937      30.20
 C       1.281075     0.283413    -0.831533      48.51
 H       1.762675     1.283635    -0.888527      25.52
 C       1.101647    -2.156902    -1.048929      63.85
 H       1.678839    -2.992764    -1.219319      25.57
 C      -0.270899    -2.188470    -0.675371     -12.12
 O      -1.099187    -3.373954    -0.527570     162.67
 C      -1.572996    -3.857844    -1.903594      98.35
 H      -2.660542    -3.200681    -1.920676      24.90
 H      -0.711794    -3.422749    -2.507310      25.67
 H      -1.881212    -4.824285    -2.107229      28.12
 C      -0.769977    -0.871140    -0.141991     -27.20
 O      -1.901871    -0.903612     0.567143     155.92
 C       0.009339     0.359373    -0.293428      62.96
 H      -0.605327     1.278179    -0.365708      24.68
 C       1.791219    -0.991307    -1.191349      36.30
 C       3.312080    -1.113555    -1.299680      79.41
 H       3.750476    -1.999826    -1.932948      23.31
 O       3.877311    -0.004023    -2.110967     300.17
 H       4.624444     0.435007    -1.792909      30.12
 C       3.868564    -1.579702     0.178530      34.68
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 H       2.772968    -2.260191     0.531778      26.52
 O       5.004475    -2.513325     0.047573     109.98
 H       5.753812    -2.312251    -0.742640      24.54
 C       4.001688    -0.327225     1.229991     105.53
 O       5.263399     0.434259     0.962920     206.91
 H       5.084527     1.303088     1.357199      26.51
 H       3.973311    -0.939970     2.163647      29.00
 H       2.885094    -0.038572     1.171613      28.76
55
name = lig-Water-frame_408
 C      -1.404490     2.393517     2.844349      69.06
 H      -1.981073     3.156608     2.191654      26.97
 C      -0.709786     0.120801     3.301783     -27.10
 H      -0.955400    -1.084055     3.021652      29.35
 C       0.581109     0.537593     3.888768       0.90
 O       1.578550    -0.219036     4.446486     118.30
 C       1.361906    -1.744381     4.251536     108.59
 H       2.133080    -2.399546     4.606775      30.08
 H       1.638123    -1.733036     3.059544      26.36
 H       0.451381    -2.080294     4.611543      26.62
 C       0.786405     1.891935     3.868825      16.23
 O       1.941408     2.354257     4.500852     213.30
 H       2.374249     3.314356     4.333855      15.14
 C      -0.243681     2.768251     3.408947      75.69
 H       0.087031     3.712007     3.736187      20.02
 C      -1.726773     1.095419     2.786962       2.56
 C      -2.920032     0.461278     2.157103      95.68
 H      -3.654646     1.434830     2.093056      27.17
 O      -3.424105    -0.615640     2.878966     202.92
 H      -4.411732    -0.330127     2.961866      19.49
 C      -2.808843     0.179500     0.487786      81.65
 H      -2.189159     1.014757    -0.046822      27.44
 C      -4.084364     0.152428    -0.358423     105.34
 O      -4.934176    -0.970253    -0.145530     198.19
 H      -4.489516    -1.766908     0.142248      29.34
 H      -3.771109     0.138481    -1.462823      28.03
 H      -4.978178     0.947452    -0.255111      24.52
 C       1.279266     0.260489    -0.878196      54.74
 H       1.679493     1.214403    -1.165894      24.28
 C       1.114590    -2.182409    -1.079311      30.01
 H       1.729382    -3.157082    -1.268155      22.62
 C      -0.253341    -2.148322    -0.599202     -16.16
 O      -1.097205    -3.349038    -0.521239     138.11
 C      -1.542069    -3.862423    -1.951741      92.97
 H      -2.348993    -3.311540    -1.891442      27.05
 H      -0.839842    -3.565660    -2.953716      23.63
 H      -1.822496    -4.995375    -1.928182      26.57
 C      -0.751874    -0.885714    -0.167138       1.82
 O      -1.886643    -0.928808     0.563296     153.76
 C      -0.000377     0.375028    -0.319006      57.38
 H      -0.406478     1.451884    -0.179293      24.10
 C       1.835165    -0.938665    -1.213179      25.86
 C       3.338730    -1.121846    -1.328060      86.83
 H       3.422178    -2.133723    -1.777946      23.68
 O       3.868886     0.017975    -2.080125     270.02
 H       4.804636     0.499612    -1.771180      24.59
 C       3.886793    -1.564297     0.165040      89.42
 H       3.132330    -2.186569     0.357050      29.30
 O       4.981883    -2.534786     0.095679     170.66
 H       5.617690    -2.223036    -0.615372      27.88
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 C       3.969795    -0.412408     1.138621     115.11
 O       5.291937     0.464247     1.005593     201.62
 H       4.937734     1.378652     1.433153      25.30
 H       3.957043    -0.655434     2.233598      27.73
 H       3.104100     0.308286     1.078791      26.02
55
name = lig-Water-frame_409
 C      -1.490623     2.433411     2.788935      48.34
 H      -2.142774     3.150934     2.388029      23.84
 C      -0.708701     0.088700     3.379567       3.75
 H      -1.418645    -0.614371     3.038463      20.80
 C       0.558455     0.560486     3.820842      12.09
 O       1.596373    -0.234179     4.489476     123.35
 C       1.424945    -1.700973     4.234717     122.34
 H       2.129369    -2.383143     4.804081      25.78
 H       1.167968    -1.852121     3.231834      24.87
 H       0.334911    -1.955248     4.653239      24.97
 C       0.729582     1.932904     3.851121      30.01
 O       1.955800     2.333653     4.481519     171.81
 H       2.174014     3.173609     4.106442      29.38
 C      -0.212111     2.824866     3.398749      76.29
 H      -0.217755     3.913346     3.784758      18.86
 C      -1.711455     1.051772     2.779324     -40.07
 C      -2.924990     0.452309     2.105733     125.31
 H      -3.676504     1.259442     2.045514      26.40
 O      -3.438683    -0.575743     2.848990     230.43
 H      -4.376881    -0.453050     3.050140      22.41
 C      -2.819298     0.173379     0.548665      96.56
 H      -2.397842     1.060917     0.141184      28.17
 C      -4.081668     0.125257    -0.411966     111.68
 O      -4.935688    -0.986239    -0.156223     225.67
 H      -4.458508    -1.787029     0.326605      24.33
 H      -3.804191     0.438389    -1.486260      26.13
 H      -4.617657     1.062509    -0.285194      27.90
 C       1.243253     0.290068    -0.934034      36.33
 H       1.855100     1.138598    -1.372752      20.82
 C       1.106787    -2.196625    -1.100594      48.87
 H       1.484816    -3.202834    -1.341047      21.26
 C      -0.203577    -2.122677    -0.541299       9.08
 O      -1.064305    -3.318377    -0.531802     132.54
 C      -1.502087    -3.869964    -1.989328      74.06
 H      -2.589675    -3.234229    -2.241377      23.26
 H      -0.974355    -3.746551    -2.943018      24.84
 H      -1.544971    -4.916891    -1.610848      25.00
 C      -0.709807    -0.869005    -0.196333      22.94
 O      -1.913287    -0.982191     0.541588     149.99
 C      -0.032682     0.346598    -0.369767      64.89
 H      -0.139211     1.379216     0.187543      23.51
 C       1.897135    -0.953300    -1.219104      12.04
 C       3.380902    -1.135249    -1.348741      88.50
 H       3.366775    -2.136607    -1.923153      22.70
 O       3.869465     0.037921    -2.044700     308.58
 H       4.766623     0.215621    -1.751842      28.75
 C       3.926196    -1.518482     0.091769      64.56
 H       2.979214    -2.349451     0.544516      23.20
 O       4.964150    -2.534834     0.144462     174.28
 H       5.613130    -2.188311    -0.502038      29.79
 C       3.969939    -0.447513     1.089911     131.94
 O       5.282393     0.479288     1.034793     210.32
 H       5.002510     1.261630     1.705924      24.87
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 H       4.019882    -0.526834     2.158529      25.60
 H       3.400928     0.473202     0.829861      21.32
55
name = lig-Water-frame_410
 C      -1.518097     2.460963     2.758215      31.61
 H      -2.374616     3.215273     2.568598      18.21
 C      -0.765171     0.117034     3.411608      60.16
 H      -1.282278    -0.967623     3.385130      21.14
 C       0.512610     0.505426     3.772635     -24.13
 O       1.593445    -0.257099     4.509192     165.30
 C       1.413685    -1.647795     4.244685     114.78
 H       2.216491    -2.090733     4.811765      26.01
 H       1.018711    -2.079926     3.206991      23.76
 H       0.521768    -1.825989     4.763606      25.12
 C       0.727645     2.002065     3.861164     -10.75
 O       1.951621     2.309852     4.448356     154.66
 H       1.994433     3.261498     4.001020      24.99
 C      -0.234737     2.931043     3.390708      53.86
 H      -0.327981     3.986199     3.619423      22.85
 C      -1.647854     1.004826     2.775966      17.62
 C      -2.969029     0.515309     2.014612     112.38
 H      -3.847184     1.338993     2.100540      22.40
 O      -3.469938    -0.590031     2.855394     219.23
 H      -4.509385    -0.530362     2.912982      24.55
 C      -2.808766     0.177918     0.612952      89.28
 H      -2.331802     1.238811     0.316032      20.71
 C      -4.050697     0.113926    -0.427486      88.50
 O      -4.954626    -1.012676    -0.170146     237.63
 H      -4.344956    -1.733131     0.201563      24.71
 H      -3.709523     0.239847    -1.483060      25.19
 H      -4.423652     1.190517    -0.043278      25.09
 C       1.253033     0.297188    -1.030428      18.85
 H       1.884984     1.132309    -1.227184      19.91
 C       1.090556    -2.174039    -1.106240      47.21
 H       1.351661    -3.195793    -1.436478      21.43
 C      -0.138741    -2.131062    -0.538006      11.86
 O      -1.014137    -3.267274    -0.575310     189.21
 C      -1.524421    -3.838994    -1.959154      84.93
 H      -2.405575    -3.630590    -2.435023      27.29
 H      -0.617766    -3.883664    -2.883164      23.50
 H      -1.496401    -4.835182    -1.587137      25.21
 C      -0.713229    -0.846850    -0.184907      16.44
 O      -1.948973    -1.029313     0.494645     142.95
 C      -0.032211     0.333368    -0.404210      63.31
 H      -0.249768     1.118361     0.279369      20.42
 C       1.895083    -1.012507    -1.205660      26.42
 C       3.405960    -1.167370    -1.379911      93.40
 H       3.699583    -1.935176    -2.170693      22.76
 O       3.874508     0.038941    -2.004673     292.17
 H       4.839862     0.104604    -1.773922      28.39
 C       3.900867    -1.550403     0.029620      82.87
 H       3.133371    -1.921915     0.543066      30.31
 O       4.959901    -2.513848     0.176363     169.09
 H       5.878750    -2.287901    -0.404709      26.76
 C       4.026904    -0.364639     1.064655      99.19
 O       5.280129     0.459156     1.057377     267.74
 H       5.145362     1.231469     1.837094      21.54
 H       3.831727    -0.787852     2.125569      25.31
 H       3.249235     0.347095     0.557910      22.03
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name = lig-Water-frame_411
 C      -1.471267     2.447284     2.779899      25.46
 H      -2.355885     3.040715     2.669492      22.11
 C      -0.849670     0.075089     3.414436      47.35
 H      -0.657765    -0.935389     3.826891      20.49
 C       0.495845     0.519007     3.782393     -32.80
 O       1.550186    -0.238881     4.470219     179.95
 C       1.360269    -1.628217     4.278743     116.34
 H       2.371867    -1.993901     4.625582      25.03
 H       1.386049    -2.022581     3.287787      27.15
 H       0.575605    -1.978886     5.104927      23.41
 C       0.718446     2.003592     3.864021     -15.47
 O       1.932987     2.320011     4.387014     143.86
 H       2.173842     3.338756     4.377796      20.93
 C      -0.319474     3.016038     3.364966      23.45
 H      -0.113610     4.101337     3.500998      24.64
 C      -1.647346     1.034170     2.731380      45.20
 C      -3.044055     0.577488     2.022098      95.47
 H      -3.771479     1.444403     2.145567      24.41
 O      -3.521349    -0.621378     2.869817     255.99
 H      -4.480072    -0.531375     2.662500      26.17
 C      -2.773444     0.197658     0.597517     105.24
 H      -2.198516     1.010998     0.274028      24.67
 C      -3.993882     0.133150    -0.368451      89.30
 O      -4.962720    -1.020487    -0.187416     204.10
 H      -4.381064    -1.825672    -0.044687      25.34
 H      -3.600179    -0.117186    -1.422185      25.05
 H      -4.559914     1.014705    -0.061975      26.58
 C       1.292471     0.245948    -1.112805      40.08
 H       1.847413     1.232463    -0.995229      21.52
 C       1.099310    -2.168385    -1.112130      48.36
 H       1.462176    -3.168601    -1.566500      22.24
 C      -0.146561    -2.119086    -0.568067      24.70
 O      -0.977835    -3.212312    -0.639414     223.93
 C      -1.451373    -3.840704    -1.907577      94.99
 H      -2.551799    -3.640935    -2.474942      23.07
 H      -0.542646    -3.817425    -2.495058      25.78
 H      -1.633277    -5.007349    -1.684304      24.52
 C      -0.737400    -0.882132    -0.156753       9.69
 O      -1.979447    -1.043454     0.437921     157.74
 C      -0.001797     0.318960    -0.431934      60.45
 H      -0.556902     1.206999     0.223213      16.86
 C       1.867339    -1.039238    -1.215330      21.97
 C       3.424217    -1.201303    -1.449446      91.59
 H       3.864806    -1.929057    -2.173197      22.67
 O       3.888583     0.046980    -1.954787     256.21
 H       4.944934     0.218183    -1.877059      26.65
 C       3.927380    -1.545399    -0.004165      43.54
 H       2.846592    -1.992583     0.593745      23.83
 O       4.983921    -2.499878     0.189943     240.73
 H       5.750469    -2.330596    -0.256055      32.26
 C       4.076317    -0.251641     1.015095     110.76
 O       5.281268     0.409061     1.087448     315.52
 H       5.209331     1.235620     1.727417      22.86
 H       3.670733    -0.806229     1.836938      26.65
 H       3.095625     0.197025     0.739177      25.10
55
name = lig-Water-frame_412
 C      -1.408172     2.414535     2.827248      45.70
 H      -2.311637     2.992062     2.539500      25.83
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 C      -0.824584     0.043414     3.430099      32.08
 H      -0.768523    -0.969381     3.858347      25.49
 C       0.462836     0.632802     3.822713       8.14
 O       1.469071    -0.182156     4.395152     139.30
 C       1.352350    -1.654164     4.374945     127.31
 H       2.382769    -2.004287     4.518019      28.12
 H       1.433736    -1.887480     3.241592      27.89
 H       0.763963    -2.219128     5.031524      28.66
 C       0.669317     2.000329     3.830785       9.86
 O       1.935002     2.350604     4.338886     180.89
 H       2.132369     3.323043     4.559915      21.88
 C      -0.344451     3.033239     3.366888      26.53
 H       0.097310     4.065552     3.350453      18.86
 C      -1.722102     1.039436     2.686971      36.32
 C      -3.062383     0.593980     2.121080      91.43
 H      -3.770017     1.509261     2.104653      26.69
 O      -3.568571    -0.625480     2.857738     245.16
 H      -4.547798    -0.634184     2.647391      25.62
 C      -2.750491     0.200480     0.553930      82.61
 H      -2.026754     0.951560    -0.014513      23.49
 C      -3.945198     0.099784    -0.303659      97.41
 O      -4.953794    -1.017755    -0.190699     131.09
 H      -4.532457    -1.984469    -0.258486      24.86
 H      -3.550465    -0.038040    -1.284613      27.96
 H      -4.757915     0.990445    -0.355365      24.36
 C       1.299541     0.214293    -1.118757      65.68
 H       1.853095     1.122645    -0.973831      27.46
 C       1.124165    -2.206597    -1.136750      62.39
 H       1.574686    -3.057146    -1.524461      25.15
 C      -0.200434    -2.095460    -0.634026      36.03
 O      -0.990639    -3.192155    -0.679715     221.59
 C      -1.396897    -3.890924    -1.852052     113.80
 H      -2.211374    -3.296821    -2.189383      26.97
 H      -0.345968    -3.688637    -2.555695      23.46
 H      -1.622015    -4.859093    -1.680735      29.28
 C      -0.733705    -0.915359    -0.143565      13.78
 O      -2.012709    -1.036213     0.389849     149.73
 C      -0.002284     0.288077    -0.433602      53.97
 H      -0.363344     1.241098    -0.283795      23.53
 C       1.897647    -1.029342    -1.282643     -11.93
 C       3.449787    -1.218566    -1.508034      87.41
 H       3.732583    -2.186765    -2.112550      23.49
 O       3.913423     0.079060    -1.917111     317.66
 H       4.805840     0.271019    -1.854575      30.61
 C       3.931441    -1.513603     0.017037      71.04
 H       3.174565    -2.121981     0.300304      28.89
 O       4.988042    -2.498651     0.210211     186.21
 H       5.815259    -2.192106    -0.407185      24.54
 C       4.044624    -0.216783     0.928620     108.94
 O       5.307518     0.359699     1.107734     282.72
 H       5.114843     1.302197     1.734984      20.29
 H       3.835907    -0.722743     2.001297      25.30
 H       3.098002     0.503601     0.944610      23.86
55
name = lig-Water-frame_413
 C      -1.439197     2.384212     2.836846      55.33
 H      -2.114593     3.103326     2.279575      24.28
 C      -0.768364     0.087527     3.423555      54.32
 H      -1.305076    -0.946552     3.522816      29.83
 C       0.373449     0.697750     3.865250      32.09
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 O       1.389572    -0.120157     4.341951      61.07
 C       1.412054    -1.675482     4.399948     107.78
 H       2.436807    -1.943131     4.694071      28.37
 H       1.026579    -1.880137     3.380230      26.66
 H       0.659658    -2.337302     5.005407      28.64
 C       0.639141     2.075459     3.799316      39.42
 O       1.941082     2.356024     4.301567     154.28
 H       1.838680     3.459715     4.362779      23.05
 C      -0.249965     2.980549     3.400816      16.62
 H      -0.021755     4.004247     3.240110      13.72
 C      -1.762437     0.976158     2.735193      31.08
 C      -3.039514     0.566898     2.202971      97.80
 H      -3.844660     1.414955     2.011189      25.89
 O      -3.597684    -0.602199     2.825004     258.56
 H      -4.614449    -0.657539     2.840917      25.72
 C      -2.723802     0.225721     0.539283      82.42
 H      -2.270374     0.989667     0.020563      28.46
 C      -3.971119     0.050125    -0.291470     110.23
 O      -4.943005    -1.026056    -0.183966     197.42
 H      -4.524634    -1.888473    -0.208929      27.46
 H      -3.471520     0.130186    -1.381127      25.10
 H      -4.584126     0.928933    -0.594748      24.90
 C       1.273520     0.188200    -1.060577      41.28
 H       1.946434     1.076251    -1.172610      24.80
 C       1.138621    -2.208398    -1.166204      39.70
 H       1.644490    -3.265403    -1.438329      22.25
 C      -0.207932    -2.104261    -0.738606     -10.73
 O      -1.033005    -3.210124    -0.649145     196.28
 C      -1.280395    -3.871086    -1.843460     110.57
 H      -2.115459    -3.060784    -2.229181      24.05
 H      -0.588276    -3.860791    -2.662374      25.23
 H      -1.626618    -5.018306    -1.558570      23.51
 C      -0.728526    -0.901021    -0.145982     -12.70
 O      -2.038293    -1.030235     0.353840      89.52
 C       0.014339     0.232258    -0.455027      55.11
 H      -0.210667     1.406695    -0.730183      20.77
 C       1.958600    -1.038845    -1.378616       1.11
 C       3.472341    -1.217253    -1.512490      87.80
 H       3.578433    -2.140325    -2.105677      25.14
 O       3.917274     0.107617    -1.908805     276.85
 H       4.943800     0.262606    -1.719542      25.63
 C       3.943614    -1.471939     0.009215      59.53
 H       3.051771    -2.292433     0.380684      26.27
 O       5.020160    -2.475627     0.208899     167.78
 H       5.750506    -2.165186    -0.468995      25.32
 C       3.954364    -0.241158     0.928904     121.23
 O       5.353336     0.347784     1.117514     253.51
 H       5.126511     1.116189     1.697100      27.76
 H       3.961076    -0.570574     1.926640      29.15
 H       3.375453     0.675489     0.814541      26.05
55
name = lig-Water-frame_414
 C      -1.499963     2.365607     2.810032      99.61
 H      -1.932700     3.117159     2.188641      22.35
 C      -0.826406     0.144804     3.367372      83.81
 H      -1.337626    -0.766417     3.230276      28.62
 C       0.286510     0.674871     3.913106      41.29
 O       1.349114    -0.078899     4.333607      63.99
 C       1.421133    -1.674675     4.387172      99.48
 H       2.452360    -1.829183     4.765402      28.35
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 H       0.946591    -2.056080     3.456510      29.85
 H       0.660067    -1.956792     5.115885      30.41
 C       0.708082     2.102736     3.824975      26.30
 O       1.918550     2.370943     4.261015     264.03
 H       2.089833     3.388755     4.143849      27.48
 C      -0.224284     2.931464     3.378726      77.83
 H      -0.202461     4.050016     3.213138      16.72
 C      -1.731975     0.974987     2.867522      42.57
 C      -3.039139     0.509001     2.185427      94.07
 H      -3.785114     1.305797     2.131193      26.76
 O      -3.613208    -0.591120     2.803569     255.38
 H      -4.579168    -0.370703     3.001144      24.25
 C      -2.757954     0.239622     0.581043      65.15
 H      -2.334812     1.281346     0.163837      25.30
 C      -4.006482     0.017578    -0.377281     108.40
 O      -4.935021    -1.026126    -0.166415     206.70
 H      -4.343622    -1.913059    -0.031643      22.12
 H      -3.531350    -0.073826    -1.325156      26.83
 H      -4.542828     1.072722    -0.408355      25.77
 C       1.318461     0.130810    -1.010420      41.68
 H       1.798709     1.051414    -1.413129      20.95
 C       1.170112    -2.218214    -1.222644      34.56
 H       1.445046    -3.193854    -1.279356      24.37
 C      -0.185353    -2.109920    -0.812781     -27.70
 O      -1.045059    -3.237334    -0.568897     178.40
 C      -1.246393    -3.846228    -1.867801     115.13
 H      -2.063295    -3.431343    -2.463109      27.41
 H      -0.463676    -4.171088    -2.817418      22.54
 H      -1.621812    -4.727990    -1.615044      28.60
 C      -0.738724    -0.906949    -0.187243     -13.24
 O      -2.028134    -1.015098     0.323136      71.91
 C       0.036692     0.258748    -0.516851      70.78
 H      -0.429169     1.149723    -0.609413      28.41
 C       1.967767    -1.067736    -1.442443      49.32
 C       3.476851    -1.174785    -1.461030      90.72
 H       3.734825    -1.993603    -2.287678      25.01
 O       3.939823     0.125421    -1.924416     271.30
 H       4.915724     0.226461    -1.609273      25.43
 C       3.902241    -1.503649    -0.003978      88.74
 H       3.082433    -1.952626     0.499692      29.92
 O       5.063609    -2.419484     0.186554     186.44
 H       5.804922    -2.241123    -0.402333      29.80
 C       3.924068    -0.263559     0.969693      89.85
 O       5.403990     0.322723     1.095393     193.35
 H       5.277736     1.188879     1.802571      22.21
 H       3.596737    -0.617809     2.089321      27.35
 H       3.426018     0.677183     0.433888      22.55
55
name = lig-Water-frame_415
 C      -1.495335     2.379910     2.803112      74.77
 H      -2.094204     3.088304     2.105947      25.56
 C      -0.904054     0.146555     3.324715      45.19
 H      -0.960036    -1.025027     3.225762      25.65
 C       0.277515     0.646392     3.962012      14.36
 O       1.353950    -0.084382     4.350632      98.85
 C       1.367996    -1.600719     4.384467     110.81
 H       2.398092    -1.817590     4.627346      29.20
 H       1.241456    -2.279830     3.446971      29.95
 H       0.759811    -1.647395     5.330756      26.97
 C       0.741218     2.030852     3.870552      -2.88
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 O       1.941497     2.379227     4.233291     166.02
 H       2.417749     3.289741     4.105622      21.90
 C      -0.318464     2.925747     3.286986      50.27
 H      -0.157320     3.983406     3.299344      24.03
 C      -1.795389     1.093670     2.937186      64.80
 C      -3.016024     0.460110     2.101930      88.91
 H      -3.729491     1.441096     2.320068      24.91
 O      -3.641395    -0.611789     2.808667     250.12
 H      -4.503570    -0.168953     3.080914      24.56
 C      -2.837870     0.265657     0.629420      91.21
 H      -2.323891     1.138151     0.410333      29.86
 C      -4.029555     0.045612    -0.460061      98.24
 O      -4.924100    -1.042836    -0.129799     167.03
 H      -4.425812    -1.861323     0.095286      25.67
 H      -3.581967    -0.315625    -1.488154      26.07
 H      -4.556041     0.984255    -0.139390      27.42
 C       1.392319     0.099858    -1.018653      51.83
 H       1.675585     1.044000    -1.431240      25.52
 C       1.163778    -2.227528    -1.282622      18.32
 H       1.488115    -3.372659    -1.289841      22.93
 C      -0.179094    -2.085071    -0.808118       2.34
 O      -1.012321    -3.256621    -0.521179     107.26
 C      -1.242372    -3.876414    -1.941923      85.36
 H      -2.115443    -3.486175    -2.628419      25.65
 H      -0.281191    -4.129215    -2.392274      23.37
 H      -1.782334    -4.935792    -1.603872      24.25
 C      -0.725859    -0.931472    -0.285984      26.39
 O      -1.985346    -0.980382     0.298971      50.92
 C       0.023935     0.264151    -0.568818      43.81
 H      -0.700401     1.210953    -0.304065      27.29
 C       1.942832    -1.109184    -1.455246      58.37
 C       3.482232    -1.122725    -1.443077     102.44
 H       3.953296    -1.780907    -2.156644      28.63
 O       3.973902     0.134767    -1.938818     298.49
 H       4.835115     0.317613    -1.660076      29.80
 C       3.896908    -1.528239     0.011528      71.09
 H       2.921619    -2.057174     0.563588      29.39
 O       5.077085    -2.359289     0.174089     139.19
 H       5.967324    -2.133619    -0.477221      23.85
 C       3.953618    -0.248017     1.006312     129.88
 O       5.423904     0.292011     1.087709     227.85
 H       5.451475     1.133368     1.646365      25.19
 H       3.319059    -0.460352     1.831967      32.70
 H       3.339213     0.371304     0.430046      29.22
55
name = lig-Water-frame_416
 C      -1.505888     2.481558     2.770607      64.54
 H      -2.287026     2.963062     2.276282      28.50
 C      -0.907084     0.104200     3.351765       5.59
 H      -0.670439    -0.937915     3.267395      24.51
 C       0.302624     0.637214     3.977903      -5.03
 O       1.396718    -0.129540     4.364590     181.07
 C       1.320381    -1.504151     4.410217     133.40
 H       2.401331    -1.789993     4.577333      27.74
 H       1.232950    -2.149080     3.569459      31.14
 H       0.799867    -1.851825     5.372102      26.19
 C       0.623911     1.986178     3.865518       0.14
 O       2.028751     2.340723     4.226175     107.70
 H       2.081148     3.396406     4.139369      20.52
 C      -0.335752     2.909502     3.236644      36.61
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 H      -0.028969     3.968063     3.292405      24.41
 C      -1.935195     1.118812     2.915570      34.47
 C      -3.021564     0.479488     2.077957     103.36
 H      -3.666699     1.319997     2.101891      29.76
 O      -3.668257    -0.642224     2.827184     235.29
 H      -4.588350    -0.306086     3.092514      21.37
 C      -2.894523     0.249586     0.618568      83.13
 H      -2.214581     1.163890     0.345263      28.09
 C      -4.027573     0.058718    -0.474147     103.24
 O      -4.935214    -1.048423    -0.080990     157.89
 H      -4.455066    -1.955259     0.069974      23.07
 H      -3.695638    -0.044359    -1.468561      29.57
 H      -4.733580     0.964684    -0.392103      28.54
 C       1.377584     0.137740    -1.058113      27.98
 H       1.923975     1.130444    -1.314678      24.13
 C       1.116411    -2.291992    -1.324486      39.24
 H       1.609212    -3.198751    -1.469177      25.65
 C      -0.175740    -2.115163    -0.768673      32.74
 O      -0.965026    -3.268031    -0.531979     150.48
 C      -1.290921    -3.986660    -1.972499      70.26
 H      -1.833027    -3.206086    -2.623396      26.08
 H      -0.104667    -3.974674    -1.979397      21.69
 H      -1.690972    -4.897988    -1.723240      28.20
 C      -0.717944    -0.897842    -0.397857      25.54
 O      -1.936252    -0.944383     0.288508      53.76
 C      -0.011441     0.248428    -0.599851      64.07
 H      -0.314669     1.160667    -0.150437      28.05
 C       1.949393    -1.135918    -1.443459      14.76
 C       3.500226    -1.082704    -1.444879      75.61
 H       4.100076    -1.962582    -2.017352      27.53
 O       3.987735     0.156417    -1.954361     251.10
 H       4.984507     0.496097    -1.681632      24.27
 C       3.904078    -1.528338     0.088663      82.03
 H       3.157976    -2.317217     0.298781      28.88
 O       5.093193    -2.308683     0.158261     215.87
 H       5.684200    -1.927560    -0.424178      32.03
 C       4.022137    -0.234094     0.985273     119.28
 O       5.409193     0.237329     1.083019     239.31
 H       5.346593     1.154856     1.585189      24.81
 H       3.310161    -0.293345     1.979139      28.44
 H       3.232741     0.492083     0.396746      25.69
55
name = lig-Water-frame_417
 C      -1.600953     2.522107     2.729470     108.68
 H      -2.470929     3.255559     2.422903      26.58
 C      -0.875290     0.134991     3.416874      45.20
 H      -0.915835    -0.986254     3.199434      22.65
 C       0.308555     0.618151     3.955659      14.04
 O       1.438208    -0.138067     4.372619     169.48
 C       1.327124    -1.489360     4.484766     120.55
 H       2.350896    -1.762155     4.662254      26.43
 H       0.826575    -1.887005     3.438680      25.32
 H       0.720357    -2.073060     5.191522      26.53
 C       0.530149     1.993898     3.850268     -12.16
 O       2.060957     2.301236     4.207226     152.97
 H       1.861103     3.270520     4.277308      22.48
 C      -0.251844     2.914988     3.243770      40.04
 H       0.056597     3.971565     3.145825      22.30
 C      -1.970537     1.036767     2.870836      30.90
 C      -3.097443     0.507990     2.108931      68.32
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 H      -4.011324     1.298824     1.759570      19.65
 O      -3.687463    -0.667786     2.848544     228.98
 H      -4.681002    -0.511676     2.928518      22.86
 C      -2.852961     0.233655     0.520054      73.38
 H      -2.384151     1.118404     0.128515      24.44
 C      -4.056761     0.074629    -0.402245     100.81
 O      -4.951886    -1.050959    -0.039636     190.28
 H      -4.414836    -1.942480    -0.120758      22.83
 H      -3.612566     0.207356    -1.519695      25.09
 H      -4.811820     0.867839    -0.765087      23.76
 C       1.327532     0.188576    -1.124665      22.71
 H       2.062333     0.937743    -1.045657      18.42
 C       1.093599    -2.310035    -1.352338      57.53
 H       1.656032    -3.271200    -1.673343      21.47
 C      -0.165822    -2.207213    -0.745013      17.58
 O      -0.946742    -3.284937    -0.553036     166.53
 C      -1.257585    -4.031190    -1.945812      80.35
 H      -1.580829    -3.166807    -2.572799      23.60
 H      -0.294375    -4.184812    -2.303356      26.06
 H      -1.804724    -5.076024    -1.782388      23.91
 C      -0.759729    -0.850029    -0.480743      13.75
 O      -1.905007    -0.921255     0.290346     105.26
 C       0.042451     0.257536    -0.633321      65.43
 H      -0.047671     1.278870    -0.117584      21.22
 C       1.956509    -1.108391    -1.416546      10.69
 C       3.550576    -1.101655    -1.439805      67.98
 H       3.894667    -2.000965    -1.920113      24.28
 O       4.002571     0.193422    -1.971461     319.73
 H       4.890797     0.470431    -1.700646      29.78
 C       3.925233    -1.505387     0.149293      73.79
 H       3.166325    -2.392149     0.333192      23.07
 O       5.098442    -2.271871     0.162867     185.49
 H       5.778745    -1.727538    -0.500191      25.37
 C       4.013511    -0.208162     0.958300     127.57
 O       5.378845     0.187825     1.088226     285.26
 H       5.164980     1.144361     1.525408      24.30
 H       3.800791    -0.272620     2.008247      24.30
 H       3.589797     0.617109     0.511750      22.45
55
name = lig-Water-frame_418
 C      -1.693922     2.490076     2.732493      59.00
 H      -2.238476     3.371059     2.578315      22.27
 C      -0.898669     0.158495     3.447972      76.95
 H      -1.371267    -0.826679     3.270156      26.01
 C       0.317236     0.591905     3.926323      24.72
 O       1.450024    -0.083047     4.396968     106.24
 C       1.322715    -1.568087     4.501036     114.87
 H       2.356595    -1.969144     4.650104      25.52
 H       0.835056    -1.688237     3.593557      26.50
 H       0.482558    -1.984979     5.217488      25.97
 C       0.571831     1.999484     3.856492      -3.16
 O       2.005198     2.256903     4.174671     148.21
 H       2.160428     3.314461     4.440637      20.01
 C      -0.248448     2.944090     3.221776      69.96
 H       0.120891     3.934497     3.021538      20.62
 C      -1.896387     1.022316     2.829202       9.89
 C      -3.250843     0.514862     2.092241      91.15
 H      -4.016208     1.160302     1.967545      28.30
 O      -3.700176    -0.683881     2.862109     233.01
 H      -4.704909    -0.591131     2.695110      26.87
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 C      -2.779211     0.224273     0.429352      80.11
 H      -2.413390     1.209027    -0.026892      24.70
 C      -4.107256     0.081224    -0.377469     103.35
 O      -4.954906    -1.052719    -0.026405     260.23
 H      -4.435706    -1.852569    -0.123948      27.64
 H      -3.558439    -0.070088    -1.288215      28.59
 H      -4.768545     0.934822    -0.522788      27.43
 C       1.342497     0.164124    -1.206205      39.59
 H       2.084205     0.962220    -0.807561      18.38
 C       1.143024    -2.282208    -1.375577      51.63
 H       1.427705    -3.280202    -1.741795      22.19
 C      -0.152825    -2.227838    -0.756888      -4.62
 O      -0.968015    -3.353646    -0.585306     146.89
 C      -1.182433    -4.052854    -1.891010      96.40
 H      -1.659666    -3.232656    -2.613726      23.72
 H      -0.404102    -4.624334    -2.709920      22.39
 H      -2.036028    -4.808851    -1.795489      25.35
 C      -0.788318    -0.858664    -0.539461       1.99
 O      -1.904061    -0.900573     0.299290     159.62
 C       0.104417     0.316744    -0.649757      44.89
 H      -0.159494     1.326515    -0.169642      20.34
 C       1.940052    -1.055109    -1.393374      22.92
 C       3.554963    -1.122855    -1.397831      63.02
 H       3.789038    -2.064853    -2.121384      22.34
 O       4.002360     0.204487    -1.987303     292.94
 H       4.920644     0.429088    -1.668026      28.10
 C       3.924514    -1.479741     0.141218      77.01
 H       3.040226    -2.068446     0.648214      24.44
 O       5.121960    -2.229599     0.176148     230.55
 H       5.950334    -1.944983    -0.306375      29.36
 C       3.990730    -0.199572     0.966109     103.48
 O       5.387545     0.170830     1.092070     266.92
 H       5.370135     1.014672     1.499367      30.45
 H       3.872543    -0.456641     2.116483      22.62
 H       3.566332     0.833402     0.527501      19.01
55
name = lig-Water-frame_419
 C      -1.655545     2.428435     2.797146      55.00
 H      -2.283540     3.340679     2.497814      21.84
 C      -0.997458     0.164440     3.433626      72.57
 H      -1.433178    -0.825897     3.559605      28.03
 C       0.338785     0.594026     3.904153     -15.14
 O       1.447678    -0.044882     4.448807      77.81
 C       1.285482    -1.633139     4.510015      98.92
 H       2.224668    -2.178746     4.612952      26.35
 H       0.946590    -1.933498     3.369489      24.52
 H       0.571768    -1.708076     5.289013      26.72
 C       0.675364     2.024836     3.843501      -2.64
 O       1.927777     2.242747     4.152438     168.55
 H       2.291850     3.065829     4.255243      22.64
 C      -0.322602     2.927751     3.187184      80.17
 H       0.104682     3.953175     2.964333      27.85
 C      -1.850636     1.101473     2.773921      21.56
 C      -3.292147     0.470241     2.067552      69.08
 H      -4.167936     1.371987     2.328571      24.26
 O      -3.716321    -0.688074     2.850219     223.23
 H      -4.678871    -0.693481     2.670959      26.08
 C      -2.764520     0.254040     0.403381      86.85
 H      -2.284971     1.191083     0.034080      25.25
 C      -4.128015     0.049398    -0.378015      79.01
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 O      -4.965486    -1.041597    -0.019389     210.59
 H      -4.382703    -1.957484     0.038154      23.80
 H      -3.748383    -0.418238    -1.394610      25.81
 H      -4.621341     1.090789    -0.077242      26.56
 C       1.408450     0.173007    -1.230588      45.77
 H       1.954104     1.016837    -0.974651      22.01
 C       1.172445    -2.228009    -1.375375      62.64
 H       1.421629    -3.235189    -1.722267      23.74
 C      -0.139840    -2.158465    -0.806113     -12.74
 O      -0.980975    -3.445161    -0.641174     147.27
 C      -1.149916    -4.061496    -1.910639     133.51
 H      -1.649324    -3.371388    -2.555317      26.11
 H      -0.579664    -4.768992    -2.355403      29.10
 H      -2.151292    -4.631087    -1.643472      25.49
 C      -0.749116    -0.882092    -0.566311       2.82
 O      -1.917697    -0.882496     0.302500     154.01
 C       0.076838     0.338525    -0.656093      38.49
 H      -0.340829     1.263591    -0.318850      22.33
 C       1.958424    -1.063944    -1.401862      32.85
 C       3.495990    -1.141872    -1.380939      88.58
 H       3.825064    -1.839686    -2.080327      24.90
 O       3.997487     0.177076    -1.987193     250.57
 H       4.992155     0.417568    -1.646786      25.65
 C       3.925164    -1.417648     0.081582      74.83
 H       3.068923    -1.913630     0.702735      25.50
 O       5.132154    -2.223368     0.235297     244.29
 H       5.936229    -1.983200    -0.289000      30.19
 C       3.992461    -0.161001     1.028128     108.97
 O       5.439625     0.160073     1.082396     241.80
 H       5.635612     1.101810     1.632960      24.14
 H       3.462859    -0.526459     1.911272      26.77
 H       3.296598     0.550246     0.718226      26.60
55
name = lig-Water-frame_420
 C      -1.550434     2.463101     2.857928      79.70
 H      -2.371176     2.941508     2.319338      21.75
 C      -1.052509     0.174597     3.423501      42.60
 H      -1.255852    -0.864136     3.843197      26.89
 C       0.319832     0.638579     3.875538     -38.28
 O       1.439371    -0.075350     4.503102      55.29
 C       1.239473    -1.655793     4.455913     104.75
 H       2.180525    -2.156941     4.756572      27.12
 H       0.971057    -2.120209     3.605114      29.31
 H       0.548917    -1.663132     5.425062      24.20
 C       0.657273     2.039155     3.754847      12.91
 O       1.912577     2.234834     4.147671     112.02
 H       2.231166     3.278295     3.973793      21.07
 C      -0.348293     2.878020     3.187912      80.70
 H      -0.157388     3.908715     3.008746      29.80
 C      -1.891222     1.103578     2.725856     -31.50
 C      -3.247557     0.480453     2.077584      87.64
 H      -3.893137     1.180690     2.234789      29.81
 O      -3.719127    -0.692079     2.816898     224.49
 H      -4.730717    -0.734677     2.752338      23.81
 C      -2.820096     0.279404     0.432372      85.58
 H      -2.245810     1.172586     0.172953      26.51
 C      -4.092119     0.006391    -0.394553     111.62
 O      -4.982624    -1.055630     0.015109     290.89
 H      -4.466979    -1.827417     0.187276      29.55
 H      -4.088978    -0.073682    -1.492435      28.77
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 H      -4.549977     0.902672    -0.150027      29.83
 C       1.402767     0.231768    -1.182402      21.10
 H       2.056001     1.199199    -1.361341      21.57
 C       1.153531    -2.190052    -1.356120      68.49
 H       1.677949    -3.190643    -1.631120      24.64
 C      -0.143189    -2.099260    -0.877895      -9.38
 O      -0.944341    -3.475706    -0.691823     113.74
 C      -1.228996    -4.092742    -1.931294     105.16
 H      -1.463269    -3.274395    -2.861957      22.28
 H      -0.318984    -4.941144    -2.038536      24.97
 H      -2.173421    -4.659322    -1.580779      25.59
 C      -0.703658    -0.873331    -0.527047      10.28
 O      -1.915383    -0.881093     0.288817     140.36
 C       0.042118     0.281022    -0.699947      60.84
 H      -0.514232     1.336452    -0.520509      22.76
 C       2.009379    -1.093506    -1.433089       9.47
 C       3.440324    -1.114570    -1.389263      92.81
 H       4.012134    -1.948496    -2.080575      22.35
 O       3.998462     0.134343    -1.971636     297.91
 H       4.828213     0.363329    -1.672079      31.52
 C       3.947538    -1.343530     0.038292      73.18
 H       3.137338    -2.114919     0.462564      25.87
 O       5.115848    -2.235874     0.314509     156.29
 H       5.795648    -1.882102    -0.465870      25.74
 C       4.013338    -0.141804     1.083428     105.66
 O       5.487386     0.179399     1.095873     245.86
 H       5.539584     0.971983     1.613876      28.17
 H       3.368937    -0.543203     1.965261      27.10
 H       3.133750     0.594998     0.728333      25.11
55
name = lig-Water-frame_421
 C      -1.561434     2.445079     2.832609      38.99
 H      -2.270246     3.006025     2.221667      24.81
 C      -1.014615     0.185462     3.452300      69.17
 H      -1.211346    -0.793498     3.764493      32.23
 C       0.261764     0.683928     3.844716       1.26
 O       1.395007    -0.149192     4.518233      23.64
 C       1.205944    -1.625983     4.486168     106.46
 H       2.186317    -1.905508     4.911347      27.63
 H       0.717523    -2.230579     3.520805      27.70
 H       0.506639    -1.939515     5.193447      29.64
 C       0.585927     1.986327     3.644804      33.94
 O       1.954202     2.296856     4.142416     103.83
 H       1.954236     3.228835     3.844837      26.58
 C      -0.285669     2.893706     3.221516      73.90
 H      -0.279286     4.011013     3.153576      22.59
 C      -1.944009     1.010597     2.738453     -59.04
 C      -3.122637     0.479726     2.078907      66.57
 H      -4.064499     1.396289     1.940488      23.09
 O      -3.705022    -0.699479     2.775309     192.79
 H      -4.711132    -0.526190     2.766358      22.28
 C      -2.882414     0.260273     0.488789      76.03
 H      -2.375333     1.275447     0.232940      26.49
 C      -4.067632    -0.015816    -0.419913     102.75
 O      -4.999994    -1.063117     0.059916     235.00
 H      -4.432722    -1.928315     0.245058      24.32
 H      -4.085038     0.381867    -1.526440      25.39
 H      -4.848866     0.941305    -0.312517      24.31
 C       1.380380     0.281043    -1.130867      39.60
 H       1.882092     1.048811    -1.653558      22.44
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 C       1.169903    -2.189964    -1.344555      59.02
 H       1.692296    -3.076305    -1.450010      26.74
 C      -0.179854    -2.116854    -0.946152       9.17
 O      -0.880030    -3.411903    -0.725969     132.36
 C      -1.294877    -4.160577    -1.980202     117.88
 H      -1.202372    -3.568491    -2.834692      28.14
 H      -0.454391    -4.730071    -2.040769      27.48
 H      -2.229721    -4.808444    -1.843079      26.66
 C      -0.717503    -0.863512    -0.429003      14.07
 O      -1.893522    -0.893842     0.263087     123.63
 C       0.037509     0.268936    -0.775279      79.75
 H      -0.418500     1.142628    -0.703225      31.03
 C       1.989325    -1.039346    -1.450512       8.26
 C       3.511434    -1.095270    -1.443700      98.57
 H       3.854547    -1.986592    -1.863063      28.92
 O       3.974576     0.095434    -1.969909     268.66
 H       4.905682     0.356592    -1.565842      26.40
 C       3.952855    -1.327585     0.066642      79.95
 H       3.135836    -2.123766     0.281693      29.79
 O       5.099543    -2.220097     0.343708     201.70
 H       5.732914    -2.085606    -0.309461      32.08
 C       3.994815    -0.151620     1.091673     116.06
 O       5.494239     0.204969     1.128647     190.64
 H       5.423388     1.104011     1.691563      26.91
 H       3.866753    -0.473802     2.143460      30.01
 H       3.583909     0.761249     0.739222      27.64
55
name = lig-Water-frame_422
 C      -1.632943     2.363227     2.740304      14.20
 H      -2.079004     3.327450     2.294404      19.99
 C      -0.958945     0.182131     3.485069      93.79
 H      -1.275654    -0.912057     3.561301      32.25
 C       0.220997     0.639678     3.842312      36.45
 O       1.288668    -0.210034     4.487569      43.21
 C       1.162013    -1.602943     4.525794     133.14
 H       2.173913    -1.861875     4.833084      28.99
 H       0.922718    -1.900425     3.576524      32.74
 H       0.315854    -2.171315     5.176283      28.02
 C       0.644497     1.937281     3.598036     -21.01
 O       1.954724     2.374464     4.107802     161.84
 H       2.019933     3.340691     3.927486      19.95
 C      -0.296956     2.969840     3.226294      35.98
 H      -0.064135     4.036709     3.373569      16.36
 C      -1.919388     0.965675     2.819504      24.05
 C      -3.089649     0.484354     2.030715     103.18
 H      -3.735661     1.170020     1.852493      31.73
 O      -3.686872    -0.687470     2.729492     235.82
 H      -4.624508    -0.373453     2.736118      27.22
 C      -2.899884     0.241396     0.537442      81.14
 H      -2.573714     1.184365     0.184975      30.97
 C      -4.139915     0.045391    -0.422677     107.13
 O      -4.983088    -1.074870     0.083292     190.08
 H      -4.476017    -1.957987     0.070553      25.63
 H      -3.713717     0.183837    -1.442103      29.58
 H      -4.816860     0.775528    -0.216738      30.30
 C       1.367427     0.255010    -1.141748      69.07
 H       1.734438     1.181228    -1.679211      25.06
 C       1.201623    -2.163391    -1.334927      14.88
 H       1.659217    -3.275587    -1.332288      23.61
 C      -0.229145    -2.155774    -0.984487       7.81
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 O      -0.836463    -3.317210    -0.761524      98.36
 C      -1.320736    -4.221272    -1.998153      74.96
 H      -1.112361    -3.582776    -3.053484      25.27
 H      -0.419683    -5.010604    -2.221997      23.77
 H      -2.360818    -4.819698    -2.144680      24.56
 C      -0.728440    -0.893224    -0.358967      21.20
 O      -1.891306    -0.907730     0.248244     100.62
 C       0.032637     0.275536    -0.834860      55.67
 H      -0.509372     1.374299    -0.773200      28.76
 C       1.938884    -0.949109    -1.434210      25.41
 C       3.586518    -1.089726    -1.453689      78.69
 H       3.788919    -2.191421    -1.939987      24.79
 O       3.982202     0.091179    -1.993629     247.21
 H       4.877388     0.389762    -1.561636      26.41
 C       3.939170    -1.356423     0.125273      73.90
 H       2.939337    -1.993707     0.367962      29.78
 O       5.076536    -2.198038     0.359869     167.41
 H       5.916370    -2.240821    -0.280549      26.65
 C       4.033285    -0.171465     1.088021     115.38
 O       5.496807     0.250569     1.174797     211.70
 H       5.402291     1.166474     1.685501      28.24
 H       4.091472    -0.379382     2.180046      28.40
 H       3.728804     0.890281     0.816820      25.65
55
name = lig-Water-frame_423
 C      -1.624160     2.363012     2.664607      55.63
 H      -2.235130     3.173498     2.354082      25.95
 C      -0.987122     0.106834     3.486852     101.86
 H      -1.180262    -0.936222     3.411353      30.61
 C       0.291452     0.552761     3.884767      13.37
 O       1.150953    -0.210775     4.455568     143.26
 C       1.105698    -1.619562     4.566937     128.05
 H       2.110349    -2.064048     4.774747      28.29
 H       1.180510    -1.819886     3.334391      27.92
 H       0.374658    -2.023522     5.161126      29.12
 C       0.741492     1.997885     3.594892     -33.48
 O       1.926990     2.435227     4.052395     177.95
 H       2.176525     3.485591     4.115805      17.42
 C      -0.350851     2.945737     3.220115      29.01
 H       0.054251     3.948542     3.424080      19.98
 C      -1.872690     1.006474     2.882505      71.31
 C      -3.062276     0.419806     1.988089      81.37
 H      -3.898518     1.474800     2.010778      26.48
 O      -3.670242    -0.657190     2.682512     210.07
 H      -4.696993    -0.490048     2.765812      23.63
 C      -2.875257     0.211563     0.538882      85.32
 H      -2.468671     1.204112     0.040246      28.49
 C      -4.194791     0.070288    -0.362698      87.65
 O      -4.952372    -1.089028     0.064683     159.57
 H      -4.451774    -1.925796    -0.113500      27.08
 H      -3.594349    -0.300727    -1.302328      26.95
 H      -4.898117     1.059841    -0.132645      25.73
 C       1.336649     0.268382    -1.219024      57.71
 H       1.736252     1.292554    -1.372778      26.07
 C       1.201154    -2.143870    -1.314086      32.69
 H       1.580387    -3.076476    -1.375249      26.30
 C      -0.206628    -2.115554    -0.997243      14.34
 O      -0.855520    -3.298661    -0.805682     118.99
 C      -1.263583    -4.257415    -2.082816      90.69
 H      -1.261965    -3.622742    -2.855332      28.68
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 H      -0.714819    -5.172497    -2.097816      26.07
 H      -2.365279    -4.559776    -2.021070      26.10
 C      -0.690439    -0.916094    -0.384923       7.39
 O      -1.940765    -0.921001     0.259122      98.61
 C      -0.044479     0.304308    -0.837555      62.85
 H      -0.429043     1.224359    -0.718569      30.63
 C       1.965526    -0.953811    -1.407143      47.01
 C       3.573453    -1.136140    -1.410388      93.64
 H       3.864706    -1.907720    -2.041008      29.02
 O       4.035088     0.118846    -2.038251     285.41
 H       4.808705     0.458267    -1.691356      32.01
 C       3.913517    -1.385867     0.154597      73.01
 H       2.970385    -1.900131     0.613145      30.19
 O       5.064095    -2.199349     0.381309     170.07
 H       5.805098    -2.114822    -0.351006      28.03
 C       4.131971    -0.144565     1.104966     120.83
 O       5.527611     0.307640     1.209018     235.03
 H       5.482995     1.121183     1.713481      30.18
 H       3.677716    -0.474648     2.100975      30.09
 H       3.345539     0.649803     0.886009      29.04
55
name = lig-Water-frame_424
 C      -1.543265     2.424034     2.650081      65.87
 H      -2.577476     2.868552     2.263034      22.45
 C      -1.001693     0.048255     3.472453      60.79
 H      -1.121277    -1.049513     3.363339      26.35
 C       0.317636     0.569254     3.867310     -12.10
 O       1.101446    -0.222050     4.498185     184.71
 C       1.091105    -1.660710     4.500522     119.79
 H       1.993019    -2.066044     4.987041      26.96
 H       1.066036    -2.088427     3.567386      28.95
 H       0.174542    -1.978377     5.183210      23.74
 C       0.725125     2.060865     3.608911       9.07
 O       1.941495     2.498518     4.013014     222.73
 H       2.000922     3.424391     4.100411      27.71
 C      -0.367041     2.832872     3.212208      58.67
 H      -0.158509     3.951874     3.225418      24.17
 C      -1.862012     1.042125     2.867557      25.24
 C      -3.079819     0.450260     2.011450     106.05
 H      -3.672065     1.177236     2.119816      33.93
 O      -3.669068    -0.647365     2.654162     260.60
 H      -4.633328    -0.614570     2.694575      25.19
 C      -2.821622     0.221193     0.478371     106.37
 H      -2.305849     1.032952     0.131047      29.78
 C      -4.198189     0.057235    -0.264792     118.36
 O      -4.946903    -1.100742     0.034929     187.53
 H      -4.327069    -1.923583    -0.216094      24.02
 H      -3.922593    -0.339904    -1.238167      28.66
 H      -4.658236     0.948098    -0.414325      30.92
 C       1.270607     0.316140    -1.297144      32.57
 H       1.879416     1.218412    -1.149526      24.97
 C       1.173187    -2.097692    -1.297186      73.30
 H       1.704888    -3.145854    -1.541227      24.00
 C      -0.138539    -2.056642    -0.985399      31.22
 O      -0.910861    -3.343800    -0.857395     106.54
 C      -1.226169    -4.267552    -2.123237      80.35
 H      -1.235948    -3.443878    -3.090222      23.48
 H      -0.714504    -5.244121    -1.974952      23.43
 H      -2.308613    -4.164919    -1.626021      20.14
 C      -0.697743    -0.886631    -0.463138      18.63
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 O      -1.995373    -0.953955     0.270535     109.18
 C      -0.089663     0.289401    -0.811602      63.31
 H      -0.547453     1.333986    -0.504095      24.35
 C       2.038707    -1.005793    -1.381857       8.84
 C       3.506093    -1.130578    -1.340641      79.47
 H       4.015288    -1.858133    -2.146965      23.73
 O       4.084645     0.140482    -2.087438     182.76
 H       4.980126     0.590854    -1.676639      25.73
 C       3.918251    -1.384884     0.162022      67.82
 H       3.095133    -1.894619     0.867323      27.56
 O       5.066280    -2.221679     0.386675     215.59
 H       5.567839    -1.975492    -0.342955      32.51
 C       4.170068    -0.114908     1.138256     122.67
 O       5.549751     0.353362     1.229561     223.98
 H       5.524101     1.208533     1.958826      24.16
 H       3.583047    -0.568488     1.941865      29.22
 H       3.261002     0.472305     0.819073      29.22
55
name = lig-Water-frame_425
 C      -1.540464     2.406571     2.659610      43.41
 H      -2.385540     2.868751     2.218995      19.24
 C      -0.972048     0.073570     3.434154      45.02
 H      -1.133116    -1.028485     3.384860      28.25
 C       0.249095     0.663377     3.785429     -35.13
 O       1.154976    -0.263158     4.589370     106.07
 C       1.052382    -1.719980     4.477391      98.01
 H       1.857749    -1.909756     5.210550      22.40
 H       0.849506    -2.404079     3.471941      24.03
 H       0.129973    -1.971354     4.966601      21.91
 C       0.643883     2.020331     3.653048      27.54
 O       1.971255     2.548139     3.983268      69.13
 H       1.822713     3.612952     3.976246      29.52
 C      -0.345210     2.815889     3.186006      49.01
 H      -0.346388     3.861117     3.004280      22.46
 C      -1.855093     1.008389     2.797180     -13.44
 C      -3.056391     0.500898     2.055900      76.30
 H      -4.008492     1.459793     2.072100      23.94
 O      -3.655328    -0.681939     2.651851     194.81
 H      -4.680451    -0.532013     2.574756      18.27
 C      -2.783717     0.228084     0.446370      95.73
 H      -2.149904     1.154028     0.101272      21.59
 C      -4.126130     0.010690    -0.226952     112.57
 O      -4.969525    -1.132004     0.025673     237.85
 H      -4.395702    -1.878789    -0.087028      27.85
 H      -3.980251     0.021882    -1.452215      25.08
 H      -4.727329     1.019801    -0.537027      24.96
 C       1.239392     0.307904    -1.335760      33.06
 H       1.947574     1.166347    -1.123137      23.37
 C       1.221911    -2.109938    -1.317023      81.18
 H       1.594141    -3.028236    -1.621461      26.72
 C      -0.133710    -2.073332    -0.944441       3.29
 O      -0.934851    -3.365112    -0.903353     153.19
 C      -1.228082    -4.178002    -2.121183     115.80
 H      -1.036672    -3.845748    -3.035899      28.57
 H      -0.618268    -5.151039    -2.054091      25.78
 H      -2.196581    -4.364844    -1.926393      27.57
 C      -0.800127    -0.854779    -0.533334       6.39
 O      -2.012806    -1.008979     0.259394     121.46
 C      -0.083913     0.326503    -0.783252      58.29
 H      -0.536649     1.207420    -0.301402      22.26
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 C       2.025402    -0.972288    -1.364336      -5.35
 C       3.499997    -1.092897    -1.311099      79.53
 H       3.868872    -1.916118    -1.822441      25.28
 O       4.135631     0.161077    -2.115420     253.61
 H       4.921731     0.497992    -1.624822      28.26
 C       3.955761    -1.358682     0.213568      76.70
 H       3.097853    -1.921230     0.700525      26.78
 O       5.070916    -2.254753     0.365292     174.52
 H       5.744891    -1.961204    -0.459218      25.54
 C       4.134122    -0.117516     1.139388     100.68
 O       5.547253     0.412437     1.268747     268.63
 H       5.453794     1.059170     1.915796      31.76
 H       4.001839    -0.520322     2.224709      25.08
 H       3.544077     0.774241     0.689138      25.14
55
name = lig-Water-frame_426
 C      -1.580721     2.298577     2.682779      45.25
 H      -2.153449     3.234027     2.151079      22.09
 C      -0.948459     0.152488     3.358920     104.56
 H      -1.105936    -0.872989     3.445851      32.26
 C       0.236083     0.674811     3.770213       1.05
 O       1.205239    -0.274044     4.629594       0.42
 C       0.984158    -1.780635     4.479346     106.92
 H       1.771222    -2.082296     5.173039      23.65
 H       1.060069    -2.235031     3.520466      27.68
 H      -0.031957    -2.066222     4.955671      24.20
 C       0.624013     1.973091     3.723037      -3.28
 O       1.955650     2.589821     3.952530     109.56
 H       1.859496     3.592168     3.804596      25.12
 C      -0.351066     2.886343     3.123009      73.25
 H      -0.133532     4.011151     2.905392      23.35
 C      -1.850115     0.950616     2.713002      45.85
 C      -3.090179     0.580875     2.068375     103.91
 H      -3.754243     1.235184     1.956204      31.79
 O      -3.640165    -0.718023     2.658080     222.45
 H      -4.605080    -0.471674     2.629139      23.78
 C      -2.762996     0.241382     0.471166      90.79
 H      -2.348551     1.092593     0.019075      28.99
 C      -4.070514     0.019798    -0.326584     103.68
 O      -4.990544    -1.144538     0.027858     179.68
 H      -4.452327    -2.072112     0.038435      24.01
 H      -3.769341     0.180736    -1.306299      30.96
 H      -4.771269     0.794878     0.007691      28.63
 C       1.261200     0.268751    -1.308824      64.48
 H       1.778614     1.196401    -1.322720      26.90
 C       1.246741    -2.139632    -1.342925      33.29
 H       1.629896    -3.184665    -1.672546      23.21
 C      -0.177753    -2.128339    -0.912589     -22.21
 O      -0.929005    -3.346140    -0.936775     178.86
 C      -1.213502    -4.112803    -2.084865     117.12
 H      -0.774858    -3.875061    -3.250364      23.35
 H      -0.576749    -4.991002    -2.068838      26.96
 H      -2.330144    -4.730188    -2.451467      22.74
 C      -0.903566    -0.868298    -0.592134      -2.70
 O      -1.997626    -1.051631     0.227616     116.39
 C      -0.065991     0.354148    -0.747513      50.77
 H      -0.393286     1.287974    -0.289118      24.50
 C       1.942781    -0.876046    -1.365323      -4.28
 C       3.539432    -1.007476    -1.292992      62.07
 H       3.746678    -2.145892    -1.667362      20.34
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 O       4.166563     0.148572    -2.113953     279.74
 H       4.929576     0.401401    -1.594583      28.30
 C       4.003427    -1.311820     0.272997      71.69
 H       3.001924    -1.973015     0.388651      24.22
 O       5.094152    -2.275481     0.297058     217.46
 H       5.896932    -2.185724    -0.222460      29.08
 C       4.119113    -0.106142     1.165220     122.81
 O       5.542588     0.437071     1.275551     208.18
 H       5.365002     1.269539     2.026461      24.51
 H       4.111854    -0.241794     2.208557      25.57
 H       3.709014     0.840584     0.868488      25.29
55
name = lig-Water-frame_427
 C      -1.590915     2.306229     2.688806      55.42
 H      -2.030273     3.134020     2.165365      24.23
 C      -0.926316     0.196559     3.278950      79.26
 H      -1.095635    -0.913564     3.507796      27.63
 C       0.321370     0.600280     3.850778      -1.74
 O       1.211432    -0.280683     4.606426     107.49
 C       0.921374    -1.795141     4.528794      95.35
 H       1.697685    -2.402619     5.045351      26.13
 H       1.287899    -2.014085     3.378753      25.48
 H      -0.078278    -2.122537     4.900287      25.31
 C       0.644275     2.057419     3.753055     -20.16
 O       1.905968     2.593122     3.923041     140.78
 H       1.925540     3.541419     3.746855      23.80
 C      -0.350680     2.921080     3.068653      55.86
 H       0.048540     3.878375     2.933643      28.08
 C      -1.865316     0.942816     2.639229      54.42
 C      -3.096584     0.523213     2.014553      82.22
 H      -3.974902     1.544546     1.939031      25.17
 O      -3.619997    -0.721158     2.665874     187.96
 H      -4.623170    -0.607993     2.825655      21.20
 C      -2.797130     0.210398     0.520239      86.18
 H      -2.363719     1.099064    -0.047001      28.48
 C      -4.059242     0.039535    -0.369394      81.96
 O      -4.976692    -1.155241     0.014226     116.60
 H      -4.551492    -2.053141     0.006699      27.13
 H      -3.702579     0.114843    -1.505838      27.88
 H      -4.701911     0.684677     0.331643      25.86
 C       1.236882     0.298875    -1.229380      51.98
 H       1.658719     1.315604    -1.577829      25.30
 C       1.189280    -2.166080    -1.351183      45.01
 H       1.752647    -3.095082    -1.588371      27.16
 C      -0.199550    -2.163488    -0.938200      -8.59
 O      -0.936765    -3.313963    -0.943767     179.36
 C      -1.182632    -4.125952    -2.166746     127.94
 H      -0.759106    -3.519870    -2.873506      25.97
 H      -0.494645    -5.032656    -1.888006      25.86
 H      -2.054241    -4.417633    -2.447469      30.71
 C      -0.904427    -0.892716    -0.636473      -1.40
 O      -1.986629    -1.056438     0.197468      73.99
 C      -0.078289     0.321660    -0.713496      50.09
 H      -0.262334     1.462456    -0.431894      24.55
 C       1.931005    -0.876405    -1.385705     -13.88
 C       3.568627    -0.929636    -1.295450      88.51
 H       3.715790    -1.876597    -1.689973      24.63
 O       4.177442     0.098084    -2.084005     275.75
 H       5.124860     0.388114    -1.633468      25.11
 C       4.034015    -1.272162     0.250604      79.36
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 H       3.184735    -1.877334     0.500904      27.43
 O       5.107202    -2.302030     0.246428     215.69
 H       5.962024    -2.128834    -0.180768      28.17
 C       4.163443    -0.064352     1.226374     100.88
 O       5.549937     0.468835     1.284899     259.92
 H       5.497478     1.273106     1.780170      30.10
 H       3.670280    -0.242524     2.321382      24.79
 H       3.356997     0.809370     0.936339      24.85
55
name = lig-Water-frame_428
 C      -1.557124     2.403046     2.666097      53.50
 H      -2.399655     3.021900     2.035020      22.62
 C      -0.852239     0.154103     3.252794      56.96
 H      -1.115983    -0.846598     3.368844      29.77
 C       0.410506     0.567595     3.942004       4.73
 O       1.190946    -0.298787     4.569754     171.39
 C       0.908758    -1.790369     4.530981     110.44
 H       1.621155    -2.423976     5.075622      28.23
 H       1.100633    -1.837554     3.457746      29.70
 H      -0.077127    -2.057235     4.769798      28.47
 C       0.641060     2.138146     3.731254       3.55
 O       1.866901     2.572206     3.908712     144.05
 H       1.976415     3.655766     3.771099      22.06
 C      -0.317817     2.856847     3.068628      57.96
 H       0.001112     3.962693     2.869431      30.90
 C      -1.864204     1.006947     2.601585      -8.10
 C      -3.153230     0.440720     1.928671     113.09
 H      -3.712762     1.192986     2.050965      34.10
 O      -3.601255    -0.707859     2.682159     219.71
 H      -4.594240    -0.683477     2.903289      20.82
 C      -2.851365     0.149825     0.500641     106.98
 H      -2.244255     1.026733     0.170657      29.96
 C      -4.075582     0.028469    -0.338148     108.44
 O      -4.950876    -1.153187    -0.022458     136.57
 H      -4.407484    -2.012597    -0.160463      23.80
 H      -4.045903     0.066910    -1.402601      31.29
 H      -4.704281     0.953963    -0.073029      30.11
 C       1.197145     0.361955    -1.159839       3.69
 H       1.595504     1.239297    -1.558716      21.80
 C       1.133309    -2.136804    -1.342108      71.01
 H       1.757306    -3.026275    -1.472122      29.65
 C      -0.198646    -2.155919    -1.012979      23.42
 O      -0.981772    -3.302335    -0.915533     129.75
 C      -1.054179    -4.131934    -2.224323      93.58
 H      -0.632009    -3.209850    -2.872516      24.24
 H      -0.580887    -5.045492    -2.057596      26.63
 H      -2.402542    -4.149235    -2.340434      22.98
 C      -0.821988    -0.905280    -0.640415      -5.43
 O      -1.990588    -1.038821     0.178621      46.06
 C      -0.107480     0.291031    -0.696068      72.94
 H      -0.471521     1.225571    -0.540640      30.78
 C       1.964995    -0.939118    -1.401285     -94.66
 C       3.552079    -0.881410    -1.288668      88.66
 H       3.899996    -1.855039    -1.946552      21.49
 O       4.205072     0.064164    -2.040113     316.40
 H       5.068927     0.331994    -1.824386      30.43
 C       4.072165    -1.223896     0.182987      68.52
 H       3.251840    -1.822585     0.894968      26.95
 O       5.106488    -2.323674     0.205892     137.35
 H       5.953624    -1.817186    -0.258329      24.68
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 C       4.168815    -0.000816     1.312462     113.01
 O       5.547618     0.476360     1.281572     246.96
 H       5.589376     1.459308     1.797093      22.19
 H       3.652376    -0.404119     2.123596      28.97
 H       3.353514     0.576808     0.874861      28.71
55
name = lig-Water-frame_429
 C      -1.584092     2.473014     2.583394      55.57
 H      -2.492575     2.944593     2.193026      24.26
 C      -0.762406     0.130020     3.250289      12.43
 H      -1.094310    -0.949875     3.160622      29.84
 C       0.380436     0.621229     3.946680      14.31
 O       1.200616    -0.326228     4.572272     142.31
 C       0.914218    -1.756269     4.493204     108.15
 H       1.630279    -2.180194     5.200732      28.35
 H       0.886596    -2.056771     3.324817      30.68
 H      -0.243200    -1.918979     4.761013      27.79
 C       0.622418     2.082418     3.708005      19.64
 O       1.889566     2.588449     3.912719     175.47
 H       1.891686     3.511487     3.889195      30.29
 C      -0.292506     2.853712     3.066442      55.43
 H      -0.181767     3.858912     2.851125      28.82
 C      -1.796164     1.070516     2.616463     -67.61
 C      -3.132399     0.326001     1.902413      76.27
 H      -4.032317     1.300403     2.058063      25.65
 O      -3.582678    -0.714754     2.716274     201.05
 H      -4.561953    -0.539939     2.729253      20.34
 C      -2.868109     0.086908     0.418008     114.80
 H      -2.297189     0.995063     0.290005      28.75
 C      -4.165991     0.027147    -0.307091     125.50
 O      -4.920852    -1.144115    -0.067499     149.26
 H      -4.261105    -1.925106    -0.271219      21.33
 H      -4.086996     0.040210    -1.478967      29.20
 H      -4.727570     1.052840    -0.448238      26.67
 C       1.207345     0.337573    -1.124886     -23.56
 H       1.662550     1.371865    -1.356410      22.53
 C       1.167003    -2.081132    -1.343436       7.33
 H       1.641266    -3.160858    -1.357843      21.47
 C      -0.231427    -2.116806    -1.075833     -16.43
 O      -1.021956    -3.314750    -0.879805     115.70
 C      -0.999315    -4.048281    -2.259031      96.46
 H      -0.549096    -3.534223    -3.099174      25.03
 H      -0.613601    -5.160756    -2.406541      25.27
 H      -1.936656    -4.031435    -2.320268      31.16
 C      -0.756283    -0.935055    -0.587946      -6.71
 O      -1.995626    -1.028378     0.158509      92.21
 C      -0.124710     0.273888    -0.704006      95.55
 H      -0.961005     1.135604    -0.505608      28.17
 C       1.960142    -0.927924    -1.385769     -42.83
 C       3.531416    -0.967904    -1.297353     102.60
 H       3.883792    -1.796372    -1.803978      25.88
 O       4.218173     0.092573    -2.022877     283.17
 H       5.157205     0.302537    -1.754692      28.38
 C       4.073309    -1.208356     0.185394      91.04
 H       3.327366    -1.661240     0.701642      32.42
 O       5.112705    -2.291909     0.150689     203.28
 H       5.832847    -1.869015    -0.251186      30.27
 C       4.183049     0.016442     1.310660      93.96
 O       5.533292     0.502630     1.304932     222.13
 H       5.563707     1.347516     1.841053      26.30
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 H       3.987959    -0.586553     2.343130      26.60
 H       3.431142     0.769319     0.755481      26.28
55
name = lig-Water-frame_430
 C      -1.611933     2.450920     2.517945      36.23
 H      -2.426267     3.263296     2.253076      21.84
 C      -0.741390     0.155718     3.221218      55.79
 H      -0.855163    -0.912978     3.017616      29.75
 C       0.300925     0.667237     3.898955      18.78
 O       1.232135    -0.316984     4.577591      15.87
 C       0.877275    -1.703292     4.425587     124.46
 H       1.605779    -2.056531     5.165083      28.02
 H       0.897953    -2.395593     3.544394      32.12
 H      -0.006272    -1.790211     4.920832      31.28
 C       0.636216     1.970797     3.694189      -7.38
 O       1.935082     2.588194     3.936161     107.95
 H       1.790403     3.645053     3.958992      22.43
 C      -0.340378     2.898888     3.037670      47.46
 H      -0.050670     4.024045     2.919481      19.26
 C      -1.710613     1.060004     2.643597       3.91
 C      -3.077509     0.322368     1.945694      80.08
 H      -3.832154     0.909241     1.779775      31.20
 O      -3.578356    -0.745388     2.759180     202.93
 H      -4.570953    -0.533775     2.621530      25.26
 C      -2.866191     0.056806     0.353766      81.52
 H      -2.476184     1.138098     0.102660      29.64
 C      -4.258652     0.043895    -0.392369     129.18
 O      -4.908272    -1.142009    -0.108267     165.51
 H      -4.343818    -1.919504    -0.173562      22.85
 H      -3.734533    -0.060487    -1.384710      28.58
 H      -4.885669     1.024235    -0.321961      27.07
 C       1.242954     0.311510    -1.112899      65.20
 H       1.712459     1.265010    -1.003744      28.56
 C       1.214865    -2.079152    -1.347078       2.99
 H       1.556432    -3.045530    -1.367767      24.65
 C      -0.254483    -2.091483    -1.098580     -13.22
 O      -1.009317    -3.331549    -0.883178     120.21
 C      -0.931836    -3.991770    -2.285201      74.38
 H      -0.383771    -3.592629    -3.240777      22.71
 H      -0.649332    -4.998133    -2.358432      27.29
 H      -2.262581    -4.058365    -2.626956      22.58
 C      -0.761328    -0.968545    -0.501696      24.70
 O      -1.998844    -1.044623     0.127221     107.86
 C      -0.149386     0.292614    -0.723230      73.96
 H      -0.801671     1.018736    -0.500351      30.96
 C       1.944606    -0.853838    -1.345200      45.14
 C       3.526699    -1.058523    -1.297039      62.19
 H       3.795199    -2.157292    -1.736383      23.53
 O       4.215266     0.151042    -2.019163     182.72
 H       5.137359     0.225323    -1.477800      25.39
 C       4.064482    -1.201545     0.210428      71.35
 H       2.994953    -1.838918     0.519916      28.66
 O       5.103302    -2.231257     0.105427     172.66
 H       5.968617    -1.976780    -0.361918      26.22
 C       4.213810    -0.019051     1.253936     121.39
 O       5.529460     0.525424     1.339814     263.14
 H       5.486064     1.369154     1.920648      27.65
 H       4.187446    -0.338485     2.233894      28.67
 H       3.579411     0.851897     1.086709      26.44
55
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name = lig-Water-frame_431
 C      -1.588743     2.428386     2.500524      54.34
 H      -2.164167     3.381365     2.247732      21.60
 C      -0.798582     0.192290     3.147894      73.91
 H      -0.719599    -0.869800     3.000176      29.34
 C       0.305971     0.643835     3.881040       7.83
 O       1.251770    -0.248603     4.533381      57.22
 C       0.858958    -1.674394     4.427007     112.59
 H       1.626583    -2.197329     5.034296      27.70
 H       0.997547    -2.365220     3.512649      28.54
 H      -0.085327    -1.823033     5.163361      25.97
 C       0.662802     1.992206     3.647937     -34.33
 O       1.958463     2.573993     3.972476     145.92
 H       1.774571     3.582708     3.933923      21.43
 C      -0.378844     2.939935     3.016119      30.18
 H       0.059065     3.901410     3.065019      19.19
 C      -1.717636     0.986456     2.622952      63.19
 C      -2.940037     0.336016     1.976919      71.52
 H      -3.924599     1.131595     1.701666      25.53
 O      -3.581457    -0.782204     2.790784     163.25
 H      -4.576402    -0.721342     2.767463      26.56
 C      -2.871277     0.101568     0.357096      75.45
 H      -2.553457     0.975958    -0.128874      30.29
 C      -4.246962     0.035231    -0.503562      95.78
 O      -4.950233    -1.153426    -0.144887     184.80
 H      -4.354959    -2.061596    -0.002864      21.18
 H      -3.712522    -0.003373    -1.491837      28.36
 H      -4.984908     0.873164    -0.168993      26.03
 C       1.238230     0.331170    -1.074058      56.52
 H       1.847011     1.226017    -0.812437      25.87
 C       1.188638    -2.068548    -1.345563      32.80
 H       1.788460    -3.127550    -1.535529      22.36
 C      -0.212640    -2.103572    -1.072329      -0.38
 O      -0.949415    -3.343883    -0.950339     192.15
 C      -0.979365    -3.956947    -2.335682      92.77
 H      -0.221285    -3.344894    -2.931445      24.76
 H      -0.590921    -5.025626    -1.988635      23.94
 H      -1.789417    -4.018347    -2.834219      29.75
 C      -0.802184    -0.949432    -0.439443      21.05
 O      -2.020209    -1.079471     0.087554     137.83
 C      -0.128785     0.269109    -0.744499      64.15
 H      -0.544268     1.367051    -0.432278      25.43
 C       1.967601    -0.839198    -1.307225      26.01
 C       3.524583    -1.090973    -1.305449      70.83
 H       3.629646    -2.075411    -1.685677      26.44
 O       4.208594     0.169085    -1.989575     257.55
 H       4.922178     0.308505    -1.434312      29.82
 C       3.995308    -1.236256     0.206788      86.81
 H       3.270828    -1.817602     0.550921      30.38
 O       5.096202    -2.166113     0.089739     177.04
 H       5.974340    -2.004960    -0.513544      25.09
 C       4.255146    -0.059583     1.185221     117.78
 O       5.568444     0.547169     1.366199     245.24
 H       5.387766     1.470414     1.916207      24.54
 H       3.930835    -0.417076     2.317100      24.73
 H       3.456703     0.815763     1.373435      22.71
55
name = lig-Water-frame_432
 C      -1.513637     2.423722     2.525191      55.94
 H      -2.243786     3.141014     2.078684      24.78
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 C      -0.805860     0.174688     3.112123      38.32
 H      -0.889526    -0.966881     2.994896      26.06
 C       0.373274     0.639735     3.856458      -7.29
 O       1.250467    -0.176684     4.453054     122.65
 C       0.861646    -1.682286     4.509403     104.71
 H       1.698277    -2.235353     4.946351      28.48
 H       0.848050    -1.862058     3.349134      28.86
 H      -0.050595    -1.887851     4.942015      29.31
 C       0.678482     2.080940     3.591163     -10.54
 O       1.943478     2.543569     4.008178     232.26
 H       1.954012     3.513036     3.914975      23.61
 C      -0.340724     2.901722     3.036118      44.79
 H      -0.077150     4.004335     3.044883      20.10
 C      -1.816529     0.966700     2.542587      56.61
 C      -2.913066     0.385168     1.936187      98.80
 H      -3.498099     1.180403     2.155694      28.51
 O      -3.558033    -0.811456     2.803085     142.08
 H      -4.555859    -0.656044     2.788512      23.15
 C      -2.884108     0.143082     0.390571      67.99
 H      -2.267042     0.966450    -0.222061      24.84
 C      -4.165326    -0.024909    -0.553150      90.07
 O      -5.005511    -1.195823    -0.181811     231.82
 H      -4.416507    -1.928807    -0.033175      28.54
 H      -4.098361     0.196020    -1.690072      27.71
 H      -4.943354     0.796321    -0.209207      25.32
 C       1.258877     0.349397    -1.017077      34.69
 H       1.851377     1.273379    -0.834949      23.65
 C       1.179392    -2.074593    -1.354276      61.48
 H       1.727122    -2.834671    -1.674609      26.24
 C      -0.154675    -2.122688    -0.984978      10.12
 O      -0.887146    -3.330584    -1.040420     210.63
 C      -0.941225    -3.953117    -2.331952      91.64
 H      -0.134384    -3.347239    -2.739917      25.31
 H      -0.601979    -4.914206    -2.000228      26.15
 H      -2.051377    -3.938903    -3.145101      22.69
 C      -0.812218    -0.906871    -0.451974      12.27
 O      -2.078662    -1.112081     0.054367     149.18
 C      -0.114568     0.291650    -0.726345      75.58
 H      -0.221604     1.299192    -0.398794      23.34
 C       1.986645    -0.886116    -1.282695      10.19
 C       3.479801    -1.011034    -1.295107      80.68
 H       3.722849    -2.014333    -1.912695      24.45
 O       4.179099     0.135244    -1.949352     246.32
 H       4.956937     0.524510    -1.358043      24.91
 C       3.971363    -1.257099     0.141397      61.29
 H       3.247490    -1.993781     0.933523      23.83
 O       5.119142    -2.125625     0.095344     218.96
 H       5.682929    -1.794379    -0.541653      30.15
 C       4.243046    -0.075029     1.220481     110.34
 O       5.603286     0.567830     1.390272     292.62
 H       5.452809     1.402450     1.806803      29.36
 H       3.921295    -0.698832     1.995554      27.11
 H       3.423660     0.591830     1.081944      26.63
55
name = lig-Water-frame_433
 C      -1.489498     2.376890     2.544228      61.37
 H      -2.350330     2.827813     1.878028      17.93
 C      -0.773664     0.125882     3.113344      30.13
 H      -1.107253    -0.855097     3.063911      27.64
 C       0.389618     0.696306     3.752011      11.24
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 O       1.262178    -0.139497     4.403394     129.53
 C       0.899057    -1.650493     4.525260      96.81
 H       1.785855    -2.163015     4.940555      26.49
 H       0.682066    -1.666198     3.466508      27.56
 H      -0.189292    -1.893145     4.898788      25.82
 C       0.705110     2.114864     3.571883      25.20
 O       1.910076     2.509882     4.043151     198.64
 H       2.191351     3.544284     3.886039      24.57
 C      -0.257182     2.891276     3.068003      70.04
 H      -0.352816     3.970019     2.925393      21.25
 C      -1.773545     1.010005     2.502608      -8.47
 C      -3.010127     0.401358     1.866529      80.42
 H      -3.665263     1.325300     2.401536      21.87
 O      -3.521361    -0.807751     2.777408     161.49
 H      -4.485964    -0.502269     2.680292      17.44
 C      -2.873194     0.164525     0.351329      89.23
 H      -2.226566     0.910774     0.106476      27.32
 C      -4.129029    -0.068376    -0.538163     103.27
 O      -5.038688    -1.222800    -0.225068     232.58
 H      -4.368896    -2.082225    -0.140616      23.25
 H      -4.221844     0.185530    -1.579140      27.18
 H      -4.768021     0.864730    -0.298859      25.32
 C       1.328401     0.308232    -0.969428      51.38
 H       1.746491     1.304734    -0.985548      21.75
 C       1.197545    -2.046549    -1.359968      56.02
 H       1.711080    -3.024239    -1.911745      21.66
 C      -0.125716    -2.115693    -0.876053      13.04
 O      -0.853748    -3.293943    -1.092141     247.11
 C      -0.908430    -3.948187    -2.363045     112.76
 H       0.004046    -3.605004    -3.094415      25.03
 H      -0.672942    -5.098577    -2.338922      26.74
 H      -1.763651    -3.791054    -2.770034      30.19
 C      -0.804984    -0.894990    -0.508284      14.42
 O      -2.133689    -1.125161     0.030647     155.89
 C      -0.078412     0.333521    -0.673172      55.14
 H      -0.476222     1.333723    -0.256124      18.90
 C       1.952937    -0.892777    -1.261227      43.10
 C       3.440588    -0.938065    -1.295586      98.56
 H       3.837944    -1.649549    -1.994803      23.77
 O       4.152840     0.099630    -1.898988     300.88
 H       4.853982     0.631320    -1.357528      25.81
 C       3.971370    -1.308288     0.131051      80.69
 H       3.287000    -1.775002     0.636147      29.34
 O       5.152800    -2.099164     0.107388     217.04
 H       5.665084    -1.573229    -0.639202      25.54
 C       4.221046    -0.092163     1.245462      77.04
 O       5.601481     0.547747     1.404825     207.22
 H       5.473004     1.557000     1.906283      23.33
 H       4.140089    -0.857842     2.141793      23.36
 H       3.410082     0.617536     0.768301      20.36
55
name = lig-Water-frame_434
 C      -1.503655     2.310038     2.529129      61.57
 H      -2.136036     2.934307     1.964136      22.16
 C      -0.758594     0.135439     3.110414      56.84
 H      -1.128020    -0.949162     3.263931      26.50
 C       0.369047     0.718679     3.614364       7.74
 O       1.289359    -0.115143     4.394409     118.37
 C       0.914472    -1.564717     4.493035     103.73
 H       1.764908    -2.061664     4.921527      26.22
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 H       0.690341    -2.052354     3.372769      25.85
 H       0.038104    -1.723784     5.163185      27.27
 C       0.748297     2.092674     3.584896      25.60
 O       1.915093     2.493262     4.088254     195.71
 H       2.017585     3.405653     3.884653      32.44
 C      -0.268768     2.937163     3.043931      90.54
 H      -0.232986     4.014954     2.932449      22.82
 C      -1.642337     1.000701     2.497731       1.58
 C      -3.134598     0.432499     1.877273      83.42
 H      -3.977953     1.052103     1.907074      27.37
 O      -3.491296    -0.753922     2.700453     182.55
 H      -4.500344    -0.681362     2.702614      24.79
 C      -2.880187     0.120232     0.289384      91.55
 H      -2.288652     1.153104     0.139189      20.94
 C      -4.163441    -0.060328    -0.479205      88.62
 O      -5.014481    -1.246291    -0.258915     207.54
 H      -4.534399    -2.107450    -0.257797      25.19
 H      -3.853211    -0.053523    -1.654577      26.54
 H      -4.700451     0.954754    -0.228163      26.26
 C       1.337170     0.294375    -0.915201      49.53
 H       1.833919     1.290935    -1.163405      22.49
 C       1.220630    -2.069813    -1.373443      53.20
 H       1.499439    -2.917868    -1.826263      25.02
 C      -0.093594    -2.096248    -0.823378      10.79
 O      -0.835823    -3.270575    -1.106547     172.08
 C      -0.782244    -3.966471    -2.414240      96.24
 H      -0.151435    -3.782094    -3.248965      26.83
 H      -0.929278    -5.066989    -2.507469      26.85
 H      -2.069985    -3.567106    -2.769935      22.09
 C      -0.804150    -0.900086    -0.548721       1.66
 O      -2.141494    -1.106112     0.007469     166.90
 C      -0.041898     0.366208    -0.583490      44.41
 H      -0.788212     1.160772    -0.306296      20.02
 C       1.934893    -0.866695    -1.252005      37.71
 C       3.442339    -0.911368    -1.286047      92.08
 H       3.726105    -1.813120    -2.000430      23.21
 O       4.144804     0.136653    -1.869998     307.86
 H       4.675602     0.547995    -1.250546      30.37
 C       4.019179    -1.309160     0.140125      68.48
 H       2.915354    -1.935439     0.483629      23.53
 O       5.197110    -2.075853     0.095232     196.59
 H       5.929707    -1.647252    -0.512826      25.38
 C       4.207621    -0.131318     1.243370     114.07
 O       5.565025     0.536017     1.421710     269.15
 H       5.409306     1.257684     1.965640      33.32
 H       4.135040    -0.427169     2.261229      25.70
 H       3.528658     0.658871     1.087419      26.08
55
name = lig-Water-frame_435
 C      -1.458574     2.342888     2.508229      58.02
 H      -2.085123     3.260540     2.062892      24.80
 C      -0.768872     0.125828     3.106988      79.83
 H      -0.857202    -0.859221     3.415028      27.19
 C       0.414799     0.686153     3.537990      12.38
 O       1.304330    -0.098065     4.373965     174.88
 C       0.935256    -1.478436     4.437365     122.59
 H       1.823693    -1.971278     4.920084      25.28
 H       0.807738    -2.190232     3.627325      27.99
 H       0.216697    -1.537410     5.350781      24.72
 C       0.722500     2.071919     3.569527     -12.62
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 O       1.946299     2.477018     4.143345     167.33
 H       1.853587     3.528184     3.952066      24.57
 C      -0.311213     2.963530     3.003167      61.53
 H       0.029939     4.039962     3.006178      20.47
 C      -1.639187     0.924229     2.463137      21.27
 C      -3.175786     0.424104     1.888698      72.85
 H      -4.186283     1.052414     1.500405      23.34
 O      -3.483859    -0.687129     2.609142     233.43
 H      -4.424982    -0.959405     2.726450      26.02
 C      -2.889312     0.078087     0.281558      95.59
 H      -2.662753     1.007037    -0.164213      28.47
 C      -4.195313    -0.036722    -0.466060     101.06
 O      -4.986282    -1.236364    -0.278161     220.90
 H      -4.418897    -2.121096    -0.264263      23.17
 H      -3.669418    -0.171056    -1.386050      28.20
 H      -4.861550     0.826573    -0.284153      27.67
 C       1.284849     0.367488    -0.865333      53.10
 H       1.948672     1.149068    -1.106247      25.34
 C       1.208039    -2.066027    -1.346224      38.12
 H       1.612016    -3.093846    -1.829419      23.37
 C      -0.062952    -2.091224    -0.855627      16.84
 O      -0.812505    -3.279417    -1.101462     139.67
 C      -0.790694    -3.958305    -2.483225     112.30
 H      -0.025748    -3.616561    -3.379391      24.55
 H      -1.021632    -5.030693    -2.260590      27.75
 H      -1.591568    -3.617458    -2.836126      28.51
 C      -0.792949    -0.891804    -0.539262       8.38
 O      -2.095108    -1.057056    -0.027264     155.99
 C      -0.062002     0.330362    -0.488737      67.87
 H      -0.642723     1.217835    -0.438553      26.20
 C       1.960184    -0.863069    -1.257914      -5.77
 C       3.478444    -0.956522    -1.291873      93.86
 H       3.511162    -1.951450    -1.735566      24.38
 O       4.143866     0.215448    -1.866493     243.75
 H       4.669788     0.586668    -1.028931      26.30
 C       4.017655    -1.288662     0.176361      89.17
 H       3.384387    -1.978421     0.435558      29.51
 O       5.256275    -2.072796     0.083026     228.15
 H       6.008074    -1.770826    -0.333780      28.21
 C       4.202514    -0.155579     1.254862     125.50
 O       5.528019     0.497703     1.409593     204.24
 H       5.291751     1.186280     2.220645      26.09
 H       3.833473    -0.300761     2.366955      22.98
 H       3.459627     0.774200     1.336930      21.80
55
name = lig-Water-frame_436
 C      -1.421164     2.434657     2.458609      43.75
 H      -2.157332     3.069704     2.141936      30.65
 C      -0.759067     0.098834     3.108493      -0.15
 H      -0.809088    -0.987488     3.410214      30.73
 C       0.510042     0.661233     3.527465      19.97
 O       1.315009    -0.073094     4.309415     216.90
 C       1.000655    -1.421401     4.475575     118.27
 H       1.920903    -1.809077     4.907578      26.85
 H       0.701988    -2.198004     3.572735      27.84
 H       0.221195    -1.493699     5.301937      26.05
 C       0.673245     2.057452     3.533761      -2.79
 O       1.950615     2.487103     4.177715      96.22
 H       1.917394     3.516771     4.234823      26.55
 C      -0.272754     2.946097     2.997047      36.35
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 H      -0.045363     3.978444     2.971712      26.64
 C      -1.778948     0.920225     2.400839     -58.05
 C      -3.143972     0.429620     1.812202     107.26
 H      -3.853555     1.217871     1.747674      28.43
 O      -3.484229    -0.671763     2.557130     236.42
 H      -4.462419    -0.941994     2.517226      21.04
 C      -2.931246     0.068215     0.328035      91.13
 H      -2.644945     0.967187    -0.386788      29.40
 C      -4.210311    -0.067265    -0.463040      96.10
 O      -4.966647    -1.229896    -0.280700     189.60
 H      -4.266468    -1.976883    -0.171045      22.72
 H      -3.764222    -0.053722    -1.588664      26.94
 H      -5.070976     0.779664    -0.519852      24.19
 C       1.257572     0.387718    -0.843254      23.77
 H       1.930184     1.337767    -0.841552      28.06
 C       1.240692    -2.061376    -1.325101      64.24
 H       1.773923    -2.941949    -1.616726      27.73
 C      -0.092623    -2.097046    -0.935984      24.15
 O      -0.787084    -3.307507    -1.092884     148.14
 C      -0.783592    -3.935592    -2.532456      87.00
 H       0.101746    -3.677661    -2.993936      26.51
 H      -0.824577    -4.983027    -2.060302      25.66
 H      -1.875089    -3.466583    -3.235983      22.88
 C      -0.764036    -0.889944    -0.487129      16.96
 O      -2.030445    -1.009297    -0.072234     136.53
 C      -0.096879     0.298783    -0.419562      61.46
 H      -0.435991     1.420297    -0.448528      26.66
 C       1.970438    -0.839546    -1.244011     -28.34
 C       3.496284    -0.999934    -1.270573      78.23
 H       3.762401    -2.002904    -1.780030      25.02
 O       4.147381     0.280616    -1.851298     231.59
 H       4.714891     0.690772    -1.120999      29.47
 C       4.068640    -1.238108     0.194591      55.07
 H       3.507888    -2.276966     0.742693      26.46
 O       5.302355    -2.092474     0.092880     131.57
 H       6.167804    -1.616539    -0.373487      22.55
 C       4.142701    -0.118990     1.329923     126.98
 O       5.483341     0.452392     1.404645     241.66
 H       5.434904     1.062966     2.220124      26.67
 H       3.769372    -0.719521     2.159547      29.60
 H       3.452762     0.631767     1.012155      30.70
55
name = lig-Water-frame_437
 C      -1.444762     2.426625     2.389578      35.51
 H      -2.384898     3.061492     2.028447      29.63
 C      -0.764146     0.101117     3.078291     -14.75
 H      -1.009603    -0.974462     3.148713      33.53
 C       0.512287     0.656723     3.513700      27.26
 O       1.362248    -0.045521     4.233760     191.30
 C       1.074390    -1.428785     4.548357     127.32
 H       2.041512    -1.795408     4.938708      27.14
 H       0.720030    -1.838490     3.620854      29.63
 H       0.159031    -1.544698     5.234157      27.95
 C       0.706354     2.060258     3.525350      15.70
 O       1.913015     2.495733     4.197781     116.31
 H       1.925086     3.445788     4.312857      36.27
 C      -0.210705     2.917727     2.993973      40.02
 H      -0.195501     4.034303     2.929111      24.84
 C      -1.851454     0.992047     2.392771     -86.28
 C      -3.021647     0.455761     1.724939      70.14
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 H      -3.712911     1.501165     2.052759      20.96
 O      -3.509915    -0.707779     2.537302     197.87
 H      -4.455024    -0.655961     2.270250      19.75
 C      -2.964532     0.128785     0.308958     104.65
 H      -2.389342     0.959314    -0.071614      30.60
 C      -4.240173    -0.097196    -0.535154     127.74
 O      -4.950717    -1.246163    -0.263222     204.83
 H      -4.365349    -2.047770    -0.114946      18.92
 H      -4.050037     0.054799    -1.611309      28.43
 H      -4.862999     0.774726    -0.493227      28.66
 C       1.286187     0.362191    -0.830759      67.97
 H       1.594544     1.339748    -0.575721      34.33
 C       1.288440    -2.018517    -1.292449       1.21
 H       1.926691    -2.953493    -1.479754      24.96
 C      -0.137467    -2.092716    -1.028349       4.08
 O      -0.778569    -3.338254    -1.093877     174.48
 C      -0.828230    -3.889992    -2.531540      80.11
 H       0.363516    -3.772191    -2.723613      20.29
 H      -0.757331    -4.934617    -2.352386      29.31
 H      -1.549545    -3.739351    -3.154322      29.50
 C      -0.725343    -0.907958    -0.433565      -9.07
 O      -2.020036    -0.993204    -0.097047      33.02
 C      -0.062304     0.349821    -0.399318      62.62
 H      -0.530786     1.244356    -0.158099      34.67
 C       1.972597    -0.798555    -1.211981      55.91
 C       3.520217    -1.008266    -1.224687      85.32
 H       4.088274    -1.660214    -1.929080      26.89
 O       4.145253     0.311774    -1.827087     248.27
 H       4.788903     0.732854    -1.313791      31.30
 C       4.133388    -1.276287     0.227700      93.38
 H       3.506761    -1.863326     0.695242      33.54
 O       5.369252    -2.094106     0.104029     164.62
 H       5.994755    -1.517206    -0.373572      27.12
 C       4.073670    -0.107324     1.360042     125.80
 O       5.436713     0.399025     1.414697     228.52
 H       5.550467     1.037762     2.106507      27.75
 H       3.880773    -0.884252     2.143571      30.42
 H       3.340883     0.575157     0.815355      32.87
55
name = lig-Water-frame_438
 C      -1.514859     2.364564     2.329437      69.88
 H      -2.112149     3.133226     1.947955      24.68
 C      -0.805193     0.159598     2.998051      88.09
 H      -1.101949    -0.864499     2.917802      33.02
 C       0.409016     0.652582     3.489131     -22.08
 O       1.452006    -0.030894     4.187946     113.44
 C       1.144413    -1.440249     4.617549     108.03
 H       2.040173    -1.934094     4.992128      27.84
 H       0.864332    -1.756012     3.480899      28.09
 H       0.191536    -1.536785     5.279938      26.09
 C       0.793923     2.082008     3.538497       0.72
 O       1.856269     2.477769     4.209707      81.84
 H       1.772277     3.609303     4.164064      24.32
 C      -0.228794     2.910550     2.942122     112.53
 H      -0.160492     4.006403     2.992841      21.05
 C      -1.744217     1.078097     2.447918      60.70
 C      -2.942190     0.498839     1.732263      85.51
 H      -3.649125     1.225867     1.904501      29.16
 O      -3.546165    -0.732075     2.502678     169.01
 H      -4.517317    -0.527867     2.314088      20.21
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 C      -2.939046     0.205711     0.205108      81.15
 H      -2.349852     1.174555     0.020635      29.96
 C      -4.243705    -0.085702    -0.613185     105.70
 O      -4.958395    -1.282613    -0.232694     143.84
 H      -4.453134    -2.219757    -0.168795      18.52
 H      -4.100176     0.013538    -1.782681      28.74
 H      -4.810355     0.899260    -0.110838      25.77
 C       1.300679     0.365601    -0.790868      58.58
 H       1.705395     1.397144    -0.532326      31.32
 C       1.298944    -1.983025    -1.259096      11.16
 H       1.914789    -2.937274    -1.370559      24.83
 C      -0.130053    -2.066423    -1.097219      12.41
 O      -0.801252    -3.362875    -1.105959     155.72
 C      -0.747882    -3.892952    -2.445809      96.12
 H       0.163817    -3.693889    -2.910398      25.83
 H      -0.915807    -5.072749    -2.627719      26.16
 H      -1.735997    -3.622873    -3.347891      23.86
 C      -0.690187    -0.914352    -0.413475     -39.77
 O      -2.068555    -1.009281    -0.094840     -25.46
 C      -0.004301     0.354474    -0.406702      59.39
 H      -0.638335     1.112635     0.220228      33.88
 C       2.018910    -0.784934    -1.179031      60.50
 C       3.594879    -0.926988    -1.175095      84.00
 H       3.972627    -1.558626    -1.989038      29.59
 O       4.125116     0.324798    -1.800089     195.78
 H       5.019882     0.739581    -1.381620      25.62
 C       4.196583    -1.319407     0.230210      93.08
 H       3.144916    -1.959153     0.673184      29.49
 O       5.416396    -2.072495     0.127789     211.73
 H       5.990983    -1.521674    -0.386098      27.37
 C       4.048973    -0.148316     1.322460     113.30
 O       5.392079     0.347390     1.420139     228.51
 H       5.545080     1.206107     2.098551      24.48
 H       3.846781    -0.481725     2.386589      30.19
 H       3.218297     0.563674     1.123089      32.04
55
name = lig-Water-frame_439
 C      -1.482777     2.417645     2.318526      73.39
 H      -2.012676     3.236583     1.753476      22.49
 C      -0.819268     0.216299     2.927479      85.17
 H      -1.059024    -0.891328     2.795850      30.56
 C       0.356310     0.663220     3.508361     -13.14
 O       1.529514    -0.029346     4.161255      87.10
 C       1.193714    -1.440918     4.606107     111.11
 H       2.036379    -1.983579     5.076224      28.29
 H       1.046021    -2.056064     3.752190      31.57
 H       0.365297    -1.459224     5.338104      28.60
 C       0.757847     2.075781     3.497160     -17.72
 O       1.816706     2.507331     4.226007     175.70
 H       1.756384     3.454177     4.060807      27.94
 C      -0.274457     2.891582     2.877930      84.33
 H      -0.120474     3.948059     2.970650      22.15
 C      -1.652084     1.071039     2.468973      55.76
 C      -2.924233     0.477141     1.769713      69.04
 H      -3.954403     1.284856     1.703986      26.47
 O      -3.570942    -0.725427     2.450950     150.24
 H      -4.579999    -0.622442     2.603553      21.44
 C      -2.846378     0.259187     0.096594      58.44
 H      -2.565722     1.259807    -0.369099      30.11
 C      -4.235869    -0.026734    -0.626888      97.82
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 O      -4.976717    -1.319746    -0.209693     152.95
 H      -4.364015    -2.092243    -0.285726      24.17
 H      -4.103023     0.026819    -1.674109      31.91
 H      -4.890396     0.638854    -0.192902      30.53
 C       1.351908     0.430635    -0.733016      28.09
 H       2.057504     1.250178    -0.719342      25.90
 C       1.294880    -1.972587    -1.235676      34.62
 H       1.799063    -2.908548    -1.379814      25.40
 C      -0.095439    -2.029784    -1.109152      -4.69
 O      -0.821534    -3.367033    -1.121654     148.53
 C      -0.724890    -3.946349    -2.446446     113.07
 H       0.120674    -3.542458    -3.187172      23.21
 H      -0.963522    -4.938113    -2.427608      29.35
 H      -1.483970    -3.373910    -2.794787      28.42
 C      -0.700929    -0.921880    -0.446142     -10.25
 O      -2.110571    -1.022974    -0.087623      57.70
 C      -0.010084     0.301383    -0.384128      71.56
 H      -0.322263     1.037539     0.334142      32.03
 C       2.087203    -0.782111    -1.135553      -8.47
 C       3.676346    -0.811665    -1.154117      87.87
 H       3.647257    -1.775753    -1.834476      25.10
 O       4.122131     0.357988    -1.758904     258.36
 H       5.055536     0.528655    -1.488258      28.26
 C       4.151953    -1.365839     0.248575      95.63
 H       3.527384    -2.122668     0.387893      30.00
 O       5.434813    -2.042967     0.172887     190.53
 H       6.198157    -1.576705    -0.447826      23.60
 C       4.051710    -0.208080     1.320888     129.74
 O       5.377502     0.339751     1.420503     298.15
 H       5.285689     1.112768     1.938048      31.79
 H       3.714502    -0.275469     2.379427      28.34
 H       3.246281     0.577649     1.239599      27.21
55
name = lig-Water-frame_440
 C      -1.407645     2.537860     2.316499      64.22
 H      -2.095535     3.077835     1.641487      19.87
 C      -0.735369     0.154934     2.922596      33.08
 H      -0.920605    -0.858789     2.830502      29.03
 C       0.423195     0.695673     3.569213      17.66
 O       1.558623    -0.058007     4.126570     107.21
 C       1.260019    -1.437039     4.574859     105.00
 H       2.149911    -1.714994     5.210104      27.63
 H       1.035011    -2.438316     3.924416      27.61
 H       0.413295    -1.304164     5.415175      28.08
 C       0.621546     2.030277     3.438999      21.86
 O       1.778865     2.530403     4.228571     141.18
 H       1.872187     3.655706     4.126941      21.08
 C      -0.272830     2.896036     2.839654      63.93
 H      -0.098515     4.019862     2.788990      24.00
 C      -1.739085     1.074129     2.383275     -29.05
 C      -3.011849     0.476316     1.769975      85.98
 H      -3.702654     1.213319     1.657547      30.49
 O      -3.571842    -0.708829     2.404723     207.61
 H      -4.514522    -0.579116     2.652873      22.46
 C      -2.789786     0.267418     0.033335      62.33
 H      -2.503385     1.046257    -0.670545      27.12
 C      -4.225720    -0.009750    -0.562038      75.80
 O      -4.979413    -1.322044    -0.214404     159.15
 H      -4.229263    -2.050631    -0.314893      23.50
 H      -4.101867     0.098073    -1.769651      28.19
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 H      -5.231103     0.729529    -0.409043      23.56
 C       1.444618     0.434358    -0.701091      37.86
 H       2.134560     1.306750    -0.775095      23.88
 C       1.321983    -1.959389    -1.225619      33.45
 H       1.760816    -3.035594    -1.529191      22.45
 C      -0.084633    -2.027347    -1.065299     -21.28
 O      -0.788544    -3.329545    -1.110195     125.66
 C      -0.714580    -3.952681    -2.475878      82.36
 H       0.132544    -3.701131    -3.105799      23.13
 H      -0.935153    -5.091911    -2.213040      23.61
 H      -1.738596    -3.194664    -2.822748      21.98
 C      -0.762910    -0.929137    -0.511621       8.82
 O      -2.109316    -1.017342    -0.099244     133.58
 C       0.014571     0.261954    -0.334147      47.49
 H      -0.238090     1.139678     0.290030      26.68
 C       2.114885    -0.750285    -1.067957     -46.06
 C       3.666930    -0.789696    -1.153012     103.60
 H       3.792186    -1.715973    -1.665990      23.74
 O       4.148937     0.400195    -1.713143     273.87
 H       5.098559     0.422230    -1.591501      28.86
 C       4.122185    -1.360204     0.244788      59.63
 H       3.573488    -2.523445     0.323056      23.95
 O       5.459206    -2.009126     0.223457     236.63
 H       6.177424    -1.712109    -0.316519      27.54
 C       4.042334    -0.253649     1.360827     116.16
 O       5.376362     0.347224     1.404768     260.94
 H       5.154521     1.201449     1.936913      27.39
 H       3.648364    -0.695794     2.344815      26.92
 H       3.423549     0.560833     0.840258      25.28
55
name = lig-Water-frame_441
 C      -1.451987     2.527452     2.261089      56.90
 H      -2.131823     3.131676     1.687665      22.28
 C      -0.661740     0.122393     2.932108     -15.45
 H      -0.792270    -1.037464     2.936689      24.24
 C       0.503789     0.653534     3.607429      30.23
 O       1.549516    -0.097122     4.065284     191.39
 C       1.323375    -1.443557     4.601640     120.74
 H       2.227459    -1.432806     5.184467      25.88
 H       1.075706    -2.225241     3.990644      29.95
 H       0.502482    -1.295828     5.267868      28.20
 C       0.572265     2.050614     3.462751      25.01
 O       1.723450     2.551849     4.198400     204.64
 H       1.668444     3.531228     4.236737      22.73
 C      -0.210565     2.990216     2.816173      -9.77
 H       0.060949     3.975695     2.639654      22.53
 C      -1.809938     1.076879     2.304353     -74.71
 C      -3.064595     0.492980     1.709999      61.58
 H      -3.893044     1.510386     1.732941      24.33
 O      -3.551878    -0.686682     2.364200     196.91
 H      -4.571945    -0.474309     2.394845      19.71
 C      -2.823503     0.224730     0.034799      67.75
 H      -2.152376     0.879880    -0.701567      22.15
 C      -4.288880    -0.005220    -0.529333     108.58
 O      -4.943421    -1.290542    -0.245700     255.66
 H      -4.364715    -2.091248    -0.179826      25.03
 H      -4.107939     0.032325    -1.567000      30.51
 H      -4.913223     0.771148    -0.459796      29.88
 C       1.497459     0.391420    -0.676630      55.09
 H       1.837728     1.439982    -0.614540      25.48
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 C       1.360348    -1.962717    -1.232307      75.05
 H       1.786394    -2.809833    -1.582430      28.24
 C      -0.073084    -2.062896    -0.996933       4.29
 O      -0.709118    -3.268080    -1.090373     205.21
 C      -0.796766    -3.921733    -2.474587     109.49
 H       0.262874    -3.897294    -2.988629      25.57
 H      -0.854581    -4.948624    -2.302759      28.68
 H      -1.588027    -3.771713    -3.170171      26.99
 C      -0.807967    -0.894794    -0.569540     -15.55
 O      -2.082515    -1.008115    -0.129611     155.94
 C       0.095792     0.261776    -0.284471      30.18
 H      -0.484695     1.207816     0.067737      22.52
 C       2.123642    -0.747343    -1.015834      10.66
 C       3.600924    -0.851673    -1.140564      91.45
 H       4.193796    -1.588914    -1.911688      21.03
 O       4.190446     0.448663    -1.660011     208.33
 H       5.266343     0.408308    -1.706327      23.45
 C       4.126793    -1.381517     0.232109      87.01
 H       3.494408    -2.160974     0.424886      28.10
 O       5.477192    -1.986996     0.289106     219.72
 H       6.170139    -1.641535    -0.307949      27.30
 C       4.025787    -0.312542     1.365255     126.61
 O       5.367745     0.363197     1.406716     233.60
 H       5.286335     1.299265     1.935760      24.28
 H       3.694946    -0.907247     2.191288      28.26
 H       3.469407     0.385987     0.816939      26.08
55
name = lig-Water-frame_442
 C      -1.520930     2.435142     2.197227      56.73
 H      -2.141446     3.316554     1.791813      24.95
 C      -0.645416     0.120572     2.933562      52.12
 H      -0.745818    -0.922280     2.986912      27.19
 C       0.489895     0.586961     3.564537       5.56
 O       1.544840    -0.123569     3.993000     180.23
 C       1.388127    -1.405697     4.663176     100.09
 H       2.382618    -1.569965     5.208367      25.16
 H       1.248337    -2.156374     3.710136      25.45
 H       0.364276    -1.403242     5.342117      24.48
 C       0.627199     2.121073     3.552770      -4.04
 O       1.662229     2.535066     4.157676      68.84
 H       1.456120     3.621250     4.275297      19.83
 C      -0.203086     3.046312     2.766672      89.11
 H       0.289080     4.073777     2.532432      15.42
 C      -1.770550     1.071085     2.287994       9.02
 C      -3.089306     0.578700     1.597522      91.95
 H      -3.833312     1.253729     1.797968      28.56
 O      -3.554054    -0.644619     2.324211     237.25
 H      -4.516952    -0.673132     2.119398      26.48
 C      -2.896973     0.173722     0.072949      92.90
 H      -2.314522     0.942597    -0.314804      27.17
 C      -4.303810    -0.039700    -0.537858      89.93
 O      -4.927068    -1.240126    -0.274073     260.35
 H      -4.342163    -2.078189    -0.088453      23.18
 H      -4.077072    -0.072437    -1.727020      27.40
 H      -4.824742     1.070287    -0.178181      24.61
 C       1.448322     0.389292    -0.616203      50.65
 H       1.735007     1.414230    -0.425208      26.05
 C       1.357328    -1.937927    -1.223879      64.00
 H       2.046089    -2.840912    -1.701125      23.78
 C      -0.022940    -2.054154    -0.934774      26.36
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 O      -0.651340    -3.239462    -1.098625     178.77
 C      -0.826204    -3.912527    -2.457124      97.38
 H       0.239743    -3.939493    -2.837883      26.13
 H      -0.889615    -5.065376    -2.214777      26.01
 H      -1.665215    -3.938386    -3.443676      23.30
 C      -0.748239    -0.840454    -0.598130      -1.50
 O      -2.063164    -1.017824    -0.161246     142.12
 C       0.128846     0.272396    -0.273262      56.68
 H      -0.446928     1.112970    -0.146032      27.16
 C       2.142568    -0.815536    -1.019635      16.32
 C       3.633003    -0.930011    -1.170905      95.95
 H       4.010355    -1.414876    -1.977709      25.51
 O       4.231223     0.492752    -1.594991     243.19
 H       5.171469     0.420776    -1.656125      27.48
 C       4.184834    -1.371730     0.220454      75.44
 H       3.209766    -2.147404     0.625183      24.26
 O       5.482519    -1.980717     0.353706     190.29
 H       6.091159    -1.463210    -0.386480      25.04
 C       4.050436    -0.362305     1.312196     107.47
 O       5.353829     0.382635     1.432586     236.99
 H       5.313716     1.189008     1.862567      27.06
 H       3.741681    -0.844644     2.337542      26.55
 H       3.101540     0.412051     1.201701      24.56
55
name = lig-Water-frame_443
 C      -1.505440     2.406872     2.168633      51.92
 H      -2.206115     3.115912     1.834588      26.18
 C      -0.704612     0.150918     2.907079      89.74
 H      -0.904466    -0.965400     2.891208      28.95
 C       0.421397     0.616612     3.476773     -19.68
 O       1.564553    -0.135191     3.943475     172.52
 C       1.426218    -1.397294     4.683911     133.56
 H       2.274238    -1.754115     5.217360      27.83
 H       1.475620    -2.053240     3.911840      28.52
 H       0.611339    -1.512514     5.292380      28.55
 C       0.596508     2.139653     3.557105     -19.36
 O       1.666385     2.559346     4.171999      99.04
 H       1.715015     3.567780     4.197246      23.59
 C      -0.232700     3.004294     2.718649      79.14
 H       0.165315     3.943155     2.441681      24.61
 C      -1.691452     1.036817     2.294742      18.34
 C      -3.043785     0.584867     1.522924      72.98
 H      -4.005594     1.427247     1.671783      22.86
 O      -3.560868    -0.598750     2.287873     163.54
 H      -4.445150    -0.924526     1.984465      24.24
 C      -2.968629     0.133036     0.133405      93.43
 H      -2.683928     1.302475    -0.178428      23.80
 C      -4.259924    -0.012961    -0.602426     123.03
 O      -4.953348    -1.214874    -0.280046     253.34
 H      -4.212559    -1.892170    -0.166507      25.56
 H      -4.196102     0.100478    -1.626911      30.93
 H      -4.806024     0.686228    -0.173995      31.01
 C       1.413902     0.374335    -0.548632      39.21
 H       2.011543     1.297500    -0.331261      26.60
 C       1.386783    -1.956891    -1.237659      73.21
 H       1.874540    -2.745471    -1.579162      28.18
 C       0.036237    -1.995830    -0.908907      35.68
 O      -0.642984    -3.250365    -1.122370     166.66
 C      -0.815582    -3.975799    -2.441093     109.26
 H       0.174906    -3.849920    -2.929464      26.60
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 H      -1.021671    -4.930451    -1.991080      27.58
 H      -1.598201    -3.584959    -3.099173      27.00
 C      -0.640231    -0.827769    -0.579670      21.35
 O      -2.041657    -1.024482    -0.193871      96.48
 C       0.075823     0.276188    -0.303518      61.60
 H      -0.398495     1.372517    -0.131778      25.20
 C       2.153054    -0.832074    -1.038122     -13.36
 C       3.716897    -0.934042    -1.196002      80.94
 H       3.767490    -1.700959    -2.184528      22.02
 O       4.236451     0.514024    -1.517283     232.53
 H       5.226676     0.468165    -1.510833      26.46
 C       4.193056    -1.400177     0.231315      96.70
 H       3.522787    -2.075962     0.570188      29.20
 O       5.484487    -1.973043     0.385119     255.83
 H       6.001220    -1.539530    -0.235260      31.66
 C       4.056126    -0.328030     1.317473     127.72
 O       5.333736     0.376972     1.449756     226.17
 H       5.114833     1.361915     1.941967      21.27
 H       4.016410    -0.775727     2.282005      28.77
 H       3.190199     0.188657     1.478370      28.44
55
name = lig-Water-frame_444
 C      -1.412631     2.411861     2.182167      68.28
 H      -2.330393     2.901399     1.685728      24.08
 C      -0.823557     0.146951     2.852584      79.60
 H      -1.056960    -0.913530     2.740689      33.15
 C       0.396329     0.712934     3.422585     -36.68
 O       1.577755    -0.115426     3.911759      61.18
 C       1.474086    -1.404717     4.655648      95.89
 H       2.382140    -1.589039     5.385828      23.61
 H       1.469160    -2.378006     3.911151      24.20
 H       0.477061    -1.556382     5.411271      22.94
 C       0.506031     2.103974     3.476573       5.52
 O       1.727412     2.579288     4.218875      89.06
 H       1.893371     3.614676     4.079799      22.51
 C      -0.289493     2.889532     2.683084      78.56
 H      -0.074031     3.968777     2.424819      29.89
 C      -1.665146     1.001219     2.272283     -25.98
 C      -3.027369     0.536595     1.563990      98.92
 H      -3.588508     1.412770     1.349544      28.94
 O      -3.556313    -0.561274     2.281934     162.65
 H      -4.366145    -0.966349     1.828024      22.30
 C      -2.971576     0.175443     0.125513      94.41
 H      -2.827751     1.085410    -0.380089      29.12
 C      -4.221227     0.001389    -0.650344      93.22
 O      -4.986525    -1.215951    -0.285832     162.06
 H      -4.306442    -1.955775    -0.337094      24.07
 H      -4.229128     0.394427    -1.813719      25.79
 H      -5.132939     0.757376    -0.187624      23.00
 C       1.470575     0.320191    -0.504063      36.61
 H       2.180767     1.103191    -0.303749      26.69
 C       1.426226    -1.972068    -1.249014      32.94
 H       1.814371    -3.096898    -1.586868      21.92
 C       0.076494    -1.988548    -0.943572      17.53
 O      -0.650914    -3.255173    -1.126306     147.09
 C      -0.767020    -4.003744    -2.367127      99.94
 H       0.095869    -3.935162    -3.212361      24.48
 H      -1.127687    -4.998777    -2.009532      26.29
 H      -1.747751    -3.239106    -2.834341      22.87
 C      -0.620180    -0.860504    -0.516465      23.44
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 O      -2.011176    -1.001313    -0.232216      78.51
 C       0.014077     0.389660    -0.343061      76.61
 H      -0.382481     1.238006    -0.009242      32.31
 C       2.163516    -0.768966    -1.038189      12.41
 C       3.767905    -0.899286    -1.239356      82.49
 H       3.833824    -1.670442    -1.883693      26.59
 O       4.226325     0.487857    -1.440712     273.81
 H       5.284848     0.616417    -1.275673      26.32
 C       4.200774    -1.403819     0.232699      60.43
 H       3.474850    -2.455864     0.529581      24.79
 O       5.490103    -1.980783     0.402794     206.17
 H       6.191940    -1.607067    -0.231384      27.44
 C       4.098090    -0.299750     1.380166     105.68
 O       5.308547     0.418774     1.468630     232.12
 H       5.074575     1.268518     1.814315      26.38
 H       4.266267    -1.090608     2.249414      26.40
 H       3.050316     0.335543     1.431691      24.79
55
name = lig-Water-frame_445
 C      -1.425726     2.349170     2.155487      76.25
 H      -2.087874     2.934384     1.533756      24.39
 C      -0.871984     0.110853     2.829458      43.44
 H      -1.058619    -0.951437     2.709828      31.17
 C       0.377770     0.723864     3.396528     -22.35
 O       1.561812    -0.078033     3.884666      55.53
 C       1.492065    -1.449891     4.631365     114.04
 H       2.308533    -1.221165     5.250857      25.92
 H       1.429675    -2.303294     4.089955      27.63
 H       0.651802    -1.407837     5.174154      27.52
 C       0.539824     2.072764     3.437607      12.82
 O       1.762671     2.569345     4.230246      53.04
 H       1.667898     3.548561     4.087619      24.21
 C      -0.308222     2.869508     2.656912      68.52
 H      -0.249994     3.968044     2.645184      28.81
 C      -1.733029     1.005273     2.204443     -24.00
 C      -2.964567     0.472734     1.615790      91.21
 H      -3.574806     1.629025     1.444194      26.11
 O      -3.559526    -0.539902     2.308467     168.75
 H      -4.276168    -0.833159     1.726470      24.59
 C      -2.903894     0.220454     0.047868      75.71
 H      -2.386779     1.040419    -0.687359      26.26
 C      -4.302895     0.034726    -0.674328     111.81
 O      -5.005823    -1.229049    -0.314013     184.43
 H      -4.548394    -2.143592    -0.482844      22.09
 H      -4.118764     0.248198    -1.658182      31.26
 H      -4.888657     0.791250    -0.405822      30.94
 C       1.521843     0.287871    -0.477132      44.01
 H       2.150243     1.170449    -0.239880      27.20
 C       1.475682    -2.012110    -1.267392      60.01
 H       1.814255    -2.942767    -1.528794      26.15
 C       0.094667    -2.039995    -1.015129      11.23
 O      -0.634168    -3.247871    -1.083345     214.07
 C      -0.768784    -3.965809    -2.326475     127.14
 H      -0.058701    -4.091320    -3.084303      28.44
 H      -1.145786    -5.036073    -2.275684      26.64
 H      -1.635143    -3.463865    -2.651751      26.63
 C      -0.662356    -0.846964    -0.437825     -11.67
 O      -1.993267    -0.968158    -0.274119      72.35
 C       0.041505     0.459556    -0.393190      45.59
 H      -0.560066     1.330601     0.190705      27.97
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 C       2.196570    -0.754353    -1.054989      44.80
 C       3.758659    -0.820215    -1.185542      76.73
 H       4.220352    -1.698947    -1.988370      24.15
 O       4.233978     0.450570    -1.376677     316.64
 H       5.086424     0.625518    -1.118890      32.68
 C       4.181008    -1.417388     0.230815      82.21
 H       3.579987    -2.239125     0.297518      29.88
 O       5.519201    -1.994638     0.400971     188.94
 H       6.320051    -1.720670    -0.256631      25.52
 C       4.113771    -0.350087     1.469607     132.88
 O       5.302109     0.481061     1.468128     197.98
 H       5.130152     1.473695     1.828315      21.45
 H       4.099925    -1.074084     2.202199      31.13
 H       3.345640     0.264148     1.391789      29.23
55
name = lig-Water-frame_446
 C      -1.501095     2.292054     2.073574      67.76
 H      -1.941055     3.116974     1.440352      21.95
 C      -0.839533     0.096698     2.836157      70.93
 H      -0.940130    -1.041442     2.804979      27.30
 C       0.355469     0.603912     3.382043     -10.29
 O       1.514101    -0.036255     3.844974      97.47
 C       1.495382    -1.421734     4.595250      74.10
 H       2.457932    -1.180812     5.201852      23.10
 H       1.562116    -2.418340     3.930777      24.27
 H       0.443891    -1.248247     5.254605      22.39
 C       0.661160     2.077600     3.437033     -21.15
 O       1.742450     2.540581     4.193746     127.57
 H       1.519314     3.563385     4.271059      22.15
 C      -0.279379     2.914177     2.682807      55.72
 H      -0.237306     3.989967     2.826352      24.73
 C      -1.786231     0.970250     2.168246      36.89
 C      -2.935925     0.517719     1.569374     101.37
 H      -3.633979     1.215108     1.817492      27.08
 O      -3.573265    -0.542374     2.347675     190.43
 H      -4.330931    -0.821360     1.771922      25.56
 C      -2.795711     0.258465    -0.069550      81.66
 H      -2.163436     0.959622    -0.462255      28.45
 C      -4.345651     0.017576    -0.671364      80.76
 O      -5.042700    -1.230016    -0.353358     199.41
 H      -4.501219    -2.042553    -0.528902      25.27
 H      -4.024179    -0.116767    -1.850657      25.42
 H      -4.939553     1.081441    -0.392946      24.29
 C       1.529105     0.330364    -0.465399      45.39
 H       2.017131     1.273540    -0.201062      25.38
 C       1.491097    -2.004299    -1.273883      53.29
 H       2.119332    -2.973364    -1.640415      23.82
 C       0.089382    -2.051336    -1.060055       6.08
 O      -0.599505    -3.254525    -1.008629     192.39
 C      -0.819207    -3.950862    -2.301476      88.59
 H       0.236392    -4.001726    -3.004292      22.99
 H      -1.084423    -4.987225    -2.158894      25.65
 H      -1.860721    -3.488729    -2.990999      22.80
 C      -0.643972    -0.794984    -0.417005     -22.83
 O      -2.012026    -0.949383    -0.310792     118.70
 C       0.096688     0.440009    -0.409233      57.33
 H      -0.336259     1.250045     0.097989      27.13
 C       2.238042    -0.816612    -1.092540      27.22
 C       3.755395    -0.806030    -1.100986     109.32
 H       4.240823    -1.275605    -1.847230      26.40
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 O       4.233624     0.458690    -1.338901     283.87
 H       5.180833     0.560648    -0.927449      27.77
 C       4.209257    -1.373552     0.224190      72.24
 H       3.354951    -2.339531     0.348409      25.14
 O       5.569073    -2.015949     0.379585     216.25
 H       6.101341    -1.769747    -0.317909      32.82
 C       4.139613    -0.435539     1.510020     104.32
 O       5.316301     0.540549     1.459232     182.65
 H       5.138822     1.496008     1.907631      21.31
 H       3.895914    -0.958860     2.581804      26.35
 H       3.186309     0.331102     1.430807      24.55
55
name = lig-Water-frame_447
 C      -1.490901     2.332879     2.012707      63.76
 H      -2.087656     3.100834     1.410014      23.83
 C      -0.786093     0.074061     2.847888     116.65
 H      -0.889458    -0.960525     2.897996      30.38
 C       0.369293     0.533697     3.373384     -12.70
 O       1.465922    -0.034777     3.809550     207.15
 C       1.472969    -1.343095     4.563103     121.36
 H       2.364723    -1.486797     5.121861      28.52
 H       1.624879    -2.133656     3.898988      29.53
 H       0.698477    -1.420846     5.167104      29.79
 C       0.708737     2.071153     3.395593     -12.83
 O       1.700365     2.525863     4.145652     258.24
 H       1.641788     3.476712     4.424746      24.53
 C      -0.251180     2.905230     2.744551      61.12
 H      -0.164729     4.045738     2.858575      22.10
 C      -1.733874     0.925892     2.192678      35.94
 C      -3.000472     0.530983     1.466361      73.44
 H      -3.931442     1.276417     1.794433      23.84
 O      -3.578266    -0.578772     2.374600     129.71
 H      -4.461406    -0.907938     2.007008      24.81
 C      -2.746810     0.251442    -0.120643      83.09
 H      -2.176714     1.291377    -0.398282      25.63
 C      -4.310203     0.008137    -0.720688     105.24
 O      -5.089537    -1.205711    -0.381201     241.20
 H      -4.302413    -1.873393    -0.404243      25.71
 H      -4.241653    -0.166004    -1.705704      29.72
 H      -4.920813     0.814216    -0.543842      29.47
 C       1.536752     0.365900    -0.508617      55.58
 H       2.033152     1.293909    -0.244283      26.24
 C       1.501682    -2.007693    -1.294984      57.46
 H       2.161170    -2.768012    -1.688804      25.93
 C       0.078424    -1.989131    -1.046611       0.24
 O      -0.584654    -3.276161    -0.953942     168.93
 C      -0.869261    -3.927329    -2.319514     109.55
 H       0.048201    -3.779877    -2.700992      27.64
 H      -1.022790    -4.959981    -1.830627      23.96
 H      -1.506381    -3.614165    -3.085461      28.11
 C      -0.574336    -0.795411    -0.487901      -7.12
 O      -2.030651    -0.938896    -0.344227     128.41
 C       0.173281     0.352220    -0.395083      64.53
 H      -0.153798     1.385968     0.010757      25.71
 C       2.236005    -0.831810    -1.088926      21.74
 C       3.756332    -0.804844    -1.009121      83.21
 H       4.164484    -1.462332    -1.998889      23.75
 O       4.248602     0.539503    -1.305261     251.66
 H       5.186004     0.552869    -0.853865      26.97
 C       4.239077    -1.388734     0.301021     105.57
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 H       3.536025    -2.117175     0.563113      30.71
 O       5.598825    -2.032875     0.340480     145.74
 H       6.007256    -1.790975    -0.609925      27.74
 C       4.119201    -0.454376     1.544511     125.72
 O       5.329864     0.556207     1.443256     197.24
 H       5.070519     1.454028     1.984964      19.96
 H       4.057321    -0.749609     2.525859      31.51
 H       3.244408     0.057157     1.436939      31.10
55
name = lig-Water-frame_448
 C      -1.394210     2.378071     2.021160      62.14
 H      -2.206821     2.905894     1.513976      24.72
 C      -0.763886     0.041959     2.845418      47.87
 H      -0.998518    -1.090388     2.936278      26.32
 C       0.413342     0.614978     3.359242       6.76
 O       1.473900    -0.090148     3.817769     209.50
 C       1.475506    -1.263261     4.499824     115.79
 H       2.389011    -1.507841     5.161632      26.66
 H       1.459734    -2.071340     3.630701      28.75
 H       0.546840    -1.636100     5.286053      25.82
 C       0.633744     2.029281     3.308119      30.42
 O       1.696305     2.508571     4.123048     161.33
 H       1.646508     3.491720     4.289467      25.63
 C      -0.264273     2.879841     2.782081      69.06
 H      -0.071074     3.903257     2.783752      21.80
 C      -1.679105     0.955104     2.197885       5.26
 C      -3.109835     0.511978     1.418837      70.19
 H      -3.737855     1.384752     1.239071      28.50
 O      -3.576676    -0.633194     2.379845     153.42
 H      -4.495980    -0.905699     2.239491      24.73
 C      -2.790003     0.262642    -0.108948      90.29
 H      -2.534816     1.174821    -0.502099      28.77
 C      -4.236322    -0.015031    -0.788170      81.24
 O      -5.101322    -1.178877    -0.391260     221.00
 H      -4.436053    -1.918635    -0.114134      25.89
 H      -4.286757     0.037474    -2.035180      25.81
 H      -5.022755     0.888810    -0.580316      25.22
 C       1.591884     0.350684    -0.601309      56.50
 H       2.181197     1.264126    -0.377549      26.00
 C       1.493465    -1.971318    -1.316692      55.98
 H       2.019340    -2.899143    -1.747993      25.73
 C       0.084220    -1.949326    -0.999876      12.29
 O      -0.601105    -3.254686    -0.925243     175.01
 C      -0.869675    -3.938164    -2.268313      80.84
 H       0.293646    -3.759098    -2.766107      23.44
 H      -1.037126    -4.928940    -1.952389      26.89
 H      -1.688117    -3.459601    -3.157499      23.97
 C      -0.543040    -0.856468    -0.607164      21.90
 O      -1.999178    -0.920655    -0.385719      88.52
 C       0.236663     0.312658    -0.344648      55.65
 H      -0.202045     1.348825    -0.181116      25.93
 C       2.213654    -0.776089    -1.030045       0.73
 C       3.777218    -0.810537    -0.998810      89.84
 H       3.955206    -1.582738    -1.645413      29.24
 O       4.262293     0.616672    -1.263060     251.82
 H       5.105911     0.746433    -0.945877      30.23
 C       4.301892    -1.413704     0.437710      80.11
 H       3.474185    -2.333150     0.750109      27.72
 O       5.618203    -2.031589     0.266635     130.74
 H       5.964238    -1.979770    -0.701989      25.87
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 C       4.149135    -0.406897     1.539722     108.11
 O       5.317169     0.533962     1.417964     176.19
 H       5.114725     1.413056     1.976948      21.17
 H       4.355468    -0.948212     2.589246      28.63
 H       3.051853     0.059868     1.361282      28.65
55
name = lig-Water-frame_449
 C      -1.299160     2.357829     2.074845      74.17
 H      -2.225402     2.932357     1.665794      25.04
 C      -0.773963     0.028137     2.827081      34.04
 H      -1.030047    -0.975768     2.934098      27.79
 C       0.438422     0.683202     3.330826      19.60
 O       1.518338    -0.095516     3.843726     177.96
 C       1.446796    -1.326652     4.453833     133.95
 H       2.358207    -1.264721     5.001622      27.34
 H       1.298749    -2.041499     3.680868      31.11
 H       0.636696    -1.426957     5.026606      31.54
 C       0.589015     1.986042     3.278725      26.08
 O       1.699199     2.489766     4.096877      96.63
 H       1.554334     3.500043     3.989693      27.18
 C      -0.329170     2.885576     2.753585      68.81
 H       0.049023     3.982785     2.726496      19.11
 C      -1.667459     1.004090     2.165229     -10.23
 C      -3.125121     0.472294     1.419715      63.49
 H      -3.741368     1.485061     1.115197      24.86
 O      -3.573659    -0.662254     2.353464     157.02
 H      -4.577154    -0.802117     2.300105      22.68
 C      -2.917576     0.209281    -0.081443      73.62
 H      -2.620296     1.196368    -0.709011      24.32
 C      -4.215448    -0.020616    -0.898100     100.62
 O      -5.078670    -1.148243    -0.390004     267.74
 H      -4.683454    -1.972838    -0.100985      27.23
 H      -4.058268     0.163547    -1.888803      30.19
 H      -4.762837     0.847412    -0.543366      28.69
 C       1.631729     0.372003    -0.672127      61.21
 H       2.267154     1.218081    -0.562309      26.73
 C       1.477623    -1.916523    -1.327702      69.22
 H       1.739351    -2.983533    -1.662200      26.91
 C       0.135670    -2.030627    -0.978756      18.66
 O      -0.639775    -3.201802    -0.927371     200.51
 C      -0.799526    -3.912289    -2.248275     115.40
 H      -0.015972    -4.017871    -2.836472      28.91
 H      -1.132411    -5.029089    -2.212176      26.48
 H      -1.690387    -3.409707    -2.598757      25.83
 C      -0.583942    -0.824918    -0.682967      17.00
 O      -1.928644    -0.896370    -0.438042      42.19
 C       0.256525     0.307961    -0.322719      56.61
 H      -0.350957     1.188477    -0.208751      27.42
 C       2.256289    -0.775211    -0.987335      27.36
 C       3.780555    -0.790480    -0.954866      58.99
 H       4.125977    -1.739540    -1.671323      26.04
 O       4.243387     0.651240    -1.236270     165.14
 H       5.253532     0.910726    -1.003422      22.88
 C       4.325256    -1.457707     0.519963      90.51
 H       3.622016    -2.263454     0.646557      30.43
 O       5.635950    -2.031555     0.197049     142.43
 H       5.914324    -2.052886    -0.672484      29.81
 C       4.218071    -0.352533     1.562197     142.90
 O       5.289823     0.502906     1.378497     224.05
 H       5.204855     1.406718     1.892320      20.64
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 H       4.376212    -0.968653     2.384157      32.56
 H       3.226731     0.023733     1.528151      31.74
55
name = lig-Water-frame_450
 C      -1.363870     2.313768     2.079714      67.30
 H      -1.971700     3.091632     1.735901      27.66
 C      -0.792755     0.102820     2.788046      63.56
 H      -1.014572    -1.006333     2.927468      31.14
 C       0.428181     0.583579     3.297932      -2.28
 O       1.561747    -0.014086     3.844250     130.51
 C       1.411971    -1.423649     4.403961      89.25
 H       2.408231    -1.411426     4.949922      25.84
 H       1.348025    -2.330254     3.677604      28.44
 H       0.413746    -1.246832     5.157855      23.36
 C       0.621424     2.033835     3.321227     -22.14
 O       1.680800     2.485259     4.039314     139.15
 H       1.655564     3.456795     3.923677      27.87
 C      -0.294658     2.952847     2.741073      55.11
 H      -0.079316     3.971332     2.683429      20.46
 C      -1.686311     0.970910     2.124380      55.50
 C      -3.061590     0.464269     1.445951      93.56
 H      -3.841484     1.238469     1.659543      27.32
 O      -3.581775    -0.659063     2.298231     185.35
 H      -4.577403    -0.620630     2.211547      22.69
 C      -3.011740     0.141156    -0.106290      87.77
 H      -2.551279     1.010398    -0.472823      28.84
 C      -4.207697    -0.058203    -0.921078      89.95
 O      -5.068738    -1.090233    -0.407672     247.91
 H      -4.553275    -2.044228    -0.388562      22.91
 H      -3.852933     0.016722    -2.096087      26.57
 H      -4.739646     0.944564    -0.583497      26.20
 C       1.619987     0.428943    -0.698037      45.22
 H       2.243888     1.358011    -0.658767      28.42
 C       1.462613    -1.916444    -1.317793      77.90
 H       1.883196    -2.887531    -1.572760      29.85
 C       0.149034    -2.079994    -0.964484      12.75
 O      -0.663942    -3.172312    -0.951168     188.04
 C      -0.773113    -3.910919    -2.196340      99.18
 H       0.080502    -4.044866    -3.160324      23.94
 H      -1.205996    -4.891864    -2.119765      27.49
 H      -1.769361    -3.274199    -2.524498      23.42
 C      -0.582198    -0.754716    -0.704747      24.94
 O      -1.883498    -0.877464    -0.490764      28.84
 C       0.237469     0.311923    -0.364576      63.85
 H      -0.453561     1.252259    -0.053162      28.88
 C       2.343256    -0.830168    -0.991150      18.45
 C       3.813395    -0.798843    -0.907814      79.52
 H       4.309408    -1.300370    -1.671455      31.64
 O       4.215141     0.652504    -1.218856     188.41
 H       5.220715     0.743021    -1.118336      25.08
 C       4.335720    -1.448407     0.462474      88.07
 H       3.537322    -2.375218     0.663514      29.09
 O       5.653787    -2.038390     0.180020      70.47
 H       5.864247    -1.972699    -0.879921      23.28
 C       4.300859    -0.366935     1.594725     133.77
 O       5.296138     0.503605     1.321617     182.72
 H       5.241711     1.442059     1.887390      18.03
 H       4.333566    -0.891162     2.682241      31.49
 H       3.251762     0.150830     1.689014      31.87
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name = lig-Water-frame_451
 C      -1.466628     2.324448     2.080174      49.54
 H      -2.003401     3.212846     1.515696      23.67
 C      -0.796035     0.137970     2.757053      87.39
 H      -0.986580    -0.927729     2.818238      35.37
 C       0.421560     0.530734     3.265446      -4.61
 O       1.590233     0.036934     3.833231      97.06
 C       1.365289    -1.485586     4.384755     101.94
 H       2.227377    -1.806741     4.970459      28.19
 H       1.349641    -2.331202     3.711562      29.23
 H       0.634764    -1.388174     5.070794      27.83
 C       0.630675     2.084826     3.359394      -7.62
 O       1.691363     2.497896     3.986208     123.28
 H       1.815082     3.490971     4.062670      30.05
 C      -0.229199     2.955275     2.731896      53.91
 H      -0.226233     4.117487     2.663790      23.79
 C      -1.739463     0.916503     2.070528      48.01
 C      -2.994498     0.434773     1.513451      98.20
 H      -3.817111     1.170336     1.925165      23.10
 O      -3.591779    -0.652678     2.238074     175.16
 H      -4.536534    -0.553030     2.069823      24.53
 C      -2.985198     0.102311    -0.105070      88.25
 H      -2.481855     1.125655    -0.346757      27.18
 C      -4.222325    -0.076855    -0.925281     116.59
 O      -5.059635    -1.060404    -0.447168     318.66
 H      -4.506108    -1.776057    -0.721482      28.33
 H      -3.970051    -0.311445    -1.911110      29.28
 H      -4.784505     0.894670    -0.994692      27.96
 C       1.617483     0.438191    -0.708182      35.94
 H       2.026304     1.435569    -0.627348      30.98
 C       1.504562    -1.976615    -1.285648      28.95
 H       2.279137    -2.845465    -1.527416      25.56
 C       0.107329    -2.004432    -0.950887      31.07
 O      -0.654836    -3.175704    -0.970802     189.91
 C      -0.806905    -3.896821    -2.217492     115.23
 H      -0.015490    -3.786705    -2.783675      28.72
 H      -1.198462    -4.871335    -1.778015      26.85
 H      -1.563851    -3.388075    -2.901239      26.30
 C      -0.514210    -0.749992    -0.696649      42.21
 O      -1.902414    -0.878890    -0.535545      20.69
 C       0.202608     0.389878    -0.437641      70.24
 H      -0.181509     1.218195    -0.014044      33.37
 C       2.344161    -0.821828    -1.012123     -37.18
 C       3.873422    -0.779876    -0.878350      94.40
 H       4.482556    -1.125038    -1.857272      26.77
 O       4.184079     0.631055    -1.198966     217.21
 H       5.116434     0.593050    -1.199442      29.02
 C       4.319296    -1.432496     0.361596     105.55
 H       3.616529    -2.232068     0.703495      29.05
 O       5.666300    -2.047869     0.173974      83.41
 H       5.891087    -1.870401    -0.773705      27.71
 C       4.320126    -0.443178     1.664109     134.80
 O       5.356339     0.551710     1.265328     186.60
 H       5.205733     1.330533     1.848115      22.01
 H       4.445072    -0.709528     2.673863      33.92
 H       3.397339     0.173119     1.633268      32.42
55
name = lig-Water-frame_452
 C      -1.524860     2.390003     2.081871      62.25
 H      -2.159774     2.892414     1.417609      24.91
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 C      -0.778411     0.096750     2.731435      51.46
 H      -0.997822    -0.977505     2.693561      34.16
 C       0.444797     0.630225     3.250586      10.08
 O       1.598876    -0.001462     3.830663      41.92
 C       1.367703    -1.516449     4.365298      94.80
 H       2.182376    -1.922545     5.011131      27.26
 H       1.126825    -2.184913     3.444767      28.23
 H       0.400032    -1.550190     5.169995      24.62
 C       0.585436     2.080838     3.351464      14.95
 O       1.773485     2.528138     3.972968     102.10
 H       1.737996     3.531766     4.196388      27.90
 C      -0.262433     2.919907     2.673917      64.64
 H      -0.211103     3.998403     2.750127      26.52
 C      -1.749500     0.945569     2.046225     -36.06
 C      -3.006039     0.383107     1.558929      98.60
 H      -3.600428     1.405373     1.537557      26.49
 O      -3.597202    -0.684091     2.201404     193.63
 H      -4.590056    -0.655970     1.951422      22.12
 C      -2.850364     0.158619    -0.073697      85.53
 H      -2.616177     1.163972    -0.447877      28.45
 C      -4.234825    -0.052801    -0.935910      88.97
 O      -5.079792    -1.060982    -0.486423     260.95
 H      -4.640157    -1.950330    -0.793861      22.80
 H      -3.946242    -0.514652    -2.004850      24.94
 H      -4.796859     0.885063    -1.237423      26.75
 C       1.600716     0.404444    -0.713702      26.40
 H       2.008546     1.407983    -0.528983      29.37
 C       1.608185    -2.031840    -1.218527      26.37
 H       2.165329    -2.857421    -1.447746      27.98
 C       0.110649    -1.927904    -0.978083      -2.16
 O      -0.640353    -3.162634    -0.973125     132.08
 C      -0.876598    -3.880439    -2.237218      86.77
 H       0.376043    -3.801408    -2.574829      22.80
 H      -1.046962    -4.899417    -1.790152      26.05
 H      -1.623272    -3.514759    -3.125995      24.37
 C      -0.497778    -0.764420    -0.657324       3.74
 O      -1.950927    -0.896772    -0.574243      34.22
 C       0.227799     0.478659    -0.541178      49.38
 H      -0.116803     1.495837     0.063356      30.99
 C       2.275464    -0.766993    -1.039192      10.59
 C       3.906240    -0.733161    -0.960257     120.50
 H       4.303273    -1.377878    -1.706631      31.91
 O       4.154661     0.615362    -1.165089     226.87
 H       5.244970     0.722361    -1.269152      22.19
 C       4.346442    -1.413660     0.346095      83.42
 H       3.539406    -2.294751     0.597977      28.45
 O       5.660628    -2.056539     0.180357     130.33
 H       6.105522    -1.869165    -0.664156      26.78
 C       4.341107    -0.475777     1.647802     126.63
 O       5.426565     0.586122     1.222338      87.85
 H       5.205339     1.470226     1.897153      18.86
 H       4.649538    -0.968538     2.657405      31.38
 H       3.361199     0.047747     1.572360      30.37
55
name = lig-Water-frame_453
 C      -1.536283     2.406052     2.080596      63.87
 H      -2.363632     2.864643     1.425695      21.87
 C      -0.748434     0.066253     2.695344      22.93
 H      -0.914150    -1.057900     2.624359      33.21
 C       0.472010     0.735651     3.260001       3.83
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 O       1.582670    -0.093026     3.842033      63.36
 C       1.324212    -1.523786     4.344417     137.37
 H       2.264985    -1.802298     4.842722      28.44
 H       1.004610    -1.858704     3.368064      28.01
 H       0.434937    -1.611517     4.892952      30.27
 C       0.575619     2.060471     3.335479      16.79
 O       1.853979     2.570261     3.970884      82.13
 H       1.562463     3.472432     4.200746      26.54
 C      -0.382434     2.884448     2.595597      62.67
 H      -0.098138     3.956850     2.757631      28.32
 C      -1.685346     0.997038     2.106495     -47.79
 C      -3.031805     0.383415     1.488588      84.00
 H      -3.659462     1.368978     1.213189      27.81
 O      -3.618978    -0.736735     2.191549     179.67
 H      -4.558015    -0.837404     1.907652      23.73
 C      -2.752589     0.242090    -0.066293      77.64
 H      -2.479865     1.213912    -0.566902      27.05
 C      -4.194942    -0.047532    -0.981296      79.32
 O      -5.133599    -1.087843    -0.514797     245.56
 H      -4.868766    -2.056870    -0.578399      24.47
 H      -3.709503    -0.360662    -1.908477      27.48
 H      -4.795179     0.934354    -1.187775      26.15
 C       1.573907     0.405880    -0.717549      48.65
 H       2.290590     1.220103    -0.460413      28.45
 C       1.645204    -2.004021    -1.122948      33.49
 H       2.001956    -3.138174    -1.400538      23.80
 C       0.198338    -1.941542    -1.038857     -22.81
 O      -0.643428    -3.116518    -0.963594     163.49
 C      -0.833425    -3.864427    -2.255385     120.25
 H       0.042767    -4.099723    -2.613120      29.36
 H      -1.052077    -4.924585    -2.085527      27.34
 H      -1.680216    -3.654143    -3.011175      25.75
 C      -0.551503    -0.715885    -0.608160     -43.64
 O      -1.980456    -0.904689    -0.599776      23.79
 C       0.227683     0.558530    -0.614207      80.20
 H      -0.171909     1.383230    -0.255036      34.14
 C       2.256480    -0.759408    -1.069472      60.88
 C       3.851434    -0.712239    -1.055672      80.45
 H       4.133474    -1.652852    -1.738231      25.93
 O       4.175503     0.628856    -1.151595     263.48
 H       5.065543     0.923949    -1.191296      29.90
 C       4.387643    -1.405571     0.382554      77.37
 H       3.622305    -2.235239     0.331490      29.39
 O       5.646043    -2.074284     0.199290     125.12
 H       6.378761    -1.831119    -0.579717      21.37
 C       4.402335    -0.473550     1.555878     156.80
 O       5.459810     0.618184     1.231833     125.54
 H       5.365419     1.421533     1.733234      21.17
 H       4.717289    -1.186300     2.311697      35.43
 H       3.297558    -0.141744     1.777285      28.28
55
name = lig-Water-frame_454
 C      -1.575846     2.373319     2.043881      51.58
 H      -2.307030     3.086811     1.698361      28.50
 C      -0.692054     0.100909     2.661771      77.83
 H      -0.778443    -0.936600     2.622127      30.50
 C       0.483328     0.677361     3.288210      -7.74
 O       1.546342    -0.155869     3.860756     112.89
 C       1.272515    -1.476724     4.260032     127.39
 H       2.270245    -1.786577     4.613283      29.26
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 H       1.100469    -2.064426     3.284604      30.68
 H       0.296648    -1.579779     5.008994      24.88
 C       0.615986     2.102472     3.311082       5.29
 O       1.875882     2.609948     3.948559     118.15
 H       1.590471     3.573269     4.243041      17.28
 C      -0.433408     2.896815     2.583214      87.49
 H      -0.103490     3.986727     2.543296      24.48
 C      -1.660021     0.971986     2.192393      33.09
 C      -3.007182     0.436279     1.363243      73.00
 H      -3.989349     1.095030     1.350311      26.51
 O      -3.631662    -0.778484     2.182901     167.34
 H      -4.545174    -0.913590     1.865629      26.82
 C      -2.745483     0.280872    -0.111529      84.30
 H      -2.182299     1.190105    -0.524831      29.16
 C      -4.124329    -0.055677    -0.993698      79.78
 O      -5.201782    -1.093331    -0.538233     205.10
 H      -4.762675    -1.963759    -0.489509      26.84
 H      -3.562720    -0.232965    -1.969471      27.68
 H      -4.731271     0.837445    -0.981005      28.03
 C       1.601325     0.432982    -0.727315      49.06
 H       2.375214     1.120364    -0.483301      29.47
 C       1.598263    -2.005857    -1.053216      64.10
 H       1.960409    -2.919441    -1.249708      30.18
 C       0.250162    -1.943361    -1.056414     -14.20
 O      -0.643574    -3.074831    -0.977534     124.54
 C      -0.792186    -3.887003    -2.241721      95.53
 H       0.230071    -4.173170    -3.062761      24.18
 H      -1.288673    -4.920787    -2.060203      25.85
 H      -1.689217    -3.427264    -2.870456      25.21
 C      -0.573105    -0.676557    -0.617157     -32.81
 O      -1.965118    -0.882993    -0.601408      54.45
 C       0.161025     0.551200    -0.668636      71.45
 H      -0.406562     1.632308    -0.499618      30.99
 C       2.307183    -0.774373    -1.082249      57.08
 C       3.769794    -0.756561    -1.100295      92.08
 H       4.130740    -1.355055    -1.914821      30.29
 O       4.189793     0.666887    -1.175043     245.70
 H       5.167036     0.876628    -1.051963      27.55
 C       4.416068    -1.377624     0.313820      69.05
 H       3.648892    -2.260311     0.465663      30.11
 O       5.665346    -2.103132     0.221085     193.75
 H       6.166251    -1.750824    -0.471322      29.11
 C       4.466134    -0.450902     1.457030     149.95
 O       5.461020     0.605947     1.254878     165.50
 H       5.332508     1.569978     1.855928      17.20
 H       4.862428    -1.107969     2.274319      34.47
 H       3.534449    -0.178428     1.900474      30.85
55
name = lig-Water-frame_455
 C      -1.592639     2.333066     2.037215      79.06
 H      -2.293551     3.154064     1.830747      26.85
 C      -0.608444     0.163555     2.655916      70.91
 H      -0.736166    -0.995348     2.599859      27.54
 C       0.497342     0.594975     3.321638      21.85
 O       1.494478    -0.154175     3.865828     189.45
 C       1.200694    -1.463160     4.144528     136.34
 H       2.128930    -1.886095     4.606275      29.80
 H       1.120900    -2.328272     3.463771      30.73
 H       0.569139    -1.543968     5.022305      30.19
 C       0.670947     2.144333     3.275946       1.49
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 O       1.837491     2.656904     3.909475     182.03
 H       1.825258     3.601218     4.202876      27.38
 C      -0.370832     2.937147     2.627214      51.87
 H      -0.283450     3.980208     2.352638      19.49
 C      -1.746967     0.925737     2.208244      43.73
 C      -2.985194     0.457994     1.318303      79.12
 H      -3.950514     1.082679     1.566486      25.95
 O      -3.613037    -0.805063     2.155766     148.05
 H      -4.580877    -0.858758     1.823881      26.32
 C      -2.786968     0.260117    -0.200438      96.80
 H      -2.253944     1.149912    -0.455754      29.93
 C      -4.050361    -0.055400    -0.971692      87.06
 O      -5.227553    -1.074000    -0.572761     179.51
 H      -4.562433    -1.882924    -0.510237      24.35
 H      -3.809943    -0.178954    -2.114460      27.13
 H      -4.734649     0.913272    -0.841105      25.69
 C       1.635908     0.436473    -0.758791      -0.56
 H       2.224676     1.405895    -0.554310      27.89
 C       1.552688    -1.990966    -1.020225      40.70
 H       2.204494    -2.998310    -1.166306      27.49
 C       0.171334    -1.901636    -1.004877      18.78
 O      -0.616448    -3.061593    -1.016432     158.94
 C      -0.761780    -3.934074    -2.274745     125.68
 H      -0.039852    -3.893027    -2.914194      30.24
 H      -1.307732    -4.718764    -1.831843      27.72
 H      -1.433867    -3.071464    -2.648293      24.70
 C      -0.537469    -0.677607    -0.696094      10.28
 O      -1.911845    -0.847686    -0.579386      81.60
 C       0.089565     0.537567    -0.696542      70.16
 H      -0.319389     1.480968    -0.768652      31.71
 C       2.307588    -0.769321    -1.051561      45.47
 C       3.768852    -0.778532    -1.103455      95.81
 H       4.238778    -1.092347    -2.145657      25.72
 O       4.200130     0.707521    -1.224128     190.14
 H       5.197569     0.526264    -0.886752      25.28
 C       4.393212    -1.389749     0.175959      79.57
 H       3.747478    -2.082862     0.854595      29.66
 O       5.685349    -2.127752     0.236354     170.16
 H       6.131341    -1.738772    -0.637689      24.83
 C       4.546416    -0.421870     1.415240     129.16
 O       5.450553     0.623176     1.295647     173.98
 H       5.175749     1.310722     1.847805      25.43
 H       4.975468    -0.967383     2.298590      32.74
 H       3.529494     0.047716     1.883328      28.88
55
name = lig-Water-frame_456
 C      -1.538942     2.302506     2.104962      75.88
 H      -2.369005     2.988809     1.725915      26.90
 C      -0.589354     0.156732     2.645293      50.04
 H      -0.703794    -0.859985     2.568549      25.12
 C       0.509416     0.651357     3.332929      29.03
 O       1.459005    -0.122252     3.850976     178.54
 C       1.184080    -1.537041     4.092193     110.77
 H       2.058663    -1.850779     4.656061      29.28
 H       0.835152    -2.285382     3.325373      28.77
 H       0.459629    -1.555821     5.044194      27.16
 C       0.707732     2.164811     3.243353      27.45
 O       1.794022     2.685587     3.864073     194.24
 H       1.749832     3.693955     4.042497      29.70
 C      -0.295319     2.933556     2.664207      47.33
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 H      -0.340106     4.059337     2.364452      15.37
 C      -1.847078     0.919285     2.154132      27.89
 C      -2.985377     0.410293     1.369513      76.82
 H      -3.652936     1.408047     1.600430      24.06
 O      -3.579648    -0.816384     2.102178     192.82
 H      -4.527606    -0.778124     1.879041      27.26
 C      -2.820753     0.197287    -0.260398      83.84
 H      -2.551336     1.310358    -0.613194      24.10
 C      -4.084828    -0.000889    -0.968206     114.29
 O      -5.172592    -1.048084    -0.609600     220.15
 H      -4.728330    -1.926933    -0.594154      26.82
 H      -4.062016    -0.163786    -2.028084      28.70
 H      -4.557722     0.908312    -0.886879      30.37
 C       1.602153     0.471637    -0.799672      20.20
 H       1.933156     1.459921    -0.766945      30.37
 C       1.545073    -1.971232    -1.021524      37.06
 H       2.104858    -2.861363    -1.048499      25.87
 C       0.084126    -1.893318    -0.933030      40.16
 O      -0.570785    -3.072748    -1.029016     212.81
 C      -0.790254    -3.866035    -2.269505     102.36
 H       0.310498    -3.925591    -2.961529      23.31
 H      -1.328489    -4.821701    -1.778158      26.37
 H      -1.467639    -3.194955    -2.821541      25.62
 C      -0.522442    -0.690455    -0.798149      37.14
 O      -1.855736    -0.826267    -0.548898      52.66
 C       0.152411     0.503935    -0.731793      47.61
 H      -0.374072     1.532032    -0.846059      23.29
 C       2.254213    -0.754585    -0.987123      21.39
 C       3.829128    -0.758124    -1.131012     132.81
 H       4.177735    -1.141224    -2.083395      26.69
 O       4.226667     0.711046    -1.260921     246.03
 H       5.098432     0.635579    -0.978495      28.58
 C       4.376857    -1.410905     0.140795      80.71
 H       3.642877    -2.027374     0.702811      29.79
 O       5.699100    -2.125948     0.200729     163.22
 H       6.294800    -2.128515    -0.676983      20.97
 C       4.568386    -0.389413     1.415743     136.68
 O       5.468457     0.658396     1.314312     183.01
 H       5.079700     1.490302     1.961904      19.99
 H       4.812064    -1.104960     2.222023      32.56
 H       3.629634     0.053375     1.556828      30.12
55
name = lig-Water-frame_457
 C      -1.475822     2.286372     2.197499      48.81
 H      -2.204909     2.822881     1.647656      18.75
 C      -0.660440     0.151594     2.622539      31.46
 H      -0.675886    -1.010345     2.556073      23.66
 C       0.474208     0.792159     3.289378      24.00
 O       1.460241    -0.105238     3.838881     134.36
 C       1.158322    -1.622084     4.112143     104.08
 H       2.168975    -1.918933     4.519003      26.68
 H       0.684477    -1.926105     3.151395      28.51
 H       0.233828    -1.582481     4.750737      27.42
 C       0.718225     2.149841     3.224452      40.28
 O       1.781461     2.718760     3.828764     129.45
 H       1.463363     3.686830     3.899431      20.90
 C      -0.292436     2.914239     2.648501      27.28
 H      -0.136157     3.947305     2.665576      23.15
 C      -1.798458     0.926558     2.110447      20.46
 C      -3.009950     0.348583     1.434664      86.42
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 H      -3.639975     1.418979     1.404862      25.89
 O      -3.538595    -0.800116     2.032879     220.64
 H      -4.530353    -0.770652     1.934983      25.20
 C      -2.826516     0.174789    -0.260787      81.61
 H      -2.687542     1.101436    -0.715797      25.22
 C      -4.201177     0.019207    -0.981621      79.79
 O      -5.096663    -1.009178    -0.634679     271.71
 H      -4.804023    -1.957097    -0.736052      26.54
 H      -4.026759    -0.137222    -2.200605      24.41
 H      -4.662322     1.151961    -0.858297      25.42
 C       1.513143     0.518193    -0.852511      60.23
 H       2.023580     1.537165    -0.996571      24.53
 C       1.501335    -1.908854    -1.019550      62.95
 H       1.980285    -2.966873    -1.021554      23.92
 C       0.121773    -1.937720    -0.898435      19.94
 O      -0.552968    -3.123782    -1.010634     253.14
 C      -0.784841    -3.758111    -2.272507     134.73
 H       0.086917    -4.173519    -2.555537      28.88
 H      -1.133481    -4.725523    -2.109877      30.07
 H      -1.608358    -3.612044    -3.164951      24.54
 C      -0.551832    -0.676256    -0.876690       8.63
 O      -1.840247    -0.819101    -0.524230      95.08
 C       0.255946     0.498502    -0.786554      70.86
 H      -0.409821     1.400694    -0.712599      23.82
 C       2.241324    -0.728231    -0.926592       9.03
 C       3.859594    -0.702891    -1.151171      99.28
 H       4.121518    -1.446773    -2.059159      24.77
 O       4.245057     0.690636    -1.300068     212.68
 H       5.242634     0.948779    -1.124337      23.18
 C       4.422070    -1.402764     0.177752      70.12
 H       3.480599    -2.188108     0.210330      24.38
 O       5.708733    -2.134406     0.144935     206.80
 H       6.224193    -2.292457    -0.624502      25.69
 C       4.532266    -0.394810     1.397341     135.19
 O       5.501260     0.721084     1.345217     160.29
 H       5.346196     1.554919     1.802539      21.46
 H       4.576201    -1.164023     2.220501      30.95
 H       3.401735     0.028787     1.313918      27.00
55
name = lig-Water-frame_458
 C      -1.452004     2.300007     2.249386      79.80
 H      -2.111955     3.011083     1.614261      19.40
 C      -0.742285     0.143281     2.616602      69.41
 H      -0.691918    -0.902421     2.587462      27.62
 C       0.416768     0.806322     3.218781      12.32
 O       1.472134    -0.082409     3.836012      76.09
 C       1.106952    -1.625967     4.101094     111.04
 H       2.035393    -2.147259     4.304031      28.45
 H       0.915532    -1.849038     3.041811      27.89
 H       0.168621    -1.726390     4.739041      27.08
 C       0.709619     2.130227     3.213617      18.02
 O       1.784148     2.762496     3.798079     101.21
 H       1.488547     3.697906     4.019768      21.50
 C      -0.311928     2.887430     2.625381      85.83
 H      -0.046165     3.993921     2.899378      26.11
 C      -1.652047     0.899846     2.098262      38.55
 C      -3.021269     0.356429     1.432234      98.02
 H      -3.917021     1.064477     1.238363      25.68
 O      -3.511248    -0.788006     1.980218     233.90
 H      -4.522838    -0.827873     1.956368      26.12
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 C      -2.854644     0.169583    -0.213648      78.72
 H      -2.390026     1.158494    -0.758492      23.95
 C      -4.293152     0.046575    -1.037924     111.64
 O      -5.064213    -0.978859    -0.637672     301.29
 H      -4.554254    -1.851658    -0.923498      25.30
 H      -3.932494     0.022728    -2.033045      29.91
 H      -4.821290     0.885049    -0.836504      29.72
 C       1.590782     0.564864    -0.931387      52.36
 H       2.201867     1.410308    -1.077876      26.77
 C       1.495987    -1.875595    -1.002109      64.62
 H       1.896953    -2.920653    -1.092913      25.19
 C       0.167445    -1.942171    -0.911046       8.91
 O      -0.576828    -3.191541    -0.971696     194.91
 C      -0.793558    -3.711119    -2.306304     114.03
 H       0.337503    -4.210587    -2.607549      23.02
 H      -1.207892    -4.830905    -2.092419      25.40
 H      -1.422396    -3.492069    -3.102666      26.34
 C      -0.552008    -0.682644    -0.912782       7.37
 O      -1.869662    -0.830774    -0.511933     108.94
 C       0.157477     0.501653    -0.837753      67.48
 H      -0.339638     1.418430    -0.602776      24.47
 C       2.277867    -0.664815    -0.900784      -5.86
 C       3.876428    -0.664366    -1.146166     100.14
 H       4.032243    -1.465486    -1.861315      25.99
 O       4.263478     0.671091    -1.357485     234.32
 H       5.260968     0.989959    -1.326080      23.40
 C       4.488575    -1.385134     0.171863     102.18
 H       3.776121    -2.176004     0.168173      25.44
 O       5.696915    -2.151266     0.129675     182.22
 H       6.116343    -2.160897    -0.921671      20.18
 C       4.411726    -0.403175     1.359812     140.46
 O       5.547038     0.727512     1.354928      69.82
 H       5.244999     1.640819     1.951367      17.25
 H       4.515391    -0.855536     2.360928      31.86
 H       3.490042    -0.001057     1.363132      27.52
55
name = lig-Water-frame_459
 C      -1.503498     2.350912     2.207182      55.30
 H      -2.141855     3.074965     1.829435      19.88
 C      -0.712240     0.097138     2.670946      72.99
 H      -0.822979    -1.004473     2.617690      27.53
 C       0.408926     0.681597     3.175561      17.01
 O       1.469247    -0.067868     3.847271      87.40
 C       1.058733    -1.558355     4.020748     118.19
 H       1.885247    -2.271572     4.352748      27.53
 H       1.012674    -2.045975     3.023518      28.41
 H       0.275476    -1.926791     4.827716      26.33
 C       0.694345     2.132336     3.207937      -6.11
 O       1.797112     2.786697     3.771879     133.80
 H       1.650657     3.742355     4.175046      23.17
 C      -0.282999     2.912120     2.655060      58.83
 H      -0.324020     3.960661     2.757030      30.02
 C      -1.637427     0.934037     2.042439      27.14
 C      -3.006900     0.408469     1.342065      93.04
 H      -4.063292     1.130779     1.417191      23.44
 O      -3.495350    -0.819487     1.968729     239.39
 H      -4.453868    -0.843482     1.899117      27.25
 C      -2.865312     0.235447    -0.178263      93.96
 H      -2.336439     1.057591    -0.446077      27.46
 C      -4.288478     0.099486    -1.056072      79.69
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 O      -5.064879    -1.013342    -0.643618     260.70
 H      -4.477172    -1.744015    -0.823403      27.78
 H      -3.841192     0.144147    -2.221575      24.36
 H      -5.065579     1.005898    -0.821582      24.57
 C       1.675993     0.571781    -1.012381      21.17
 H       2.303389     1.514470    -1.041554      27.72
 C       1.563228    -1.868603    -0.976456      42.31
 H       2.080905    -2.822275    -1.141362      27.33
 C       0.142358    -1.922733    -0.954347      10.45
 O      -0.608396    -3.227517    -0.930765     111.00
 C      -0.732607    -3.808581    -2.326919      97.40
 H       0.174438    -3.767782    -2.854152      25.43
 H      -1.329077    -4.582333    -2.037282      26.65
 H      -1.307229    -2.838378    -2.989944      23.66
 C      -0.568154    -0.706973    -0.895009      11.13
 O      -1.922185    -0.878488    -0.515200      86.46
 C       0.055893     0.536002    -0.897328      38.18
 H      -0.354158     1.581899    -0.525453      22.41
 C       2.339141    -0.602872    -0.918407      14.25
 C       3.875230    -0.660359    -1.081145     109.34
 H       4.100185    -1.359189    -2.032890      25.56
 O       4.288759     0.672742    -1.440871     256.00
 H       5.204673     0.669910    -1.354899      28.02
 C       4.538327    -1.341716     0.151284     100.45
 H       3.776605    -2.258901     0.538279      25.15
 O       5.700993    -2.168278     0.097051     220.63
 H       6.095100    -1.878072    -0.691697      27.82
 C       4.334609    -0.393082     1.348857     108.77
 O       5.560199     0.712607     1.372701     127.12
 H       5.115494     1.295145     1.957172      26.05
 H       4.538081    -0.624035     2.419519      29.69
 H       3.289094     0.245417     1.383513      26.15
55
name = lig-Water-frame_460
 C      -1.540418     2.383210     2.129889      33.92
 H      -2.431758     3.108251     1.940970      20.05
 C      -0.681766     0.027680     2.703056      34.90
 H      -0.999843    -1.040297     2.682853      26.37
 C       0.496155     0.583344     3.188737      14.97
 O       1.441754    -0.098162     3.868248     185.42
 C       1.063779    -1.518114     3.935840     127.42
 H       1.895175    -1.936162     4.507938      27.03
 H       0.789192    -2.097780     3.028461      26.00
 H       0.274292    -1.722280     4.667755      27.38
 C       0.683132     2.132065     3.213650     -19.09
 O       1.826917     2.767779     3.754294     137.76
 H       1.579561     3.702796     4.052472      27.13
 C      -0.307898     2.949667     2.686662      16.53
 H      -0.417022     4.075619     2.603507      23.15
 C      -1.723249     1.009887     1.975409     -18.72
 C      -3.021659     0.458922     1.265083     114.06
 H      -3.596381     1.281062     1.725604      23.61
 O      -3.465930    -0.859413     1.974274     215.07
 H      -4.465357    -0.850194     1.815217      24.48
 C      -2.886535     0.306024    -0.166834      76.30
 H      -2.309438     1.359463    -0.386246      20.73
 C      -4.236876     0.193231    -1.049899      99.71
 O      -5.068849    -1.055417    -0.662760     218.81
 H      -4.488779    -1.987400    -0.582277      20.35
 H      -4.047990     0.050885    -2.023684      28.51
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 H      -4.828479     1.016436    -0.961196      28.86
 C       1.648240     0.600147    -1.076463      22.68
 H       2.116204     1.593252    -0.949945      25.67
 C       1.622865    -1.856629    -0.953737      29.63
 H       2.362664    -2.768769    -1.116671      21.37
 C       0.145413    -1.938852    -1.000396      -8.12
 O      -0.606397    -3.224153    -0.902698     116.84
 C      -0.702202    -3.790141    -2.340264     104.67
 H       0.251252    -3.741144    -3.052815      24.93
 H      -1.555860    -4.661794    -2.292320      24.06
 H      -1.140466    -2.898249    -2.564102      26.26
 C      -0.632821    -0.697814    -0.837187     -22.74
 O      -1.987141    -0.938544    -0.527695      69.30
 C       0.078944     0.599178    -0.954206      42.36
 H      -0.418851     1.437878    -0.674504      22.39
 C       2.386132    -0.607395    -0.966709      19.47
 C       3.866519    -0.700350    -1.057539     103.73
 H       4.138359    -1.129974    -2.003982      24.65
 O       4.329461     0.675572    -1.512706     220.45
 H       5.355847     0.497600    -1.302991      24.45
 C       4.498638    -1.332908     0.206358      96.49
 H       3.746931    -1.971461     0.611225      27.80
 O       5.700667    -2.166420     0.080514     172.46
 H       6.530371    -1.742863    -0.660413      20.32
 C       4.312731    -0.307276     1.369033     119.95
 O       5.534789     0.647174     1.379820     153.04
 H       5.182846     1.412874     2.041740      21.16
 H       4.419514    -0.866131     2.313374      28.51
 H       3.459633     0.217145     1.220333      25.88
55
name = lig-Water-frame_461
 C      -1.566137     2.410337     2.061462      27.94
 H      -2.417955     3.004125     1.864909      26.13
 C      -0.718808     0.031641     2.666409       6.65
 H      -1.030183    -0.980371     2.747233      26.90
 C       0.558187     0.591467     3.203313       3.27
 O       1.424172    -0.157202     3.888082     173.85
 C       1.099904    -1.511923     3.905058     121.29
 H       2.005922    -1.744608     4.506048      27.51
 H       0.753465    -1.955640     2.960583      28.55
 H       0.049665    -1.324563     4.500041      25.99
 C       0.674144     2.122611     3.214681       4.74
 O       1.849591     2.710745     3.736206      93.76
 H       1.514840     3.659345     3.866670      29.63
 C      -0.399067     2.975036     2.692787      42.89
 H      -0.139527     4.064050     2.628721      18.41
 C      -1.759237     1.020569     1.960275      -5.04
 C      -3.005374     0.469581     1.311172      90.58
 H      -3.637152     1.460715     1.662483      23.70
 O      -3.436764    -0.866334     1.967411     186.27
 H      -4.428175    -0.901721     1.797502      23.93
 C      -2.905696     0.394063    -0.231625      83.48
 H      -2.492434     1.248349    -0.578349      26.89
 C      -4.155959     0.212411    -0.991277      77.43
 O      -5.063824    -1.080798    -0.675305     164.30
 H      -4.545553    -1.872759    -0.523120      24.93
 H      -4.059386    -0.116451    -2.203452      23.28
 H      -4.780752     1.238073    -0.938583      25.42
 C       1.527914     0.625325    -1.104068      55.66
 H       1.938467     1.616089    -0.974127      25.99
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 C       1.659423    -1.847630    -0.953394      41.59
 H       2.244524    -2.697949    -0.987948      24.23
 C       0.183961    -1.950706    -1.011107     -31.01
 O      -0.556124    -3.209763    -0.883191     135.57
 C      -0.699985    -3.741224    -2.339763      92.39
 H       0.222838    -4.116512    -2.831544      25.97
 H      -1.287808    -4.537560    -2.623898      28.06
 H      -1.432876    -2.790204    -2.740346      24.37
 C      -0.660247    -0.682688    -0.786196     -45.00
 O      -2.049155    -0.953857    -0.541841      17.40
 C       0.169464     0.582180    -1.003219      53.10
 H      -0.521335     1.561421    -0.894356      24.18
 C       2.352361    -0.627500    -1.031474      32.73
 C       3.871887    -0.713155    -1.085387      89.22
 H       4.167390    -1.399602    -1.973425      24.78
 O       4.406156     0.659301    -1.539051     238.97
 H       5.395450     0.752268    -1.341307      27.57
 C       4.454530    -1.309168     0.263393      58.69
 H       3.520343    -2.071738     0.552729      27.13
 O       5.703825    -2.135611     0.069060     212.58
 H       6.414615    -1.912627    -0.450526      30.59
 C       4.393774    -0.225410     1.394707     133.65
 O       5.473055     0.578937     1.412349     212.98
 H       5.512549     1.489129     1.818612      22.78
 H       4.160776    -1.034021     2.195016      27.95
 H       3.360565     0.332930     1.115746      26.21
55
name = lig-Water-frame_462
 C      -1.567074     2.418465     2.020245      50.71
 H      -2.371608     3.098736     1.602046      28.83
 C      -0.761424     0.142665     2.596063      55.48
 H      -0.995120    -0.969919     2.743454      26.82
 C       0.507302     0.678012     3.182222      15.23
 O       1.447579    -0.166389     3.887499     160.17
 C       1.094065    -1.507976     3.935044     128.66
 H       1.893807    -2.134635     4.416602      29.38
 H       1.045215    -1.876524     2.863477      30.14
 H       0.134827    -1.515097     4.412359      28.24
 C       0.647484     2.088396     3.197456      21.90
 O       1.841007     2.639172     3.709288     117.33
 H       1.726612     3.656475     3.858259      27.90
 C      -0.449494     2.957686     2.693233      49.98
 H      -0.041172     3.956178     2.713687      13.24
 C      -1.708371     0.967046     2.009587      52.36
 C      -3.002055     0.485918     1.409727      82.53
 H      -3.938069     1.115218     1.253657      25.92
 O      -3.407948    -0.830325     1.943859     211.82
 H      -4.362743    -0.931306     1.825575      26.71
 C      -2.910675     0.402940    -0.283200      58.33
 H      -2.396561     1.316853    -0.905090      24.79
 C      -4.145021     0.167035    -0.994426     114.29
 O      -5.061449    -1.041734    -0.672282     191.69
 H      -4.368657    -1.866767    -0.660853      22.11
 H      -3.862538     0.103672    -1.930246      30.62
 H      -4.722265     1.026001    -0.850952      29.23
 C       1.464100     0.605817    -1.110257      54.27
 H       1.941566     1.647634    -1.145391      25.22
 C       1.629535    -1.834121    -0.976572      17.22
 H       2.123210    -2.939622    -0.838489      21.62
 C       0.202384    -1.907928    -0.966071     -20.23
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 O      -0.483399    -3.199947    -0.895277     151.66
 C      -0.731603    -3.640058    -2.343511     104.71
 H       0.319477    -4.065495    -2.607906      24.84
 H      -1.336331    -4.696454    -2.485409      25.43
 H      -1.196966    -3.045775    -3.048985      29.09
 C      -0.611540    -0.719732    -0.774692     -23.84
 O      -2.074971    -0.902760    -0.563101      30.56
 C       0.126599     0.531794    -1.020037      72.71
 H      -0.261292     1.469871    -1.181683      29.77
 C       2.275993    -0.601593    -1.103693      16.76
 C       3.909651    -0.703880    -1.157305      77.06
 H       4.146363    -1.653460    -1.703164      23.12
 O       4.484714     0.627513    -1.536633     290.63
 H       5.370366     0.819581    -1.343557      30.73
 C       4.408900    -1.291370     0.264661      79.96
 H       3.761249    -2.065845     0.470171      27.27
 O       5.640886    -2.116005     0.129837     148.44
 H       6.345211    -1.695620    -0.768158      20.87
 C       4.383526    -0.208326     1.403243     156.91
 O       5.482548     0.533520     1.446877     241.45
 H       5.405475     1.456264     1.717725      26.64
 H       4.101742    -0.701709     2.342425      30.72
 H       3.517834     0.366301     1.234324      28.42
55
name = lig-Water-frame_463
 C      -1.551291     2.417738     2.003543      69.82
 H      -2.154511     3.089145     1.347164      25.18
 C      -0.745038     0.235782     2.564805      88.55
 H      -0.911882    -0.778713     2.614030      26.76
 C       0.405726     0.740690     3.159643      23.47
 O       1.479910    -0.112329     3.874414      98.42
 C       1.091475    -1.547776     3.938712     126.54
 H       1.690787    -2.350860     4.400968      29.54
 H       1.245724    -1.886633     2.920392      30.60
 H       0.075056    -2.041392     4.439568      26.16
 C       0.610208     2.074269     3.177844      26.66
 O       1.820441     2.569150     3.678531     189.75
 H       1.834750     3.489993     3.951317      31.14
 C      -0.438967     2.900510     2.687109      67.22
 H      -0.237442     4.050558     2.754447      16.36
 C      -1.698169     0.979234     2.055624      46.77
 C      -3.028342     0.468800     1.427415      80.45
 H      -4.057756     1.000922     1.386008      26.10
 O      -3.370429    -0.782500     1.921532     216.21
 H      -4.377011    -0.885840     1.828055      26.41
 C      -2.828666     0.360660    -0.289752      84.79
 H      -2.406879     1.137515    -0.811164      28.79
 C      -4.202755     0.089046    -0.996933      92.80
 O      -5.011744    -0.984363    -0.663484     233.54
 H      -4.493960    -1.817676    -0.902635      25.75
 H      -3.710063     0.266016    -2.180396      25.47
 H      -4.921127     0.986918    -0.800448      26.49
 C       1.495258     0.562556    -1.122226      38.76
 H       1.938542     1.481042    -1.346732      23.79
 C       1.567794    -1.858663    -1.004345      30.86
 H       1.980976    -2.747671    -0.846837      25.47
 C       0.188188    -1.862319    -0.882540      24.67
 O      -0.423807    -3.168318    -0.937426     191.51
 C      -0.736070    -3.633126    -2.326883     105.52
 H       0.373918    -3.769570    -2.576119      24.58
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 H      -1.312176    -4.421266    -1.956798      26.54
 H      -0.974215    -2.983172    -3.297796      25.04
 C      -0.575956    -0.756333    -0.792771      27.17
 O      -2.045125    -0.819270    -0.597616     123.78
 C       0.005370     0.461155    -1.022591      53.92
 H      -0.406624     1.510160    -1.300936      25.39
 C       2.252247    -0.567432    -1.167942      -5.01
 C       3.925654    -0.695165    -1.180976      85.35
 H       4.203618    -1.575978    -1.817838      23.03
 O       4.532158     0.574042    -1.537413     236.92
 H       5.575138     0.617865    -1.204273      25.59
 C       4.386734    -1.254449     0.239008      80.78
 H       3.650924    -2.214580     0.551613      23.46
 O       5.596505    -2.060448     0.165197     250.55
 H       5.959637    -1.765161    -0.570819      31.37
 C       4.283571    -0.253044     1.412512     112.87
 O       5.576811     0.530729     1.476055     221.14
 H       5.121608     1.422917     1.774437      24.76
 H       4.195286    -0.479524     2.537540      27.71
 H       3.413538     0.543874     1.228898      26.11
55
name = lig-Water-frame_464
 C      -1.516439     2.402845     1.992168      59.75
 H      -2.039589     3.029707     1.308745      22.94
 C      -0.697654     0.242330     2.573525      41.81
 H      -0.853580    -0.887238     2.493919      24.22
 C       0.364806     0.731321     3.178982      26.59
 O       1.468819    -0.058013     3.862674      69.49
 C       1.081506    -1.637935     3.919004     104.52
 H       1.889899    -2.073043     4.619058      28.29
 H       1.172402    -1.980290     2.852871      28.79
 H       0.139167    -1.955316     4.227936      28.64
 C       0.587889     2.122818     3.175811      29.24
 O       1.808263     2.492985     3.651578      65.33
 H       1.638926     3.454529     4.059127      27.28
 C      -0.404202     2.899881     2.667176      31.15
 H      -0.460509     3.921412     2.736903      22.01
 C      -1.802228     1.090004     2.039664      15.38
 C      -3.044395     0.460641     1.356998      93.98
 H      -3.792365     1.268790     1.809480      26.30
 O      -3.344424    -0.774392     1.920818     223.16
 H      -4.321791    -0.846430     1.808063      25.35
 C      -2.772530     0.278825    -0.242042      88.96
 H      -2.354895     1.328035    -0.647190      22.69
 C      -4.226488     0.102879    -1.047921     114.09
 O      -4.955716    -0.965059    -0.664578     286.73
 H      -4.636320    -1.857158    -0.925460      26.56
 H      -4.099637     0.095458    -2.029799      31.01
 H      -4.885290     0.945305    -0.842561      28.86
 C       1.472462     0.525984    -1.149936      33.21
 H       1.958700     1.523300    -1.499032      22.35
 C       1.518364    -1.820323    -1.035666      33.29
 H       2.139865    -2.865575    -0.942990      21.88
 C       0.177054    -1.899374    -0.803867      43.97
 O      -0.390112    -3.098723    -0.963963     259.19
 C      -0.665882    -3.632467    -2.293514     112.67
 H       0.326219    -3.931897    -2.784160      26.69
 H      -1.429290    -4.408431    -1.870839      26.60
 H      -1.194127    -2.867470    -2.839810      26.70
 C      -0.645095    -0.720266    -0.809440      19.52
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 O      -1.971891    -0.768012    -0.640430     203.17
 C      -0.022535     0.461006    -1.043010      61.14
 H      -0.780619     1.262404    -1.137792      22.17
 C       2.296922    -0.612446    -1.201151      10.74
 C       3.896536    -0.700155    -1.167392      92.61
 H       4.227213    -1.283123    -2.104629      22.90
 O       4.591038     0.514210    -1.528651     274.76
 H       5.468194     0.341715    -1.197656      28.42
 C       4.311923    -1.277113     0.246358      97.72
 H       3.531889    -1.893508     0.485662      27.77
 O       5.537859    -1.993765     0.224041     169.73
 H       6.178147    -1.775523    -0.717532      23.15
 C       4.193797    -0.257971     1.425459     102.26
 O       5.646350     0.553099     1.499951     159.57
 H       5.286058     1.404475     1.852016      27.24
 H       4.125023    -0.723829     2.417660      28.71
 H       3.452861     0.490140     1.171145      28.03
55
name = lig-Water-frame_465
 C      -1.494516     2.412478     1.971909      78.10
 H      -2.150137     3.172493     1.378487      23.90
 C      -0.755686     0.188798     2.554440      12.02
 H      -0.817794    -0.872040     2.416708      25.89
 C       0.415966     0.700229     3.242197       8.28
 O       1.401490    -0.036038     3.839353     101.43
 C       1.135174    -1.691306     3.885502      90.44
 H       1.912619    -1.662560     4.610811      27.21
 H       1.191876    -2.108321     2.883946      27.56
 H      -0.069391    -1.602735     4.194465      21.40
 C       0.581603     2.138107     3.186468      48.28
 O       1.805796     2.467831     3.657200     181.46
 H       1.601946     3.333641     4.046801      28.93
 C      -0.376740     2.951796     2.631025      15.69
 H      -0.411617     4.130062     2.741301      18.64
 C      -1.863566     1.108822     2.015862      29.04
 C      -3.011301     0.498202     1.286819      97.09
 H      -3.645261     1.367421     1.635221      25.31
 O      -3.338633    -0.798575     1.942754     206.90
 H      -4.300606    -0.908222     1.773059      24.71
 C      -2.804424     0.284246    -0.213874      99.40
 H      -2.467939     1.287651    -0.341702      24.56
 C      -4.187806     0.169075    -1.073503      80.61
 O      -4.946397    -0.997498    -0.644754     203.40
 H      -4.517788    -1.966300    -0.880615      22.47
 H      -4.248093    -0.021815    -2.347220      23.60
 H      -4.766788     1.106615    -0.824829      26.89
 C       1.422021     0.533832    -1.210705      47.32
 H       1.831248     1.468013    -1.418700      26.67
 C       1.561515    -1.802382    -1.052714      51.23
 H       2.049019    -2.696298    -1.193148      25.06
 C       0.164739    -1.898514    -0.762599      38.16
 O      -0.386451    -3.079281    -0.952165     262.85
 C      -0.607841    -3.635236    -2.221870     121.08
 H       0.029347    -4.198179    -3.031386      26.66
 H      -1.364932    -4.449444    -2.298170      29.27
 H      -1.417958    -2.798110    -2.525545      25.24
 C      -0.666059    -0.684746    -0.817827      16.22
 O      -1.931982    -0.773654    -0.675889     182.06
 C       0.025834     0.498437    -1.067407      70.43
 H      -0.754642     1.264081    -1.007876      23.22
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 C       2.327015    -0.665302    -1.197509      22.21
 C       3.837668    -0.712887    -1.178537     113.74
 H       4.087782    -1.339747    -2.017318      25.66
 O       4.635529     0.468944    -1.507444     258.06
 H       5.542447     0.307125    -1.194018      28.39
 C       4.236470    -1.280266     0.238732      67.80
 H       3.213942    -1.954212     0.466533      25.04
 O       5.499688    -1.929377     0.261615     211.06
 H       6.256903    -1.857535    -0.368707      27.18
 C       4.190433    -0.241376     1.412626      92.92
 O       5.661683     0.561597     1.526798      74.75
 H       5.601793     1.473083     1.907970      26.30
 H       3.965641    -0.967183     2.264308      28.15
 H       3.360514     0.507842     1.211670      29.07
55
name = lig-Water-frame_466
 C      -1.510817     2.483951     1.943493     121.41
 H      -2.218714     3.175861     1.632639      35.47
 C      -0.830925     0.167106     2.546186      44.82
 H      -0.922849    -0.920548     2.362315      26.42
 C       0.395913     0.676749     3.250289      24.43
 O       1.332180    -0.053071     3.807284     128.61
 C       1.144708    -1.632778     3.858737     105.98
 H       1.930028    -1.759758     4.691722      28.53
 H       1.388339    -2.253759     2.948852      27.99
 H       0.246911    -1.569523     4.244251      28.40
 C       0.575006     2.085288     3.195660      27.07
 O       1.822896     2.490821     3.694675     218.53
 H       1.816009     3.447952     4.054684      20.67
 C      -0.361115     3.048606     2.590147      10.44
 H      -0.115140     4.049295     2.680761      14.83
 C      -1.798601     1.028311     2.009099      51.12
 C      -2.980229     0.506994     1.261263      73.26
 H      -3.947770     1.245160     1.041255      22.56
 O      -3.348652    -0.811467     1.974203     166.93
 H      -4.325483    -0.980500     1.698594      24.94
 C      -2.888542     0.333082    -0.236614      76.54
 H      -2.401044     1.386266    -0.484309      21.90
 C      -4.137432     0.205085    -1.112425     100.87
 O      -4.950532    -1.042607    -0.618636     238.84
 H      -4.351947    -1.753192    -0.768415      28.38
 H      -3.976415     0.183822    -2.102481      30.69
 H      -4.679050     1.149901    -0.832208      28.05
 C       1.418381     0.537902    -1.272959      48.78
 H       1.845755     1.606380    -1.321646      26.00
 C       1.598394    -1.808751    -1.060365      42.72
 H       2.050276    -2.850296    -1.406423      21.57
 C       0.192219    -1.812383    -0.777413      23.17
 O      -0.397145    -3.151833    -0.885997     218.22
 C      -0.651522    -3.633094    -2.222782     120.53
 H       0.111235    -3.924029    -2.950255      28.68
 H      -1.323250    -4.547564    -2.211180      28.85
 H      -1.293481    -2.896555    -2.738703      28.90
 C      -0.561125    -0.684473    -0.822604      20.36
 O      -1.976948    -0.803997    -0.691705     107.74
 C       0.070214     0.533854    -1.080161      60.72
 H      -0.339724     1.643223    -0.994127      22.26
 C       2.281750    -0.612223    -1.180870      22.48
 C       3.798132    -0.736888    -1.196324     100.36
 H       3.997400    -1.746213    -1.803478      26.15
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 O       4.653646     0.437706    -1.487253     202.47
 H       5.671320     0.383168    -1.126733      24.30
 C       4.152707    -1.260915     0.205227      83.45
 H       3.526274    -2.025302     0.469443      28.86
 O       5.459706    -1.900561     0.333203     180.82
 H       6.154364    -1.686853    -0.349078      26.83
 C       4.230586    -0.204618     1.383074     113.40
 O       5.634356     0.533418     1.550002      91.09
 H       5.632148     1.474889     1.998592      24.71
 H       3.996613    -0.867220     2.261909      29.90
 H       3.352904     0.540444     1.418460      28.82
55
name = lig-Water-frame_467
 C      -1.516931     2.538278     1.956064     101.11
 H      -2.472634     3.196917     1.757393      30.87
 C      -0.859231     0.148723     2.566527      72.06
 H      -1.082713    -0.934554     2.411008      26.27
 C       0.267097     0.679732     3.181654      25.78
 O       1.306267    -0.121174     3.782324     147.88
 C       1.203792    -1.514561     3.862744     133.52
 H       1.810529    -2.034000     4.605288      28.77
 H       1.475996    -2.165303     3.024673      28.79
 H       0.084399    -1.908673     4.407085      26.11
 C       0.565571     2.062183     3.196959      15.37
 O       1.851710     2.532835     3.749734     122.08
 H       1.857805     3.546505     3.945832      26.52
 C      -0.334749     3.059081     2.555237      65.83
 H       0.132812     4.132394     2.560744      16.25
 C      -1.701931     1.016716     1.981424      50.77
 C      -3.014767     0.473569     1.239071      92.28
 H      -3.975784     1.052658     1.104842      22.54
 O      -3.376642    -0.799510     1.994577     215.49
 H      -4.272394    -0.976229     1.664452      26.25
 C      -2.895146     0.393756    -0.307788      86.29
 H      -2.391550     1.220447    -0.817976      23.14
 C      -4.117014     0.215982    -1.067134      81.10
 O      -4.942021    -1.034202    -0.617609     165.48
 H      -4.211912    -1.818263    -0.690466      22.57
 H      -3.633651     0.306185    -2.266511      23.88
 H      -4.794195     1.061690    -0.932111      26.49
 C       1.497173     0.584582    -1.314648      71.43
 H       1.967500     1.545071    -1.291604      28.06
 C       1.604207    -1.845320    -1.072293      56.50
 H       2.023581    -2.793757    -1.405501      23.86
 C       0.263567    -1.810193    -0.842652       5.64
 O      -0.403669    -3.216714    -0.799414     110.48
 C      -0.732640    -3.642385    -2.270826      78.53
 H       0.437730    -3.475327    -2.592203      23.39
 H      -1.196068    -4.602162    -1.865247      24.09
 H      -1.267075    -2.901200    -3.001285      25.27
 C      -0.533755    -0.645150    -0.814803       1.94
 O      -2.019786    -0.837475    -0.701899      59.79
 C       0.102252     0.607947    -1.081943      54.77
 H      -0.096790     1.605189    -1.013331      23.10
 C       2.227749    -0.523040    -1.180467      18.37
 C       3.794087    -0.796289    -1.197985      91.96
 H       4.010704    -1.693248    -1.698156      28.85
 O       4.655175     0.402137    -1.483282     244.64
 H       5.465046     0.371194    -1.038515      31.24
 C       4.131127    -1.199683     0.204484      80.79
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 H       3.575977    -2.210013     0.578901      24.90
 O       5.438706    -1.896502     0.400154     130.13
 H       5.940844    -1.388587    -0.466878      24.94
 C       4.265231    -0.143990     1.380448     121.70
 O       5.584909     0.482839     1.560152     208.12
 H       5.285246     1.237775     2.065538      31.30
 H       4.236636    -0.653814     2.372988      28.30
 H       3.506012     0.618206     1.470297      28.19
55
name = lig-Water-frame_468
 C      -1.529337     2.545172     1.999297      44.67
 H      -2.392662     3.066597     1.763322      18.21
 C      -0.878993     0.105337     2.581820      73.45
 H      -1.125792    -0.917435     2.593154      29.51
 C       0.200014     0.679669     3.139838      10.27
 O       1.289395    -0.167464     3.762369     134.55
 C       1.198955    -1.477704     3.913474     157.81
 H       1.930703    -1.948055     4.644754      28.74
 H       1.390269    -1.889242     2.858390      27.24
 H       0.365021    -1.988861     4.105189      29.74
 C       0.568070     2.102751     3.184043      -1.97
 O       1.859708     2.564082     3.794227      90.42
 H       1.623113     3.515079     3.895226      27.49
 C      -0.279138     3.017836     2.536186      58.75
 H       0.038880     4.035115     2.409405      28.29
 C      -1.698363     1.115816     1.902510      18.47
 C      -3.038945     0.434198     1.231718      95.82
 H      -3.888422     1.173301     1.758281      21.95
 O      -3.399180    -0.770682     1.989339     192.91
 H      -4.348059    -0.972569     1.714876      23.09
 C      -2.818611     0.400766    -0.366127      87.90
 H      -2.352055     1.266818    -0.911707      23.69
 C      -4.137090     0.197792    -1.065549     107.19
 O      -4.887539    -0.992645    -0.651944     220.20
 H      -4.477085    -1.898627    -0.651090      24.86
 H      -3.784882     0.146909    -2.023924      30.29
 H      -4.969718     0.981182    -1.069487      25.82
 C       1.579329     0.677620    -1.321492      79.74
 H       2.192850     1.602672    -1.394904      29.06
 C       1.609495    -1.828815    -1.094240      61.81
 H       2.169496    -2.788496    -1.275129      24.53
 C       0.270291    -1.896128    -0.904906     -17.75
 O      -0.418671    -3.197346    -0.739923     137.17
 C      -0.730879    -3.633935    -2.267690      95.03
 H       0.227367    -3.571120    -2.471771      29.21
 H      -1.029621    -4.623164    -2.071677      27.59
 H      -1.484170    -3.025280    -2.918191      25.92
 C      -0.586630    -0.573961    -0.812735     -30.27
 O      -2.017692    -0.859145    -0.709176     103.16
 C       0.145582     0.646638    -1.081099      51.29
 H      -0.420871     1.736645    -0.953928      21.46
 C       2.256789    -0.546626    -1.204150      26.18
 C       3.788913    -0.809076    -1.160458      91.68
 H       4.112610    -1.609918    -2.005717      25.12
 O       4.623007     0.357193    -1.505662     235.20
 H       5.398109     0.341319    -0.863157      30.51
 C       4.135611    -1.190513     0.313898      96.81
 H       3.361738    -1.823589     0.572081      29.04
 O       5.439850    -1.871162     0.409231     202.98
 H       5.995972    -1.556809    -0.220293      32.41
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 C       4.269266    -0.109071     1.407540     111.98
 O       5.542132     0.447583     1.546154     198.47
 H       5.169996     1.113308     2.211288      27.36
 H       4.225000    -0.665250     2.419700      27.08
 H       3.508160     0.814039     1.330590      26.94
55
name = lig-Water-frame_469
 C      -1.517719     2.485174     2.044236      66.78
 H      -2.316103     3.224725     1.620823      18.30
 C      -0.927926     0.125149     2.554118      54.79
 H      -1.166755    -0.992562     2.748425      28.16
 C       0.256920     0.670993     3.166531       9.30
 O       1.256838    -0.103494     3.759780      98.89
 C       1.223092    -1.554167     3.907184     147.18
 H       2.070005    -1.633655     4.592220      28.75
 H       1.431100    -1.787413     2.863617      27.96
 H       0.047117    -2.027799     4.043252      26.10
 C       0.601927     2.127559     3.168413      -0.06
 O       1.818666     2.576951     3.810420     127.19
 H       1.507539     3.565877     4.075433      21.10
 C      -0.244203     2.964781     2.516361      67.76
 H      -0.087408     4.060029     2.370996      30.71
 C      -1.754140     1.165272     1.838000      34.21
 C      -3.032599     0.480431     1.289442     103.26
 H      -3.661127     1.251312     1.740966      27.68
 O      -3.410572    -0.751222     1.959541     205.89
 H      -4.414826    -0.888833     1.844628      23.73
 C      -2.770891     0.369294    -0.380074      84.61
 H      -2.309618     1.378549    -0.686570      24.18
 C      -4.183298     0.154871    -1.076398      99.34
 O      -4.854904    -0.951723    -0.689459     181.43
 H      -4.479352    -1.865981    -0.724592      24.05
 H      -3.984857    -0.105224    -2.375353      25.87
 H      -4.852555     0.981781    -1.036431      28.91
 C       1.642527     0.745366    -1.292615      31.25
 H       2.267835     1.653126    -1.538119      23.91
 C       1.616450    -1.801853    -1.129417      52.67
 H       2.342942    -2.705335    -0.986229      25.27
 C       0.179064    -1.942394    -0.933707     -14.42
 O      -0.447914    -3.114925    -0.737432     200.40
 C      -0.729242    -3.635809    -2.198689      79.58
 H       0.356790    -3.748606    -2.912916      23.46
 H      -0.988943    -4.806136    -2.424145      25.23
 H      -1.586887    -3.094287    -2.611880      25.91
 C      -0.600418    -0.568520    -0.840323     -50.32
 O      -1.976434    -0.837403    -0.710121     120.74
 C       0.153142     0.698518    -1.066233      65.65
 H      -0.511649     1.428033    -0.997045      25.36
 C       2.325168    -0.599608    -1.247407       1.71
 C       3.804106    -0.793608    -1.137706     114.03
 H       4.044808    -1.441519    -1.889554      28.05
 O       4.587567     0.319180    -1.534146     262.96
 H       5.301988     0.452404    -0.761362      30.20
 C       4.168468    -1.189033     0.414895      82.31
 H       3.112801    -1.681121     0.735844      28.19
 O       5.430996    -1.871430     0.427061     135.96
 H       6.241370    -1.682738    -0.260181      23.55
 C       4.205137    -0.091746     1.449111     133.03
 O       5.527751     0.455699     1.529780     175.31
 H       5.617448     1.109849     2.328905      24.04
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 H       3.852241    -0.685287     2.330673      29.44
 H       3.497730     0.643373     1.212047      31.32
55
name = lig-Water-frame_470
 C      -1.511325     2.461482     2.046346      65.10
 H      -1.983401     3.289918     1.553303      19.18
 C      -0.931709     0.211677     2.533184      65.91
 H      -1.217321    -0.778161     2.653828      29.58
 C       0.313625     0.670274     3.184903      23.69
 O       1.226399    -0.013093     3.789058      98.02
 C       1.206083    -1.619765     3.850299     112.62
 H       2.033867    -1.656926     4.592202      28.26
 H       1.613108    -2.079276     2.901514      28.05
 H       0.326561    -1.843856     4.240239      29.54
 C       0.660995     2.096823     3.161788      10.01
 O       1.742488     2.592609     3.815427     170.19
 H       1.695720     3.494438     4.237832      21.52
 C      -0.257804     2.939522     2.486842      77.19
 H      -0.130297     4.070675     2.489192      31.09
 C      -1.799616     1.076129     1.849948      49.16
 C      -3.004245     0.557012     1.331139      80.77
 H      -3.893122     1.477482     1.225008      26.07
 O      -3.415580    -0.732880     1.925129     218.69
 H      -4.396337    -0.738327     1.894583      26.04
 C      -2.797749     0.335682    -0.354182      90.23
 H      -2.345137     1.275159    -0.528714      25.24
 C      -4.148720     0.123383    -1.187427     116.31
 O      -4.884019    -0.957656    -0.694217     197.52
 H      -4.185625    -1.762845    -0.820325      23.42
 H      -4.160226     0.029905    -2.165677      31.86
 H      -4.676227     1.127866    -0.923525      28.71
 C       1.659861     0.729596    -1.251385      28.71
 H       2.135999     1.638941    -1.528853      21.79
 C       1.588407    -1.797642    -1.137594      30.81
 H       2.194916    -2.622371    -0.877284      28.10
 C       0.129963    -1.845135    -0.950302      23.12
 O      -0.496716    -3.064230    -0.789258     229.23
 C      -0.679367    -3.700645    -2.171767     115.83
 H      -0.081392    -3.494947    -2.928091      28.98
 H      -1.014382    -4.662951    -2.209820      30.82
 H      -1.638434    -3.000300    -2.355032      24.95
 C      -0.528732    -0.639479    -0.897752      12.37
 O      -1.919956    -0.770553    -0.703808     135.44
 C       0.184569     0.673863    -1.049128      37.84
 H      -0.569366     1.637814    -1.099980      19.23
 C       2.344412    -0.577009    -1.289523      -8.24
 C       3.826341    -0.763824    -1.086836     104.94
 H       4.092600    -1.791868    -1.723059      22.87
 O       4.574060     0.318363    -1.551439     334.10
 H       5.134199     0.647801    -0.912104      34.33
 C       4.182164    -1.187287     0.437083      91.24
 H       3.471543    -1.877244     0.816326      29.41
 O       5.432945    -1.910450     0.467311     123.56
 H       6.043368    -1.727655    -0.414605      26.27
 C       4.141800    -0.079787     1.501034     112.72
 O       5.536483     0.479375     1.528235     185.14
 H       5.859526     1.004043     2.226531      25.83
 H       3.582226    -0.478613     2.444334      28.40
 H       3.281521     0.670473     1.066638      28.16
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name = lig-Water-frame_471
 C      -1.485121     2.458019     1.995538      58.76
 H      -2.022924     3.264100     1.446373      19.88
 C      -0.865018     0.299212     2.545273      82.70
 H      -1.213911    -0.795298     2.522047      29.03
 C       0.300395     0.736679     3.140332      37.54
 O       1.244747    -0.008464     3.854201      74.28
 C       1.242909    -1.606962     3.793932     104.46
 H       1.924669    -1.884346     4.618459      28.06
 H       1.534560    -2.290529     2.984666      28.02
 H       0.248543    -1.897494     4.496457      25.75
 C       0.660840     2.069869     3.132911      19.61
 O       1.702935     2.579338     3.828621     121.85
 H       1.631386     3.586209     4.142467      21.58
 C      -0.280486     2.918470     2.488318      74.64
 H      -0.090364     3.949555     2.599031      28.78
 C      -1.796959     1.031416     1.937817      47.54
 C      -3.061968     0.606875     1.263348     100.96
 H      -3.875735     1.300868     1.017848      28.31
 O      -3.418321    -0.689027     1.895003     223.30
 H      -4.449523    -0.732135     1.869700      24.57
 C      -2.839643     0.302403    -0.320109      86.50
 H      -2.349698     1.347370    -0.658069      24.90
 C      -4.086800     0.173304    -1.227528      91.65
 O      -4.916300    -1.002657    -0.695033     154.52
 H      -4.306184    -1.710931    -0.704892      28.90
 H      -4.008385     0.239579    -2.541371      25.88
 H      -4.584583     1.052218    -0.931825      29.30
 C       1.606499     0.652720    -1.215267      33.12
 H       2.045461     1.708465    -1.402797      19.90
 C       1.534958    -1.754088    -1.131076     -17.39
 H       1.997414    -2.847444    -0.887749      24.29
 C       0.188879    -1.756042    -0.973997      26.40
 O      -0.532970    -3.044971    -0.852234     181.79
 C      -0.716448    -3.702969    -2.130254      98.78
 H      -0.023134    -3.130562    -3.018042      21.35
 H      -1.044389    -4.819816    -1.741083      24.63
 H      -1.590806    -3.218208    -2.485750      26.55
 C      -0.476928    -0.618911    -0.951054      39.57
 O      -1.859048    -0.704203    -0.696163     121.70
 C       0.219587     0.623441    -1.043411      72.09
 H      -0.162963     1.558377    -1.162786      25.13
 C       2.314243    -0.545740    -1.301603     -26.61
 C       3.850158    -0.796682    -1.031943      93.46
 H       4.144851    -1.713221    -1.359409      23.93
 O       4.571729     0.338080    -1.582248     306.47
 H       5.124342     0.865056    -0.901935      29.53
 C       4.201786    -1.194269     0.437331      83.39
 H       3.624793    -2.187373     0.749595      25.71
 O       5.451433    -1.961353     0.494997     153.55
 H       5.767741    -1.778356    -0.318827      34.69
 C       4.068246    -0.025439     1.533735     114.66
 O       5.535597     0.482063     1.513092     170.78
 H       5.700293     1.054362     2.343266      24.77
 H       3.764980    -0.202728     2.562536      29.35
 H       3.453882     0.686537     1.139186      30.26
55
name = lig-Water-frame_472
 C      -1.472826     2.460055     1.899660      66.83
 H      -2.280245     3.076460     1.415556      26.30
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 C      -0.806023     0.267648     2.570216      62.17
 H      -0.906051    -0.794863     2.510371      28.97
 C       0.322704     0.777997     3.108015      -2.24
 O       1.281412    -0.076435     3.913628     122.68
 C       1.245381    -1.563630     3.835839     104.37
 H       2.015448    -1.940153     4.538091      29.94
 H       1.277356    -2.139827     2.859824      31.48
 H       0.351409    -1.932473     4.172240      28.57
 C       0.611540     2.095690     3.090275      40.75
 O       1.698063     2.561650     3.848776     114.51
 H       1.426277     3.548224     3.883151      26.99
 C      -0.294567     2.904564     2.514567      57.77
 H      -0.034515     4.050998     2.612710      18.12
 C      -1.813218     1.132384     2.007658      25.17
 C      -3.101803     0.560215     1.142584      78.72
 H      -4.070391     1.419171     1.253359      24.41
 O      -3.440417    -0.627721     1.868102     228.90
 H      -4.396120    -0.875032     1.838865      24.77
 C      -2.814282     0.335520    -0.338261     102.96
 H      -2.505475     1.241595    -0.745597      28.69
 C      -4.038735     0.209785    -1.247067      85.72
 O      -4.939880    -1.017536    -0.723315      91.65
 H      -4.435764    -1.968531    -0.573898      22.83
 H      -3.727562     0.295376    -2.204758      30.55
 H      -4.784534     1.073012    -1.029572      26.57
 C       1.572301     0.597386    -1.198355      74.99
 H       2.019865     1.522134    -1.179660      28.90
 C       1.550198    -1.739355    -1.118138      56.85
 H       1.856007    -2.697663    -1.110192      27.49
 C       0.231773    -1.782510    -1.004183     -26.97
 O      -0.538334    -2.993265    -0.890390     204.65
 C      -0.787460    -3.675352    -2.110745     130.04
 H       0.067457    -3.523694    -2.659200      28.14
 H      -0.688661    -4.641704    -1.778926      30.14
 H      -1.825237    -3.615752    -2.786726      25.10
 C      -0.520735    -0.479952    -0.972561       9.52
 O      -1.807534    -0.667000    -0.687658     143.01
 C       0.256743     0.571684    -1.051604      91.52
 H      -0.139131     1.658286    -1.109887      27.92
 C       2.309821    -0.585270    -1.264652      19.42
 C       3.849646    -0.795926    -0.964863      59.44
 H       4.271935    -1.781811    -1.588068      22.19
 O       4.583064     0.356643    -1.607049     247.09
 H       5.064708     0.915604    -0.853130      27.88
 C       4.178305    -1.233225     0.501595      96.63
 H       3.400666    -1.996576     0.570759      28.24
 O       5.481686    -2.001490     0.531281      12.89
 H       5.944967    -1.845549    -0.510260      21.63
 C       4.070098     0.012541     1.532381      97.44
 O       5.523898     0.481039     1.512072     174.08
 H       5.297577     1.148657     2.252448      27.54
 H       3.995482    -0.127856     2.695810      28.35
 H       3.457417     0.987425     1.125084      28.19
55
name = lig-Water-frame_473
 C      -1.492211     2.486084     1.804380      83.80
 H      -2.305180     3.063965     1.448468      28.24
 C      -0.802460     0.203083     2.567655      33.23
 H      -0.738522    -0.906815     2.545507      26.20
 C       0.403022     0.708741     3.130322      -8.03
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 O       1.308639    -0.139481     3.944320     135.04
 C       1.239360    -1.518482     3.869898     129.04
 H       2.162897    -1.893438     4.347558      28.40
 H       1.238105    -1.632660     2.747290      31.05
 H       0.105632    -1.983778     4.118433      24.69
 C       0.603571     2.132666     3.088005      24.47
 O       1.683369     2.541851     3.840704     124.96
 H       1.604601     3.593042     3.956953      23.66
 C      -0.329435     2.987334     2.515068      60.39
 H      -0.126916     3.979300     2.499554      22.39
 C      -1.839215     1.191478     2.021711      16.00
 C      -3.117133     0.531040     1.096810      93.64
 H      -3.905238     1.321858     1.328645      27.07
 O      -3.453974    -0.583983     1.847921     248.58
 H      -4.406916    -0.890150     1.755823      25.09
 C      -2.778639     0.406381    -0.391557      93.07
 H      -2.428397     1.489859    -0.802720      25.35
 C      -4.041287     0.198891    -1.170174      74.70
 O      -4.943109    -1.021132    -0.771601     108.67
 H      -4.506829    -1.920312    -0.699405      27.01
 H      -3.518390     0.113169    -2.374216      25.95
 H      -4.807615     0.941596    -1.202241      26.69
 C       1.645031     0.543257    -1.190976      67.35
 H       2.220112     1.538255    -1.011058      31.30
 C       1.592101    -1.778916    -1.117629      36.94
 H       2.161367    -2.848287    -1.374700      23.87
 C       0.154432    -1.764820    -1.034202      -9.83
 O      -0.544841    -2.909558    -0.900340     241.51
 C      -0.857769    -3.687686    -2.129344     114.69
 H       0.237185    -3.833631    -2.718989      24.85
 H      -0.501002    -4.839149    -1.886055      25.52
 H      -1.700322    -3.768167    -2.661487      28.62
 C      -0.560375    -0.468068    -0.972345      -2.71
 O      -1.812542    -0.644401    -0.669732     157.32
 C       0.229503     0.657707    -1.072828      76.58
 H      -0.316057     1.603429    -0.900570      25.88
 C       2.361098    -0.640990    -1.186358       7.76
 C       3.861150    -0.792529    -0.967176     107.63
 H       4.120153    -1.444711    -1.691745      29.94
 O       4.596016     0.367438    -1.596772     272.40
 H       4.988446     0.827932    -0.929527      32.67
 C       4.135498    -1.253231     0.553764      88.69
 H       3.143777    -1.847628     0.700409      27.28
 O       5.504693    -2.023215     0.549782      82.96
 H       6.075430    -1.963935    -0.214637      25.91
 C       4.134535     0.042576     1.508462     126.03
 O       5.490753     0.497374     1.528763     243.21
 H       5.337780     1.384144     1.938685      30.04
 H       3.847164    -0.287844     2.467129      31.57
 H       3.479492     0.766104     1.226102      32.86
55
name = lig-Water-frame_474
 C      -1.503103     2.533250     1.765623      94.58
 H      -2.245876     3.341187     1.368806      28.44
 C      -0.801083     0.174545     2.557369      38.62
 H      -0.996344    -0.942486     2.515993      25.42
 C       0.455264     0.605930     3.168851      -1.81
 O       1.321140    -0.117853     3.971262     185.72
 C       1.191629    -1.502404     3.835098     133.79
 H       2.113065    -1.957484     4.197897      30.13
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 H       1.354297    -1.530263     2.753744      31.87
 H       0.350952    -1.914822     4.279897      29.54
 C       0.600882     2.133715     3.113564       4.42
 O       1.685634     2.546695     3.823265     177.92
 H       1.779837     3.517211     4.180320      24.37
 C      -0.380912     3.065264     2.478484      51.60
 H      -0.165301     4.239221     2.402082      20.15
 C      -1.839839     1.117509     1.975200      22.87
 C      -3.053606     0.558278     1.136782      82.16
 H      -3.945250     1.478094     1.161457      24.43
 O      -3.456742    -0.587572     1.837300     253.77
 H      -4.460319    -0.716729     1.696778      25.20
 C      -2.750920     0.521859    -0.432805      99.49
 H      -2.361387     1.418117    -0.683695      30.08
 C      -4.051845     0.120779    -1.165261     106.78
 O      -4.928694    -1.003610    -0.823300     193.10
 H      -4.321718    -1.813553    -0.905205      27.85
 H      -3.797662    -0.209219    -2.096277      30.51
 H      -4.743034     0.997396    -1.294911      27.51
 C       1.729380     0.559843    -1.159874      38.58
 H       2.343700     1.402592    -1.016806      31.20
 C       1.601629    -1.900329    -1.148042      55.57
 H       2.184785    -2.667403    -1.395417      30.60
 C       0.124725    -1.693865    -1.077058      46.59
 O      -0.592942    -2.866313    -0.915440     172.25
 C      -0.773897    -3.794911    -2.136021     103.62
 H      -0.125864    -3.573185    -2.978360      26.56
 H      -0.864136    -4.777837    -1.752090      27.72
 H      -1.921771    -3.614034    -2.623862      24.77
 C      -0.521312    -0.522680    -0.971544      19.73
 O      -1.888433    -0.625013    -0.644397     148.99
 C       0.200779     0.765243    -1.085576      43.66
 H      -0.313728     1.683996    -0.805733      23.23
 C       2.407514    -0.676283    -1.092388      -4.40
 C       3.870637    -0.763542    -0.996227     104.27
 H       4.124013    -1.631665    -1.826971      27.52
 O       4.599306     0.366605    -1.567586     214.91
 H       5.084273     0.914800    -0.829393      27.27
 C       4.122393    -1.236190     0.526467      64.82
 H       3.311579    -1.848875     1.045895      27.59
 O       5.483571    -2.046798     0.613118      73.51
 H       6.090218    -1.876082    -0.184040      26.20
 C       4.217636    -0.010420     1.476786     118.45
 O       5.467957     0.547017     1.550442     242.71
 H       5.560563     1.551813     1.623331      26.69
 H       3.646939    -0.492366     2.409327      28.87
 H       3.280007     0.690216     1.114647      31.01
55
name = lig-Water-frame_475
 C      -1.516736     2.564213     1.785120      59.24
 H      -2.067792     3.298321     1.289658      26.21
 C      -0.814052     0.168951     2.541320      55.74
 H      -1.289477    -0.787468     2.506545      28.05
 C       0.425122     0.598920     3.182746      17.32
 O       1.324676    -0.042875     4.003445     193.41
 C       1.197525    -1.506250     3.758938     104.95
 H       2.059200    -2.036077     4.244901      29.24
 H       1.202364    -1.928901     2.682787      30.31
 H       0.300795    -1.968906     4.436943      27.05
 C       0.554479     2.111309     3.130233      -1.09
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 O       1.727328     2.553378     3.813582     190.08
 H       1.526674     3.539122     4.210674      13.97
 C      -0.391526     3.105790     2.437488       7.28
 H      -0.185482     4.117472     2.425148      21.08
 C      -1.775907     1.048601     1.891429      39.95
 C      -2.967143     0.652554     1.196539      93.09
 H      -3.863462     1.487516     1.125244      25.07
 O      -3.464137    -0.611960     1.822944     244.77
 H      -4.455515    -0.592180     1.769142      26.24
 C      -2.762648     0.561183    -0.406380      75.83
 H      -2.248977     1.604973    -0.768100      25.39
 C      -4.093425     0.072892    -1.195444      86.64
 O      -4.898625    -0.996543    -0.843688     165.65
 H      -4.192661    -1.790711    -0.986504      24.19
 H      -3.813199    -0.383124    -2.376920      24.93
 H      -4.617441     1.040946    -1.324747      26.96
 C       1.735049     0.606044    -1.102917      26.15
 H       2.455836     1.491375    -1.111464      28.59
 C       1.574376    -1.918881    -1.181102      56.38
 H       2.119865    -3.002570    -1.389858      24.80
 C       0.204434    -1.715555    -1.133433      18.46
 O      -0.664251    -2.871909    -0.948285     143.49
 C      -0.758081    -3.856147    -2.145220     123.01
 H      -0.237625    -3.408503    -3.128305      23.97
 H      -1.061360    -4.849587    -1.601418      24.99
 H      -1.655921    -3.469042    -2.375663      27.14
 C      -0.502260    -0.460882    -0.959247      -5.35
 O      -1.943669    -0.613412    -0.634738      89.88
 C       0.243814     0.778669    -1.080861      60.58
 H      -0.147667     1.862900    -0.843608      22.75
 C       2.364863    -0.708563    -1.026502      -8.82
 C       3.899248    -0.799999    -1.048117     114.29
 H       4.194163    -1.654510    -1.515629      30.69
 O       4.603348     0.367444    -1.517979     242.90
 H       5.111494     0.913635    -0.798757      27.44
 C       4.196384    -1.209399     0.472964      87.84
 H       3.552554    -1.945514     0.984318      29.67
 O       5.434373    -2.070899     0.685687      76.11
 H       5.994132    -1.641213    -0.186804      25.03
 C       4.193940    -0.084753     1.448698     134.25
 O       5.492056     0.599812     1.555762     273.56
 H       5.413521     1.597878     1.560464      30.48
 H       3.965063    -0.368723     2.429248      32.53
 H       3.490117     0.553495     1.083013      33.82
55
name = lig-Water-frame_476
 C      -1.499907     2.531047     1.840726      65.64
 H      -2.160209     3.162144     1.112728      18.40
 C      -0.848816     0.185865     2.516713      56.59
 H      -1.352632    -0.857764     2.639027      27.30
 C       0.326588     0.708261     3.170927      15.47
 O       1.312080    -0.002727     3.999223     130.24
 C       1.212760    -1.555473     3.721613     112.26
 H       2.070651    -1.919080     4.263033      29.22
 H       0.943750    -2.028667     2.799769      29.69
 H       0.325254    -1.806051     4.291079      28.61
 C       0.502632     2.084415     3.137424      13.75
 O       1.746673     2.569892     3.800865     119.21
 H       1.485081     3.535715     4.011509      20.88
 C      -0.356075     3.041935     2.429007      47.50
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 H      -0.097507     4.175201     2.488516      28.54
 C      -1.632816     1.097459     1.823958      29.51
 C      -2.930989     0.708386     1.214074     101.72
 H      -3.785020     1.554289     1.419976      26.85
 O      -3.457134    -0.616606     1.802289     199.98
 H      -4.497084    -0.617307     1.849933      23.48
 C      -2.788638     0.548653    -0.365022      95.86
 H      -2.461621     1.387654    -0.845975      28.32
 C      -4.096731     0.091933    -1.310988     102.65
 O      -4.863496    -1.020338    -0.833837     227.60
 H      -4.397672    -1.850971    -0.760886      27.32
 H      -3.636405     0.024749    -2.242767      29.97
 H      -4.745928     0.971438    -1.372703      27.52
 C       1.709160     0.624691    -1.034993      42.45
 H       2.339049     1.501552    -1.228550      24.38
 C       1.584495    -1.908959    -1.218044      73.07
 H       1.757271    -2.922094    -1.213981      25.44
 C       0.229490    -1.780560    -1.166484     -48.36
 O      -0.706337    -2.885623    -0.987709     171.36
 C      -0.791117    -3.854374    -2.125228      98.81
 H       0.022693    -3.759483    -2.947857      24.56
 H      -0.830240    -4.916703    -1.814242      25.88
 H      -1.883188    -3.448551    -2.478755      22.56
 C      -0.507634    -0.369354    -0.940374     -32.31
 O      -1.921398    -0.600303    -0.647037     100.72
 C       0.337095     0.757900    -1.046968      65.24
 H       0.021772     1.728960    -1.032264      26.84
 C       2.300241    -0.708734    -1.021036      18.39
 C       3.918153    -0.852094    -1.026419      96.39
 H       4.372460    -1.834498    -1.583211      23.54
 O       4.605029     0.367774    -1.475239     274.68
 H       5.024021     0.735434    -0.760138      32.87
 C       4.300713    -1.223141     0.448531     101.43
 H       3.413153    -2.030569     0.568980      26.99
 O       5.402977    -2.061601     0.712058     190.59
 H       6.041092    -1.779334     0.162749      33.89
 C       4.186573    -0.123859     1.442535     100.33
 O       5.540184     0.646350     1.524610     258.60
 H       5.097823     1.490230     1.776662      30.89
 H       4.200476    -0.339902     2.587642      26.35
 H       3.404013     0.704811     1.087451      26.67
55
name = lig-Water-frame_477
 C      -1.460563     2.493544     1.862709      91.16
 H      -2.161744     2.939971     1.227836      15.56
 C      -0.871196     0.198388     2.513914      64.60
 H      -1.093245    -0.780224     2.712526      25.74
 C       0.229299     0.784514     3.181409       8.99
 O       1.264494     0.003778     3.932559     105.47
 C       1.209794    -1.563494     3.740937      97.70
 H       2.200239    -1.869825     4.172880      26.79
 H       0.944801    -1.847408     2.648629      27.62
 H       0.239495    -1.790304     4.360327      25.68
 C       0.501052     2.119904     3.146165      27.38
 O       1.720586     2.575755     3.765171      90.08
 H       1.725958     3.681920     3.879971      21.30
 C      -0.288183     2.969880     2.458573      64.87
 H      -0.044801     4.028607     2.514044      31.23
 C      -1.530966     1.175257     1.770668      42.64
 C      -2.946573     0.702479     1.206535      88.04
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 H      -3.735986     1.620322     1.612516      24.42
 O      -3.433233    -0.593434     1.789167     209.46
 H      -4.413958    -0.666003     1.734796      24.98
 C      -2.863392     0.482445    -0.341930      84.95
 H      -2.534168     1.461045    -0.939008      22.51
 C      -4.071037     0.160059    -1.360502      67.96
 O      -4.850034    -1.036690    -0.832960     148.44
 H      -4.351140    -1.960328    -0.534562      20.97
 H      -3.411365     0.202269    -2.448411      23.60
 H      -4.986878     0.853604    -1.376076      23.65
 C       1.730258     0.575365    -0.988339      69.87
 H       2.270139     1.484212    -1.195445      24.02
 C       1.557954    -1.876526    -1.236342      38.50
 H       1.901167    -3.004202    -1.092404      21.55
 C       0.124259    -1.771856    -1.158393     -35.52
 O      -0.706416    -2.900532    -1.027836     216.23
 C      -0.866124    -3.823060    -2.119701     114.48
 H       0.190868    -3.938845    -2.754731      22.44
 H      -0.679824    -4.937465    -1.868065      24.77
 H      -1.691052    -3.840756    -2.782629      25.87
 C      -0.501462    -0.386971    -0.930684      -2.96
 O      -1.839761    -0.568573    -0.670051     123.46
 C       0.377221     0.729308    -0.994289      61.03
 H      -0.065794     1.820575    -1.234211      21.91
 C       2.317129    -0.681569    -1.063339      17.99
 C       3.948619    -0.909999    -0.986875     104.69
 H       4.241428    -1.594083    -1.714850      25.04
 O       4.588863     0.352820    -1.452393     244.89
 H       5.058320     0.651299    -0.552692      28.05
 C       4.316388    -1.283149     0.428367     112.72
 H       3.401509    -1.868239     0.445887      26.64
 O       5.406881    -2.060379     0.732202     147.85
 H       6.401421    -1.856528     0.296294      24.08
 C       4.207851    -0.108063     1.471518     106.68
 O       5.567795     0.698857     1.465136     192.09
 H       5.109931     1.363698     2.161377      26.18
 H       4.061415    -0.531740     2.449706      29.28
 H       3.381382     0.542118     1.311080      28.27
55
name = lig-Water-frame_478
 C      -1.383705     2.502673     1.857827      60.20
 H      -2.183815     3.155117     1.366788      16.95
 C      -0.837147     0.248382     2.533924      69.86
 H      -0.971673    -0.910409     2.618982      24.20
 C       0.190829     0.757128     3.234056      23.96
 O       1.192480    -0.006867     3.833870     187.68
 C       1.172226    -1.502116     3.764333     118.98
 H       2.148665    -1.885184     4.004047      29.84
 H       1.175240    -1.615500     2.716298      31.22
 H       0.408577    -2.013664     4.452776      27.76
 C       0.574783     2.183348     3.183931      20.43
 O       1.692385     2.592108     3.720221     138.28
 H       1.708728     3.551016     3.901077      27.83
 C      -0.251470     2.971865     2.481015      48.06
 H      -0.000302     4.029808     2.485736      30.20
 C      -1.566284     1.125998     1.719453      41.23
 C      -2.979218     0.662249     1.180861      93.07
 H      -3.644783     1.553736     1.545464      26.14
 O      -3.389166    -0.554813     1.792235     221.78
 H      -4.360920    -0.680887     1.498184      23.52
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 C      -2.931747     0.473780    -0.383413      86.49
 H      -2.539768     1.429792    -0.656047      24.67
 C      -4.041201     0.196513    -1.353601     105.73
 O      -4.841955    -1.047467    -0.853083     245.55
 H      -4.145046    -1.719177    -0.722639      25.98
 H      -3.648760     0.082299    -2.339280      28.15
 H      -4.845447     0.862928    -1.384686      26.52
 C       1.782664     0.529985    -0.972888      20.61
 H       2.408097     1.499627    -1.011316      24.14
 C       1.481259    -1.856659    -1.222830       1.46
 H       2.177521    -2.694156    -1.145165      25.82
 C       0.028952    -1.711194    -1.136076      28.65
 O      -0.715468    -2.913789    -1.058434     199.25
 C      -0.867995    -3.850075    -2.159643      91.01
 H       0.184343    -3.745137    -2.602691      22.34
 H      -0.849435    -4.831917    -1.498496      24.03
 H      -1.609023    -3.962669    -3.035870      23.95
 C      -0.470188    -0.480572    -0.932929      30.44
 O      -1.778152    -0.526877    -0.687414     132.17
 C       0.326756     0.725197    -0.952283      64.73
 H      -0.087985     1.615985    -1.177724      22.56
 C       2.403276    -0.704997    -1.117590     -26.07
 C       3.952752    -0.891216    -0.992706     118.31
 H       4.132828    -1.631649    -1.879794      25.49
 O       4.574697     0.330900    -1.409721     260.79
 H       5.105536     0.742394    -0.643895      28.86
 C       4.282505    -1.308752     0.417947      85.10
 H       3.369880    -1.996456     0.876960      26.60
 O       5.468740    -2.093939     0.749839     109.54
 H       6.342763    -1.673936     0.297955      25.34
 C       4.260672    -0.115981     1.485993     106.86
 O       5.534490     0.742993     1.429990     145.26
 H       5.576281     1.323605     2.206105      27.23
 H       4.019199    -0.750787     2.424858      28.50
 H       3.298259     0.520013     1.389617      28.44
55
name = lig-Water-frame_479
 C      -1.343420     2.513945     1.806663      78.96
 H      -1.974591     3.397929     1.605379      26.56
 C      -0.818882     0.256477     2.532715      62.15
 H      -0.976443    -0.762826     2.390352      27.93
 C       0.233771     0.756568     3.304136      28.80
 O       1.138292    -0.034905     3.769973     199.94
 C       1.149381    -1.414260     3.771826     133.50
 H       2.183696    -1.778302     4.060497      30.03
 H       1.118364    -1.721350     2.631167      30.82
 H       0.489380    -2.099300     4.385957      30.17
 C       0.595879     2.151165     3.204395      21.82
 O       1.731001     2.609566     3.707480      76.61
 H       1.526723     3.672851     4.062653      23.71
 C      -0.234341     3.048936     2.493744      39.91
 H       0.003732     4.188807     2.401736      18.56
 C      -1.677884     1.052610     1.693208      26.31
 C      -2.979333     0.597285     1.128694      81.14
 H      -3.851806     1.638415     1.355678      22.26
 O      -3.360875    -0.523814     1.809677     216.97
 H      -4.223759    -0.810589     1.385301      24.20
 C      -2.921180     0.524605    -0.421769      83.75
 H      -2.500184     1.572473    -0.570109      23.39
 C      -4.064928     0.168344    -1.295870      94.05
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 O      -4.824670    -1.011862    -0.900025     263.85
 H      -4.119732    -1.779082    -0.976707      22.94
 H      -3.765356    -0.117883    -2.441621      23.82
 H      -4.677485     1.197843    -1.339968      24.89
 C       1.802020     0.545882    -0.976137      -7.85
 H       2.445608     1.350691    -0.799117      28.09
 C       1.447438    -1.792816    -1.195691      30.45
 H       2.045663    -2.736296    -1.296962      24.01
 C       0.055224    -1.750193    -1.135519      52.97
 O      -0.758738    -2.900849    -1.068531     171.61
 C      -0.814113    -3.914885    -2.186713      91.36
 H       0.241503    -3.750418    -2.750454      22.39
 H      -1.093338    -4.735785    -1.492303      25.24
 H      -1.613404    -3.689011    -2.921848      25.19
 C      -0.462245    -0.480930    -0.928555       7.35
 O      -1.796287    -0.496722    -0.696653     111.26
 C       0.330702     0.659306    -0.920452      54.92
 H      -0.223088     1.710975    -0.986778      22.83
 C       2.433575    -0.756126    -1.158078     -41.27
 C       3.923331    -0.872690    -1.052274     119.01
 H       4.223095    -1.714926    -1.686443      30.36
 O       4.575139     0.324415    -1.372044     296.62
 H       5.092233     0.759833    -0.763383      29.79
 C       4.236370    -1.334152     0.480003      80.83
 H       3.611500    -1.983452     1.016594      29.07
 O       5.543079    -2.108792     0.743184     139.84
 H       6.121228    -1.589597     0.247438      30.45
 C       4.299408    -0.134023     1.497538     115.82
 O       5.483912     0.749748     1.397749     173.17
 H       5.785494     1.305258     2.124745      25.65
 H       4.350921    -0.686312     2.456207      30.99
 H       3.406159     0.519319     1.382795      29.44
55
name = lig-Water-frame_480
 C      -1.331552     2.517427     1.757242      99.54
 H      -1.979574     3.367485     1.514528      28.60
 C      -0.848848     0.271325     2.481786      58.29
 H      -0.980962    -0.850116     2.336291      22.94
 C       0.237237     0.805602     3.303058      28.42
 O       1.151024    -0.064520     3.779226     191.01
 C       1.167673    -1.399123     3.719255     131.44
 H       2.140178    -1.533146     4.181143      28.68
 H       0.933013    -1.913411     2.817537      31.85
 H       0.321070    -1.946531     4.357010      28.72
 C       0.550428     2.114747     3.188340      25.71
 O       1.805321     2.658965     3.745860     162.71
 H       1.663557     3.545530     4.055099      28.39
 C      -0.225977     3.097634     2.496057      22.59
 H      -0.027135     4.107451     2.416019      14.90
 C      -1.739485     1.083597     1.738919      30.81
 C      -3.009703     0.603951     1.070762     105.49
 H      -3.775385     1.274916     1.007186      25.38
 O      -3.360187    -0.532004     1.834026     270.70
 H      -4.112785    -0.997933     1.449673      26.65
 C      -2.819507     0.588999    -0.443616      78.24
 H      -2.559206     1.643199    -0.783241      22.80
 C      -4.111347     0.158459    -1.279110     106.69
 O      -4.810573    -0.954569    -0.946365     339.56
 H      -4.423393    -1.880445    -1.082045      25.24
 H      -3.760371    -0.039171    -2.338207      25.82
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 H      -4.574219     1.076044    -1.263325      27.80
 C       1.785372     0.541762    -0.987280      43.20
 H       2.461099     1.427683    -0.646641      24.03
 C       1.496567    -1.792137    -1.185788      56.14
 H       1.593451    -2.911677    -1.466938      25.86
 C       0.124314    -1.818443    -1.139182     -14.56
 O      -0.798152    -2.878661    -1.073161     148.08
 C      -0.746299    -3.923475    -2.191620      98.17
 H       0.186716    -4.172391    -2.886738      23.18
 H      -1.270517    -4.956771    -1.843342      24.76
 H      -1.581049    -3.424076    -2.713818      23.50
 C      -0.501747    -0.442488    -0.920145     -10.68
 O      -1.858845    -0.481975    -0.710046     114.20
 C       0.389509     0.630506    -0.903991      81.61
 H      -0.097036     1.532585    -0.605876      24.43
 C       2.369983    -0.736628    -1.180503      40.84
 C       3.896414    -0.907586    -1.052935      83.24
 H       4.425202    -1.777597    -1.582786      26.55
 O       4.574230     0.331837    -1.374719     193.84
 H       5.187144     0.706641    -0.549041      22.86
 C       4.248978    -1.330152     0.562025      57.18
 H       3.428970    -2.174224     1.001498      26.22
 O       5.585999    -2.088104     0.714871      60.81
 H       6.242946    -1.491251    -0.029589      21.07
 C       4.347110    -0.144394     1.528255     118.50
 O       5.451542     0.727007     1.330634     160.97
 H       5.585429     1.268721     2.207458      24.47
 H       4.560012    -0.507426     2.585408      29.10
 H       3.425531     0.472250     1.448623      28.53
55
name = lig-Water-frame_481
 C      -1.345052     2.541653     1.735925      66.52
 H      -2.135667     3.125578     1.130267      25.88
 C      -0.890208     0.280344     2.427588      70.17
 H      -0.968940    -0.808590     2.488598      22.66
 C       0.185294     0.793376     3.220152      25.88
 O       1.192862    -0.024593     3.814996     134.27
 C       1.165368    -1.467545     3.700861     109.65
 H       2.130698    -1.700929     4.206114      27.28
 H       0.958140    -2.016470     2.708139      29.01
 H       0.291931    -1.699441     4.430454      27.37
 C       0.555969     2.197639     3.186821      14.55
 O       1.840251     2.646098     3.785265      63.29
 H       1.824996     3.791903     4.074289      20.51
 C      -0.257803     3.046099     2.472752      35.09
 H       0.028419     4.207507     2.494775      17.38
 C      -1.748603     1.205100     1.823878      24.53
 C      -3.011026     0.623233     1.019153      61.31
 H      -4.109017     1.488900     1.034967      20.24
 O      -3.368611    -0.566088     1.854031     225.41
 H      -4.136455    -1.128237     1.489781      24.23
 C      -2.724696     0.601144    -0.484670      88.83
 H      -2.495543     1.542725    -0.953949      22.26
 C      -4.074991     0.186714    -1.290933      81.13
 O      -4.860587    -0.912579    -0.968286     279.17
 H      -4.395162    -1.769285    -1.065987      28.11
 H      -3.626105     0.203805    -2.416175      24.24
 H      -4.955322     1.035343    -1.204964      23.60
 C       1.787553     0.536550    -0.984011      74.93
 H       2.304315     1.391007    -0.736842      25.09
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 C       1.519737    -1.915131    -1.215740      47.76
 H       1.758438    -2.898988    -1.508228      26.33
 C       0.125190    -1.771218    -1.116096     -11.78
 O      -0.784467    -2.882956    -1.075750     142.10
 C      -0.750913    -3.932257    -2.201531     100.14
 H       0.205869    -4.299011    -2.808461      25.51
 H      -1.155395    -4.899992    -2.045945      26.59
 H      -1.456119    -3.346425    -2.884026      23.77
 C      -0.528320    -0.474649    -0.925184      -0.86
 O      -1.899616    -0.479090    -0.741808     140.95
 C       0.416428     0.628492    -0.866986      64.04
 H       0.082208     1.564547    -0.317435      22.81
 C       2.339558    -0.690451    -1.194840      36.17
 C       3.888839    -0.956278    -0.984880      75.51
 H       4.399178    -1.747415    -1.595189      26.28
 O       4.586251     0.348942    -1.374183     210.52
 H       5.074273     0.492526    -0.556573      26.81
 C       4.275081    -1.352747     0.632368      86.93
 H       3.496945    -1.981382     0.811973      27.97
 O       5.610414    -2.010496     0.644189     161.03
 H       6.252546    -1.854217    -0.017047      28.64
 C       4.369523    -0.166412     1.590410     114.55
 O       5.448012     0.713082     1.261427     221.13
 H       5.231869     1.255417     2.030355      28.02
 H       4.468203    -0.447310     2.690134      28.54
 H       3.318372     0.338559     1.611044      27.60
55
name = lig-Water-frame_482
 C      -1.414385     2.584950     1.706758      41.17
 H      -1.975757     3.034054     0.945773      25.37
 C      -0.901739     0.294396     2.428761      72.07
 H      -1.144279    -0.751585     2.522567      23.05
 C       0.180902     0.773368     3.119203      18.75
 O       1.232321     0.045105     3.830120     101.42
 C       1.146079    -1.547809     3.717950     101.86
 H       2.043398    -2.072985     4.094437      28.80
 H       1.104275    -1.833142     2.696858      30.01
 H       0.289836    -1.680891     4.495881      26.34
 C       0.598498     2.276538     3.208501       2.37
 O       1.808137     2.636699     3.826070     139.79
 H       1.794476     3.632928     4.024987      25.77
 C      -0.288935     3.041233     2.435433      57.37
 H      -0.047692     4.019680     2.472835      26.99
 C      -1.780878     1.296964     1.876754      37.67
 C      -3.044847     0.713673     1.032581      93.57
 H      -3.765804     1.300321     1.231901      26.62
 O      -3.372060    -0.594197     1.846119     219.87
 H      -4.176609    -0.997619     1.444258      26.53
 C      -2.725336     0.572201    -0.514927      82.59
 H      -2.234374     1.551395    -1.015210      22.16
 C      -4.043098     0.291327    -1.332711     101.70
 O      -4.916497    -0.895418    -0.986386     218.23
 H      -4.196320    -1.650180    -0.934554      25.45
 H      -3.702550     0.414017    -2.415675      26.89
 H      -4.823799     0.908231    -1.206509      25.78
 C       1.777210     0.528366    -0.978366      39.19
 H       2.398313     1.500061    -0.867042      23.13
 C       1.514963    -1.998302    -1.262068      27.60
 H       2.272485    -2.909998    -1.474586      23.00
 C       0.092061    -1.714536    -1.096558      20.69
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 O      -0.732646    -2.921595    -1.077943     142.99
 C      -0.779749    -3.887171    -2.253615      85.07
 H       0.418019    -4.005425    -2.481514      23.60
 H      -1.299277    -4.935297    -1.811951      23.29
 H      -1.243648    -3.571880    -3.149338      25.10
 C      -0.508960    -0.502967    -0.930321      32.19
 O      -1.885563    -0.514413    -0.795481     195.31
 C       0.359832     0.639015    -0.799261      41.26
 H       0.170044     1.602366    -0.243827      23.92
 C       2.375378    -0.751352    -1.195949     -14.24
 C       3.886749    -0.947010    -0.899694      78.46
 H       4.178820    -1.775329    -1.602201      26.31
 O       4.589243     0.335412    -1.368763     184.10
 H       5.122393     0.578394    -0.579908      25.59
 C       4.345075    -1.340907     0.624814      78.77
 H       3.392392    -2.150689     0.882055      25.73
 O       5.609601    -1.951026     0.596794     125.57
 H       6.247351    -1.921000    -0.312256      20.39
 C       4.334485    -0.219892     1.664563     114.09
 O       5.429142     0.708691     1.224136     188.15
 H       5.149313     1.596705     1.707727      26.09
 H       4.420537    -0.585964     2.706154      29.14
 H       3.369987     0.253352     1.655036      29.65
55
name = lig-Water-frame_483
 C      -1.480073     2.634718     1.692967      49.30
 H      -1.812217     3.370661     0.832427      20.89
 C      -0.919554     0.331582     2.464661      53.80
 H      -1.404262    -0.707699     2.439058      22.46
 C       0.288321     0.804211     3.071894      18.71
 O       1.261811     0.080733     3.822080      77.33
 C       1.123465    -1.574917     3.763624      97.33
 H       2.006866    -2.158703     4.072401      27.83
 H       0.990957    -1.661492     2.621126      26.93
 H       0.258465    -1.934140     4.330242      26.98
 C       0.586956     2.259172     3.192222       5.01
 O       1.728957     2.609801     3.856177      87.66
 H       1.700481     3.719067     4.120438      22.18
 C      -0.288845     3.074097     2.410799      87.01
 H      -0.097620     4.257956     2.317252      30.43
 C      -1.846187     1.287681     1.875080      43.04
 C      -2.998721     0.754661     1.103410      73.43
 H      -4.051523     1.617862     1.393034      22.41
 O      -3.372656    -0.593125     1.802533     195.33
 H      -4.242293    -0.782096     1.394595      26.26
 C      -2.765215     0.561336    -0.531883      86.75
 H      -2.217785     1.391462    -0.805436      25.39
 C      -4.036540     0.390894    -1.371779      76.67
 O      -4.906378    -0.884426    -1.015228     203.66
 H      -4.269572    -1.608609    -0.739852      26.28
 H      -3.821527     0.391657    -2.535740      25.39
 H      -4.718677     1.398236    -1.135253      24.92
 C       1.749539     0.506222    -0.973019      40.14
 H       2.435438     1.329431    -1.003981      28.82
 C       1.551346    -1.975797    -1.301700      61.03
 H       2.147902    -2.805022    -1.304887      25.21
 C       0.114474    -1.786410    -1.120685       0.12
 O      -0.691939    -2.962653    -1.085153     190.49
 C      -0.766342    -3.846910    -2.249580      99.03
 H       0.418462    -3.905445    -2.343571      24.57
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 H      -1.259764    -4.567332    -1.764902      27.94
 H      -1.192599    -3.724452    -3.327747      24.18
 C      -0.491907    -0.467310    -0.913397       6.74
 O      -1.847932    -0.582067    -0.856925     160.65
 C       0.327066     0.655750    -0.723947      58.18
 H      -0.066037     1.584638    -0.359148      23.48
 C       2.392171    -0.848316    -1.158406     -24.12
 C       3.891535    -0.893331    -0.836957      95.07
 H       4.095550    -1.815731    -1.498858      25.39
 O       4.586216     0.289591    -1.356959     186.40
 H       5.198796     0.805891    -0.644895      23.61
 C       4.347705    -1.344272     0.573805     100.37
 H       3.757591    -2.092593     0.969280      29.97
 O       5.643673    -1.920293     0.552425     143.37
 H       5.869304    -1.712729    -0.456600      21.52
 C       4.302925    -0.276460     1.711776      92.67
 O       5.378515     0.719280     1.235653     163.37
 H       5.212015     1.704377     1.231929      27.80
 H       4.591222    -0.770609     2.736774      26.59
 H       3.291003     0.330067     1.638008      26.86
55
name = lig-Water-frame_484
 C      -1.490398     2.699528     1.696720      24.61
 H      -1.817719     3.478545     1.093825      22.34
 C      -0.951853     0.398395     2.513570      40.72
 H      -1.295294    -0.582146     2.447757      27.54
 C       0.402616     0.840442     3.062065      17.49
 O       1.281588     0.060066     3.813099      81.56
 C       1.094561    -1.539238     3.767355     101.23
 H       2.072694    -1.907688     4.128323      26.65
 H       0.847196    -1.642317     2.734732      26.83
 H       0.127414    -2.146510     4.168666      25.02
 C       0.521222     2.202722     3.120657      26.30
 O       1.636928     2.611481     3.894605     135.50
 H       1.674203     3.652810     4.154795      21.91
 C      -0.288074     3.150345     2.381712      46.42
 H      -0.083969     4.157125     2.229138      28.40
 C      -1.866848     1.271288     1.845212      34.25
 C      -3.031370     0.769161     1.195027     115.55
 H      -3.736888     1.397739     1.151600      30.98
 O      -3.379390    -0.554433     1.729955     190.63
 H      -4.356635    -0.657619     1.433112      24.42
 C      -2.800095     0.530287    -0.517651      64.09
 H      -2.206693     1.578786    -0.729465      20.60
 C      -4.077248     0.489164    -1.387445      89.53
 O      -4.860247    -0.830838    -1.047244     226.10
 H      -4.297886    -1.578344    -0.702340      25.46
 H      -3.945573     0.272357    -2.527278      26.33
 H      -4.404157     1.429970    -1.165510      30.11
 C       1.711189     0.429962    -0.964091      58.82
 H       2.438851     1.268463    -1.006389      29.40
 C       1.565920    -1.908036    -1.306446      62.99
 H       1.863286    -3.090568    -1.201557      22.72
 C       0.181359    -1.869353    -1.165047      -0.70
 O      -0.670899    -2.964259    -1.089668     226.33
 C      -0.696354    -3.804659    -2.242593     106.62
 H       0.415073    -4.311177    -2.502534      23.53
 H      -1.351424    -4.764081    -1.753909      22.45
 H      -1.252002    -3.555524    -3.094420      26.72
 C      -0.468648    -0.483940    -0.892168     -12.44
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 O      -1.831188    -0.637535    -0.908944     129.06
 C       0.346795     0.667247    -0.668194      62.85
 H      -0.343838     1.625040    -0.606810      21.14
 C       2.362205    -0.837354    -1.081325      39.21
 C       3.889535    -0.865632    -0.813052     107.61
 H       4.318734    -1.746769    -1.381923      26.08
 O       4.586075     0.246966    -1.354076     259.52
 H       5.040465     0.661829    -0.660447      31.48
 C       4.318854    -1.322304     0.563414      77.15
 H       3.731370    -2.314859     1.040238      26.42
 O       5.678439    -1.896433     0.500937     106.57
 H       6.079128    -1.634177    -0.338917      24.57
 C       4.286908    -0.287191     1.709441     110.50
 O       5.335892     0.719777     1.250445     230.41
 H       4.985968     1.603579     1.197398      32.57
 H       4.665879    -0.699698     2.606034      29.63
 H       3.379211     0.181703     1.829478      29.42
55
name = lig-Water-frame_485
 C      -1.447586     2.733916     1.744696      35.68
 H      -2.188483     3.506750     1.236533      22.57
 C      -0.941088     0.490129     2.564386      43.85
 H      -1.052050    -0.668662     2.572438      25.77
 C       0.404550     0.820529     3.045249      10.85
 O       1.284850     0.001132     3.811810     135.08
 C       1.049081    -1.465697     3.742557     123.88
 H       2.040505    -1.667246     4.150847      28.00
 H       0.963984    -1.777185     2.635084      28.44
 H       0.278810    -1.882496     4.305143      29.52
 C       0.490752     2.219101     3.050234      18.52
 O       1.545017     2.617482     3.931367     138.60
 H       1.594163     3.703613     4.070455      20.52
 C      -0.316031     3.169837     2.343474      35.25
 H       0.099467     4.256287     2.271364      24.87
 C      -1.800707     1.322535     1.834509      40.21
 C      -3.060545     0.685912     1.195876      78.22
 H      -4.060695     1.625929     1.018601      22.17
 O      -3.416292    -0.500883     1.663887     213.12
 H      -4.351743    -0.695161     1.536280      26.06
 C      -2.771447     0.531390    -0.501014      84.31
 H      -2.401679     1.419006    -0.775677      24.92
 C      -4.079530     0.485551    -1.377792      84.26
 O      -4.825831    -0.734087    -1.074439     278.49
 H      -4.106558    -1.444273    -0.815638      25.47
 H      -3.887506     0.419830    -2.467172      27.00
 H      -4.655056     1.560523    -1.160146      25.82
 C       1.696621     0.393568    -0.932715      68.56
 H       2.354257     1.302483    -0.896007      29.98
 C       1.550810    -1.955957    -1.270276      63.36
 H       1.761493    -2.964683    -1.275158      26.32
 C       0.215840    -1.836266    -1.190189      19.39
 O      -0.641487    -2.954447    -1.095642     219.71
 C      -0.646617    -3.872720    -2.209552     118.00
 H       0.321221    -4.428892    -2.652248      24.22
 H      -1.160081    -4.702309    -2.050069      29.34
 H      -1.303582    -3.170380    -2.920004      23.82
 C      -0.431879    -0.578583    -0.880026      -3.95
 O      -1.841116    -0.651270    -0.943822     127.54
 C       0.328255     0.641989    -0.663492      69.57
 H      -0.114332     1.553730    -0.794820      25.49
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 C       2.353115    -0.760091    -0.995995      27.41
 C       3.866852    -0.900502    -0.836147      97.04
 H       4.411100    -1.725359    -1.400727      24.90
 O       4.581133     0.222723    -1.364607     253.11
 H       4.960712     0.599747    -0.479327      26.60
 C       4.283791    -1.341172     0.619180      82.44
 H       3.643696    -2.119722     0.764121      30.61
 O       5.689298    -1.885392     0.487293      15.19
 H       6.565614    -1.545545    -0.239154      13.28
 C       4.314706    -0.276910     1.660320     115.12
 O       5.292921     0.715194     1.259453     239.10
 H       4.658568     1.520029     1.519510      27.02
 H       4.786660    -0.699572     2.692989      27.49
 H       3.242089     0.108367     2.085064      26.03
55
name = lig-Water-frame_486
 C      -1.475081     2.750242     1.761152      40.38
 H      -2.351293     3.251865     1.475785      20.68
 C      -0.881500     0.507856     2.602681      63.31
 H      -1.055836    -0.522691     2.670432      27.01
 C       0.324911     0.815116     3.031838      18.83
 O       1.256986    -0.033666     3.790680     181.02
 C       1.045084    -1.377195     3.688198     128.50
 H       1.978115    -1.802095     4.184826      28.65
 H       1.115097    -1.922716     2.740575      30.04
 H       0.277667    -1.546270     4.638258      24.56
 C       0.531152     2.263592     3.018224      18.28
 O       1.458148     2.641375     3.953342     176.71
 H       1.550862     3.693110     4.024003      22.14
 C      -0.289585     3.193154     2.328321      27.10
 H       0.134692     4.204827     2.417351      24.28
 C      -1.737889     1.384981     1.840141      30.96
 C      -3.097129     0.706717     1.071083     101.24
 H      -3.810099     1.316879     1.194945      27.45
 O      -3.474127    -0.497141     1.651765     247.55
 H      -4.415033    -0.752659     1.508848      25.96
 C      -2.739716     0.531225    -0.482408      79.52
 H      -2.247401     1.562268    -0.936363      23.29
 C      -4.068988     0.474688    -1.341145     103.95
 O      -4.793266    -0.639851    -1.093826     277.28
 H      -4.130169    -1.321916    -1.019536      29.72
 H      -3.641281     0.765656    -2.458441      26.38
 H      -4.839121     1.152263    -1.178602      26.80
 C       1.690430     0.470716    -0.860895      66.84
 H       2.266082     1.354457    -0.775373      32.59
 C       1.569220    -1.985602    -1.202177      41.26
 H       2.093759    -3.047858    -1.401405      23.86
 C       0.181267    -1.776410    -1.186139      35.47
 O      -0.595094    -2.964195    -1.082324     189.61
 C      -0.631252    -3.907456    -2.221338     112.27
 H       0.421554    -4.113011    -2.849248      23.73
 H      -1.351374    -4.909672    -2.061175      25.19
 H      -1.059204    -3.215132    -2.875776      27.06
 C      -0.438702    -0.632287    -0.870480      28.05
 O      -1.861070    -0.633970    -0.961644     159.26
 C       0.299581     0.531587    -0.716977      58.00
 H       0.041209     1.680431    -0.846306      23.11
 C       2.367069    -0.789425    -0.945912     -16.01
 C       3.854437    -0.958526    -0.881692     100.67
 H       4.112348    -1.845960    -1.494861      25.49
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 O       4.582289     0.225261    -1.358726     233.32
 H       4.866994     0.726927    -0.491453      26.31
 C       4.295488    -1.346143     0.618213      69.55
 H       3.431340    -2.225079     0.706614      27.66
 O       5.711216    -1.897527     0.524548      85.10
 H       6.096591    -1.531321    -0.284776      22.39
 C       4.344634    -0.298536     1.688860     148.41
 O       5.211573     0.747353     1.267312     193.00
 H       4.903071     1.498674     1.879914      26.70
 H       4.744342    -0.751498     2.533840      34.01
 H       3.429143     0.037984     1.962269      30.03
55
name = lig-Water-frame_487
 C      -1.531954     2.738012     1.772883      58.59
 H      -2.431952     3.376367     1.489499      18.72
 C      -0.890079     0.464601     2.574872      60.15
 H      -1.327509    -0.569745     2.685662      25.19
 C       0.309911     0.881619     3.067716      26.15
 O       1.223863     0.021694     3.727775     184.72
 C       1.060972    -1.365314     3.731734     139.05
 H       1.869789    -1.923248     4.189135      30.71
 H       0.899646    -1.906929     2.747424      30.30
 H       0.268335    -1.544762     4.342547      31.42
 C       0.583764     2.279391     3.001222      30.60
 O       1.401793     2.676504     3.977396     184.62
 H       1.603903     3.765633     4.056469      19.03
 C      -0.224353     3.214094     2.345504      45.17
 H      -0.013547     4.296595     2.484368      23.81
 C      -1.724513     1.379239     1.847972      32.47
 C      -3.022657     0.737891     0.942625      80.16
 H      -4.025907     1.599742     1.253925      20.78
 O      -3.532560    -0.532740     1.675977     187.06
 H      -4.480558    -0.720071     1.339406      24.73
 C      -2.706023     0.590391    -0.496883     105.13
 H      -2.149175     1.371010    -0.793483      27.57
 C      -4.002844     0.518014    -1.328711      94.90
 O      -4.775875    -0.611879    -1.119249     272.05
 H      -4.283149    -1.534110    -1.148559      25.61
 H      -3.622174     0.762950    -2.342936      27.90
 H      -4.857080     1.310308    -1.036926      25.05
 C       1.703890     0.517776    -0.765780      31.61
 H       2.266149     1.530761    -0.656421      23.51
 C       1.621271    -1.974178    -1.121309      66.37
 H       2.235414    -2.792657    -1.485497      25.65
 C       0.166958    -1.834776    -1.166825       9.61
 O      -0.555686    -3.002306    -1.054827     201.75
 C      -0.626067    -3.912802    -2.266546     106.86
 H       0.515418    -4.004821    -2.722335      22.07
 H      -1.206038    -4.682650    -1.956747      27.22
 H      -1.131889    -3.415969    -3.193787      25.94
 C      -0.532429    -0.605212    -0.866336       6.40
 O      -1.892689    -0.602167    -0.960549     160.84
 C       0.309221     0.482763    -0.804998      63.56
 H      -0.150616     1.417765    -0.679100      25.83
 C       2.355523    -0.843548    -0.924518       7.16
 C       3.862716    -0.991266    -0.902030      94.65
 H       3.892717    -1.917589    -1.594335      26.02
 O       4.580630     0.227958    -1.350495     236.80
 H       4.720044     0.807549    -0.641439      27.97
 C       4.304201    -1.400652     0.559250      87.78
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 H       3.701145    -2.122046     0.961185      30.71
 O       5.702084    -1.919795     0.590306     125.81
 H       5.718413    -1.653546    -0.440420      22.49
 C       4.366692    -0.345954     1.715869     110.99
 O       5.139649     0.806606     1.283722     158.35
 H       5.228111     1.551222     1.937547      25.32
 H       4.816720    -0.984665     2.658711      28.42
 H       3.256175     0.111316     1.854823      26.84
55
name = lig-Water-frame_489
 C      -1.476755     2.742192     1.843043      56.41
 H      -2.007296     3.514332     1.294904      21.91
 C      -0.968171     0.381427     2.448163      48.60
 H      -1.277335    -0.636745     2.592535      24.78
 C       0.221049     0.921511     3.080290      16.76
 O       1.249842     0.190444     3.642552      55.07
 C       0.975028    -1.413166     3.769251     112.96
 H       1.916640    -1.695136     4.157413      29.49
 H       0.878163    -1.581657     2.691007      28.06
 H       0.191248    -1.699751     4.384988      30.49
 C       0.603889     2.354719     3.015798      17.91
 O       1.460992     2.767465     4.080807     159.74
 H       1.563467     3.840871     4.183788      20.24
 C      -0.313548     3.222009     2.333249      77.61
 H      -0.213563     4.239865     2.527044      27.08
 C      -1.851553     1.282848     1.789253      44.97
 C      -2.893217     0.780680     1.040697      62.50
 H      -3.757477     1.788544     0.766881      21.39
 O      -3.610911    -0.514048     1.667507     132.28
 H      -4.368212    -0.717451     1.039825      23.68
 C      -2.606903     0.660818    -0.568485      87.79
 H      -2.180871     1.594809    -0.794321      24.95
 C      -3.895439     0.656887    -1.360061      86.81
 O      -4.798305    -0.640738    -1.168965     237.97
 H      -4.133543    -1.384518    -1.089532      26.01
 H      -3.818148     0.657029    -2.386499      28.01
 H      -4.330403     1.683687    -1.011309      26.53
 C       1.720685     0.435839    -0.622073      43.51
 H       2.315652     1.414027    -0.406703      24.25
 C       1.548820    -1.907190    -1.028329      46.30
 H       1.977240    -2.971963    -1.224077      23.60
 C       0.167554    -1.924796    -1.024774      18.86
 O      -0.570865    -3.144449    -1.075413     212.56
 C      -0.570049    -3.870163    -2.314003     121.89
 H       0.554299    -4.297303    -2.495889      24.21
 H      -0.863799    -4.840144    -1.997119      27.67
 H      -1.247315    -3.609770    -3.159923      26.12
 C      -0.531723    -0.669120    -0.964220      -0.32
 O      -1.983541    -0.548916    -0.922593     126.96
 C       0.282287     0.537079    -0.885708      47.49
 H      -0.175112     1.488593    -0.525826      22.23
 C       2.376154    -0.698731    -0.856929      48.54
 C       3.867208    -0.977874    -0.851689      85.98
 H       4.444573    -1.704797    -1.548305      24.61
 O       4.558570     0.176041    -1.369801     228.51
 H       4.441281     0.806942    -0.644757      29.26
 C       4.363475    -1.470390     0.600430     100.00
 H       3.683096    -2.235583     0.830928      27.61
 O       5.682045    -1.997520     0.620519     166.99
 H       6.389162    -2.069677     0.027720      26.59
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 C       4.310229    -0.360325     1.689550     108.42
 O       5.087413     0.835574     1.269318     221.01
 H       4.877727     1.453054     1.964500      28.29
 H       4.864764    -0.787346     2.720666      27.65
 H       3.190548    -0.186611     2.086205      25.69
55
name = lig-Water-frame_490
 C      -1.468077     2.677942     1.822646      32.34
 H      -2.112283     3.364240     1.170245      22.57
 C      -0.955589     0.398518     2.419030      56.54
 H      -1.030356    -0.750824     2.465703      22.33
 C       0.150499     0.939949     3.024469      24.48
 O       1.263461     0.199679     3.651736      78.36
 C       0.935189    -1.338903     3.733288     109.70
 H       1.978871    -1.657851     4.125923      27.70
 H       1.059094    -1.827108     2.688658      26.23
 H       0.209926    -1.574609     4.643513      26.93
 C       0.552604     2.384442     3.085879      12.66
 O       1.506442     2.773008     4.099063     162.38
 H       1.701808     3.954770     4.197525      18.21
 C      -0.347213     3.210688     2.384799      76.65
 H      -0.102904     4.375473     2.410058      24.39
 C      -1.828239     1.318774     1.816904      45.38
 C      -2.974532     0.771030     1.033746     102.98
 H      -3.597691     1.506630     1.156959      28.45
 O      -3.611092    -0.432552     1.623262     207.65
 H      -4.322058    -0.745628     0.983123      25.61
 C      -2.566593     0.662299    -0.568563      83.82
 H      -2.083671     1.670768    -0.918683      23.18
 C      -3.894904     0.681354    -1.386581      80.49
 O      -4.796392    -0.603695    -1.180129     206.79
 H      -3.988085    -1.201201    -0.956546      24.90
 H      -3.650383     0.819118    -2.614543      24.14
 H      -4.640701     1.487718    -1.157451      25.11
 C       1.657584     0.459630    -0.593252      36.66
 H       2.249984     1.275426    -0.294245      24.05
 C       1.506966    -1.893789    -0.998295      41.01
 H       1.917538    -2.865399    -0.987610      24.16
 C       0.123685    -1.913765    -0.948700      24.11
 O      -0.596983    -3.195809    -1.091828     172.41
 C      -0.512173    -3.964221    -2.276987     104.94
 H       0.460460    -3.938419    -3.023279      24.06
 H      -0.971507    -5.023148    -2.127160      25.63
 H      -1.097927    -3.265359    -3.015865      24.10
 C      -0.477237    -0.657634    -1.022071      11.72
 O      -1.956815    -0.565144    -0.916454     174.97
 C       0.259265     0.540582    -0.848010      58.27
 H      -0.027222     1.581090    -0.668606      22.13
 C       2.399487    -0.755305    -0.838846      12.03
 C       3.923709    -0.954828    -0.810808      97.39
 H       4.144343    -1.798383    -1.439619      26.40
 O       4.551090     0.175596    -1.366997     228.72
 H       4.510311     0.890474    -0.720822      29.56
 C       4.385028    -1.455909     0.631485      92.68
 H       3.580886    -2.325261     0.601240      24.70
 O       5.716218    -2.087070     0.664830      73.61
 H       6.448034    -1.697968    -0.149562      20.55
 C       4.289966    -0.371935     1.689656     122.29
 O       5.055732     0.812847     1.258155     253.47
 H       4.601946     1.501135     1.909044      26.66
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 H       4.804700    -0.639452     2.493175      31.70
 H       3.296169    -0.144838     1.989039      27.55
55
name = lig-Water-frame_491
 C      -1.522943     2.626147     1.744769      98.67
 H      -2.210572     3.187138     1.201636      25.64
 C      -0.914237     0.402535     2.409852      69.34
 H      -0.964992    -0.615017     2.270928      21.64
 C       0.195807     0.991511     3.016829      11.33
 O       1.225905     0.168673     3.648748     171.17
 C       0.988143    -1.237516     3.717506     129.60
 H       1.867141    -1.623383     4.159287      27.99
 H       0.778372    -1.934139     2.906797      27.05
 H       0.184747    -1.424780     4.458901      27.52
 C       0.469367     2.382324     3.190259      18.53
 O       1.542139     2.782603     4.080431     140.67
 H       1.776018     3.692822     4.112397      36.87
 C      -0.317083     3.248953     2.473414      42.53
 H      -0.152442     4.226778     2.245009      13.85
 C      -1.781683     1.320362     1.857712      28.87
 C      -3.052712     0.755133     0.995770      73.89
 H      -3.987664     1.667188     1.315157      20.37
 O      -3.591867    -0.349361     1.565822     236.61
 H      -4.295325    -0.675265     1.011303      25.72
 C      -2.605109     0.683434    -0.550168      89.14
 H      -1.881479     1.463911    -0.877881      18.65
 C      -3.939063     0.684317    -1.457380      95.65
 O      -4.742188    -0.533830    -1.187609     277.61
 H      -4.221871    -1.348239    -0.980330      27.00
 H      -3.570592     0.806332    -2.388004      28.87
 H      -4.742901     1.390038    -1.199811      25.08
 C       1.624890     0.456147    -0.597575      37.69
 H       2.138499     1.398702    -0.220529      21.31
 C       1.513878    -1.891886    -0.956391      40.55
 H       2.065916    -2.960644    -0.841568      21.05
 C       0.070542    -1.927370    -0.922743      13.70
 O      -0.598663    -3.218179    -1.056987     159.19
 C      -0.474432    -4.007445    -2.324986      94.47
 H       0.511187    -3.814076    -3.023081      23.57
 H      -1.043428    -4.973532    -2.275991      24.86
 H      -1.112280    -3.349640    -2.860092      25.72
 C      -0.509146    -0.595255    -1.042363      10.39
 O      -1.880910    -0.598330    -0.923445     196.28
 C       0.285139     0.536084    -0.781947      69.25
 H      -0.207161     1.608488    -0.922308      18.51
 C       2.353859    -0.836350    -0.806586      21.47
 C       3.962715    -0.945362    -0.762902      92.43
 H       3.876520    -1.879034    -1.428677      23.88
 O       4.560787     0.189244    -1.379785     201.03
 H       4.683695     1.001242    -0.693278      22.61
 C       4.390274    -1.450766     0.615909      93.64
 H       3.741612    -2.269565     0.822954      26.93
 O       5.773648    -2.152047     0.681313     166.59
 H       5.988071    -1.564337     0.046209      33.28
 C       4.285907    -0.392178     1.682954      87.04
 O       5.001165     0.802673     1.249199     260.23
 H       4.698619     1.623945     1.763870      27.03
 H       4.855944    -0.782825     2.715901      23.29
 H       3.197566    -0.043192     1.869721      23.27
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name = lig-Water-frame_492
 C      -1.513913     2.652860     1.712700      76.57
 H      -2.345847     3.287744     1.185535      24.98
 C      -0.835554     0.425400     2.420031      60.42
 H      -1.000237    -0.686714     2.127161      18.76
 C       0.298784     0.996666     3.063007      17.03
 O       1.175632     0.157539     3.619658     194.74
 C       1.042330    -1.168193     3.730690     132.22
 H       1.933139    -1.646372     4.265963      24.26
 H       0.466388    -1.747073     2.913537      22.52
 H       0.054543    -1.311880     4.395153      24.36
 C       0.412386     2.394341     3.313471      23.14
 O       1.560877     2.731120     4.034685      68.87
 H       1.670676     3.869287     4.017551      27.66
 C      -0.366653     3.255834     2.502905      87.07
 H      -0.119756     4.373019     2.211864      19.54
 C      -1.814161     1.258623     1.840689      24.66
 C      -3.104510     0.857833     0.981324      91.51
 H      -3.810432     1.532515     0.904204      24.73
 O      -3.572743    -0.322968     1.521682     270.72
 H      -4.406224    -0.619577     1.049318      25.00
 C      -2.694744     0.694073    -0.536421      76.01
 H      -1.954300     1.435281    -0.736646      18.72
 C      -3.968916     0.654476    -1.481878      76.61
 O      -4.690460    -0.475026    -1.194808     320.90
 H      -4.394883    -1.436380    -1.183156      24.30
 H      -3.511645     0.719086    -2.645201      22.69
 H      -4.623147     1.614339    -1.207525      23.35
 C       1.671517     0.429809    -0.607029      47.65
 H       2.070428     1.413192    -0.330674      20.39
 C       1.518663    -1.981233    -0.897512      47.37
 H       2.011289    -2.860062    -0.892512      22.80
 C       0.061901    -1.935337    -0.948890       7.26
 O      -0.579108    -3.223818    -0.990348     159.19
 C      -0.474066    -3.975718    -2.407696      64.49
 H       0.732041    -3.977158    -2.621403      23.32
 H      -0.852844    -4.974700    -2.257557      24.80
 H      -1.370417    -3.518819    -3.052998      22.65
 C      -0.558731    -0.585000    -1.014542      10.62
 O      -1.842090    -0.617388    -0.929635     174.42
 C       0.278719     0.554876    -0.747765      87.06
 H      -0.232643     1.400060    -0.932516      21.15
 C       2.295840    -0.814633    -0.734157      35.64
 C       3.923267    -0.969611    -0.743295      90.38
 H       4.123911    -1.717268    -1.501261      26.24
 O       4.586405     0.209686    -1.396500     240.50
 H       4.791076     0.752050    -0.650857      26.98
 C       4.395674    -1.466637     0.631830      81.45
 H       3.735484    -2.273715     1.123923      24.95
 O       5.795197    -2.178257     0.688805     110.26
 H       6.208433    -1.512852    -0.042895      28.48
 C       4.296791    -0.395971     1.730830      93.52
 O       4.958515     0.807912     1.229293     339.84
 H       4.808897     1.576085     1.798850      27.52
 H       4.550886    -0.802924     2.613972      26.71
 H       3.212013    -0.158186     1.785880      24.67
55
name = lig-Water-frame_493
 C      -1.489096     2.702288     1.737505      35.03
 H      -2.127313     3.388665     1.288790      26.05
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 C      -0.786144     0.442292     2.406825      51.25
 H      -0.887771    -0.591708     2.254459      20.64
 C       0.323871     0.976572     3.101501      18.91
 O       1.200684     0.196626     3.601093     211.75
 C       1.002598    -1.190945     3.779791     127.69
 H       1.902134    -1.628606     4.149793      26.05
 H       0.706713    -1.488451     2.781480      23.55
 H       0.200505    -1.253792     4.528383      25.92
 C       0.374797     2.406787     3.391989      -5.32
 O       1.579951     2.722167     3.982311     160.05
 H       1.524759     3.650244     4.119299      21.58
 C      -0.466481     3.254268     2.480321      91.32
 H      -0.129539     4.252598     2.477889      26.21
 C      -1.860645     1.258619     1.784037      30.25
 C      -3.061483     0.925790     0.949367      66.95
 H      -3.910730     1.923218     0.650119      20.38
 O      -3.578801    -0.340798     1.498981     209.03
 H      -4.490514    -0.537891     1.133200      24.82
 C      -2.771319     0.686997    -0.549578      75.68
 H      -2.165498     1.714818    -0.737673      15.88
 C      -3.912505     0.653029    -1.523183     120.73
 O      -4.707809    -0.448514    -1.193876     348.74
 H      -4.182763    -1.303294    -1.450150      25.60
 H      -3.732947     0.650220    -2.495611      29.54
 H      -4.398893     1.594445    -1.356922      28.99
 C       1.698588     0.435057    -0.619190      20.46
 H       2.310269     1.335560    -0.514249      19.36
 C       1.479419    -2.041333    -0.833720      27.47
 H       2.049100    -3.114084    -1.008129      22.66
 C       0.114789    -1.938098    -0.994255      33.85
 O      -0.563851    -3.214827    -0.954429     100.23
 C      -0.509340    -3.921976    -2.437075      71.10
 H       0.692596    -4.006663    -2.554178      22.64
 H      -0.527113    -5.044331    -2.047951      21.77
 H      -1.138216    -3.629466    -3.204957      24.28
 C      -0.522531    -0.631123    -0.941255      22.15
 O      -1.905755    -0.612628    -0.926964     127.04
 C       0.262992     0.518005    -0.747946      75.78
 H      -0.244378     1.646765    -0.787726      16.58
 C       2.291512    -0.792524    -0.655674      40.33
 C       3.844653    -1.001793    -0.766758      67.26
 H       4.334736    -1.679493    -1.530585      24.48
 O       4.609490     0.211610    -1.391900     200.47
 H       4.910163     0.667534    -0.535408      24.27
 C       4.412491    -1.500830     0.697268      67.66
 H       3.716266    -2.262375     1.115297      25.31
 O       5.793114    -2.143433     0.659426     109.53
 H       6.660879    -1.930069     0.116192      26.03
 C       4.284176    -0.377819     1.731235      81.15
 O       4.933528     0.811938     1.217069     295.90
 H       4.828103     1.544416     1.995439      22.92
 H       4.538094    -0.799032     2.871432      22.66
 H       3.166594    -0.260781     1.791208      23.70
55
name = lig-Water-frame_494
 C      -1.502062     2.710559     1.782220      31.31
 H      -2.046718     3.566269     1.221683      22.49
 C      -0.816873     0.480981     2.357614      50.60
 H      -0.807799    -0.647373     2.406284      21.45
 C       0.232705     1.015634     3.114539       6.31
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 O       1.319894     0.234468     3.628023     134.76
 C       0.940203    -1.221620     3.813457     114.63
 H       1.968993    -1.664499     4.049462      25.07
 H       0.974780    -1.614512     2.732775      23.69
 H       0.218881    -1.414550     4.685013      24.47
 C       0.326631     2.378671     3.373301      -5.01
 O       1.592043     2.730131     3.942067     133.60
 H       1.608988     3.769690     4.268444      19.38
 C      -0.493649     3.222425     2.530825     110.61
 H      -0.276843     4.325404     2.657563      31.45
 C      -1.826048     1.343098     1.738725      35.51
 C      -3.050364     0.947141     0.884738     110.49
 H      -3.579009     1.770480     0.975732      28.85
 O      -3.603402    -0.343317     1.490812     237.57
 H      -4.490611    -0.475894     1.161851      26.88
 C      -2.755813     0.712931    -0.595661      99.90
 H      -2.360567     1.621904    -0.913205      25.74
 C      -3.853340     0.660617    -1.533261      89.14
 O      -4.764640    -0.449818    -1.202409     303.50
 H      -4.131788    -1.090333    -1.453435      29.89
 H      -3.623011     0.609429    -2.746791      24.23
 H      -4.476486     1.705074    -1.464552      26.12
 C       1.686388     0.463418    -0.634808      32.32
 H       2.527464     1.233861    -0.736211      19.60
 C       1.502589    -2.063529    -0.777696      58.01
 H       1.873835    -2.967203    -0.975916      28.48
 C       0.160803    -1.952432    -1.017705      12.43
 O      -0.566912    -3.182804    -0.990341     126.84
 C      -0.495278    -3.919109    -2.348918      82.14
 H       0.645709    -3.704767    -2.843277      23.46
 H      -0.618374    -4.869052    -2.026259      25.30
 H      -1.037802    -3.583852    -3.345119      23.08
 C      -0.491533    -0.680006    -0.848993       5.16
 O      -1.994162    -0.589410    -0.916304      78.46
 C       0.264463     0.516266    -0.759679      61.24
 H      -0.082737     1.414817    -0.574043      26.00
 C       2.320523    -0.863888    -0.615200       9.59
 C       3.809687    -1.019144    -0.789970      63.52
 H       4.091746    -1.876331    -1.451405      26.12
 O       4.615279     0.198844    -1.352041     169.04
 H       5.023104     0.720417    -0.530537      21.92
 C       4.451876    -1.507288     0.728734      77.51
 H       3.798340    -2.396991     0.962503      25.91
 O       5.797252    -2.124276     0.642347     160.54
 H       6.534062    -1.945395     0.165139      30.09
 C       4.263636    -0.379545     1.747113     101.89
 O       4.914103     0.820279     1.246450     328.83
 H       4.796026     1.515393     1.879271      27.98
 H       4.677072    -0.503373     2.683172      26.74
 H       3.129172    -0.236608     1.817913      24.88
55
name = lig-Water-frame_495
 C      -1.557890     2.748801     1.806874      87.43
 H      -2.052760     3.450093     1.172586      18.08
 C      -0.886598     0.511824     2.309826      50.92
 H      -0.968248    -0.589664     2.363369      26.23
 C       0.146899     1.033301     3.136134      -7.93
 O       1.410895     0.253663     3.667620      35.77
 C       0.963985    -1.241289     3.817213     119.62
 H       1.905647    -1.638894     4.183928      29.56
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 H       0.750947    -1.845448     2.943387      29.99
 H       0.174796    -1.604534     4.568343      28.23
 C       0.327183     2.375524     3.309583      14.58
 O       1.583467     2.764738     3.918808      48.56
 H       1.659941     3.756610     4.169606      35.34
 C      -0.457070     3.221754     2.655471      65.62
 H      -0.524794     4.324199     2.705502      25.07
 C      -1.749253     1.403583     1.691669      22.82
 C      -3.010961     0.879754     0.859345      89.67
 H      -3.779411     1.867438     1.263014      22.75
 O      -3.619947    -0.312432     1.483607     212.43
 H      -4.544767    -0.452940     1.095658      25.26
 C      -2.681992     0.731505    -0.648922      84.65
 H      -2.043595     1.629407    -1.182783      22.54
 C      -3.896379     0.693695    -1.589581     106.57
 O      -4.822200    -0.430028    -1.230279     255.14
 H      -4.292579    -1.344097    -1.258699      24.75
 H      -3.379767     0.618250    -2.471106      30.55
 H      -4.455998     1.534579    -1.501151      29.71
 C       1.707943     0.418111    -0.668188      41.49
 H       2.342132     1.239443    -0.820493      25.73
 C       1.562317    -2.022480    -0.729536      56.54
 H       1.988116    -3.148092    -0.885496      24.79
 C       0.150486    -1.951582    -0.995497     -11.51
 O      -0.583816    -3.138253    -1.086877     164.12
 C      -0.454385    -3.877277    -2.267026     105.30
 H       0.667848    -3.600434    -2.870503      22.52
 H      -0.829234    -5.027058    -2.083049      23.39
 H      -1.186998    -3.517148    -2.938008      25.94
 C      -0.523537    -0.701573    -0.772672     -14.33
 O      -2.034293    -0.563626    -0.895996      88.16
 C       0.313466     0.493072    -0.756482      37.91
 H      -0.262144     1.525665    -0.420200      23.79
 C       2.327007    -0.920753    -0.617982      27.39
 C       3.847575    -1.026718    -0.765479      80.85
 H       3.819788    -1.949799    -1.402705      28.42
 O       4.600728     0.161118    -1.299127     207.60
 H       4.907925     0.627372    -0.558483      28.06
 C       4.485296    -1.500717     0.699990      89.17
 H       3.922279    -2.477032     0.879760      27.78
 O       5.793861    -2.123727     0.654056      90.93
 H       6.327495    -1.489926    -0.113231      23.13
 C       4.241032    -0.369441     1.745679     107.65
 O       4.902265     0.830064     1.268112     287.90
 H       4.668988     1.688513     1.810044      25.87
 H       4.843888    -0.501812     2.783229      25.85
 H       3.191967    -0.187222     1.890777      28.66
55
name = lig-Water-frame_496
 C      -1.564831     2.817855     1.855487      53.57
 H      -2.214086     3.445966     1.185138      21.95
 C      -0.920842     0.516655     2.318057      55.42
 H      -1.234986    -0.509033     2.147566      29.81
 C       0.127959     0.984795     3.158350       0.40
 O       1.402317     0.236682     3.689486      42.17
 C       1.038220    -1.261214     3.829353     115.62
 H       1.901990    -1.697301     4.379495      30.79
 H       0.518423    -1.827816     2.969677      30.54
 H       0.147037    -1.411287     4.510728      31.23
 C       0.425829     2.395482     3.278975       9.77
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 O       1.562005     2.798186     3.902670     128.59
 H       1.508435     3.824368     3.954405      28.52
 C      -0.523326     3.287839     2.719754      55.45
 H      -0.466759     4.348144     2.844167      23.88
 C      -1.723894     1.407115     1.619704      20.24
 C      -2.982404     0.868350     0.898167      99.62
 H      -3.772472     1.485568     0.948205      27.75
 O      -3.624512    -0.276237     1.467029     222.13
 H      -4.483726    -0.401692     0.989188      26.26
 C      -2.607551     0.766729    -0.710383      89.89
 H      -1.871510     1.381509    -1.024326      26.60
 C      -3.943131     0.673178    -1.608767      78.48
 O      -4.860402    -0.411293    -1.277194     245.13
 H      -4.653043    -1.332652    -0.939425      24.79
 H      -3.318963     0.554695    -2.601248      24.58
 H      -4.648909     1.707644    -1.528520      23.56
 C       1.728519     0.320404    -0.713338      80.05
 H       2.186717     1.387926    -0.761740      29.72
 C       1.576509    -2.045285    -0.713571      65.70
 H       2.090137    -2.960041    -0.660063      32.39
 C       0.124868    -1.924002    -0.928745      -7.87
 O      -0.605698    -3.082548    -1.149494     187.35
 C      -0.439022    -3.862101    -2.230829     127.80
 H       0.585117    -3.796070    -2.789796      25.72
 H      -0.659506    -4.839572    -2.155350      30.22
 H      -1.403288    -3.412361    -2.752260      23.55
 C      -0.580218    -0.686028    -0.732729     -44.03
 O      -2.010530    -0.559196    -0.870070      97.58
 C       0.326199     0.472985    -0.711301      43.36
 H      -0.180713     1.361156    -0.590823      30.94
 C       2.356472    -0.878265    -0.639806      34.84
 C       3.918122    -1.044607    -0.696126     114.03
 H       3.973466    -1.857384    -1.502060      29.82
 O       4.565841     0.086349    -1.261319     203.62
 H       4.742342     0.635768    -0.325046      22.25
 C       4.467268    -1.510950     0.653102     100.64
 H       3.838589    -2.326376     0.991513      29.61
 O       5.827807    -2.078296     0.627943     182.24
 H       5.988449    -1.366577    -0.013204      28.99
 C       4.268984    -0.357157     1.773068     106.27
 O       4.899019     0.864169     1.278925     282.51
 H       4.457690     1.711033     1.678411      28.50
 H       4.685313    -0.794401     2.670980      31.05
 H       3.137296    -0.184101     2.038473      29.98
55
name = lig-Water-frame_497
 C      -1.564025     2.865501     1.888409      50.98
 H      -2.331336     3.567764     1.464678      26.04
 C      -0.928085     0.499639     2.353385      44.77
 H      -1.320905    -0.532867     2.061440      28.73
 C       0.195353     0.937441     3.175545       5.68
 O       1.314874     0.186726     3.683868      93.52
 C       1.085862    -1.269583     3.867432     123.84
 H       1.902045    -1.839113     4.373781      29.55
 H       0.743348    -1.607123     2.892768      30.69
 H       0.231869    -0.991899     4.591277      28.74
 C       0.479463     2.380692     3.233358      -5.46
 O       1.551640     2.851579     3.901609     133.21
 H       1.476141     3.922488     3.762092      22.18
 C      -0.613963     3.364233     2.749586      46.99
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 H      -0.284784     4.440286     3.024111      21.18
 C      -1.739268     1.432063     1.587078      34.60
 C      -2.936015     0.888144     0.886927      85.73
 H      -3.907290     1.741195     0.639023      23.91
 O      -3.611510    -0.266253     1.450482     187.12
 H      -4.403751    -0.340296     0.925033      28.82
 C      -2.602525     0.745196    -0.715691      73.09
 H      -1.751746     1.574896    -0.950397      23.01
 C      -3.948060     0.662112    -1.617497     111.26
 O      -4.912286    -0.385432    -1.318020     241.70
 H      -4.539098    -1.160140    -0.841867      27.61
 H      -3.787376     0.517973    -2.702995      27.63
 H      -4.479635     1.484528    -1.620345      29.28
 C       1.712268     0.315353    -0.758170     115.44
 H       2.209741     1.225722    -0.642960      35.27
 C       1.536667    -2.039536    -0.705153      41.90
 H       2.118135    -3.032778    -0.536777      25.67
 C       0.125912    -1.898666    -0.839163      26.72
 O      -0.631548    -3.009492    -1.114738     167.08
 C      -0.489241    -3.840729    -2.288226      93.93
 H       0.709900    -3.813595    -2.887868      23.77
 H      -0.537050    -5.030505    -1.960289      25.52
 H      -1.236239    -3.604311    -3.049092      27.06
 C      -0.604721    -0.641611    -0.727564      23.06
 O      -1.945365    -0.588521    -0.846390     111.04
 C       0.305644     0.394255    -0.662639      32.45
 H      -0.037491     1.535674    -0.746474      25.30
 C       2.420679    -0.866178    -0.666672     -20.20
 C       3.952678    -1.091677    -0.665796     114.40
 H       4.305545    -1.799728    -1.440973      25.87
 O       4.549484     0.034248    -1.193564     258.02
 H       4.572769     0.672745    -0.493039      28.92
 C       4.405648    -1.520927     0.663726      93.09
 H       3.630600    -2.236207     1.182894      26.40
 O       5.847370    -1.999603     0.587612     132.34
 H       6.316543    -1.402825    -0.047740      23.93
 C       4.281091    -0.372282     1.781772     106.00
 O       4.892141     0.905999     1.292580     284.28
 H       4.404889     1.609350     1.642943      32.26
 H       4.726582    -0.924933     2.714938      27.97
 H       3.285673    -0.215694     2.019503      30.84
55
name = lig-Water-frame_498
 C      -1.605724     2.896354     1.901426      61.22
 H      -2.366351     3.641100     1.722363      24.74
 C      -0.934058     0.498257     2.368413      44.71
 H      -1.075036    -0.549612     2.297255      27.42
 C       0.283765     0.921161     3.155265      13.39
 O       1.233362     0.149758     3.662807     178.80
 C       1.078084    -1.233076     3.920564     132.79
 H       1.954516    -1.783409     4.271109      29.81
 H       0.963045    -1.656349     2.873144      29.05
 H       0.273961    -1.260401     4.650568      30.54
 C       0.421546     2.357758     3.165251      -0.04
 O       1.558025     2.929070     3.896724     205.79
 H       1.647545     3.870435     3.881494      26.01
 C      -0.600126     3.383574     2.800991      42.33
 H      -0.412170     4.386493     3.027871      21.67
 C      -1.738088     1.479799     1.650007      32.15
 C      -2.958883     0.970964     0.793183      99.18
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 H      -3.474932     1.837223     0.728429      28.26
 O      -3.579510    -0.253505     1.431524     190.80
 H      -4.453413    -0.346657     0.918779      26.55
 C      -2.614859     0.695816    -0.697799      88.89
 H      -2.175088     1.580247    -0.997037      26.47
 C      -3.921334     0.629282    -1.638102      94.06
 O      -4.957572    -0.364844    -1.330287     228.76
 H      -4.310043    -1.077211    -0.975108      25.84
 H      -3.942489     0.541643    -2.703727      26.16
 H      -4.478966     1.776010    -1.524234      24.52
 C       1.703959     0.330797    -0.777971      44.21
 H       2.363690     1.260147    -0.628057      30.20
 C       1.522967    -2.005632    -0.686346      60.57
 H       1.818379    -3.092461    -0.586813      25.34
 C       0.138972    -1.876353    -0.757801      32.99
 O      -0.681003    -2.960406    -1.060936     150.76
 C      -0.501622    -3.871282    -2.377428      81.85
 H       0.534083    -3.631005    -2.720526      27.11
 H      -0.539107    -4.741226    -1.803885      26.52
 H      -1.127298    -3.800914    -3.305164      26.06
 C      -0.561879    -0.633358    -0.739655      33.50
 O      -1.892717    -0.623566    -0.832334     111.62
 C       0.284701     0.396179    -0.631842      42.72
 H       0.126031     1.458741    -0.828656      23.62
 C       2.440859    -0.935664    -0.707702       5.61
 C       3.928960    -1.152911    -0.683459     106.26
 H       4.436762    -2.018192    -1.282038      24.32
 O       4.567136     0.029053    -1.143544     238.79
 H       4.525522     0.816406    -0.541282      25.43
 C       4.371823    -1.504061     0.746731      89.63
 H       3.806431    -2.325207     1.111096      29.06
 O       5.839964    -1.918490     0.556564      83.72
 H       6.648825    -1.569671    -0.059545      19.58
 C       4.314229    -0.409892     1.768435     105.59
 O       4.889080     0.921777     1.313391     232.50
 H       4.355182     1.674676     1.839947      27.18
 H       4.922914    -0.670774     2.689630      28.22
 H       3.173462    -0.184295     2.006304      27.69
55
name = lig-Water-frame_499
 C      -1.640810     2.918081     1.950099      57.28
 H      -2.513726     3.652947     1.756190      22.12
 C      -0.891801     0.537813     2.391051      51.63
 H      -0.937817    -0.603509     2.476308      23.77
 C       0.275907     0.960447     3.059885      18.78
 O       1.202585     0.137599     3.661602     195.85
 C       1.039048    -1.223557     3.942438     134.17
 H       2.125968    -1.424951     4.298590      26.85
 H       0.926843    -1.912370     3.065747      27.58
 H       0.260876    -1.874288     4.588570      26.69
 C       0.375014     2.403077     3.148052      15.63
 O       1.564182     2.957203     3.879996     148.50
 H       1.670565     4.085231     3.985480      22.86
 C      -0.553827     3.306847     2.815049      56.80
 H      -0.570200     4.436401     3.045751      20.09
 C      -1.745098     1.498914     1.748160      30.01
 C      -2.943309     1.025761     0.724045      81.61
 H      -3.608025     2.135732     0.850321      21.04
 O      -3.551990    -0.207362     1.394605     188.03
 H      -4.455305    -0.414860     1.049441      26.01
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 C      -2.673520     0.615564    -0.698880      84.67
 H      -2.255891     1.600485    -1.238705      20.54
 C      -3.941351     0.661429    -1.637366      92.39
 O      -4.957182    -0.346064    -1.314269     251.30
 H      -4.545690    -1.255250    -1.221624      26.19
 H      -3.612586     0.659261    -2.800298      24.61
 H      -4.223195     1.559259    -1.360620      30.05
 C       1.754252     0.313201    -0.762006      45.33
 H       2.309178     1.248155    -0.776135      29.75
 C       1.510573    -2.012216    -0.663622      63.15
 H       1.692744    -3.085600    -0.705916      23.59
 C       0.122900    -1.866910    -0.715056      29.28
 O      -0.755495    -2.936432    -1.024134     123.74
 C      -0.497844    -3.865714    -2.408102      39.51
 H       0.736261    -3.494532    -2.725583      22.44
 H      -0.608306    -4.852115    -1.829504      23.20
 H      -1.270776    -3.854653    -3.279686      23.37
 C      -0.492183    -0.666177    -0.747590       8.60
 O      -1.876104    -0.638634    -0.827697     103.68
 C       0.345778     0.495985    -0.636297      31.60
 H      -0.125123     1.518617    -0.747876      20.22
 C       2.391944    -0.993602    -0.764112      20.13
 C       3.900254    -1.195743    -0.689171     103.27
 H       4.198134    -2.085837    -1.189878      27.02
 O       4.608214     0.039226    -1.131341     238.82
 H       4.474030     0.768210    -0.366780      23.71
 C       4.414298    -1.467290     0.791133      92.30
 H       4.111246    -2.579876     1.050930      25.90
 O       5.845301    -1.875626     0.562849     137.01
 H       6.334619    -1.475873    -0.147164      27.38
 C       4.328681    -0.389903     1.778928     121.87
 O       4.870325     0.934283     1.340053     256.56
 H       4.535267     1.568512     2.027359      29.04
 H       4.975848    -0.543060     2.666798      28.14
 H       3.336373    -0.281750     2.041323      29.56
55
name = lig-Water-frame_500
 C      -1.672537     2.898028     2.033525      -3.81
 H      -2.439091     3.504480     1.691918      20.02
 C      -0.838864     0.567585     2.409105      66.97
 H      -1.097866    -0.456798     2.379148      26.76
 C       0.231961     1.049155     2.957529      29.05
 O       1.168401     0.160734     3.670533      79.98
 C       1.034153    -1.311859     3.955946     125.27
 H       1.991009    -1.255371     4.401904      24.77
 H       0.935516    -1.962245     3.062850      25.95
 H       0.347058    -1.780312     4.588704      28.25
 C       0.442821     2.462556     3.208534      16.51
 O       1.563602     2.970605     3.855935     151.89
 H       1.455415     3.919637     3.878684      30.85
 C      -0.580689     3.278318     2.770839      55.93
 H      -0.522719     4.287131     3.128570      27.61
 C      -1.794537     1.496991     1.805314      32.51
 C      -2.935120     1.082864     0.747253      99.69
 H      -3.719305     1.757848     0.723011      24.84
 O      -3.524134    -0.134793     1.362315     237.47
 H      -4.399602    -0.392335     1.077722      28.35
 C      -2.706803     0.585418    -0.750778      93.35
 H      -2.050196     1.240221    -1.278161      24.03
 C      -3.933958     0.634706    -1.627606      90.05
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 O      -4.941429    -0.320206    -1.305342     301.21
 H      -4.826384    -1.295115    -1.398658      27.55
 H      -3.444473     0.771985    -2.510709      28.34
 H      -4.385492     1.754105    -1.226917      24.58
 C       1.800512     0.305236    -0.736699      60.40
 H       2.390401     1.216008    -0.919692      24.79
 C       1.465255    -2.089935    -0.648772      56.27
 H       1.914954    -3.192456    -0.824416      21.96
 C       0.085675    -1.912260    -0.717955      22.32
 O      -0.836912    -2.941414    -1.014169     141.09
 C      -0.471674    -3.839579    -2.369263      74.58
 H       0.555569    -3.573526    -2.764887      26.25
 H      -0.532136    -4.948304    -2.157120      24.71
 H      -1.301557    -3.643723    -2.990878      25.48
 C      -0.447242    -0.611808    -0.734763     -26.60
 O      -1.877236    -0.639397    -0.829726      99.38
 C       0.422520     0.593260    -0.677092      54.78
 H      -0.323004     1.459594    -0.524797      22.13
 C       2.342623    -0.987254    -0.805630      30.95
 C       3.865053    -1.184617    -0.655977      89.39
 H       4.029947    -2.130018    -1.372592      25.15
 O       4.642278     0.035965    -1.129520     289.66
 H       4.555602     0.499821    -0.334688      29.06
 C       4.512796    -1.493942     0.760099     100.26
 H       4.117504    -2.368526     1.174861      28.86
 O       5.866569    -1.844046     0.585267     175.56
 H       5.944338    -1.222916    -0.268721      23.97
 C       4.351457    -0.333113     1.825693     112.72
 O       4.844011     0.943227     1.365104     269.95
 H       4.704823     1.550256     2.096311      29.98
 H       4.975471    -0.730726     2.780329      27.33
 H       3.236117    -0.318814     2.215335      26.26
55
name = lig-Water-frame_501
 C      -1.718444     2.811016     2.105654      42.42
 H      -2.428838     3.579447     1.578697      24.50
 C      -0.903863     0.596766     2.350155      51.51
 H      -1.215938    -0.470243     2.231144      26.39
 C       0.289195     1.135087     2.957223      25.57
 O       1.118022     0.204981     3.675431      49.30
 C       1.048869    -1.390333     3.943708      85.96
 H       2.017447    -1.563075     4.594410      23.62
 H       1.096403    -1.872920     2.919841      25.58
 H       0.166597    -1.366731     4.793748      22.79
 C       0.508498     2.484622     3.251359      23.96
 O       1.559864     2.945332     3.831168      65.44
 H       1.407926     4.051435     3.854876      22.74
 C      -0.592673     3.314019     2.751406      82.51
 H      -0.462028     4.353919     3.151238      24.37
 C      -1.864668     1.492236     1.809524      34.44
 C      -2.927076     1.057275     0.804077      78.70
 H      -3.927468     1.837127     0.615885      22.78
 O      -3.492895    -0.069808     1.361341     208.76
 H      -4.374383    -0.279529     0.899968      25.10
 C      -2.648066     0.594991    -0.771220      86.25
 H      -1.859163     1.242570    -1.297056      24.01
 C      -3.934913     0.632734    -1.554082     114.42
 O      -4.948905    -0.279315    -1.309788     287.50
 H      -4.714802    -1.270416    -1.514949      27.46
 H      -3.560388     0.755086    -2.729858      25.03
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 H      -4.474816     1.466979    -1.471440      27.50
 C       1.830597     0.352143    -0.726889      48.19
 H       2.656464     1.111449    -0.949901      23.99
 C       1.447404    -2.198138    -0.668006      49.22
 H       1.981494    -3.061259    -0.772756      24.72
 C       0.040780    -1.974075    -0.753408     -13.71
 O      -0.901698    -2.979209    -1.030173     121.70
 C      -0.487793    -3.812196    -2.279766      63.89
 H       0.665282    -3.483272    -2.871599      23.38
 H      -0.465918    -4.882537    -2.239619      24.84
 H      -1.392686    -3.242516    -2.876180      21.24
 C      -0.433371    -0.511910    -0.712880     -47.30
 O      -1.875590    -0.644463    -0.829176     104.36
 C       0.423723     0.608148    -0.715293      82.88
 H       0.019400     1.547757    -0.439609      27.80
 C       2.302493    -0.971928    -0.793239      14.32
 C       3.831699    -1.178413    -0.653354      80.67
 H       4.091875    -1.878434    -1.369396      30.51
 O       4.659278    -0.004260    -1.138705     238.98
 H       4.787887     0.583931    -0.252979      23.76
 C       4.558943    -1.515737     0.749929      91.45
 H       3.824556    -2.226061     1.363341      26.68
 O       5.914836    -1.795377     0.572942     145.84
 H       6.034945    -1.115439    -0.246384      20.09
 C       4.356386    -0.319555     1.903002     122.00
 O       4.814553     0.945819     1.394673     214.86
 H       4.851125     1.746282     2.118263      24.45
 H       4.916924    -0.773901     2.727144      30.42
 H       3.358409    -0.251184     2.223095      27.61
55
name = lig-Water-frame_502
 C      -1.773314     2.800793     2.148199      60.79
 H      -2.339031     3.535812     1.695393      23.47
 C      -0.980462     0.633511     2.276671      42.58
 H      -1.032864    -0.456270     2.165599      28.65
 C       0.320618     1.108056     2.997083      18.48
 O       1.106116     0.244139     3.688606     104.34
 C       1.054699    -1.392428     3.960337      93.29
 H       1.846951    -1.811077     4.495941      28.30
 H       1.035090    -1.866631     3.015692      30.59
 H       0.170203    -1.253196     4.436291      28.32
 C       0.447831     2.492371     3.205730      30.82
 O       1.595924     2.954577     3.839075     160.63
 H       1.731674     3.916218     3.969448      27.09
 C      -0.556793     3.358749     2.782841      75.44
 H      -0.551978     4.479211     2.949613      24.54
 C      -1.925490     1.468734     1.777216      31.41
 C      -2.961397     1.046145     0.821699      98.08
 H      -3.526074     1.927525     0.673786      27.89
 O      -3.501407    -0.054534     1.390310     238.06
 H      -4.222088    -0.259464     0.750595      25.42
 C      -2.519167     0.653752    -0.748507      82.39
 H      -2.020319     1.528072    -1.237383      26.45
 C      -3.905166     0.637982    -1.566733     110.51
 O      -4.973678    -0.271766    -1.314910     306.26
 H      -4.502312    -1.098312    -1.402979      31.42
 H      -3.884971     0.531062    -2.575426      26.93
 H      -4.526110     1.722265    -1.535781      24.85
 C       1.861759     0.380507    -0.745642      88.10
 H       2.653136     1.066685    -0.787335      32.39
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 C       1.426284    -2.213124    -0.711143      30.41
 H       2.041368    -3.296160    -0.677162      22.72
 C       0.028740    -1.985490    -0.796242     -46.35
 O      -0.931820    -3.027643    -1.042677     153.96
 C      -0.532699    -3.710647    -2.224627     112.36
 H       0.432237    -3.364124    -2.654870      25.58
 H      -0.603748    -4.887068    -2.090975      25.98
 H      -1.169542    -3.386597    -2.928099      28.81
 C      -0.462008    -0.506065    -0.707106     -65.01
 O      -1.858328    -0.638073    -0.821001     112.01
 C       0.411743     0.600579    -0.736663      60.61
 H       0.415885     1.764244    -0.496366      26.59
 C       2.270321    -0.980969    -0.725896       3.66
 C       3.827157    -1.148655    -0.651241      74.58
 H       4.273304    -1.946901    -1.437344      27.05
 O       4.665683    -0.040667    -1.132480     251.41
 H       4.985997     0.629914    -0.510122      29.41
 C       4.495660    -1.493954     0.794437      79.12
 H       3.916026    -2.277776     1.234526      29.40
 O       5.972028    -1.744316     0.541575      96.84
 H       6.403700    -1.235114    -0.107299      21.98
 C       4.362111    -0.330928     1.938483     127.81
 O       4.802723     0.962294     1.434439     217.42
 H       4.788711     1.733671     1.965094      28.15
 H       5.077247    -0.727903     2.857467      29.17
 H       3.253713    -0.192721     2.232745      26.86
55
name = lig-Water-frame_503
 C      -1.772502     2.857009     2.189700      43.70
 H      -2.528309     3.646782     1.785942      21.49
 C      -0.937296     0.632353     2.261206      65.21
 H      -0.878263    -0.428725     2.072163      29.00
 C       0.230233     1.019757     3.008487     -10.02
 O       1.155508     0.260120     3.715705     135.70
 C       1.025478    -1.323337     3.933038      76.98
 H       1.888788    -1.788680     4.586449      24.52
 H       0.834456    -1.928034     2.935851      28.71
 H      -0.109282    -1.501583     4.310650      25.16
 C       0.393215     2.513610     3.155321     -19.31
 O       1.652439     2.928887     3.862053     158.50
 H       1.741111     4.012648     3.993494      21.09
 C      -0.588899     3.392421     2.791319      54.42
 H      -0.544733     4.443969     2.770092      24.72
 C      -1.944435     1.486663     1.749393      17.73
 C      -2.938914     1.056523     0.790904      82.12
 H      -3.570638     2.164620     0.677342      24.05
 O      -3.564790    -0.083756     1.421800     181.53
 H      -4.192811    -0.500288     0.799048      25.56
 C      -2.465538     0.743220    -0.703084      80.74
 H      -2.017673     1.649528    -1.127259      25.41
 C      -3.900953     0.709419    -1.603136      88.04
 O      -4.989634    -0.280193    -1.289504     239.40
 H      -4.525013    -1.197722    -1.137485      26.13
 H      -3.752746     0.386597    -2.748957      24.44
 H      -4.126815     1.698718    -1.426248      28.89
 C       1.841401     0.322815    -0.772462      43.75
 H       2.551738     1.248012    -0.568297      33.97
 C       1.429561    -2.183520    -0.752959      63.23
 H       1.728352    -3.113926    -0.649747      30.15
 C       0.040118    -1.937695    -0.827091      -7.14
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 O      -0.934336    -3.036492    -1.021668     167.38
 C      -0.612840    -3.663589    -2.192182      84.32
 H       0.651865    -3.243411    -2.515018      22.24
 H      -0.697107    -4.657655    -1.940086      27.74
 H      -1.267579    -3.604831    -3.263214      24.54
 C      -0.491193    -0.595643    -0.727875     -16.91
 O      -1.831018    -0.585986    -0.812076     112.04
 C       0.455966     0.621724    -0.740827      19.52
 H       0.216609     1.628680    -0.693503      25.96
 C       2.281140    -1.007313    -0.647852      -4.52
 C       3.875879    -1.134778    -0.637552     114.58
 H       4.129187    -1.983641    -1.164961      29.64
 O       4.663962    -0.062507    -1.163677     243.34
 H       4.967891     0.562840    -0.496931      28.06
 C       4.445643    -1.411903     0.814635      56.69
 H       4.177771    -2.560422     1.094242      30.22
 O       6.000626    -1.726816     0.549552      14.30
 H       6.665694    -1.178204    -0.159238      15.37
 C       4.364128    -0.340211     1.961972     147.53
 O       4.808652     0.961326     1.449263     213.13
 H       4.518411     1.767190     2.089395      25.57
 H       4.986153    -0.598289     2.791881      35.27
 H       3.327220    -0.290415     2.300379      29.68
55
name = lig-Water-frame_504
 C      -1.794250     2.920414     2.181676      45.50
 H      -2.619061     3.575134     2.005353      27.09
 C      -0.848379     0.587120     2.262571      61.63
 H      -0.948924    -0.474422     1.908777      24.57
 C       0.121782     1.002354     3.033789      -7.34
 O       1.210047     0.236915     3.732971     136.55
 C       0.926596    -1.245416     3.876646     116.58
 H       1.706139    -1.424434     4.529673      27.16
 H       0.972084    -1.722044     2.944874      33.21
 H       0.093042    -1.642818     4.383450      29.67
 C       0.410530     2.491108     3.151646     -33.54
 O       1.674020     2.893557     3.871510     180.88
 H       1.516806     3.879033     3.876246      24.80
 C      -0.658378     3.409575     2.777985      73.96
 H      -0.388129     4.558471     2.736545      22.16
 C      -1.878704     1.562791     1.777499      21.07
 C      -2.938190     1.095770     0.743663      93.11
 H      -3.711251     1.807483     0.667543      24.72
 O      -3.645007    -0.113882     1.442912     186.67
 H      -4.213888    -0.720501     0.872454      25.32
 C      -2.515384     0.804917    -0.661132      81.01
 H      -1.763398     1.616865    -1.035807      19.85
 C      -3.858680     0.724950    -1.652537      68.34
 O      -4.974461    -0.276469    -1.241209     252.95
 H      -4.709828    -1.203089    -0.915710      24.88
 H      -3.403891     0.633832    -2.591847      28.14
 H      -4.150260     1.869999    -1.426689      25.97
 C       1.797530     0.279571    -0.764273      63.96
 H       2.344337     1.108234    -0.544457      31.34
 C       1.427537    -2.080397    -0.778496      35.24
 H       1.663856    -3.294607    -0.650590      23.70
 C       0.035859    -1.872683    -0.842780      25.59
 O      -0.924525    -2.973251    -0.964739     193.80
 C      -0.654615    -3.661102    -2.262021     109.96
 H       0.392485    -3.552365    -2.373806      26.95
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 H      -0.629891    -4.794754    -1.891204      25.61
 H      -1.287259    -3.575290    -3.017865      28.83
 C      -0.461241    -0.650924    -0.771001      16.23
 O      -1.821490    -0.494150    -0.803723     160.32
 C       0.472708     0.563056    -0.750973      44.84
 H      -0.194196     1.533118    -0.865200      18.85
 C       2.344477    -1.040126    -0.595832       5.73
 C       3.910493    -1.128032    -0.567743     108.94
 H       4.045561    -2.206448    -1.063333      24.64
 O       4.654013    -0.072088    -1.227284     191.83
 H       4.820962     0.464068    -0.331149      24.95
 C       4.463821    -1.356352     0.812373      75.68
 H       4.395323    -2.392176     0.994158      29.59
 O       6.033147    -1.716697     0.576635      71.77
 H       6.344825    -1.109892    -0.095477      24.16
 C       4.346939    -0.346069     1.947624     138.26
 O       4.814597     0.969387     1.472182     249.02
 H       4.210864     1.577262     2.021533      27.21
 H       5.052794    -0.678374     2.920658      28.48
 H       3.313775    -0.363426     2.387634      27.27
55
name = lig-Water-frame_505
 C      -1.843210     2.950449     2.147706      38.84
 H      -2.746184     3.590606     2.072930      24.26
 C      -0.853402     0.537798     2.200995      44.53
 H      -1.060717    -0.449731     1.885790      22.47
 C       0.151055     1.066835     3.134648      -2.27
 O       1.199814     0.215507     3.716406      64.43
 C       0.855352    -1.150187     3.823290     114.61
 H       1.777732    -1.357316     4.533001      24.14
 H       1.227664    -1.604269     2.792158      27.33
 H      -0.014048    -1.493496     4.524602      26.71
 C       0.420430     2.442778     3.175668      -0.83
 O       1.624737     2.834075     3.847406     205.99
 H       1.617540     3.899901     3.879214      22.46
 C      -0.631581     3.433167     2.786244      62.60
 H      -0.392317     4.422394     2.858441      21.61
 C      -1.788967     1.606591     1.808638      18.04
 C      -2.963169     1.089960     0.772177      75.02
 H      -3.979343     1.776276     0.678134      21.86
 O      -3.707484    -0.132563     1.462560     212.54
 H      -4.178300    -0.685707     0.817772      25.29
 C      -2.575462     0.830816    -0.660244     102.86
 H      -1.889353     1.547691    -0.965687      22.82
 C      -3.785882     0.747482    -1.624696      85.06
 O      -4.934588    -0.231383    -1.199953     255.08
 H      -4.563100    -1.135359    -0.975614      26.41
 H      -3.252870     0.741613    -2.659925      24.87
 H      -4.493141     1.603318    -1.687530      25.07
 C       1.773598     0.251702    -0.717868      38.23
 H       2.505406     1.176029    -0.642081      25.11
 C       1.440485    -2.044798    -0.774934      51.57
 H       1.744594    -2.998723    -0.761953      26.49
 C       0.033261    -1.878555    -0.856162      15.87
 O      -0.899697    -2.885893    -0.917498     160.33
 C      -0.690990    -3.744579    -2.248641      53.88
 H       0.626321    -3.636419    -2.645373      22.67
 H      -0.723448    -4.757158    -2.072259      26.08
 H      -1.596592    -3.327296    -3.032132      21.92
 C      -0.444781    -0.564400    -0.819587      23.54
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 O      -1.828266    -0.406764    -0.794499     203.51
 C       0.386645     0.441084    -0.779867      83.43
 H      -0.097755     1.377008    -0.944953      20.97
 C       2.409015    -1.034639    -0.578236      12.88
 C       3.907488    -1.182911    -0.518020     103.80
 H       4.148424    -2.049920    -1.030949      26.63
 O       4.633425    -0.079007    -1.267992     217.91
 H       4.745661     0.571441    -0.574584      28.13
 C       4.570623    -1.336704     0.817407      85.21
 H       4.130025    -2.372308     1.220471      27.08
 O       6.042597    -1.690368     0.614926     142.40
 H       6.161058    -1.005288    -0.102622      25.52
 C       4.349452    -0.368483     1.955047     129.27
 O       4.794411     0.961234     1.505239     311.01
 H       4.207322     1.636953     1.808619      28.81
 H       4.959023    -0.744139     2.704852      31.92
 H       3.297022    -0.326215     2.344273      26.23
55
name = lig-Water-frame_506
 C      -1.831255     2.984231     2.145254      33.85
 H      -2.775542     3.582333     1.973954      18.79
 C      -0.872658     0.587424     2.174320      42.16
 H      -1.106454    -0.502764     1.970072      21.20
 C       0.211417     1.077039     3.196115      13.79
 O       1.143399     0.254473     3.683705     130.06
 C       0.875174    -1.103140     3.802880     137.43
 H       1.601738    -1.603508     4.391837      28.18
 H       0.996852    -1.621237     2.903589      29.23
 H      -0.141477    -1.166449     4.223164      28.82
 C       0.394739     2.449542     3.212275      28.40
 O       1.552876     2.793162     3.807579     299.65
 H       1.778249     3.714973     3.964054      28.39
 C      -0.577383     3.397403     2.796009      75.71
 H      -0.412958     4.545334     3.083276      20.38
 C      -1.771329     1.564363     1.780376      16.74
 C      -3.041762     1.068009     0.877972      83.76
 H      -3.801623     1.887239     0.821033      22.70
 O      -3.737133    -0.134106     1.476575     214.53
 H      -4.173132    -0.521348     0.693807      23.57
 C      -2.630056     0.842728    -0.656012      84.16
 H      -2.083643     1.869614    -1.015199      19.30
 C      -3.751745     0.761468    -1.604813     109.15
 O      -4.853333    -0.175692    -1.170955     278.10
 H      -4.373527    -1.090571    -1.244575      25.14
 H      -3.438763     0.493014    -2.638433      25.46
 H      -4.533003     1.552154    -1.805637      22.82
 C       1.810975     0.258877    -0.645756      57.76
 H       2.415339     1.094441    -0.845447      20.42
 C       1.457622    -2.038134    -0.755262      49.59
 H       1.966018    -3.143832    -0.864358      21.92
 C       0.058721    -1.875244    -0.859638      10.90
 O      -0.864008    -2.847207    -0.908136     160.40
 C      -0.701587    -3.785261    -2.236624      91.67
 H       0.057434    -3.584471    -2.888150      29.07
 H      -1.009983    -4.902556    -2.090741      25.07
 H      -1.448987    -3.260445    -2.690121      26.46
 C      -0.541713    -0.533145    -0.865738      26.61
 O      -1.846802    -0.356028    -0.790905     181.40
 C       0.387468     0.413746    -0.821665      72.35
 H       0.128053     1.506863    -0.938093      22.08
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 C       2.410182    -0.978498    -0.583685      31.32
 C       3.912981    -1.218181    -0.505840      69.96
 H       4.325297    -2.093751    -1.198319      23.69
 O       4.605181    -0.094266    -1.300002     219.21
 H       4.718459     0.784811    -0.834658      27.01
 C       4.671344    -1.414391     0.864694     104.66
 H       3.935864    -2.046118     1.365459      26.76
 O       6.019982    -1.642379     0.652758     181.83
 H       6.311069    -0.945083    -0.172035      22.05
 C       4.344804    -0.356613     1.939000      96.48
 O       4.778096     0.936010     1.532482     295.94
 H       4.276342     1.847223     1.732335      24.66
 H       5.094053    -0.837956     2.854028      24.61
 H       3.304455    -0.333153     2.204300      25.28
55
name = lig-Water-frame_507
 C      -1.741798     2.969283     2.157060      41.73
 H      -2.558037     3.580176     1.876224      21.01
 C      -0.846355     0.670378     2.231665      62.22
 H      -1.031468    -0.376175     2.110601      24.45
 C       0.170121     1.047755     3.131099      41.32
 O       1.133872     0.315777     3.668553     170.34
 C       0.871480    -1.101522     3.782541     120.04
 H       1.485048    -1.751393     4.498363      25.63
 H       0.628691    -1.696225     2.750783      24.82
 H      -0.251608    -1.087357     3.975825      26.15
 C       0.348275     2.483319     3.250343      27.01
 O       1.527057     2.760109     3.784087     133.97
 H       1.687572     3.779052     4.015451      21.21
 C      -0.576285     3.388343     2.798298      60.95
 H      -0.465516     4.330390     3.207934      21.84
 C      -1.853164     1.528312     1.720515       2.66
 C      -3.092158     1.038973     0.997804      79.75
 H      -3.741236     2.083203     1.010578      22.42
 O      -3.744079    -0.116488     1.471588     213.27
 H      -4.310303    -0.373614     0.653916      21.79
 C      -2.654518     0.919097    -0.621091      85.40
 H      -2.268094     1.813188    -0.883192      24.10
 C      -3.811672     0.749525    -1.621375      92.02
 O      -4.745039    -0.142963    -1.148008     328.15
 H      -4.497186    -1.055197    -1.387102      28.68
 H      -3.497290     0.249385    -2.551804      26.73
 H      -4.140298     1.901962    -1.776225      24.95
 C       1.831694     0.291825    -0.598143      56.64
 H       2.401725     1.223024    -0.898908      20.34
 C       1.503499    -2.077285    -0.730965      55.60
 H       1.898871    -3.047088    -0.908191      23.51
 C       0.089474    -1.825519    -0.855919      12.68
 O      -0.824060    -2.887009    -0.924539     155.38
 C      -0.774100    -3.799829    -2.181455      78.14
 H       0.164500    -3.514595    -3.093180      23.49
 H      -1.126194    -4.816108    -1.981568      25.29
 H      -1.740338    -3.236408    -2.704858      22.15
 C      -0.612384    -0.568887    -0.896044       7.68
 O      -1.907687    -0.335558    -0.797458     160.99
 C       0.479821     0.511020    -0.864323      39.67
 H       0.265157     1.647320    -0.863702      21.38
 C       2.389515    -0.964747    -0.590409      30.30
 C       3.961297    -1.220188    -0.537272      80.32
 H       4.195266    -2.044697    -1.171541      26.46
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 O       4.585492    -0.117364    -1.334537     232.97
 H       4.592770     0.817093    -0.884298      25.52
 C       4.666321    -1.454975     0.906329      95.17
 H       4.131048    -2.362172     1.405287      25.98
 O       6.021979    -1.598623     0.675964     239.52
 H       6.364904    -1.108420     0.037562      33.08
 C       4.379096    -0.330796     1.945285     111.33
 O       4.782492     0.927946     1.535522     340.19
 H       4.378684     1.711224     1.986009      27.78
 H       4.867004    -0.599901     2.827650      28.58
 H       3.229426    -0.444603     2.122233      25.67
55
name = lig-Water-frame_508
 C      -1.669485     2.874056     2.123245      55.54
 H      -2.366892     3.759211     1.795100      25.88
 C      -0.860312     0.710830     2.293404      61.14
 H      -0.945323    -0.370131     2.148473      28.03
 C       0.102395     1.102436     3.019665      33.79
 O       1.174485     0.334967     3.669820     121.00
 C       0.786511    -1.140533     3.723830     120.52
 H       1.359880    -1.573616     4.535066      26.72
 H       0.758221    -1.528489     2.753601      28.70
 H      -0.270659    -1.180033     4.138786      27.57
 C       0.303971     2.453395     3.274829      16.45
 O       1.552614     2.772167     3.792635      90.63
 H       1.463013     3.721355     3.947880      27.69
 C      -0.601705     3.391863     2.813406      68.40
 H      -0.524986     4.460935     3.241086      18.19
 C      -1.918949     1.549588     1.725083       2.53
 C      -3.120492     1.063785     1.054201     104.91
 H      -3.789492     1.968773     1.166381      25.46
 O      -3.753839    -0.099104     1.453127     227.65
 H      -4.462250    -0.298742     0.831364      26.41
 C      -2.697543     0.973853    -0.559413      64.48
 H      -1.977847     1.947938    -0.793770      23.89
 C      -3.836303     0.778186    -1.649769      93.29
 O      -4.700632    -0.126587    -1.105608     336.53
 H      -4.574361    -1.073397    -1.378486      28.40
 H      -3.277366     0.312562    -2.562801      26.76
 H      -4.014470     1.849381    -1.788265      26.61
 C       1.842908     0.363467    -0.600122      46.26
 H       2.527466     1.257721    -0.655099      23.07
 C       1.527234    -2.068229    -0.711841      57.69
 H       1.840884    -3.178936    -0.873706      23.68
 C       0.088722    -1.791801    -0.860154       6.28
 O      -0.773216    -2.979068    -0.947057     208.32
 C      -0.885409    -3.708483    -2.166824     127.53
 H       0.047481    -3.744089    -2.665448      28.20
 H      -0.892763    -4.756156    -1.843482      27.01
 H      -1.785735    -3.593873    -2.754863      27.31
 C      -0.528573    -0.524338    -0.898142      -5.71
 O      -1.984268    -0.338773    -0.809677      89.21
 C       0.507565     0.611134    -0.888071      56.61
 H       0.197925     1.621685    -0.880308      25.03
 C       2.406480    -1.014671    -0.584476      21.57
 C       3.977947    -1.178807    -0.568660      84.76
 H       4.091349    -2.170801    -1.162903      26.28
 O       4.579036    -0.140833    -1.362323     261.71
 H       4.464413     0.565770    -0.751686      31.09
 C       4.591828    -1.460991     0.926990      91.62
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 H       4.613969    -2.551989     1.148828      25.96
 O       6.058225    -1.598195     0.721084     100.25
 H       6.432071    -0.975403    -0.081144      25.91
 C       4.360142    -0.338965     1.947554     116.88
 O       4.804539     0.940974     1.513196     285.95
 H       4.495960     1.565833     2.240975      26.78
 H       4.750024    -0.488210     3.130779      25.47
 H       3.312226    -0.416839     2.072321      28.32
55
name = lig-Water-frame_509
 C      -1.675994     2.849600     2.044239      59.64
 H      -2.243969     3.631581     1.734235      24.98
 C      -1.004464     0.656668     2.269326      23.71
 H      -0.961049    -0.436697     2.086770      25.27
 C       0.169610     1.175190     2.998548      -9.18
 O       1.183447     0.319653     3.652665     102.20
 C       0.682047    -1.134749     3.696540      98.20
 H       1.437204    -1.502284     4.439639      24.60
 H       1.035609    -1.577470     2.630472      25.42
 H      -0.269929    -1.266249     4.236391      25.20
 C       0.310135     2.451552     3.292184      18.05
 O       1.569539     2.806182     3.812470      -4.70
 H       1.506656     3.800049     3.950004      27.57
 C      -0.608359     3.400722     2.865992      57.68
 H      -0.636598     4.498272     2.997001      23.98
 C      -1.910413     1.556239     1.812517      71.44
 C      -3.150900     1.121012     1.017078      92.08
 H      -4.036958     1.954318     1.153319      24.88
 O      -3.762792    -0.102232     1.460144     195.90
 H      -4.586683    -0.242908     0.932323      24.57
 C      -2.701410     1.029045    -0.513340      83.91
 H      -1.960980     1.680748    -0.674419      28.96
 C      -3.752241     0.828952    -1.661308      86.46
 O      -4.734309    -0.117661    -1.058302     311.48
 H      -4.416060    -1.079915    -1.260000      26.26
 H      -3.198518     0.599336    -2.517489      28.67
 H      -4.506163     1.804532    -1.978294      24.15
 C       1.877109     0.401468    -0.625960      21.12
 H       2.584790     1.189423    -0.366087      27.10
 C       1.500728    -2.053124    -0.714191      39.07
 H       1.757633    -3.168196    -0.696111      24.51
 C       0.071019    -1.803758    -0.875744     -17.59
 O      -0.720141    -3.040426    -0.938898     155.59
 C      -0.993893    -3.673880    -2.129651     102.50
 H       0.255230    -3.731086    -2.717924      21.45
 H      -0.666539    -4.713449    -1.744331      22.98
 H      -1.923570    -3.654171    -2.861744      23.77
 C      -0.421822    -0.417374    -0.874714     -34.09
 O      -2.001454    -0.355253    -0.818926      41.25
 C       0.483115     0.662468    -0.885084      79.61
 H      -0.023482     1.759014    -0.967256      24.68
 C       2.437840    -1.010111    -0.569954       3.69
 C       3.940369    -1.186526    -0.594385      97.60
 H       4.143429    -2.178265    -1.050096      27.03
 O       4.582289    -0.168077    -1.364600     217.48
 H       4.526169     0.550842    -0.643172      29.26
 C       4.587148    -1.451918     0.895538      82.76
 H       4.443218    -2.518858     1.057197      29.13
 O       6.126884    -1.590473     0.742077      93.27
 H       6.331441    -0.901749    -0.029555      25.14
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 C       4.309665    -0.381747     1.998629     113.34
 O       4.827358     0.947569     1.478661     230.31
 H       4.704125     1.629608     2.282257      25.52
 H       4.659713    -0.634818     2.881559      31.61
 H       3.148023    -0.210389     2.082158      26.42
55
name = lig-Water-frame_510
 C      -1.664050     2.938234     2.012346      45.45
 H      -2.505273     3.622621     1.492574      22.17
 C      -1.061379     0.558583     2.287123      40.69
 H      -1.189639    -0.457245     2.007183      23.83
 C       0.221212     1.115053     2.984787     -17.94
 O       1.138381     0.292377     3.609013     151.90
 C       0.665847    -1.106587     3.680120     103.56
 H       1.489686    -1.544751     4.287400      26.11
 H       0.913515    -1.663139     2.791638      30.31
 H      -0.403226    -1.332413     4.064767      26.26
 C       0.375032     2.544432     3.310856      17.25
 O       1.572683     2.860773     3.844811     153.91
 H       1.780681     3.870861     3.980753      23.26
 C      -0.658342     3.391316     2.873995      62.82
 H      -0.581523     4.474032     2.852285      27.24
 C      -1.953743     1.518048     1.878771      24.61
 C      -3.193933     1.181515     0.945642      86.68
 H      -4.075468     1.916085     0.981265      25.50
 O      -3.762548    -0.109446     1.482132     185.47
 H      -4.620906    -0.205434     0.956616      24.33
 C      -2.702681     1.030242    -0.494845      75.83
 H      -1.823694     1.826913    -0.704989      22.16
 C      -3.727360     0.926299    -1.623652      85.80
 O      -4.769860    -0.113935    -1.046357     265.37
 H      -4.292489    -0.974333    -0.950980      25.01
 H      -3.178584     0.676536    -2.660835      24.86
 H      -4.554086     1.548018    -1.921221      24.32
 C       1.911297     0.386182    -0.656534      19.93
 H       2.558690     1.222438    -0.156252      29.72
 C       1.435145    -2.031692    -0.719071      39.02
 H       1.760385    -3.066467    -0.577256      26.80
 C       0.070367    -1.812841    -0.887730       0.04
 O      -0.679474    -3.026214    -0.881785     185.13
 C      -0.968373    -3.731956    -2.143619     115.54
 H      -0.337918    -3.422709    -2.860908      29.34
 H      -0.957656    -4.760629    -1.906872      27.32
 H      -1.944548    -3.439887    -2.672172      25.76
 C      -0.402579    -0.367976    -0.846590     -40.22
 O      -1.944571    -0.361450    -0.814764      59.73
 C       0.463862     0.719292    -0.860351      85.76
 H       0.079106     1.626834    -0.979415      25.74
 C       2.413881    -0.936213    -0.567580       5.44
 C       3.904020    -1.237499    -0.583198      95.76
 H       4.210332    -2.180398    -1.112455      26.43
 O       4.594045    -0.182876    -1.336045     192.36
 H       4.824201     0.652398    -0.792493      24.84
 C       4.627497    -1.433721     0.837230      87.57
 H       3.949066    -2.332173     1.206777      28.67
 O       6.165006    -1.567727     0.739561     122.91
 H       6.359609    -0.954009     0.116733      28.39
 C       4.209743    -0.399579     1.988331      86.34
 O       4.855319     0.926741     1.460980     187.91
 H       4.786401     1.696701     1.991868      28.14
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 H       4.824077    -0.927148     2.986057      24.92
 H       3.215739    -0.152092     2.140373      28.65
55
name = lig-Water-frame_511
 C      -1.711047     2.999279     1.990413      57.56
 H      -2.418567     3.554023     1.513850      26.91
 C      -1.027098     0.501843     2.354263      29.58
 H      -1.383675    -0.535649     2.031101      20.47
 C       0.193276     1.045941     2.967454      -3.74
 O       1.074241     0.249709     3.554570     188.38
 C       0.700107    -1.102846     3.685101     102.55
 H       1.356340    -1.592078     4.393501      27.35
 H       0.644118    -1.713507     2.605891      28.28
 H      -0.336510    -1.208466     3.892477      28.50
 C       0.402899     2.581448     3.276170      -5.75
 O       1.602871     2.934754     3.898437     213.26
 H       1.769108     3.891531     3.950569      26.14
 C      -0.700232     3.414393     2.844343      50.26
 H      -0.372111     4.536799     2.887388      23.64
 C      -2.036298     1.533094     1.896958      -5.29
 C      -3.206911     1.180999     0.910734      85.17
 H      -4.017803     2.032263     0.831040      24.19
 O      -3.760299    -0.092341     1.489067     192.98
 H      -4.579242    -0.277263     1.022173      27.02
 C      -2.650037     1.030443    -0.534122      78.65
 H      -2.075776     1.882525    -0.724265      22.76
 C      -3.736079     0.963861    -1.578875      75.71
 O      -4.782275    -0.104894    -1.060834     291.54
 H      -4.298672    -0.930598    -0.703591      24.82
 H      -3.369125     0.627811    -2.463937      27.77
 H      -4.587732     1.922736    -1.757344      23.02
 C       1.914722     0.397423    -0.656735      66.43
 H       2.474791     1.195715    -0.335193      34.62
 C       1.402361    -1.972695    -0.719160      42.61
 H       1.852017    -3.066210    -0.509910      25.57
 C       0.075756    -1.796857    -0.886940      10.35
 O      -0.661192    -2.989493    -0.818174     155.29
 C      -0.961813    -3.755255    -2.154377      72.86
 H      -0.391805    -3.201219    -3.218703      23.75
 H      -1.160354    -4.883792    -2.149685      23.94
 H      -2.058941    -3.276764    -2.319842      22.03
 C      -0.480625    -0.396451    -0.828184     -26.77
 O      -1.837040    -0.340671    -0.794578      91.15
 C       0.500066     0.708852    -0.818367      40.46
 H       0.186109     1.898028    -0.934226      21.04
 C       2.342893    -0.887322    -0.584143      41.22
 C       3.914411    -1.262318    -0.545045     100.03
 H       4.094172    -2.140070    -1.284592      27.04
 O       4.625603    -0.186771    -1.318355     209.57
 H       4.987948     0.515429    -0.822049      29.11
 C       4.611659    -1.412015     0.803378     112.63
 H       4.042493    -2.152458     1.305612      31.50
 O       6.135527    -1.566428     0.743373      60.48
 H       6.504336    -0.825125    -0.004015      19.25
 C       4.208067    -0.400439     1.956316     100.91
 O       4.888236     0.867252     1.442022     157.35
 H       4.608755     1.774366     1.926608      24.52
 H       4.656648    -0.762761     2.741090      33.76
 H       3.075719    -0.264568     2.231801      28.89
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name = lig-Water-frame_512
 C      -1.790502     2.948619     1.992620     103.96
 H      -2.450776     3.833025     1.520975      26.13
 C      -1.033936     0.541832     2.402555      52.70
 H      -1.258325    -0.486410     2.284542      21.72
 C       0.105919     1.044001     2.958328       6.69
 O       1.048837     0.202550     3.510255     212.36
 C       0.727636    -1.157349     3.650388     102.25
 H       1.223502    -1.644083     4.547017      25.58
 H       0.590918    -1.563242     2.676334      30.72
 H      -0.409214    -1.022625     4.033022      25.00
 C       0.363723     2.533383     3.190841     -24.25
 O       1.620634     2.992558     3.947842     179.07
 H       1.563050     4.078522     3.911216      22.73
 C      -0.646036     3.474770     2.812249      32.04
 H      -0.417201     4.470180     2.959406      14.99
 C      -2.067104     1.588916     1.897415      23.38
 C      -3.180340     1.130987     0.923321      77.76
 H      -3.874535     2.083813     0.730390      21.48
 O      -3.756180    -0.049583     1.478854     220.57
 H      -4.613899    -0.346794     1.068524      26.36
 C      -2.599907     1.013904    -0.588296      61.34
 H      -2.039910     2.016795    -0.811635      17.24
 C      -3.825520     0.964119    -1.501473      74.10
 O      -4.784611    -0.071801    -1.083123     367.59
 H      -4.343530    -0.922136    -0.823691      27.19
 H      -3.486984     0.545911    -2.580070      23.54
 H      -4.167516     2.017250    -1.505089      24.97
 C       1.856810     0.446133    -0.646280      17.91
 H       2.646901     1.369138    -0.662311      23.41
 C       1.451960    -1.921538    -0.702052      65.37
 H       1.773446    -2.873056    -0.608756      27.31
 C       0.050046    -1.756858    -0.871279       5.32
 O      -0.656486    -2.974916    -0.774950     129.90
 C      -1.010742    -3.686810    -2.202640      90.77
 H      -0.373191    -3.380775    -2.979587      28.32
 H      -0.839696    -4.750601    -2.251739      26.45
 H      -2.029430    -3.345533    -1.958608      21.13
 C      -0.512323    -0.432798    -0.819623       2.06
 O      -1.761477    -0.285376    -0.765043     103.87
 C       0.518400     0.683067    -0.777974      75.84
 H       0.325819     1.659176    -0.764545      27.46
 C       2.320345    -0.905437    -0.599900      35.66
 C       3.918607    -1.235204    -0.546227     111.12
 H       3.937604    -2.091688    -1.177308      29.36
 O       4.664166    -0.198535    -1.321202     184.76
 H       5.052988     0.399762    -0.578945      31.16
 C       4.566966    -1.387504     0.814279     101.68
 H       4.424999    -2.488667     1.283267      29.04
 O       6.066773    -1.559592     0.732403     109.24
 H       6.464440    -0.980741     0.036389      23.69
 C       4.227753    -0.350299     1.857364     130.01
 O       4.909324     0.820495     1.439881     206.62
 H       4.366860     1.488443     1.922205      28.82
 H       4.768622    -0.675122     2.980555      27.85
 H       3.182426    -0.406279     2.079890      28.99
55
name = lig-Water-frame_513
 C      -1.848737     2.943119     2.032612     142.94
 H      -2.390863     3.770707     1.679303      22.26
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 C      -1.120418     0.664470     2.415853      62.66
 H      -1.149806    -0.453391     2.498203      23.27
 C       0.057080     1.085875     2.991524      12.96
 O       1.067786     0.188607     3.470676     199.02
 C       0.666865    -1.200729     3.660085     114.83
 H       1.287143    -1.652484     4.414079      29.31
 H       0.731075    -1.785532     2.592971      28.73
 H      -0.251739    -1.180322     4.152737      29.07
 C       0.324086     2.482709     3.118750       5.76
 O       1.577709     3.029952     3.959510     159.43
 H       1.513582     3.995901     3.967283      28.39
 C      -0.574730     3.461666     2.749312     158.63
 H      -0.570024     4.631225     3.025160      17.31
 C      -2.054726     1.606830     1.883257      25.80
 C      -3.110595     1.098661     0.929241     124.17
 H      -3.855935     1.952555     0.822182      26.35
 O      -3.757127    -0.009380     1.466360     229.34
 H      -4.635425    -0.258555     1.052295      26.69
 C      -2.549820     0.986903    -0.616294      73.01
 H      -1.939732     1.861473    -0.894484      20.67
 C      -3.882657     0.890380    -1.469550      95.14
 O      -4.807616    -0.019038    -1.096897     417.06
 H      -4.361743    -0.907501    -1.184323      30.64
 H      -3.666786     0.849634    -2.488573      29.26
 H      -3.961077     2.105966    -1.268337      24.16
 C       1.852516     0.494415    -0.644438      47.17
 H       2.499981     1.209231    -0.915234      23.52
 C       1.467843    -1.889413    -0.688739      23.19
 H       1.808655    -3.080377    -0.750798      21.98
 C       0.040724    -1.730780    -0.833980       5.24
 O      -0.652821    -2.971436    -0.756331     120.33
 C      -1.067865    -3.607175    -2.169472      70.12
 H      -0.202340    -3.126615    -3.092644      24.12
 H      -0.579083    -4.642642    -2.049964      24.03
 H      -2.188142    -3.486944    -2.217442      22.81
 C      -0.416802    -0.441670    -0.807596      11.72
 O      -1.787828    -0.208083    -0.736194     192.14
 C       0.490901     0.620346    -0.736606      63.84
 H       0.101333     1.760961    -0.631087      22.16
 C       2.395187    -0.873471    -0.601384       7.84
 C       3.878546    -1.176336    -0.582131     105.16
 H       3.959528    -2.288202    -1.047091      25.27
 O       4.707529    -0.212603    -1.309028     238.71
 H       4.999822     0.346204    -0.517491      30.61
 C       4.548100    -1.444256     0.860143     110.84
 H       4.501752    -2.460626     1.021114      30.48
 O       5.995345    -1.552984     0.717181     196.58
 H       6.387138    -1.071551     0.010659      25.73
 C       4.296457    -0.363664     1.818007     157.43
 O       4.906577     0.807097     1.439638     229.48
 H       4.384043     1.484272     1.886283      30.09
 H       4.613810    -0.573662     2.724674      36.12
 H       3.148878    -0.257806     1.848828      29.54
55
name = lig-Water-frame_514
 C      -1.815359     3.002840     2.121156      71.99
 H      -2.620206     3.727110     1.705828      19.59
 C      -1.194481     0.767946     2.441176      60.76
 H      -1.358146    -0.313420     2.456097      24.75
 C       0.060073     1.129184     3.050050      19.14
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 O       1.081540     0.190940     3.429758     164.86
 C       0.613984    -1.237339     3.652852     111.55
 H       1.557230    -1.600692     4.223082      27.85
 H       0.790607    -1.953583     2.840742      30.08
 H      -0.400588    -1.501314     4.236392      27.19
 C       0.351162     2.495660     3.109808      16.35
 O       1.489732     3.003165     3.932765     136.02
 H       1.507374     4.078542     4.027000      24.15
 C      -0.586959     3.427872     2.653482      71.98
 H      -0.573545     4.387106     2.962931      24.62
 C      -2.040973     1.589715     1.849494      44.08
 C      -3.038948     1.121349     0.907837     102.42
 H      -3.961674     1.909236     0.940460      23.54
 O      -3.761789    -0.003056     1.461963     227.88
 H      -4.579628    -0.061018     0.965321      26.22
 C      -2.527586     0.938530    -0.608064      88.64
 H      -1.909904     1.814081    -0.960580      21.92
 C      -3.843877     0.913032    -1.451990     110.05
 O      -4.863902     0.001987    -1.094485     356.31
 H      -4.564476    -0.874188    -1.521479      28.17
 H      -3.726246     1.094320    -2.628465      25.83
 H      -4.368183     1.854434    -1.191945      26.94
 C       1.881864     0.470324    -0.659631      44.35
 H       2.529595     1.425063    -1.010184      23.31
 C       1.468322    -1.927120    -0.687369      31.14
 H       1.800466    -2.841092    -0.811381      26.60
 C       0.090283    -1.766454    -0.774580      10.33
 O      -0.669493    -2.957078    -0.771531     139.89
 C      -1.058864    -3.510337    -2.111673     105.59
 H      -0.602245    -2.878035    -2.792207      28.48
 H      -0.629262    -4.473160    -1.872706      26.51
 H      -2.041871    -3.715418    -2.714455      24.46
 C      -0.386147    -0.408318    -0.774591     -11.70
 O      -1.812486    -0.182168    -0.719545     212.92
 C       0.450638     0.635270    -0.687168      89.60
 H      -0.134027     1.516514    -0.623959      23.05
 C       2.466094    -0.793625    -0.605584     -25.62
 C       3.857606    -1.172680    -0.615506     107.69
 H       4.052316    -2.090055    -1.024716      25.65
 O       4.745034    -0.231281    -1.283071     278.57
 H       4.971054     0.466690    -0.677723      31.74
 C       4.559018    -1.510928     0.837687     105.59
 H       4.012516    -2.576129     1.115116      28.43
 O       5.954391    -1.555971     0.708963     149.79
 H       6.323179    -1.026356    -0.215534      16.63
 C       4.277712    -0.414048     1.813556     122.92
 O       4.920338     0.839573     1.414033     116.10
 H       4.536627     1.714714     1.891626      25.62
 H       4.574343    -0.752067     3.005102      28.34
 H       3.252423    -0.051445     1.717691      27.54
55
name = lig-Water-frame_515
 C      -1.805314     3.054311     2.156083      53.15
 H      -2.707575     3.624073     1.876944      20.70
 C      -1.179958     0.780365     2.509145      52.01
 H      -1.589298    -0.223540     2.303891      22.31
 C       0.074913     1.157242     3.098779      23.26
 O       1.049947     0.183384     3.389568     136.25
 C       0.618367    -1.282009     3.683957     113.08
 H       1.505100    -1.473799     4.206088      28.94
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 H       0.610338    -1.964809     2.690443      27.58
 H      -0.252473    -1.519764     4.150709      30.07
 C       0.415260     2.545047     3.148052      38.80
 O       1.390922     2.961810     3.887817     192.00
 H       1.485735     3.944617     3.980593      25.02
 C      -0.626560     3.389151     2.571495      73.33
 H      -0.406169     4.513973     2.916953      24.66
 C      -2.026304     1.661102     1.823283      35.72
 C      -3.042784     1.178141     0.886824     103.20
 H      -3.772402     1.997951     0.830353      24.02
 O      -3.758390    -0.016851     1.450917     231.96
 H      -4.559738    -0.012067     0.846912      23.98
 C      -2.554463     0.946998    -0.578529      91.75
 H      -2.035525     1.903161    -0.947172      22.22
 C      -3.800855     1.020588    -1.469898      87.66
 O      -4.926333    -0.021191    -1.109547     308.50
 H      -4.875292    -0.872495    -1.567876      30.19
 H      -3.676594     1.073095    -2.526286      27.29
 H      -4.691191     1.698238    -1.121995      22.58
 C       1.916440     0.493727    -0.705535      73.40
 H       2.415503     1.403230    -0.734206      31.69
 C       1.504467    -1.913487    -0.681715      33.76
 H       1.999667    -3.036365    -0.837182      24.10
 C       0.139309    -1.804916    -0.709035       8.77
 O      -0.718826    -2.918302    -0.782541     141.26
 C      -1.046843    -3.443849    -2.048462      93.34
 H      -0.490381    -2.521972    -2.888799      21.92
 H      -0.594574    -4.508518    -2.070779      25.83
 H      -1.983098    -3.656697    -2.529909      25.10
 C      -0.456050    -0.401751    -0.717922      -2.93
 O      -1.788268    -0.258385    -0.720305     191.85
 C       0.456377     0.675583    -0.639187      54.33
 H      -0.120911     1.664608    -0.636594      21.69
 C       2.440461    -0.762502    -0.622576      17.83
 C       3.913412    -1.168668    -0.611846      88.09
 H       4.081889    -2.124569    -1.396840      21.77
 O       4.785595    -0.249402    -1.269060     219.33
 H       4.883318     0.679947    -0.799464      25.83
 C       4.522892    -1.576488     0.788036     121.58
 H       3.857650    -2.231292     1.250067      28.82
 O       5.949442    -1.579972     0.683223     202.59
 H       6.055087    -1.152824    -0.129909      26.58
 C       4.217985    -0.432745     1.873403     104.53
 O       4.961640     0.887810     1.382080     115.36
 H       4.640445     1.584587     1.949748      27.80
 H       4.418375    -0.790746     2.802204      32.21
 H       3.159522    -0.156129     1.862971      29.09
55
name = lig-Water-frame_516
 C      -1.894810     3.048559     2.106608      32.82
 H      -2.658309     3.840920     2.006642      19.23
 C      -1.150214     0.770016     2.549003      54.51
 H      -1.478267    -0.278134     2.305989      20.10
 C       0.071367     1.155628     3.119186      24.15
 O       0.996710     0.161735     3.368210     139.10
 C       0.675119    -1.308572     3.666447      98.21
 H       1.494114    -1.645714     4.399192      25.36
 H       0.391639    -1.654791     2.643600      25.35
 H      -0.356517    -1.328965     4.316139      25.41
 C       0.358221     2.544695     3.128037      44.25
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 O       1.369669     2.941033     3.884064     192.24
 H       1.426222     3.943661     3.887390      22.77
 C      -0.551944     3.445208     2.590357      77.42
 H      -0.319781     4.473014     2.676394      24.43
 C      -1.978848     1.748418     1.854357      53.34
 C      -3.080221     1.217791     0.893674      82.53
 H      -3.703268     2.257989     0.608464      22.64
 O      -3.750570    -0.005886     1.412597     232.34
 H      -4.534402    -0.256565     0.815176      23.45
 C      -2.605179     0.994726    -0.547750      80.79
 H      -2.048161     1.894062    -0.822734      21.35
 C      -3.846663     1.088980    -1.469695      66.81
 O      -4.986319    -0.051422    -1.138637     259.27
 H      -4.887744    -0.961644    -1.510409      27.95
 H      -3.538021     1.026358    -2.575840      25.17
 H      -4.325538     2.005416    -1.192535      28.82
 C       1.880977     0.548744    -0.731650      45.83
 H       2.553107     1.487000    -0.471228      26.27
 C       1.590584    -1.918923    -0.679725      60.00
 H       2.007134    -2.848833    -0.716918      27.85
 C       0.139850    -1.789407    -0.652169       0.57
 O      -0.778076    -2.869466    -0.756197     209.83
 C      -0.976041    -3.381223    -2.064209     101.77
 H      -0.545568    -2.760953    -2.742787      28.82
 H      -0.480539    -4.289648    -2.450550      25.38
 H      -2.196581    -3.324521    -1.935198      19.85
 C      -0.475481    -0.421766    -0.642297       1.64
 O      -1.789354    -0.366148    -0.732359     165.57
 C       0.465049     0.709880    -0.607597      51.95
 H       0.271873     1.847107    -0.658927      22.05
 C       2.400757    -0.804035    -0.650214      19.04
 C       3.978277    -1.198274    -0.637807     111.47
 H       3.958160    -1.901755    -1.337678      26.80
 O       4.841691    -0.239681    -1.268404     232.77
 H       4.713803     0.632827    -0.842076      29.09
 C       4.453038    -1.537391     0.762732     102.82
 H       3.949241    -2.475703     1.313891      26.98
 O       5.940316    -1.649686     0.674333     128.84
 H       6.037857    -1.130910    -0.242893      22.65
 C       4.150585    -0.400377     1.855678      91.04
 O       4.992089     0.892801     1.372983      76.14
 H       4.629626     1.563936     2.074060      24.45
 H       4.558347    -0.828631     2.986263      27.47
 H       3.018864    -0.313667     2.055044      26.44
55
name = lig-Water-frame_517
 C      -1.912699     3.115240     2.065507      57.15
 H      -2.562555     4.049001     1.944513      17.09
 C      -1.139645     0.772881     2.530131      58.37
 H      -1.208189    -0.277816     2.442222      20.31
 C       0.024585     1.099319     3.104725      21.92
 O       0.981276     0.139715     3.383513     198.95
 C       0.672947    -1.269393     3.673705     115.58
 H       1.393102    -1.888503     4.214401      27.21
 H       0.424130    -1.707647     2.680502      27.07
 H      -0.127942    -1.151487     4.291079      29.44
 C       0.253325     2.512392     3.091922      21.12
 O       1.418407     2.946760     3.914837     151.36
 H       1.438712     3.999468     3.861957      20.42
 C      -0.524013     3.519135     2.613633      85.43
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 H      -0.231370     4.623734     2.560196      20.91
 C      -1.982610     1.724005     1.898285      51.73
 C      -3.118977     1.257723     0.917463     115.54
 H      -3.768495     2.129516     0.747392      26.09
 O      -3.744387     0.030688     1.366636     266.46
 H      -4.384576    -0.399672     0.806727      26.23
 C      -2.655978     1.016904    -0.522931      63.27
 H      -1.825688     1.819445    -0.765326      17.16
 C      -3.914193     1.081571    -1.476629      60.63
 O      -5.033899    -0.042128    -1.177228     255.02
 H      -4.495016    -0.914541    -1.396698      25.18
 H      -3.499661     0.943057    -2.515030      27.08
 H      -4.008822     2.262552    -1.408608      25.62
 C       1.842228     0.572698    -0.710472      51.69
 H       2.570272     1.312730    -0.401123      25.87
 C       1.598100    -1.916203    -0.672217      41.75
 H       2.096568    -3.005650    -0.605317      23.62
 C       0.139480    -1.734158    -0.602598       2.92
 O      -0.789975    -2.814095    -0.685593     191.94
 C      -0.976248    -3.337730    -2.082037      73.03
 H      -0.519343    -2.423495    -3.036916      23.65
 H      -0.472429    -4.260617    -2.435334      23.85
 H      -1.950563    -3.267537    -1.941635      24.00
 C      -0.411345    -0.441987    -0.567613      -0.28
 O      -1.844719    -0.441231    -0.744812     139.39
 C       0.489817     0.746200    -0.598048      72.26
 H       0.304639     1.791903    -0.610853      21.97
 C       2.420791    -0.810797    -0.688529       9.40
 C       3.963699    -1.189238    -0.664057      82.66
 H       3.975819    -2.217374    -1.380541      22.86
 O       4.896665    -0.216845    -1.275562     205.08
 H       4.678919     0.575834    -0.782663      33.38
 C       4.404412    -1.486640     0.800766     104.33
 H       4.261568    -2.514515     0.982082      28.94
 O       5.908913    -1.730510     0.662020      70.95
 H       6.315401    -1.117843    -0.141938      21.20
 C       4.120616    -0.380933     1.839588     134.72
 O       4.971187     0.858792     1.406305     134.87
 H       4.676155     1.652351     2.015377      24.32
 H       4.702131    -0.626023     2.647349      32.82
 H       3.104125    -0.203535     2.057392      26.94
55
name = lig-Water-frame_518
 C      -1.811990     3.214731     2.057195      36.48
 H      -2.553637     3.901978     1.686713      19.22
 C      -1.170080     0.754224     2.466600      53.01
 H      -1.258562    -0.393400     2.407649      20.06
 C      -0.000138     1.062920     3.087758       3.10
 O       1.018740     0.138769     3.421656     207.90
 C       0.635918    -1.209049     3.660427     114.16
 H       1.510505    -1.840017     3.992997      27.49
 H       0.416901    -1.975533     2.761809      26.22
 H      -0.260944    -1.223746     4.438061      26.90
 C       0.250990     2.501427     3.131788     -26.46
 O       1.459851     2.951154     3.927060     242.03
 H       1.553659     3.898137     3.974303      22.14
 C      -0.601245     3.586535     2.599663      36.88
 H      -0.121774     4.614772     2.623166      21.01
 C      -2.068689     1.686474     1.922969      44.88
 C      -3.136785     1.259765     0.949110     101.21
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 H      -4.089318     2.048572     1.084842      21.90
 O      -3.733741     0.066157     1.356660     243.11
 H      -4.315565    -0.330612     0.625525      22.02
 C      -2.670216     1.007961    -0.517947      80.68
 H      -1.916445     1.621986    -0.841344      24.33
 C      -3.933511     1.050145    -1.486504      94.03
 O      -5.031442     0.002056    -1.229659     352.57
 H      -4.327954    -0.643585    -1.181111      30.26
 H      -3.610924     0.784320    -2.498610      27.47
 H      -4.261840     2.050768    -1.615540      26.46
 C       1.867071     0.509843    -0.655301      53.69
 H       2.553329     1.386132    -0.518274      26.07
 C       1.553670    -1.932984    -0.654565      56.13
 H       1.952541    -2.946455    -0.543958      24.19
 C       0.169438    -1.699237    -0.557244      11.59
 O      -0.754283    -2.760884    -0.615193     185.24
 C      -0.948975    -3.241250    -2.128080      79.97
 H      -0.795675    -2.451107    -2.717570      28.41
 H      -0.494753    -4.285890    -2.129892      24.53
 H      -2.176878    -3.464073    -2.420892      23.10
 C      -0.379246    -0.416900    -0.519175      -0.74
 O      -1.895282    -0.467005    -0.740309      80.41
 C       0.489870     0.751273    -0.594818      58.88
 H      -0.085896     1.811002    -0.483202      15.37
 C       2.463575    -0.781890    -0.739415      30.62
 C       3.909783    -1.191001    -0.715921      90.50
 H       4.166659    -2.085124    -1.075043      29.81
 O       4.927721    -0.204586    -1.285168     154.39
 H       4.803102     0.642879    -0.687109      32.84
 C       4.422381    -1.440615     0.791447     101.20
 H       4.109915    -2.530257     0.938997      28.38
 O       5.892419    -1.795823     0.659948     148.11
 H       6.329282    -1.244090     0.132822      28.66
 C       4.150508    -0.349599     1.800377     125.85
 O       4.918456     0.817279     1.442007     168.26
 H       4.662253     1.591532     1.922360      28.13
 H       4.815716    -0.693094     2.772789      28.36
 H       3.064538     0.029108     2.019477      26.24
55
name = lig-Water-frame_519
 C      -1.737826     3.221208     2.025676      38.28
 H      -2.532475     3.720138     1.373426      23.89
 C      -1.234766     0.689730     2.385430      30.44
 H      -1.567285    -0.285653     2.193026      21.50
 C       0.025132     1.105643     3.076614     -17.41
 O       1.057068     0.164085     3.457944     155.45
 C       0.579638    -1.212010     3.662602     119.23
 H       1.601127    -1.478438     3.986967      27.53
 H       0.253268    -1.784251     2.803331      30.36
 H      -0.133077    -1.420432     4.421792      29.45
 C       0.303380     2.527093     3.213983     -18.96
 O       1.479799     2.922878     3.918089     158.48
 H       1.574788     3.976942     4.077672      21.35
 C      -0.622826     3.605601     2.619291      31.32
 H      -0.209275     4.574039     2.735680      25.37
 C      -2.140651     1.721579     1.949064      18.49
 C      -3.187104     1.272060     0.988349      96.76
 H      -3.995410     1.988321     1.073984      23.69
 O      -3.732581     0.055915     1.375675     234.51
 H      -4.327301    -0.131091     0.608594      22.91
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 C      -2.696432     0.966075    -0.531744      67.31
 H      -1.956221     1.750373    -1.089069      21.70
 C      -3.932364     0.999665    -1.521584      94.96
 O      -4.988278     0.071908    -1.270795     278.31
 H      -4.520955    -0.840429    -1.037014      27.85
 H      -3.586444     0.618476    -2.576831      25.19
 H      -4.676187     1.902485    -1.627980      22.42
 C       1.929677     0.463735    -0.589953      55.84
 H       2.457021     1.459895    -0.810959      23.50
 C       1.524018    -1.903576    -0.631007      61.46
 H       1.825707    -2.985299    -0.579803      24.61
 C       0.186087    -1.695006    -0.522451       9.81
 O      -0.721278    -2.730196    -0.575336     176.91
 C      -1.004497    -3.198478    -2.095014      62.11
 H      -0.652384    -2.091675    -2.834488      24.18
 H      -0.350768    -4.058847    -2.047284      25.65
 H      -1.829149    -3.539020    -2.539829      27.36
 C      -0.410611    -0.353878    -0.508948      -6.96
 O      -1.918059    -0.439232    -0.708821     130.37
 C       0.429028     0.734215    -0.572646      58.56
 H      -0.051496     1.589619    -0.450136      22.24
 C       2.460130    -0.799506    -0.787441      49.38
 C       3.906556    -1.133603    -0.720401      85.90
 H       4.293949    -2.196386    -1.192452      28.38
 O       4.930267    -0.195216    -1.293966     155.61
 H       4.985945     0.583019    -0.730705      33.39
 C       4.458930    -1.440482     0.729888     109.14
 H       3.743774    -2.164066     1.210456      31.51
 O       5.861540    -1.869567     0.692113     128.35
 H       6.375292    -1.074672     0.108782      20.90
 C       4.215144    -0.322474     1.825225     149.41
 O       4.884593     0.790273     1.440788     178.28
 H       4.516836     1.606156     2.051991      22.53
 H       4.384870    -0.838062     2.769593      32.67
 H       3.205722    -0.084214     1.927421      30.95
55
name = lig-Water-frame_520
 C      -1.769263     3.116313     1.938401      67.87
 H      -2.290080     3.816380     1.315466      25.17
 C      -1.278769     0.696618     2.336942     -17.08
 H      -1.744869    -0.311301     2.019628      18.33
 C       0.038483     1.162747     3.046172     -24.82
 O       1.047051     0.222708     3.486769      97.78
 C       0.582455    -1.224282     3.679537      95.52
 H       1.548210    -1.580119     4.030736      26.30
 H       0.097682    -1.471802     2.587865      24.88
 H      -0.117900    -1.406623     4.584398      26.01
 C       0.329028     2.569668     3.280380      18.86
 O       1.497609     2.902059     3.906629     107.02
 H       1.457187     3.863182     4.076044      29.51
 C      -0.540898     3.568078     2.696654      81.65
 H      -0.377544     4.763260     2.844709      20.01
 C      -2.127744     1.784023     1.978328      24.33
 C      -3.217515     1.291695     1.002341      69.83
 H      -4.006937     2.229468     0.739378      24.38
 O      -3.749957     0.013169     1.411796     220.52
 H      -4.525708    -0.117331     0.841598      24.07
 C      -2.704697     0.957160    -0.586604      80.21
 H      -2.197441     1.737240    -0.982010      26.03
 C      -3.928557     0.933037    -1.599679      94.75
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 O      -4.951236     0.080346    -1.271455     368.49
 H      -4.988781    -0.888750    -1.186906      30.71
 H      -3.450608     0.766406    -2.537464      28.70
 H      -4.482731     1.867447    -1.547663      26.36
 C       1.923183     0.486157    -0.566605      45.59
 H       2.477391     1.311713    -0.905336      24.01
 C       1.531300    -1.873100    -0.607148      56.70
 H       1.794864    -3.013173    -0.734371      23.24
 C       0.141259    -1.660445    -0.501789      11.61
 O      -0.722501    -2.732603    -0.556471     207.06
 C      -0.981420    -3.108446    -2.043474      87.79
 H      -0.542813    -2.359064    -2.614012      29.03
 H      -0.040491    -3.753584    -2.254533      25.64
 H      -2.078467    -3.554675    -2.375555      23.76
 C      -0.496020    -0.342540    -0.528826       8.10
 O      -1.915781    -0.358729    -0.653772     188.69
 C       0.422943     0.679156    -0.534526      49.69
 H       0.106230     1.877990    -0.469210      22.96
 C       2.435240    -0.841273    -0.803511      27.94
 C       3.991914    -1.112702    -0.713862     102.40
 H       4.032418    -1.900996    -1.389843      30.46
 O       4.919902    -0.189029    -1.317678     174.32
 H       5.014613     0.578180    -0.748578      31.01
 C       4.452665    -1.434470     0.711328     118.10
 H       3.724651    -2.011344     1.241233      31.76
 O       5.826770    -1.927704     0.723206     224.42
 H       6.222130    -1.199788     0.147039      26.61
 C       4.239705    -0.369077     1.830832     125.16
 O       4.884520     0.834418     1.446131     197.92
 H       4.625115     1.518684     2.051447      25.46
 H       4.308027    -0.890779     2.923410      28.51
 H       3.059292    -0.265211     1.746887      28.17
55
name = lig-Water-frame_521
 C      -1.735010     3.060480     1.900465      61.63
 H      -2.135837     3.969226     1.396559      22.69
 C      -1.256097     0.770662     2.354542      42.32
 H      -1.511905    -0.224791     2.104502      22.69
 C       0.004853     1.163411     2.998566     -26.70
 O       1.000941     0.297120     3.518797     117.74
 C       0.592299    -1.197601     3.683530     107.60
 H       1.426479    -1.979333     3.852577      25.92
 H       0.198154    -1.398366     2.798079      28.85
 H      -0.108316    -1.167916     4.533532      26.14
 C       0.307372     2.596235     3.298285      -4.82
 O       1.521823     2.886860     3.905848     127.87
 H       1.503515     3.882623     4.095896      28.25
 C      -0.505464     3.520248     2.752086      79.37
 H      -0.468569     4.504753     2.906073      21.72
 C      -2.117181     1.785531     1.942175      50.35
 C      -3.245302     1.322542     0.944029      81.56
 H      -3.922269     2.069149     0.688478      28.11
 O      -3.783352    -0.014840     1.459691     200.65
 H      -4.776942    -0.206733     1.226718      21.81
 C      -2.723804     0.948000    -0.611097      68.81
 H      -2.080232     1.954156    -0.885679      22.20
 C      -3.872709     0.860995    -1.650327      90.76
 O      -4.985211     0.052463    -1.253672     313.74
 H      -4.927832    -0.914147    -1.513919      28.30
 H      -3.365616     0.908867    -2.730259      25.32
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 H      -4.092353     2.011874    -1.568270      25.74
 C       1.840987     0.484894    -0.591539      39.96
 H       2.636401     1.343661    -0.825831      21.50
 C       1.515449    -1.883151    -0.601116      52.47
 H       1.837740    -2.863485    -0.779899      23.45
 C       0.072905    -1.606354    -0.493362       4.91
 O      -0.751190    -2.762326    -0.556316     233.72
 C      -0.917580    -3.076511    -1.959504      80.88
 H      -0.596416    -1.965669    -2.747494      23.58
 H      -0.174897    -3.682156    -2.412748      27.17
 H      -1.936075    -3.331598    -1.922193      25.36
 C      -0.581025    -0.369316    -0.553837      16.63
 O      -1.904845    -0.248095    -0.592850     164.91
 C       0.476180     0.706770    -0.490628      69.20
 H       0.325347     1.686998    -0.560532      28.33
 C       2.436776    -0.820631    -0.761424       6.38
 C       4.039353    -1.099383    -0.719653      95.24
 H       3.979177    -1.949299    -1.508967      25.40
 O       4.912077    -0.170126    -1.352937     205.36
 H       4.948832     0.670071    -0.723688      27.91
 C       4.437461    -1.436660     0.749332     104.86
 H       3.855076    -2.432113     0.984677      27.31
 O       5.785839    -1.981503     0.749915     264.97
 H       6.263389    -1.435316     0.152022      29.78
 C       4.189821    -0.441269     1.806644     115.45
 O       4.907215     0.883780     1.455301     156.91
 H       4.749316     1.675436     2.160306      19.72
 H       4.577033    -0.667083     2.805062      29.65
 H       3.170115    -0.283948     1.681185      30.01
55
name = lig-Water-frame_522
 C      -1.618599     3.118938     1.932661      53.57
 H      -2.230903     3.931660     1.499933      25.73
 C      -1.168484     0.852697     2.424160      63.29
 H      -1.244579    -0.245074     2.284434      22.37
 C      -0.030976     1.152966     2.978041      10.39
 O       0.952558     0.350600     3.550010     170.37
 C       0.613519    -1.131351     3.700384     106.24
 H       1.317885    -1.930219     3.703870      26.30
 H      -0.001505    -1.568518     2.662880      24.26
 H      -0.146445    -1.065918     4.475722      25.82
 C       0.297831     2.550796     3.287769      -1.20
 O       1.540733     2.885837     3.913786     120.54
 H       1.654695     3.901309     4.132248      26.46
 C      -0.572346     3.454661     2.740842      54.65
 H      -0.398015     4.644717     3.025938      23.23
 C      -2.149104     1.736841     1.819115       8.29
 C      -3.251803     1.273151     0.859594      81.24
 H      -4.228121     2.105185     0.831493      22.24
 O      -3.828263    -0.018555     1.513421     224.75
 H      -4.796243    -0.138183     1.548389      24.26
 C      -2.705953     0.984006    -0.599619      92.12
 H      -2.092768     1.768956    -0.796807      24.28
 C      -3.784104     0.846556    -1.683262     109.84
 O      -5.029470     0.018319    -1.258596     344.80
 H      -4.600425    -0.751654    -1.726155      27.79
 H      -3.578005     0.663772    -2.692983      27.80
 H      -4.042537     1.913549    -1.680551      26.36
 C       1.820785     0.470195    -0.651153      68.62
 H       2.410866     1.300575    -0.552985      30.13
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 C       1.468776    -1.850154    -0.607372      33.00
 H       1.893123    -2.993639    -0.754737      21.95
 C       0.032672    -1.603041    -0.484668      11.80
 O      -0.765748    -2.787351    -0.550978     242.96
 C      -0.835435    -2.984775    -1.916177     122.68
 H      -1.193742    -2.161231    -2.372671      27.47
 H      -0.328103    -3.912240    -2.448344      25.29
 H      -1.954953    -3.331282    -1.904790      24.11
 C      -0.562366    -0.334436    -0.558234      13.01
 O      -1.909350    -0.155358    -0.534515     210.11
 C       0.493527     0.719409    -0.466784      60.09
 H       0.188784     1.888761    -0.593401      22.75
 C       2.439695    -0.779465    -0.677754      16.48
 C       4.003010    -1.102841    -0.750933      82.03
 H       4.244958    -2.084122    -1.224250      24.66
 O       4.904285    -0.124835    -1.379515     280.51
 H       4.932705     0.623261    -0.790549      30.27
 C       4.441958    -1.525685     0.756707     114.81
 H       4.012610    -2.459134     0.736858      27.48
 O       5.758513    -2.029925     0.782345     205.67
 H       6.522282    -1.641722     0.054726      22.74
 C       4.155356    -0.442731     1.776830      96.90
 O       4.935123     0.917533     1.455691     164.26
 H       4.718213     1.566976     2.197834      23.47
 H       4.700724    -0.677084     2.735713      27.36
 H       3.021021    -0.158103     1.888080      26.32
55
name = lig-Water-frame_523
 C      -1.613272     3.143597     1.932510      61.99
 H      -2.313674     3.885462     1.601025      24.17
 C      -1.181605     0.861999     2.430692      39.98
 H      -1.222240    -0.245390     2.456990      21.93
 C       0.042108     1.216719     3.049117      28.37
 O       0.921340     0.348480     3.572819     211.13
 C       0.561707    -1.052282     3.654406     111.09
 H       1.570844    -1.598150     3.817393      24.96
 H       0.031564    -1.426892     2.928275      30.47
 H      -0.141424    -1.228366     4.574260      24.87
 C       0.321054     2.492755     3.266548      17.79
 O       1.540891     2.890137     3.917286     151.86
 H       1.570861     3.832150     4.077520      28.17
 C      -0.606412     3.478378     2.758023      52.22
 H      -0.360056     4.405387     2.974792      28.43
 C      -2.106778     1.732035     1.699177     -30.16
 C      -3.321392     1.205859     0.822205     107.43
 H      -4.057486     1.859976     0.892113      23.61
 O      -3.851757    -0.002282     1.562920     254.15
 H      -4.845867     0.069030     1.510735      24.69
 C      -2.693026     1.016596    -0.573888      77.03
 H      -1.986818     1.951082    -0.879088      20.86
 C      -3.754628     0.876989    -1.679072      93.60
 O      -5.022460     0.000962    -1.299548     293.84
 H      -4.625256    -0.857806    -1.605556      25.24
 H      -3.572677     0.241619    -2.681291      21.61
 H      -4.286601     1.870250    -1.868478      23.10
 C       1.849745     0.479992    -0.692481      50.83
 H       2.382368     1.492018    -0.359818      26.71
 C       1.435586    -1.816245    -0.616206      46.36
 H       1.688953    -2.776055    -0.631729      25.48
 C       0.042372    -1.636045    -0.468368      13.44
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 O      -0.747129    -2.788479    -0.506191     232.28
 C      -0.891742    -2.990031    -1.914194     109.82
 H      -1.401455    -1.903640    -2.453107      20.27
 H      -0.262554    -3.743265    -2.327349      26.36
 H      -1.788779    -3.622657    -2.144228      25.73
 C      -0.480449    -0.243623    -0.534206       6.86
 O      -1.896670    -0.130609    -0.476318     224.74
 C       0.422976     0.752926    -0.484051      57.09
 H       0.035642     1.739097    -0.452272      23.95
 C       2.430990    -0.795600    -0.611339       7.41
 C       3.957157    -1.111981    -0.751359      83.50
 H       4.312772    -2.084555    -1.179041      22.85
 O       4.875134    -0.090170    -1.400105     275.27
 H       5.012205     0.648975    -0.745754      25.78
 C       4.453391    -1.584848     0.693325      89.88
 H       3.713773    -2.478163     0.875758      25.18
 O       5.791438    -2.081147     0.809438     247.50
 H       6.395188    -1.712798     0.198199      27.86
 C       4.141620    -0.390784     1.775266      90.18
 O       4.949706     0.903399     1.439838     233.95
 H       4.605359     1.501083     2.182757      24.98
 H       4.596667    -0.886304     2.724859      26.31
 H       3.156620    -0.163140     2.139969      26.60
55
name = lig-Water-frame_524
 C      -1.725955     3.112960     1.886022      69.49
 H      -2.380068     4.010030     1.614109      23.27
 C      -1.234649     0.839076     2.397336      46.05
 H      -1.518057    -0.186258     2.463682      23.52
 C       0.080844     1.242375     3.121553       4.54
 O       0.913616     0.316997     3.599670     149.74
 C       0.536769    -0.993974     3.678570     117.06
 H       1.550530    -1.232918     3.899420      25.59
 H      -0.048153    -1.442852     2.639170      25.63
 H       0.046672    -1.308227     4.571566      27.92
 C       0.364180     2.563148     3.247049      34.04
 O       1.523972     2.889320     3.910958     160.10
 H       1.385161     3.939140     4.027484      19.03
 C      -0.573001     3.484311     2.798442      72.61
 H      -0.306366     4.673736     2.982133      24.53
 C      -1.988771     1.746676     1.646818       3.99
 C      -3.335489     1.128126     0.861733      81.13
 H      -4.237424     2.085864     0.807456      22.98
 O      -3.869126     0.034718     1.588085     257.09
 H      -4.839755     0.086266     1.278842      24.16
 C      -2.685293     1.068530    -0.577256      83.66
 H      -2.192554     1.958314    -0.808361      24.12
 C      -3.800180     0.869153    -1.696178      83.47
 O      -4.977757    -0.006535    -1.348765     359.36
 H      -4.878869    -1.016691    -1.199197      27.08
 H      -3.237712     0.324314    -2.380499      27.81
 H      -4.354520     1.744864    -2.147410      23.50
 C       1.869276     0.561100    -0.670981      36.17
 H       2.502582     1.368664    -0.496323      29.23
 C       1.402244    -1.779020    -0.605077      46.39
 H       1.678407    -2.990076    -0.544396      22.54
 C       0.075665    -1.614362    -0.451742      25.60
 O      -0.728564    -2.779194    -0.456291     167.24
 C      -1.049835    -3.018020    -1.962383      78.02
 H      -0.979838    -2.097436    -2.482951      25.17
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 H       0.150897    -3.286539    -2.345282      24.52
 H      -1.765726    -3.835171    -2.125223      25.03
 C      -0.460970    -0.235684    -0.491170      10.74
 O      -1.847452    -0.158761    -0.425376     178.42
 C       0.408678     0.799396    -0.531857      54.68
 H      -0.028598     1.837971    -0.320575      22.21
 C       2.413994    -0.807204    -0.594866     -10.53
 C       3.953527    -1.129376    -0.723781      85.28
 H       4.022596    -1.955688    -1.567130      21.08
 O       4.812898    -0.071616    -1.402206     268.82
 H       5.159239     0.594436    -0.669422      22.62
 C       4.429671    -1.574446     0.635908     101.44
 H       3.690460    -2.190909     1.064193      27.52
 O       5.815339    -2.139585     0.844266     224.54
 H       6.366757    -1.567712     0.197680      25.20
 C       4.200176    -0.368664     1.789190      86.41
 O       4.934786     0.839347     1.433509     254.76
 H       4.601421     1.646453     2.074751      23.26
 H       4.554230    -0.915819     2.697118      26.82
 H       3.120538    -0.147520     2.098686      25.73
55
name = lig-Water-frame_525
 C      -1.797941     3.122342     1.887787      71.14
 H      -2.374837     3.920299     1.528503      24.43
 C      -1.209726     0.822629     2.396607      64.06
 H      -1.830472    -0.149357     2.418424      22.72
 C      -0.013633     1.204997     3.124468     -30.66
 O       0.920002     0.335582     3.636384     153.36
 C       0.529459    -1.014731     3.683121     113.89
 H       1.550267    -1.566878     3.811919      26.96
 H       0.259038    -1.324764     2.797797      32.81
 H      -0.065594    -1.289567     4.664416      26.40
 C       0.389352     2.657624     3.220833       2.44
 O       1.512455     2.938306     3.910824     239.44
 H       1.497384     3.902734     4.100246      20.40
 C      -0.577623     3.536665     2.779448      76.57
 H      -0.451824     4.553758     2.913923      25.62
 C      -1.926984     1.754280     1.641548      19.90
 C      -3.304220     1.177126     0.927125     101.12
 H      -3.961595     1.888786     0.773830      28.17
 O      -3.898881     0.079354     1.582765     268.94
 H      -4.750359    -0.216952     1.174669      28.06
 C      -2.752210     1.071647    -0.561007      52.73
 H      -2.198546     2.098323    -0.720985      21.71
 C      -3.843778     0.791044    -1.708826      79.45
 O      -4.938129    -0.015556    -1.392306     396.44
 H      -4.782361    -0.816393    -0.803837      28.43
 H      -2.984016     0.418526    -2.409231      24.85
 H      -4.200012     1.649839    -2.194920      24.70
 C       1.863506     0.609339    -0.616474       1.30
 H       2.729076     1.407936    -0.709606      21.48
 C       1.435958    -1.824809    -0.571219      52.55
 H       1.729105    -2.765793    -0.564562      26.82
 C       0.061204    -1.554398    -0.440791      27.66
 O      -0.732927    -2.760605    -0.429625     159.46
 C      -1.081393    -3.073569    -1.993664      71.13
 H      -1.104693    -1.987298    -2.631128      22.31
 H      -0.145195    -2.985439    -2.266286      27.26
 H      -1.806673    -3.983808    -2.067735      24.53
 C      -0.490131    -0.295606    -0.451010      20.91
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 O      -1.799600    -0.193665    -0.392344      95.23
 C       0.473703     0.878049    -0.586451      54.36
 H       0.087215     1.915460    -0.285402      22.29
 C       2.382098    -0.744700    -0.616200      12.79
 C       3.944131    -1.140946    -0.751005     108.81
 H       3.778544    -1.775020    -1.570406      24.83
 O       4.736033    -0.061540    -1.373876     277.38
 H       5.200436     0.411303    -0.720493      29.28
 C       4.426593    -1.499455     0.649846     100.05
 H       3.769837    -2.165452     1.084450      30.00
 O       5.810294    -2.183064     0.853232     165.02
 H       6.417214    -1.429775     0.307698      23.17
 C       4.265447    -0.375608     1.789137     116.15
 O       4.912319     0.782740     1.439519     262.19
 H       4.727883     1.554205     1.905114      28.54
 H       4.698782    -0.852340     2.773324      28.76
 H       3.171073    -0.166579     1.752813      26.63
55
name = lig-Water-frame_526
 C      -1.774719     3.147081     1.943809      43.70
 H      -2.465770     3.867197     1.358502      21.83
 C      -1.167569     0.795210     2.414097      77.46
 H      -1.647162    -0.113680     2.454106      25.83
 C      -0.115095     1.197410     3.100771     -32.05
 O       0.927164     0.382214     3.683558     105.28
 C       0.581693    -1.089738     3.742451     105.74
 H       1.315505    -1.862667     3.784631      30.24
 H       0.165673    -1.395426     2.567686      28.50
 H      -0.219428    -1.189979     4.416171      30.60
 C       0.336506     2.664754     3.173994     -23.38
 O       1.522787     3.010642     3.919444     204.71
 H       1.671619     4.031625     4.196714      20.31
 C      -0.648338     3.586439     2.691971      65.73
 H      -0.549282     4.743259     2.895986      23.13
 C      -1.963005     1.767111     1.679192      14.19
 C      -3.195877     1.259281     0.965081      79.48
 H      -4.091106     2.235357     0.859046      23.25
 O      -3.922355     0.110628     1.579587     247.92
 H      -4.660474    -0.411894     1.136795      27.12
 C      -2.843058     1.048697    -0.512967      63.19
 H      -2.212547     1.911354    -0.734090      23.63
 C      -3.792184     0.695188    -1.707548     102.41
 O      -4.923860    -0.033503    -1.420841     386.00
 H      -4.495474    -0.586839    -0.752139      29.26
 H      -3.268787     0.233968    -2.580916      26.44
 H      -4.101138     1.781681    -2.107972      23.93
 C       1.885839     0.643404    -0.568270      55.99
 H       2.602507     1.385361    -0.888866      24.69
 C       1.491342    -1.805850    -0.527282      33.13
 H       1.935675    -2.959144    -0.611787      24.18
 C       0.055696    -1.566410    -0.436986      16.36
 O      -0.765238    -2.733579    -0.432655     163.48
 C      -1.084932    -3.049974    -1.992503      82.84
 H      -1.908672    -2.361052    -2.359420      24.07
 H       0.066256    -3.360933    -2.496371      23.55
 H      -1.665415    -3.903694    -2.069369      28.55
 C      -0.464835    -0.262709    -0.433463      10.43
 O      -1.806862    -0.216146    -0.375145     101.95
 C       0.524303     0.914482    -0.610349      55.35
 H       0.231500     1.928439    -0.453822      24.97
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 C       2.342596    -0.676037    -0.642643      29.12
 C       3.894784    -1.086255    -0.775772      85.26
 H       3.826440    -2.100791    -1.510979      25.56
 O       4.654644    -0.061785    -1.350780     193.41
 H       5.253680     0.359877    -0.655159      27.58
 C       4.462992    -1.436770     0.716889      90.68
 H       3.808050    -2.380051     0.961895      27.90
 O       5.787589    -2.180875     0.830448     218.55
 H       6.467554    -1.682636     0.568949      29.48
 C       4.301370    -0.422425     1.767619     154.43
 O       4.936995     0.753358     1.416048     192.97
 H       4.690727     1.610452     2.050774      22.30
 H       4.667568    -0.758216     2.742706      33.68
 H       3.206714    -0.271307     1.699912      29.60
55
name = lig-Water-frame_527
 C      -1.755801     3.158830     1.966831      43.87
 H      -2.404354     3.780165     1.419569      23.53
 C      -1.199046     0.783379     2.391273      34.07
 H      -1.334062    -0.378270     2.471209      24.17
 C      -0.070671     1.252250     3.127593     -43.40
 O       0.925033     0.404545     3.733742      90.46
 C       0.587906    -1.156688     3.716765      97.81
 H       1.397764    -1.888340     4.051045      29.35
 H       0.148100    -1.304563     2.844813      33.80
 H      -0.427916    -1.194969     4.298972      27.80
 C       0.235643     2.654807     3.138022     -37.53
 O       1.523753     3.077572     3.914765     252.76
 H       1.491151     4.100220     4.087087      15.28
 C      -0.692697     3.651847     2.611044      53.98
 H      -0.578873     4.736345     2.850759      19.52
 C      -2.018906     1.774316     1.783565      24.95
 C      -3.190224     1.370935     0.959421     106.98
 H      -3.781297     2.157577     1.054983      28.41
 O      -3.908331     0.147655     1.599167     205.06
 H      -4.647368    -0.228026     1.042978      26.95
 C      -2.868759     0.980926    -0.474547      71.22
 H      -2.203509     1.787057    -0.903886      25.14
 C      -3.713321     0.677972    -1.729267     120.75
 O      -4.932059    -0.056877    -1.425139     299.51
 H      -4.588034    -0.794854    -0.817257      27.09
 H      -3.361757     0.073851    -2.632581      25.99
 H      -4.015873     1.635472    -1.908054      27.26
 C       1.910530     0.667345    -0.564109      58.35
 H       2.540047     1.533742    -0.872881      25.64
 C       1.516689    -1.776368    -0.488427      59.22
 H       1.942486    -2.702925    -0.622208      28.44
 C       0.109289    -1.620731    -0.434588       4.72
 O      -0.809455    -2.707677    -0.480192     189.19
 C      -1.066599    -3.034195    -1.957152     112.44
 H      -2.121404    -2.584698    -2.176340      24.84
 H      -0.403153    -3.366362    -2.620225      28.87
 H      -1.529291    -4.173551    -1.849592      26.02
 C      -0.399528    -0.162677    -0.439360       4.50
 O      -1.851806    -0.227251    -0.365058     116.77
 C       0.518921     0.893107    -0.590867      56.44
 H       0.209645     2.052970    -0.787142      22.50
 C       2.350750    -0.669779    -0.657847      43.06
 C       3.820062    -1.051872    -0.762248      95.53
 H       4.073294    -2.016418    -1.152941      29.68
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 O       4.593405    -0.045777    -1.352206     197.75
 H       5.210724     0.342686    -0.640847      29.07
 C       4.508022    -1.472490     0.744402     110.58
 H       3.897349    -2.285456     0.850984      31.34
 O       5.744340    -2.174765     0.803778     179.37
 H       6.718214    -1.728998     0.670477      22.15
 C       4.288072    -0.469527     1.753299     149.04
 O       4.994361     0.787965     1.390681     171.70
 H       4.667683     1.382319     2.073655      27.78
 H       4.564119    -0.802804     2.869315      32.42
 H       3.162653    -0.334352     1.951504      31.48
55
name = lig-Water-frame_528
 C      -1.791789     3.139305     1.941237      60.71
 H      -2.480893     3.907062     1.478083      22.80
 C      -1.219135     0.774115     2.397015      38.00
 H      -1.196651    -0.262912     2.258786      23.72
 C       0.019434     1.303447     3.157506      -9.09
 O       0.913672     0.397110     3.780180      75.95
 C       0.544396    -1.163782     3.720382      94.96
 H       1.408309    -1.515988     4.293445      27.91
 H       0.266523    -1.440792     2.527717      26.52
 H      -0.256831    -1.314780     4.382973      28.53
 C       0.175831     2.685892     3.151415       5.04
 O       1.471643     3.115271     3.868152     274.37
 H       1.355051     4.118841     4.073231      15.25
 C      -0.656050     3.690698     2.585321       7.44
 H      -0.521937     4.756595     2.751732      16.85
 C      -2.057645     1.748098     1.907342      40.80
 C      -3.236014     1.400310     0.954128      63.93
 H      -3.974455     2.476248     1.103694      22.73
 O      -3.870462     0.207716     1.622129     207.17
 H      -4.697524     0.150470     1.072895      25.63
 C      -2.769642     0.901314    -0.484097      91.71
 H      -2.196299     1.742112    -1.005169      23.69
 C      -3.686209     0.653469    -1.716087      82.73
 O      -4.954226    -0.080711    -1.407520     286.93
 H      -4.944113    -1.106189    -1.203512      24.98
 H      -3.040205     0.139804    -2.557047      25.09
 H      -4.088761     1.735033    -2.025131      25.69
 C       1.923876     0.676373    -0.605546      41.55
 H       2.561551     1.633779    -0.682152      25.35
 C       1.488652    -1.738093    -0.465363      58.46
 H       1.995708    -2.801823    -0.607090      25.04
 C       0.159962    -1.601500    -0.428975       9.77
 O      -0.823079    -2.674172    -0.555053     180.58
 C      -1.140167    -3.115020    -1.847650     118.07
 H      -2.064701    -2.501459    -2.351908      23.53
 H      -0.404652    -2.994000    -2.919984      24.86
 H      -1.275459    -4.090789    -1.580188      27.43
 C      -0.379348    -0.142561    -0.450053       3.23
 O      -1.878468    -0.228021    -0.356553     130.87
 C       0.488489     0.910019    -0.570436      60.51
 H       0.137066     1.777978    -0.926523      24.25
 C       2.403010    -0.669893    -0.649004      39.44
 C       3.791318    -1.020773    -0.687951      85.42
 H       4.196903    -2.062939    -1.166901      25.55
 O       4.557510    -0.007858    -1.377067     211.45
 H       5.066913     0.413839    -0.728374      31.06
 C       4.521185    -1.530476     0.723849     106.66
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 H       3.742533    -2.345816     0.968234      28.75
 O       5.733872    -2.182964     0.770773     183.91
 H       6.622952    -1.593350     0.709913      21.75
 C       4.256048    -0.478047     1.809123     135.20
 O       5.041000     0.807786     1.382618     170.56
 H       4.736024     1.482636     2.064302      26.06
 H       4.623963    -0.854300     2.774719      32.95
 H       3.233129    -0.261080     1.986524      29.61
55
name = lig-Water-frame_529
 C      -1.825352     3.153261     1.926567      60.40
 H      -2.567932     3.875941     1.561348      28.25
 C      -1.146395     0.813346     2.464429      41.67
 H      -1.335579    -0.237840     2.042893      24.84
 C       0.033006     1.290850     3.145992      -4.35
 O       0.885355     0.378811     3.812238     118.33
 C       0.502037    -1.105057     3.701216     119.71
 H       1.458211    -1.303858     4.188400      26.25
 H       0.729073    -1.603276     2.799161      29.48
 H      -0.302210    -1.426879     4.460852      26.46
 C       0.211833     2.754400     3.219784      -4.97
 O       1.376308     3.125653     3.788428     248.77
 H       1.436787     4.107568     4.248348      17.37
 C      -0.630765     3.668321     2.569095      45.41
 H      -0.372347     4.842634     2.596140      22.99
 C      -2.118449     1.738336     1.966005       6.75
 C      -3.298018     1.411604     0.992010      84.76
 H      -3.943866     2.156447     0.801484      27.35
 O      -3.845009     0.294031     1.623692     265.11
 H      -4.825201     0.256239     1.341743      26.70
 C      -2.637206     0.877646    -0.527042      96.72
 H      -2.085666     1.746905    -0.880070      26.67
 C      -3.710637     0.624823    -1.669047     102.84
 O      -4.989213    -0.101235    -1.400217     290.32
 H      -4.883032    -1.047963    -1.667015      28.68
 H      -2.998126     0.239933    -2.353927      29.03
 H      -4.037254     1.488587    -2.118976      29.22
 C       1.914695     0.678429    -0.655979      57.18
 H       2.573855     1.483052    -0.573722      28.76
 C       1.502870    -1.747116    -0.471555      55.57
 H       1.849862    -2.807013    -0.500293      26.02
 C       0.116933    -1.505108    -0.434930      20.79
 O      -0.787480    -2.608576    -0.594988     199.49
 C      -1.202231    -3.178391    -1.827429     115.44
 H      -2.099442    -2.582135    -2.322377      24.52
 H      -0.528683    -2.707877    -2.397844      27.61
 H      -1.249065    -4.386046    -1.618071      24.66
 C      -0.422809    -0.228340    -0.451973      11.80
 O      -1.853727    -0.237809    -0.347505     168.28
 C       0.485585     0.912792    -0.560678      88.36
 H      -0.070449     1.935819    -0.976543      23.23
 C       2.418453    -0.642330    -0.604181      16.71
 C       3.890130    -1.040189    -0.626755     103.90
 H       3.864934    -1.869215    -1.370889      26.87
 O       4.534117     0.031479    -1.408297     174.91
 H       4.960292     0.672492    -0.745503      26.57
 C       4.436923    -1.553566     0.720811     103.20
 H       3.749965    -2.327698     1.078795      27.86
 O       5.755230    -2.198253     0.733527     238.77
 H       6.304092    -1.501788     0.667478      29.18
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 C       4.268808    -0.453443     1.860782      93.08
 O       5.062121     0.797858     1.404034     157.17
 H       4.903367     1.701219     1.943874      24.46
 H       4.861188    -0.898173     2.781518      27.52
 H       3.155809    -0.095911     1.895458      26.24
55
name = lig-Water-frame_530
 C      -1.836196     3.170019     1.958119      44.75
 H      -2.612926     3.817122     1.559190      25.68
 C      -1.089979     0.865103     2.514132      58.60
 H      -1.383331    -0.119388     2.154826      24.86
 C      -0.005342     1.276085     3.127768      -0.89
 O       0.833122     0.369623     3.817708     186.56
 C       0.533375    -1.021765     3.742648     125.65
 H       1.476702    -1.436998     4.195679      24.41
 H       0.798138    -1.630888     2.737451      26.96
 H      -0.380341    -1.417903     4.200019      27.20
 C       0.227524     2.773992     3.263768     -25.29
 O       1.341913     3.150153     3.749133     140.82
 H       1.384676     4.041148     4.209280      22.01
 C      -0.636498     3.637170     2.540130      55.29
 H      -0.328571     4.603629     2.480943      30.34
 C      -2.161906     1.805784     1.966246      -2.78
 C      -3.268387     1.363843     1.021883      87.28
 H      -4.108966     2.138748     0.429608      21.95
 O      -3.876139     0.352319     1.636396     272.03
 H      -4.810220     0.099522     1.587612      27.53
 C      -2.573057     0.922231    -0.539268      70.58
 H      -1.890750     1.842727    -0.783170      24.54
 C      -3.740378     0.592468    -1.594424      80.39
 O      -5.011328    -0.100299    -1.418276     259.27
 H      -4.661167    -0.959640    -1.805484      26.37
 H      -3.107650    -0.072828    -2.466366      23.48
 H      -4.014608     1.590779    -2.137894      25.88
 C       1.858407     0.667498    -0.688822      53.59
 H       2.695614     1.520071    -0.615541      24.18
 C       1.512118    -1.733719    -0.487930      26.07
 H       1.773909    -2.828096    -0.430395      24.09
 C       0.070858    -1.466138    -0.478420      31.51
 O      -0.751014    -2.548175    -0.555433     211.22
 C      -1.245920    -3.221415    -1.824040      87.60
 H      -2.384460    -2.953812    -2.075053      24.17
 H      -0.278126    -2.755893    -2.434861      23.70
 H      -1.279815    -4.226142    -1.954234      28.44
 C      -0.477291    -0.256741    -0.454126      26.48
 O      -1.793760    -0.272172    -0.339931     157.36
 C       0.453622     0.906612    -0.586025      76.83
 H       0.089159     1.832664    -0.669661      28.79
 C       2.398522    -0.642818    -0.522775      -2.03
 C       3.984777    -1.055793    -0.627435     108.98
 H       3.636919    -1.703242    -1.502205      23.23
 O       4.544336     0.065758    -1.414846     170.22
 H       4.719952     0.902666    -0.845481      25.60
 C       4.350603    -1.543113     0.750933     101.50
 H       3.736575    -2.338571     1.033742      27.21
 O       5.755152    -2.213601     0.698527     172.26
 H       6.303340    -1.255867     0.553759      23.18
 C       4.317908    -0.399842     1.884033     111.31
 O       5.082194     0.780120     1.428004     257.26
 H       4.891424     1.536163     1.911993      30.83
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 H       4.767029    -0.784136     2.749331      29.91
 H       3.324562    -0.123530     2.016338      27.88
55
name = lig-Water-frame_531
 C      -1.860909     3.187439     2.003906      54.89
 H      -2.565873     3.908292     1.477236      22.22
 C      -1.182628     0.925151     2.481863      53.06
 H      -1.270617    -0.181154     2.463592      25.91
 C      -0.011197     1.310731     3.164336      -8.69
 O       0.782091     0.387815     3.811545     179.47
 C       0.628934    -0.999566     3.758045     143.26
 H       1.269654    -1.577983     4.400844      26.33
 H       0.467791    -1.206283     2.679324      27.94
 H      -0.452317    -1.266799     4.009489      25.77
 C       0.147731     2.710875     3.228734     -22.32
 O       1.404527     3.181928     3.759500     132.69
 H       1.277003     4.216328     4.132577      19.38
 C      -0.646106     3.581150     2.530380      57.82
 H      -0.256048     4.737465     2.382300      25.06
 C      -2.145191     1.885795     1.946444       3.79
 C      -3.228156     1.352247     0.954847     106.72
 H      -3.843609     2.073774     0.680611      28.39
 O      -3.934041     0.337803     1.699697     267.39
 H      -4.887412     0.073475     1.379075      24.52
 C      -2.564904     0.972168    -0.488338      83.91
 H      -1.955767     1.739954    -0.840961      29.51
 C      -3.727295     0.585316    -1.588550      99.40
 O      -5.011802    -0.080280    -1.447836     310.09
 H      -4.790106    -1.063117    -1.545997      26.61
 H      -3.372015    -0.066826    -2.323496      25.57
 H      -3.891996     1.586361    -1.941881      27.53
 C       1.814410     0.656963    -0.687521      46.32
 H       2.416213     1.460949    -0.809656      28.84
 C       1.472001    -1.697736    -0.500681      44.08
 H       1.818118    -2.819928    -0.376871      22.46
 C       0.115959    -1.518421    -0.554973      28.18
 O      -0.758631    -2.559236    -0.474939     190.67
 C      -1.226956    -3.185327    -1.844250     100.75
 H      -2.275815    -3.097427    -2.028375      26.02
 H      -0.672531    -3.070177    -2.736986      28.22
 H      -1.133365    -4.417362    -1.930734      25.07
 C      -0.467910    -0.179032    -0.471203      28.94
 O      -1.779038    -0.296128    -0.335200     155.24
 C       0.422997     0.854065    -0.608720      75.56
 H       0.158044     2.025524    -0.382165      26.14
 C       2.380254    -0.659513    -0.443552       3.50
 C       3.956037    -1.010937    -0.686548     100.14
 H       3.992168    -1.839398    -1.392646      24.10
 O       4.584343     0.095290    -1.399277     230.96
 H       4.483935     0.888194    -0.928360      29.97
 C       4.351981    -1.515036     0.787584      84.04
 H       3.595835    -2.408263     0.958631      24.66
 O       5.729650    -2.183347     0.673240     209.41
 H       6.436514    -1.500411     0.423191      24.86
 C       4.375160    -0.358114     1.862624     100.66
 O       5.109499     0.748517     1.438210     242.56
 H       4.735057     1.464384     2.117112      25.57
 H       4.728851    -0.790403     2.951769      24.84
 H       3.268577    -0.101379     2.232981      24.76
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name = lig-Water-frame_532
 C      -1.901372     3.267595     2.022929      50.97
 H      -2.416463     3.993109     1.476986      20.20
 C      -1.299541     0.965913     2.449468      72.87
 H      -1.390646    -0.120448     2.671803      26.80
 C      -0.067776     1.328136     3.201418       7.17
 O       0.773817     0.455556     3.831723     146.87
 C       0.629631    -0.995217     3.717543     139.14
 H       1.218799    -1.662130     4.389609      27.57
 H       0.536038    -1.089110     2.597068      29.63
 H      -0.415654    -1.098744     4.068967      26.86
 C       0.155287     2.662387     3.203980       4.75
 O       1.452305     3.213223     3.772085     159.99
 H       1.381127     4.113979     4.077394      23.74
 C      -0.646774     3.596349     2.527716      57.72
 H      -0.340427     4.524708     2.461539      28.45
 C      -2.124608     1.860004     1.892855       5.26
 C      -3.163732     1.336918     0.900822      82.58
 H      -3.881459     2.410874     0.921787      23.16
 O      -4.005410     0.297448     1.758541     203.52
 H      -4.725478     0.176576     1.078478      24.97
 C      -2.627172     0.938261    -0.402004      85.07
 H      -2.011308     1.762597    -1.014893      25.72
 C      -3.699845     0.608224    -1.581072      78.06
 O      -5.016567    -0.055080    -1.460387     271.60
 H      -4.985461    -1.025710    -1.094196      26.26
 H      -3.095956    -0.027122    -2.530934      21.92
 H      -3.938629     1.656140    -1.922534      26.95
 C       1.788085     0.596884    -0.661802      28.65
 H       2.297185     1.638286    -1.021255      26.31
 C       1.451156    -1.715827    -0.492118      58.66
 H       1.851443    -2.673629    -0.418756      26.85
 C       0.143969    -1.533166    -0.627915      21.13
 O      -0.790603    -2.629437    -0.429237     150.57
 C      -1.172196    -3.217140    -1.856287      81.47
 H      -2.438616    -3.024840    -2.032620      21.64
 H      -0.903986    -2.928378    -2.987221      24.01
 H      -0.965967    -4.152145    -1.475609      24.41
 C      -0.414872    -0.177900    -0.507134      19.47
 O      -1.808552    -0.281619    -0.327715     129.86
 C       0.400928     0.885118    -0.609362      79.40
 H       0.166017     1.844700    -0.299903      29.64
 C       2.387903    -0.635631    -0.435776      21.92
 C       3.855088    -0.948669    -0.725215      86.36
 H       4.400819    -1.916173    -1.149623      21.77
 O       4.635662     0.105434    -1.374243     230.01
 H       4.297416     0.931668    -0.878545      28.25
 C       4.419997    -1.472617     0.787305      91.56
 H       3.727998    -2.197985     0.978452      29.77
 O       5.682601    -2.154931     0.661315     242.06
 H       6.422412    -1.702311     0.303474      25.27
 C       4.380534    -0.393929     1.890850     127.61
 O       5.132392     0.750591     1.461424     218.59
 H       4.797981     1.437967     2.145320      27.67
 H       4.810337    -0.773219     2.752697      31.62
 H       3.424080    -0.059534     2.123517      28.04
55
name = lig-Water-frame_533
 C      -1.915276     3.320900     2.016881      37.24
 H      -2.459067     4.157258     1.420480      19.40
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 C      -1.324357     0.944540     2.508861      80.99
 H      -1.798890    -0.037316     2.492740      24.81
 C      -0.182611     1.312040     3.212395      13.00
 O       0.804103     0.534027     3.875713     135.36
 C       0.545149    -0.963705     3.646197     119.25
 H       1.362755    -1.509884     4.129251      28.66
 H       0.866476    -1.358931     2.585956      29.13
 H      -0.399421    -1.203396     4.146681      26.18
 C       0.262012     2.707450     3.204118      -8.21
 O       1.465701     3.186202     3.754321      65.93
 H       1.414268     4.242760     4.187867      19.31
 C      -0.661922     3.609508     2.549596      57.80
 H      -0.268920     4.781701     2.608603      24.35
 C      -2.137589     1.847313     1.802917      -1.13
 C      -3.168665     1.386533     0.957650      99.62
 H      -3.775032     2.130813     0.802921      28.53
 O      -4.045779     0.283819     1.766481     185.51
 H      -4.761137     0.070077     1.080840      24.95
 C      -2.703902     0.865277    -0.401612     103.42
 H      -2.203555     1.664546    -0.804786      29.11
 C      -3.668578     0.622606    -1.610012      94.46
 O      -5.016012    -0.024618    -1.455660     320.79
 H      -4.907719    -0.763683    -0.767077      27.03
 H      -2.988402     0.311837    -2.326367      29.29
 H      -4.078717     1.605919    -1.954940      26.35
 C       1.792802     0.610491    -0.653664      57.34
 H       2.338865     1.408339    -0.973307      30.05
 C       1.491183    -1.745680    -0.468486      20.23
 H       1.972404    -2.888038    -0.485456      23.38
 C       0.086678    -1.534856    -0.655666      12.62
 O      -0.800503    -2.676759    -0.438233     181.85
 C      -1.182424    -3.252747    -1.857162      99.50
 H      -2.142270    -3.126520    -1.925155      27.29
 H      -0.736411    -2.645644    -2.645630      27.71
 H      -0.866600    -4.272619    -1.436197      21.81
 C      -0.427193    -0.261011    -0.550827      26.25
 O      -1.826957    -0.252267    -0.313123     166.30
 C       0.405568     0.920602    -0.586925      58.40
 H      -0.006140     1.991674    -0.359189      24.72
 C       2.390932    -0.620585    -0.515280      37.57
 C       3.820994    -0.915441    -0.702266      93.74
 H       4.167292    -1.787954    -1.159062      26.90
 O       4.667111     0.118296    -1.331796     222.39
 H       4.317051     0.978686    -0.921908      31.72
 C       4.499484    -1.379943     0.753547      87.65
 H       3.727706    -2.220069     1.136055      27.11
 O       5.628548    -2.145844     0.669402     174.27
 H       6.437219    -1.697251    -0.009977      19.54
 C       4.392537    -0.450439     1.899563     121.59
 O       5.158259     0.783106     1.495730     183.58
 H       4.993032     1.523852     2.037341      29.88
 H       5.026622    -0.937858     2.822396      28.88
 H       3.291861    -0.073827     2.015056      25.12
55
name = lig-Water-frame_534
 C      -1.908522     3.314033     1.965340      28.01
 H      -2.503028     4.066847     1.543221      21.31
 C      -1.359258     0.895507     2.574604      61.05
 H      -1.935544    -0.017741     2.313101      22.25
 C      -0.222942     1.341995     3.244472      -5.32
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 O       0.807518     0.567034     3.897174      95.81
 C       0.511151    -0.924338     3.582173     120.52
 H       1.459444    -1.210832     4.106766      28.37
 H       0.718902    -1.332510     2.615458      30.97
 H      -0.405153    -1.442412     4.049418      27.45
 C       0.315128     2.778964     3.179768       6.46
 O       1.466870     3.159921     3.740973     162.12
 H       1.380492     4.004652     4.118024      27.40
 C      -0.633402     3.680285     2.610659      57.38
 H      -0.411736     4.670100     2.739894      26.25
 C      -2.110356     1.931340     1.775704      12.51
 C      -3.258657     1.358991     1.024281      82.78
 H      -4.098632     2.219022     0.524574      23.18
 O      -4.045336     0.298459     1.742289     242.18
 H      -4.959526    -0.048545     1.419628      27.00
 C      -2.779378     0.805384    -0.428003      88.18
 H      -2.170272     1.823044    -0.670484      22.47
 C      -3.709002     0.665935    -1.611257      85.01
 O      -4.985858     0.011795    -1.438126     338.08
 H      -4.825542    -0.639640    -0.775263      28.11
 H      -2.825475     0.314223    -2.494271      22.99
 H      -4.032495     1.649127    -1.932478      26.61
 C       1.786538     0.677981    -0.655487      51.98
 H       2.659254     1.488053    -0.855700      28.90
 C       1.535142    -1.795145    -0.466155      38.18
 H       1.857660    -2.723914    -0.497115      27.57
 C       0.058347    -1.598983    -0.622010      -5.87
 O      -0.794603    -2.693050    -0.478210     203.59
 C      -1.144245    -3.296413    -1.784114      97.06
 H      -2.475723    -3.277132    -1.931389      20.27
 H      -0.435291    -2.621068    -2.351317      27.19
 H      -0.845109    -4.385900    -2.136382      25.11
 C      -0.496828    -0.278968    -0.584204      24.79
 O      -1.829133    -0.250627    -0.294709     153.94
 C       0.400810     0.910960    -0.545126      61.83
 H      -0.097020     1.917492    -0.668660      24.96
 C       2.351459    -0.658030    -0.629210      11.99
 C       3.870664    -0.886667    -0.627618      95.51
 H       3.731318    -1.812759    -1.478937      24.06
 O       4.677265     0.135154    -1.286914     200.94
 H       4.508903     0.989404    -0.967950      35.68
 C       4.478176    -1.325707     0.717701     111.71
 H       3.815422    -2.029222     1.093818      28.95
 O       5.642735    -2.139477     0.650066     235.79
 H       6.131533    -1.833306    -0.043965      28.98
 C       4.439987    -0.441807     1.920757     153.99
 O       5.190932     0.810418     1.524942     133.03
 H       5.037977     1.700682     2.125607      24.05
 H       4.811966    -0.935529     2.722353      35.42
 H       3.390330    -0.326010     2.101172      27.88
55
name = lig-Water-frame_535
 C      -1.833661     3.288934     1.926311      66.83
 H      -2.627708     4.040849     1.608628      25.18
 C      -1.418723     0.914914     2.589658      44.58
 H      -1.637905    -0.159096     2.466048      22.18
 C      -0.179195     1.411746     3.283024     -18.20
 O       0.748372     0.559422     3.879711      81.09
 C       0.548092    -0.890205     3.575273     111.42
 H       1.395074    -1.214662     4.169303      28.82
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 H       0.381915    -1.000230     2.361724      28.50
 H      -0.320181    -1.373394     3.942290      29.68
 C       0.240394     2.802632     3.120871      30.44
 O       1.487022     3.113933     3.733877     176.05
 H       1.376451     4.152598     4.152953      20.78
 C      -0.623976     3.739894     2.671260      71.12
 H      -0.488279     4.911762     2.839998      20.14
 C      -2.089421     1.988644     1.822092      25.43
 C      -3.451219     1.313786     1.000850      98.56
 H      -4.037828     2.045866     0.691397      25.66
 O      -4.023220     0.312947     1.732748     300.95
 H      -5.026285     0.190017     1.668367      27.74
 C      -2.801300     0.843676    -0.427185      96.51
 H      -2.239866     1.667911    -0.660164      26.98
 C      -3.743840     0.711668    -1.640819      92.72
 O      -4.941867     0.054738    -1.425050     368.15
 H      -4.820197    -0.835409    -0.891776      25.73
 H      -3.259234     0.223451    -2.439505      26.60
 H      -3.885163     1.838566    -1.892768      26.15
 C       1.804184     0.734288    -0.671432      43.51
 H       2.521470     1.521650    -0.568726      27.95
 C       1.493198    -1.790956    -0.502103      52.51
 H       1.929457    -2.973995    -0.462688      23.24
 C       0.093138    -1.650095    -0.549827      -6.06
 O      -0.798996    -2.738734    -0.502112     204.29
 C      -1.130604    -3.336101    -1.757131     138.45
 H      -2.031573    -3.294604    -2.006972      30.72
 H      -0.525732    -2.714806    -2.498593      27.14
 H      -0.798400    -4.267085    -2.343196      27.29
 C      -0.532362    -0.265020    -0.593888       7.47
 O      -1.846741    -0.280547    -0.276168     148.59
 C       0.377477     0.858274    -0.538949      88.19
 H      -0.055784     1.818373    -0.819652      27.43
 C       2.298408    -0.661757    -0.708554      14.38
 C       3.910731    -0.883684    -0.606843     110.18
 H       3.805984    -1.529501    -1.361684      27.53
 O       4.688674     0.138966    -1.260844     191.93
 H       4.638075     1.047693    -0.801397      30.60
 C       4.423073    -1.329275     0.693758      94.55
 H       3.573458    -2.092366     1.022334      27.11
 O       5.672752    -2.137508     0.630474     163.08
 H       6.213833    -1.909238    -0.269376      21.16
 C       4.492428    -0.363442     1.904078     145.30
 O       5.220459     0.847883     1.571973     174.24
 H       4.895302     1.498156     2.218828      28.12
 H       4.847786    -1.018456     2.898058      29.25
 H       3.386391    -0.271805     2.254698      27.74
55
name = lig-Water-frame_536
 C      -1.732030     3.338526     1.919946      80.79
 H      -2.556102     3.982760     1.635329      25.90
 C      -1.405890     1.007814     2.606654      55.64
 H      -1.375020    -0.074002     2.701251      22.00
 C      -0.173380     1.457683     3.264855      10.73
 O       0.668494     0.547270     3.856743     171.75
 C       0.587325    -0.834525     3.546633     121.41
 H       1.415109    -1.500497     3.963610      28.06
 H       0.440564    -0.762713     2.544655      30.91
 H      -0.418295    -1.183364     4.048801      26.24
 C       0.182747     2.786349     3.114285      20.11
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 O       1.491750     3.098057     3.739868     277.55
 H       1.521780     3.984507     4.026638      26.30
 C      -0.680528     3.828624     2.683275      44.10
 H      -0.507495     4.897878     2.893207      19.61
 C      -2.147332     1.903943     1.878670      24.89
 C      -3.538267     1.284477     0.948078      69.47
 H      -4.360299     2.283731     0.814449      21.02
 O      -4.018464     0.299383     1.756336     283.03
 H      -5.002699     0.480444     1.654339      24.58
 C      -2.799956     0.900937    -0.411667      75.90
 H      -2.086978     1.786562    -0.742967      21.42
 C      -3.752865     0.774829    -1.649924      89.69
 O      -4.942089     0.082308    -1.393390     295.49
 H      -4.765859    -0.899177    -1.271602      25.57
 H      -3.439230     0.083702    -2.653847      21.72
 H      -3.918603     1.785317    -1.891230      27.64
 C       1.786334     0.696041    -0.674339      44.60
 H       2.351560     1.686148    -0.438700      24.03
 C       1.440097    -1.818863    -0.566427      75.28
 H       1.877326    -2.681748    -0.446218      26.85
 C       0.107109    -1.637619    -0.478357       8.65
 O      -0.807317    -2.809500    -0.496418     140.87
 C      -1.052990    -3.342601    -1.822219     106.56
 H      -2.359295    -3.165093    -2.137485      22.08
 H      -0.798314    -2.691954    -2.717741      22.77
 H      -0.565233    -4.428369    -1.866882      25.29
 C      -0.504754    -0.295530    -0.567513       5.77
 O      -1.894141    -0.321988    -0.261662     133.25
 C       0.352860     0.802970    -0.577782      93.54
 H      -0.056847     1.906934    -0.760752      24.75
 C       2.291021    -0.596616    -0.728307      12.71
 C       3.891432    -0.840319    -0.637589      81.58
 H       4.261773    -1.832777    -1.416761      21.94
 O       4.707502     0.162874    -1.244838     220.37
 H       4.718322     0.894808    -0.539322      29.55
 C       4.373270    -1.397700     0.720983      86.13
 H       3.600285    -2.074757     0.948051      27.25
 O       5.696416    -2.121967     0.604905     144.67
 H       6.288972    -2.042153    -0.292680      20.72
 C       4.515475    -0.320870     1.902373     129.62
 O       5.238768     0.879452     1.635569     209.61
 H       4.799569     1.497493     2.299735      26.91
 H       5.030177    -0.797047     2.645941      33.35
 H       3.554871     0.088089     2.242557      25.44
55
name = lig-Water-frame_537
 C      -1.713202     3.357123     1.912608      75.83
 H      -2.429113     4.090084     1.517953      29.79
 C      -1.336767     1.092405     2.645053      64.15
 H      -1.568499     0.009823     2.780169      22.56
 C      -0.208050     1.477706     3.203020      30.70
 O       0.627303     0.569340     3.866754     207.89
 C       0.570457    -0.795670     3.545430     122.24
 H       1.414841    -1.483917     3.643544      27.52
 H       0.581303    -0.921561     2.293548      26.85
 H      -0.285887    -1.131937     4.022396      28.40
 C       0.198236     2.813444     3.179359       7.96
 O       1.474915     3.066481     3.734382     220.24
 H       1.565380     4.092019     3.984324      23.11
 C      -0.722874     3.872638     2.681030      39.46
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 H      -0.490530     4.935874     2.907232      19.75
 C      -2.243312     1.848104     1.903699      27.22
 C      -3.513028     1.354081     0.914363      95.66
 H      -4.259782     2.021193     0.906166      24.81
 O      -4.047918     0.276048     1.782474     288.71
 H      -5.037215     0.268139     1.663941      25.85
 C      -2.768205     0.965615    -0.433717      79.27
 H      -2.088723     1.768406    -0.636897      24.59
 C      -3.736715     0.783303    -1.678282      96.07
 O      -4.984700     0.098567    -1.353642     312.59
 H      -4.711885    -0.819094    -1.469669      27.63
 H      -3.222995     0.438378    -2.526309      27.91
 H      -4.131615     1.851765    -2.014754      26.23
 C       1.729095     0.647725    -0.659960      41.37
 H       2.197458     1.668970    -0.552587      24.63
 C       1.436314    -1.762458    -0.644578      30.04
 H       1.999354    -2.851053    -0.475116      21.73
 C       0.047675    -1.618528    -0.432362      18.04
 O      -0.806353    -2.848075    -0.490764     150.03
 C      -1.039496    -3.343344    -1.913589     110.75
 H      -2.010180    -3.438581    -1.915332      29.59
 H      -0.744237    -2.650998    -2.789650      21.77
 H      -0.589551    -4.305380    -1.607435      24.12
 C      -0.497324    -0.353879    -0.501759      11.43
 O      -1.948153    -0.353470    -0.255551     119.11
 C       0.325489     0.790997    -0.643120      43.38
 H      -0.056839     1.730925    -0.540329      23.42
 C       2.342957    -0.575581    -0.715143      24.98
 C       3.864008    -0.870110    -0.741237      98.45
 H       4.299662    -1.676262    -1.072109      24.62
 O       4.724352     0.208301    -1.209491     284.46
 H       4.858594     0.747392    -0.458532      30.39
 C       4.375170    -1.427762     0.740725      58.29
 H       3.621047    -2.250362     1.097948      24.33
 O       5.697992    -2.107884     0.598180     219.93
 H       6.205904    -1.951730    -0.175017      25.69
 C       4.512838    -0.301161     1.882767     104.34
 O       5.269010     0.929863     1.686288     184.69
 H       4.837263     1.743290     2.256703      24.40
 H       5.261695    -0.829131     2.689635      26.31
 H       3.549946     0.129318     2.239722      23.31
55
name = lig-Water-frame_538
 C      -1.821191     3.324667     1.882339     109.07
 H      -2.280005     4.182626     1.282724      26.66
 C      -1.384123     1.090792     2.636832      58.07
 H      -1.797908     0.137892     2.774592      23.07
 C      -0.167202     1.516586     3.176327      19.98
 O       0.624001     0.618165     3.892931     200.77
 C       0.541308    -0.785853     3.459704     104.63
 H       1.570232    -1.188850     3.742520      25.65
 H       0.447126    -1.035805     2.492760      29.71
 H      -0.320548    -1.423184     3.978735      24.97
 C       0.217418     2.889230     3.258962      14.37
 O       1.457517     3.059089     3.739002     157.18
 H       1.472919     4.089050     3.950962      24.04
 C      -0.690208     3.842378     2.703927      62.52
 H      -0.504208     5.018504     2.813776      16.03
 C      -2.303887     1.920453     1.900450      37.51
 C      -3.383403     1.381659     0.966982      78.41
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 H      -4.327590     2.217712     0.770402      22.68
 O      -4.086289     0.256855     1.789421     262.74
 H      -5.021991    -0.120485     1.541519      24.41
 C      -2.753420     0.993270    -0.463970      78.35
 H      -2.023158     1.855752    -0.624675      23.15
 C      -3.747747     0.840610    -1.678248      89.77
 O      -5.010093     0.111057    -1.334913     260.22
 H      -4.795838    -0.919820    -1.372847      24.95
 H      -2.860460     0.626603    -2.523066      24.44
 H      -4.147012     1.743269    -1.951882      27.83
 C       1.660068     0.642026    -0.652317      49.67
 H       2.266293     1.551325    -0.741576      24.17
 C       1.487323    -1.700726    -0.697199      39.92
 H       1.814039    -2.687918    -0.715442      21.86
 C       0.004169    -1.660479    -0.427418       8.95
 O      -0.793674    -2.816315    -0.489845     185.09
 C      -1.015771    -3.332729    -1.959885      74.07
 H      -2.217759    -3.835686    -1.805279      20.73
 H      -0.515071    -2.756970    -2.685451      24.37
 H      -0.403001    -4.445379    -1.934155      23.05
 C      -0.569810    -0.376063    -0.420256      25.49
 O      -1.992613    -0.356897    -0.260831     131.88
 C       0.288839     0.749518    -0.691601      51.67
 H      -0.193288     1.801606    -0.309868      18.30
 C       2.389592    -0.641632    -0.705635      34.80
 C       3.848661    -0.885883    -0.773425      63.63
 H       4.129695    -1.971428    -1.433894      20.94
 O       4.729217     0.248827    -1.175731     219.50
 H       5.078324     0.745406    -0.324563      24.22
 C       4.405010    -1.410228     0.750068      62.26
 H       3.809354    -2.177228     1.242647      26.32
 O       5.663181    -2.100110     0.625314     154.58
 H       6.264181    -1.632592    -0.229846      20.52
 C       4.529751    -0.302411     1.900153     126.32
 O       5.311647     1.005269     1.705026     217.63
 H       4.872130     1.677857     2.191015      27.22
 H       4.976376    -0.859100     2.638149      31.08
 H       3.467889    -0.218376     2.316350      24.25
55
name = lig-Water-frame_539
 C      -1.933190     3.318752     1.870772      56.31
 H      -2.245469     4.020282     1.156622      20.52
 C      -1.485631     1.094001     2.604560      23.43
 H      -1.814894     0.029770     2.789339      20.69
 C      -0.144253     1.542211     3.175876     -23.99
 O       0.622038     0.657564     3.901352     128.41
 C       0.532782    -0.806516     3.429547      96.40
 H       1.496543    -0.903396     3.912066      23.75
 H       0.228866    -0.946202     2.219401      23.93
 H      -0.104646    -1.464013     3.940650      26.64
 C       0.185917     2.932785     3.298985       4.82
 O       1.461469     3.101544     3.770092     156.17
 H       1.532243     4.017264     4.055593      23.99
 C      -0.674513     3.786910     2.695713      78.36
 H      -0.528575     4.807739     2.669290      28.13
 C      -2.296329     2.056854     1.900102      26.61
 C      -3.318459     1.397821     1.038466     101.65
 H      -3.908050     2.154603     0.645097      28.38
 O      -4.106161     0.249178     1.783415     261.63
 H      -4.820237    -0.113786     1.167763      26.22
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 C      -2.750530     0.997166    -0.452852      79.67
 H      -2.025353     1.809089    -0.771513      24.79
 C      -3.727953     0.896201    -1.646661      85.99
 O      -4.998313     0.103794    -1.348837     315.37
 H      -4.875093    -0.812204    -1.039071      27.88
 H      -3.163996     0.519606    -2.417119      28.98
 H      -4.144876     1.979406    -1.885844      26.32
 C       1.645773     0.625034    -0.664050      43.59
 H       2.390737     1.509370    -0.941038      21.37
 C       1.469201    -1.680112    -0.722990      44.96
 H       1.826911    -2.803555    -0.989428      20.63
 C       0.028582    -1.676017    -0.463683       6.45
 O      -0.781805    -2.769175    -0.516462     177.20
 C      -1.010399    -3.409564    -1.928445      89.96
 H      -1.919462    -3.677532    -2.115025      27.62
 H      -0.483461    -2.666447    -2.693578      25.15
 H      -0.302301    -4.306725    -2.283075      24.97
 C      -0.672516    -0.391462    -0.357358      19.35
 O      -2.027648    -0.328565    -0.277388     162.91
 C       0.207286     0.727148    -0.665161      79.00
 H      -0.125741     1.641317    -0.457757      23.49
 C       2.367798    -0.666174    -0.705709      30.13
 C       3.892330    -0.949365    -0.758315      84.72
 H       3.811756    -1.538315    -1.579487      25.40
 O       4.720053     0.271895    -1.142232     213.89
 H       5.175576     0.621716    -0.338983      25.85
 C       4.461181    -1.352688     0.737932      71.24
 H       3.747236    -2.071691     1.266486      26.32
 O       5.638929    -2.077289     0.632842     230.34
 H       6.242394    -1.643045     0.103772      28.82
 C       4.522077    -0.303359     1.910764     113.84
 O       5.348128     1.034790     1.699066     160.83
 H       4.721575     1.706107     2.360925      18.82
 H       4.962189    -0.977315     2.830072      26.83
 H       3.500401    -0.250026     2.263265      23.02
55
name = lig-Water-frame_540
 C      -1.946069     3.414641     1.909407      61.43
 H      -2.409119     4.016223     1.024776      20.60
 C      -1.505506     1.137367     2.618151      75.30
 H      -1.651799     0.088286     2.664346      22.15
 C      -0.232966     1.522094     3.184444     -22.23
 O       0.600157     0.681742     3.883740     138.55
 C       0.547207    -0.799048     3.399991     106.18
 H       1.585316    -1.121374     3.710497      25.69
 H       0.404916    -0.715443     2.428551      28.81
 H      -0.170593    -1.405997     4.097333      24.15
 C       0.150930     2.903789     3.308717      -6.64
 O       1.474164     3.167927     3.816559     139.50
 H       1.614191     4.165098     4.314257      18.82
 C      -0.745442     3.739406     2.623759      64.13
 H      -0.417648     4.935168     2.511858      25.45
 C      -2.276423     2.062471     1.918576       0.25
 C      -3.291890     1.382163     1.059844      79.66
 H      -4.033022     2.326511     0.656696      25.10
 O      -4.085693     0.286034     1.739853     241.71
 H      -4.657674     0.131537     0.980460      26.19
 C      -2.734055     0.978490    -0.402059      95.90
 H      -2.044763     1.713138    -0.817150      25.11
 C      -3.752852     0.944498    -1.565651      89.51
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 O      -4.973442     0.111841    -1.370503     299.14
 H      -4.694964    -0.688091    -0.801521      26.01
 H      -3.465305     0.302117    -2.576795      22.72
 H      -4.008673     1.940564    -1.781679      27.97
 C       1.665450     0.592712    -0.705239      36.52
 H       2.189930     1.448005    -0.925694      23.71
 C       1.398003    -1.771949    -0.737853      63.82
 H       1.847398    -2.662612    -1.177261      25.29
 C       0.065090    -1.616203    -0.522346      14.77
 O      -0.785844    -2.774389    -0.572142     106.22
 C      -0.922575    -3.434530    -1.905574      92.60
 H      -2.143192    -3.549517    -2.365466      22.22
 H      -0.840033    -2.586974    -2.545736      26.25
 H      -0.163003    -4.254603    -2.317670      25.04
 C      -0.703894    -0.402631    -0.338867      14.07
 O      -2.071078    -0.297090    -0.299410     198.80
 C       0.160592     0.685174    -0.590225      81.78
 H      -0.201967     1.851129    -0.722455      20.48
 C       2.308329    -0.608522    -0.689722      21.54
 C       3.925197    -0.930174    -0.688535      76.15
 H       3.941298    -1.509287    -1.781939      21.60
 O       4.699029     0.270035    -1.120879     211.39
 H       5.156886     0.578894    -0.352750      29.34
 C       4.485034    -1.306141     0.715238      91.67
 H       3.624884    -1.945686     1.063814      25.93
 O       5.630652    -2.078534     0.659846     214.51
 H       6.468139    -1.657794     0.164883      23.81
 C       4.536427    -0.304789     1.927047     112.60
 O       5.335463     1.022591     1.715169     203.78
 H       4.942288     1.642807     2.309230      25.76
 H       5.022399    -0.790866     2.695796      29.74
 H       3.466710     0.134241     2.132906      21.99
55
name = lig-Water-frame_541
 C      -1.941597     3.508326     1.930650      55.40
 H      -2.469206     4.116378     1.277342      24.11
 C      -1.458992     1.181027     2.659914     100.39
 H      -1.624845     0.101382     2.469261      22.19
 C      -0.328747     1.513241     3.240430       4.03
 O       0.576676     0.668833     3.853899     196.71
 C       0.596437    -0.762950     3.452067     107.48
 H       1.518328    -1.393949     3.348796      26.16
 H       0.470134    -0.678811     2.229423      26.01
 H      -0.249112    -1.201601     3.973041      26.26
 C       0.117712     2.856822     3.293999     -27.36
 O       1.465133     3.250638     3.871407     117.01
 H       1.334759     4.131485     4.282169      19.46
 C      -0.789866     3.795030     2.536529      71.04
 H      -0.407614     4.691421     2.477393      28.17
 C      -2.269783     2.007650     1.940256     -29.35
 C      -3.322506     1.421404     1.021617     102.18
 H      -4.107792     2.112140     0.970596      24.94
 O      -4.026753     0.364494     1.660719     238.17
 H      -4.853910     0.198170     1.051117      24.80
 C      -2.720838     0.953736    -0.349384     102.74
 H      -1.965212     1.780396    -0.713982      22.74
 C      -3.795272     0.919612    -1.513946      98.48
 O      -4.955789     0.129603    -1.362334     375.59
 H      -4.560212    -0.646044    -0.824863      26.87
 H      -3.369250     0.606122    -2.392277      28.12
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 H      -4.039690     2.031707    -1.747597      26.05
 C       1.613376     0.577991    -0.741293      43.03
 H       2.086554     1.693723    -0.843924      23.32
 C       1.386483    -1.824611    -0.752996      46.00
 H       1.801168    -2.764458    -1.197471      24.73
 C       0.023861    -1.589733    -0.584546      15.12
 O      -0.794516    -2.816717    -0.632228     160.71
 C      -0.888261    -3.389876    -1.937121     107.18
 H      -1.857120    -3.727571    -1.996315      27.51
 H      -0.926479    -2.432682    -2.612634      24.26
 H      -0.112759    -4.250168    -2.098873      25.43
 C      -0.668853    -0.370429    -0.358862      12.57
 O      -2.106431    -0.303978    -0.315792     206.57
 C       0.168062     0.704254    -0.512343      84.00
 H      -0.211384     1.564735    -0.933111      23.94
 C       2.263968    -0.612506    -0.663120      11.65
 C       3.917564    -0.833930    -0.677105      96.09
 H       4.277573    -1.674051    -1.235848      26.28
 O       4.674067     0.264364    -1.113149     210.54
 H       5.128749     0.742135    -0.292577      23.81
 C       4.459597    -1.277583     0.691536      85.31
 H       3.660951    -1.990771     0.975800      26.50
 O       5.653818    -2.100901     0.699270     193.09
 H       6.526373    -1.778583     0.126177      21.97
 C       4.528707    -0.222807     1.898317     105.66
 O       5.336062     0.955676     1.708040     188.67
 H       4.983898     1.752420     2.400949      22.24
 H       5.077079    -0.802832     2.793255      26.38
 H       3.617992     0.228049     2.080745      24.15
55
name = lig-Water-frame_542
 C      -1.988432     3.475769     1.928911      42.84
 H      -2.595520     4.387614     1.489948      23.25
 C      -1.472844     1.149717     2.656038      77.68
 H      -1.651584     0.103523     2.387797      24.63
 C      -0.304035     1.546480     3.366157      31.08
 O       0.587197     0.627440     3.839997     183.86
 C       0.618040    -0.707063     3.422459     132.62
 H       1.510810    -1.354010     3.474465      29.15
 H       0.310814    -0.819714     2.439603      32.30
 H      -0.290460    -1.234912     3.823959      28.37
 C       0.080493     2.863516     3.255764       7.00
 O       1.390172     3.282144     3.889965     145.27
 H       1.167646     4.294354     4.243202      15.44
 C      -0.730713     3.845359     2.520732      62.53
 H      -0.240827     5.003147     2.460355      16.81
 C      -2.277515     2.040168     1.946112     -17.23
 C      -3.351182     1.469559     0.995345      99.06
 H      -4.247396     2.309032     0.904965      24.09
 O      -3.985039     0.412209     1.576949     288.48
 H      -4.960625     0.235625     1.498103      27.79
 C      -2.733034     0.986055    -0.336665     106.32
 H      -2.059321     1.734033    -0.551968      27.49
 C      -3.812753     0.943225    -1.475724      83.19
 O      -4.942358     0.134813    -1.324328     352.64
 H      -4.749790    -0.791816    -1.044581      28.65
 H      -2.961562     0.830595    -2.418292      23.99
 H      -4.212942     1.959673    -1.583474      26.38
 C       1.530004     0.636137    -0.746602      47.26
 H       2.048900     1.487028    -0.769785      27.66
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 C       1.414448    -1.800256    -0.767993      35.18
 H       1.694146    -2.928704    -0.980747      24.78
 C      -0.055015    -1.641995    -0.634244      10.90
 O      -0.794960    -2.839430    -0.665258     203.64
 C      -0.868329    -3.306076    -1.991204     112.76
 H      -1.886629    -4.152829    -1.739683      20.88
 H      -0.737174    -2.665079    -2.814618      25.13
 H      -0.018791    -4.158679    -1.970627      26.20
 C      -0.647947    -0.352481    -0.396622       9.45
 O      -2.095733    -0.348029    -0.319493     166.11
 C       0.219638     0.742059    -0.474277      73.84
 H      -0.323308     1.653260    -0.956744      22.37
 C       2.267534    -0.694598    -0.660418       0.80
 C       3.889089    -0.746791    -0.650862     103.84
 H       4.328390    -1.855755    -0.912882      20.69
 O       4.666954     0.294595    -1.120709     251.44
 H       4.920760     0.878006    -0.396688      26.75
 C       4.420019    -1.248304     0.717139      64.89
 H       3.746684    -2.096016     1.099054      25.88
 O       5.690263    -2.123602     0.734888     188.81
 H       6.307530    -1.862385     0.069660      25.29
 C       4.536257    -0.161537     1.875037     122.59
 O       5.367346     0.909617     1.688254     258.83
 H       4.951274     1.570273     2.255454      26.69
 H       4.760882    -0.781510     2.719828      29.11
 H       3.396258     0.094295     2.192536      25.84
55
name = lig-Water-frame_543
 C      -2.004560     3.440755     1.939723      62.54
 H      -2.638367     4.243241     1.702274      24.80
 C      -1.489951     1.111039     2.636089      28.24
 H      -1.673324     0.063071     2.493485      24.10
 C      -0.288117     1.548456     3.452058      -4.90
 O       0.639906     0.606100     3.861040     121.99
 C       0.575401    -0.705627     3.371170     114.43
 H       1.568621    -1.023837     3.856834      27.12
 H       0.229313    -0.834890     2.234244      28.50
 H      -0.162462    -1.391310     3.920463      27.99
 C       0.084428     2.955783     3.229036      25.72
 O       1.252745     3.272927     3.870171     318.56
 H       1.453545     4.216820     4.214113      17.60
 C      -0.644317     3.899162     2.534910      28.76
 H      -0.380851     4.846159     2.507855      21.54
 C      -2.303073     2.121235     1.938378      23.77
 C      -3.404114     1.556986     0.986820      91.39
 H      -3.933126     2.402096     0.552209      26.90
 O      -3.978008     0.393448     1.539456     287.24
 H      -4.947230     0.494913     1.756061      26.33
 C      -2.787733     1.030955    -0.338579      70.89
 H      -1.957081     1.860243    -0.636813      21.42
 C      -3.764425     0.992237    -1.464116      94.38
 O      -4.935318     0.121153    -1.290020     308.26
 H      -4.842647    -0.897744    -1.257378      27.32
 H      -3.189940     0.860437    -2.276465      30.99
 H      -4.338860     1.965668    -1.463236      27.08
 C       1.538015     0.624439    -0.716804      20.69
 H       2.299885     1.559298    -0.823222      24.47
 C       1.396887    -1.785017    -0.768562      54.11
 H       1.727957    -2.789168    -0.701139      27.16
 C      -0.077645    -1.672429    -0.656175      23.30
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 O      -0.798413    -2.821048    -0.678531     252.70
 C      -0.883884    -3.342310    -2.019709     119.17
 H      -1.548465    -4.088625    -2.067910      29.52
 H      -0.751954    -2.804621    -3.018419      24.63
 H       0.113707    -4.029908    -2.178859      25.96
 C      -0.663733    -0.403504    -0.448513      11.62
 O      -2.048659    -0.378822    -0.310868     122.63
 C       0.197638     0.809853    -0.491247      60.59
 H      -0.273570     1.826387    -0.567372      22.51
 C       2.280171    -0.718085    -0.688759     -15.29
 C       3.852073    -0.770171    -0.584719      90.85
 H       4.018145    -1.588795    -1.272972      20.82
 O       4.660460     0.347264    -1.157701     247.77
 H       4.742039     1.008654    -0.446187      27.86
 C       4.396781    -1.226132     0.815862      79.55
 H       3.716273    -1.927826     1.214500      27.27
 O       5.703136    -2.121099     0.774029     163.02
 H       6.241565    -1.870049    -0.193425      19.57
 C       4.457674    -0.185914     1.867020     120.19
 O       5.421245     0.886952     1.650698     192.83
 H       4.963806     1.678991     2.229615      22.71
 H       4.697568    -0.818349     2.842079      27.87
 H       3.477570     0.060246     2.055366      28.12
55
name = lig-Water-frame_544
 C      -1.923407     3.466235     1.998071      61.24
 H      -2.763764     4.158945     1.636349      21.26
 C      -1.457517     1.130850     2.644304      42.83
 H      -1.751768     0.036899     2.657270      23.15
 C      -0.354774     1.536340     3.424823     -21.15
 O       0.686025     0.637232     3.898938      93.67
 C       0.532405    -0.766345     3.344554     118.70
 H       1.504557    -0.915215     3.757246      28.79
 H       0.564206    -0.743847     2.264512      30.29
 H      -0.086316    -1.367930     3.994411      28.42
 C       0.095225     3.027560     3.236597      18.08
 O       1.159754     3.234012     3.851512     175.48
 H       1.473292     4.161003     4.169409      16.85
 C      -0.665730     3.892309     2.528082      37.25
 H      -0.413864     5.091670     2.564534      24.75
 C      -2.333312     2.129080     1.936555      26.38
 C      -3.391342     1.622250     0.978629      66.83
 H      -3.984310     2.523494     0.430987      22.19
 O      -4.014299     0.367034     1.530059     252.67
 H      -4.905325     0.743645     1.778548      25.50
 C      -2.780326     1.091296    -0.343106      63.57
 H      -2.113263     1.723116    -0.727926      26.78
 C      -3.770710     1.024977    -1.439926      82.60
 O      -4.938047     0.105995    -1.274255     283.47
 H      -4.544884    -0.813098    -1.245018      27.70
 H      -3.377675     0.753555    -2.604405      24.21
 H      -4.283730     2.046903    -1.466369      26.58
 C       1.643635     0.599097    -0.672327      29.13
 H       2.237243     1.427864    -0.849844      26.70
 C       1.348413    -1.779938    -0.749282      38.05
 H       1.913104    -2.809015    -0.428207      24.32
 C      -0.017664    -1.644878    -0.664284      30.54
 O      -0.828169    -2.810985    -0.703218     142.57
 C      -0.822430    -3.434217    -2.083710      95.15
 H      -1.789569    -4.297267    -2.377726      23.67
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 H      -1.099361    -2.608143    -2.838314      23.65
 H       0.213970    -3.779868    -2.370571      24.97
 C      -0.684700    -0.423355    -0.509990      18.10
 O      -2.010659    -0.377785    -0.294089      76.30
 C       0.146432     0.837832    -0.520917      58.79
 H      -0.140400     1.881699    -0.190920      23.23
 C       2.251812    -0.643774    -0.717757      10.89
 C       3.813936    -0.824382    -0.548101      70.88
 H       3.906560    -1.386225    -1.605093      19.34
 O       4.632445     0.386939    -1.190601     166.46
 H       4.610977     1.166937    -0.492359      26.95
 C       4.413173    -1.256839     0.883435      77.01
 H       3.494731    -1.892761     1.323032      25.69
 O       5.686991    -2.074939     0.786925     253.90
 H       6.180743    -1.923311     0.027215      26.30
 C       4.401239    -0.238595     1.906300     100.10
 O       5.455660     0.880995     1.623944     122.11
 H       5.155729     1.717011     2.131545      24.94
 H       4.757737    -0.649342     2.835403      29.39
 H       3.336872     0.353920     1.893375      25.05
55
name = lig-Water-frame_545
 C      -1.880553     3.501466     2.038268      64.32
 H      -2.563261     4.149180     1.475115      18.26
 C      -1.453717     1.164894     2.655003      69.30
 H      -1.763443     0.178485     2.722199      24.22
 C      -0.398009     1.570015     3.336299      11.19
 O       0.680331     0.697351     3.923393      82.81
 C       0.562717    -0.792254     3.369295     101.12
 H       1.619363    -1.313312     3.478743      27.36
 H       0.665996    -0.756082     2.261921      27.87
 H      -0.331073    -1.381324     3.912121      25.52
 C       0.010732     2.977851     3.235437       9.98
 O       1.190001     3.203771     3.885456      61.04
 H       1.187098     4.214467     4.132047      17.84
 C      -0.733207     3.945527     2.518370      28.29
 H      -0.490108     4.961290     2.609359      30.06
 C      -2.312964     2.099837     1.969202      36.76
 C      -3.334698     1.644627     0.959992      94.87
 H      -4.180032     2.360381     0.823169      24.91
 O      -4.071471     0.389758     1.525097     238.89
 H      -5.000844     0.653093     1.711670      26.24
 C      -2.740480     1.109743    -0.361610      52.73
 H      -1.903774     1.840829    -0.851111      21.27
 C      -3.842508     1.022468    -1.484087     104.90
 O      -4.922747     0.103219    -1.268844     318.63
 H      -4.397472    -0.678846    -0.994082      29.60
 H      -3.508280     0.831744    -2.428107      29.85
 H      -4.154371     2.081853    -1.554142      29.14
 C       1.664525     0.614927    -0.627904      32.53
 H       2.307365     1.574757    -0.764004      24.66
 C       1.384198    -1.783676    -0.689311      64.67
 H       1.778741    -2.665032    -0.468055      26.14
 C       0.024583    -1.636389    -0.682400      -6.54
 O      -0.866254    -2.834114    -0.740593     131.82
 C      -0.799567    -3.494725    -2.180636      96.53
 H      -1.577337    -4.195012    -2.269340      28.34
 H      -1.311727    -2.544066    -2.525357      22.88
 H       0.277202    -3.747665    -2.457560      26.81
 C      -0.671513    -0.328802    -0.567587      11.31
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 O      -2.012836    -0.351106    -0.271145     101.48
 C       0.163293     0.789900    -0.557337      65.99
 H      -0.038903     1.715524     0.109131      22.71
 C       2.213505    -0.590720    -0.717831      36.73
 C       3.783007    -0.840462    -0.589421      67.03
 H       4.115612    -1.536084    -1.382542      23.53
 O       4.576872     0.409617    -1.192892     180.55
 H       4.562427     1.173587    -0.642250      31.51
 C       4.410915    -1.361914     0.872611      89.97
 H       3.646909    -1.983125     1.247201      27.91
 O       5.623440    -2.011760     0.833341     253.16
 H       6.296841    -1.780534    -0.005424      20.55
 C       4.370950    -0.186033     1.955346      97.41
 O       5.485406     0.865176     1.597685     127.51
 H       5.181650     1.620876     2.095247      29.16
 H       4.659225    -0.589514     2.966136      29.08
 H       3.508248     0.368178     1.878864      27.67
55
name = lig-Water-frame_546
 C      -1.954953     3.484197     1.994427      76.07
 H      -2.383577     4.264539     1.349491      15.49
 C      -1.530127     1.178905     2.638415      59.25
 H      -1.791058     0.083739     2.664633      24.18
 C      -0.329013     1.625813     3.268969      19.36
 O       0.637022     0.733159     3.923608      89.06
 C       0.636050    -0.792558     3.404815     120.26
 H       1.391906    -1.526417     3.529193      29.13
 H       0.343309    -0.724709     2.279834      28.75
 H      -0.277810    -1.231775     3.622486      29.04
 C      -0.065185     2.895025     3.246330      20.09
 O       1.240153     3.198025     3.926259     171.73
 H       1.157678     4.109972     4.233914      21.72
 C      -0.748404     3.979164     2.577584      71.64
 H      -0.467930     5.103055     2.619498      32.82
 C      -2.250808     2.108142     2.012709      45.20
 C      -3.299972     1.598461     0.985758     112.51
 H      -4.181020     2.316845     1.026545      27.89
 O      -4.116377     0.435056     1.525152     272.57
 H      -5.131051     0.456524     1.491331      25.71
 C      -2.685940     1.121230    -0.433925      86.52
 H      -1.934490     1.761836    -0.701091      26.65
 C      -3.911763     1.031883    -1.508101      88.98
 O      -4.901206     0.111436    -1.264282     260.27
 H      -4.626031    -0.691700    -0.622680      23.29
 H      -3.277866     0.797101    -2.593071      24.48
 H      -4.229006     2.150986    -1.601790      26.80
 C       1.610416     0.704028    -0.607967      52.03
 H       2.263732     1.596832    -0.480937      25.94
 C       1.430562    -1.745972    -0.622408      40.69
 H       1.804953    -2.936866    -0.600500      21.80
 C      -0.011803    -1.644321    -0.712162     -25.52
 O      -0.871677    -2.869547    -0.769382     105.93
 C      -0.789479    -3.463047    -2.227436      73.71
 H      -1.540110    -4.494464    -2.124797      23.28
 H      -1.324281    -2.595719    -2.764930      23.85
 H       0.319733    -3.749485    -2.627284      25.17
 C      -0.637976    -0.261781    -0.616325       2.34
 O      -2.034614    -0.285279    -0.250138     128.06
 C       0.256211     0.751906    -0.550696      66.89
 H      -0.116275     1.545292     0.016056      24.30
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 C       2.241517    -0.618436    -0.692360      14.31
 C       3.782969    -0.812670    -0.638934      71.98
 H       4.258870    -1.823364    -1.165373      23.19
 O       4.505988     0.390068    -1.188406     149.66
 H       4.481605     1.173325    -0.608780      32.02
 C       4.363589    -1.400058     0.837236      76.00
 H       3.698254    -2.330994     1.193436      24.97
 O       5.589295    -1.959922     0.863820     237.63
 H       6.279559    -1.568833     0.189963      22.41
 C       4.410420    -0.122058     1.963183      99.33
 O       5.505815     0.829004     1.579491     112.08
 H       5.068358     1.651128     2.179633      22.73
 H       4.410318    -0.572519     3.023730      28.21
 H       3.349179     0.426246     1.982067      26.47
55
name = lig-Water-frame_547
 C      -2.001641     3.506296     1.932644      22.63
 H      -2.482111     4.250732     1.207208      16.07
 C      -1.550558     1.140978     2.669307      57.33
 H      -1.810580     0.110209     2.503468      27.43
 C      -0.272794     1.537561     3.213301      20.43
 O       0.594201     0.730178     3.910990     151.38
 C       0.644399    -0.734764     3.387221     112.59
 H       1.443218    -1.455511     3.832660      26.80
 H       0.389356    -0.643669     2.366680      30.13
 H      -0.441756    -1.188892     3.732345      25.07
 C      -0.011598     2.968898     3.297451      15.89
 O       1.255516     3.182371     3.942420     160.83
 H       1.356751     4.122065     4.451840      19.68
 C      -0.785532     3.952987     2.667060      65.21
 H      -0.415030     5.034853     2.625692      30.29
 C      -2.260278     2.135329     1.983667      50.04
 C      -3.317751     1.526598     1.032498     113.28
 H      -3.936052     2.524514     0.819085      29.30
 O      -4.141913     0.461732     1.541265     290.13
 H      -5.072472     0.470467     1.176873      26.78
 C      -2.698189     1.106783    -0.472739      86.40
 H      -1.879178     1.902586    -0.746631      22.55
 C      -3.874593     1.060122    -1.556901     104.14
 O      -4.908681     0.107587    -1.246857     267.40
 H      -4.840089    -0.553880    -0.582184      27.77
 H      -3.370204     0.785921    -2.398357      30.47
 H      -4.423527     1.991559    -1.614482      28.03
 C       1.638805     0.730672    -0.597209      53.98
 H       2.155247     1.633689    -0.266640      26.21
 C       1.421839    -1.763880    -0.577197      37.25
 H       1.812278    -2.662796    -0.759085      28.37
 C      -0.069430    -1.633401    -0.735967      -2.44
 O      -0.832939    -2.889001    -0.811490     145.27
 C      -0.823093    -3.423802    -2.242302     112.36
 H      -1.144102    -4.479325    -2.069998      26.03
 H      -1.232039    -2.864002    -3.032415      27.60
 H       0.186495    -3.652091    -2.629123      27.97
 C      -0.628242    -0.343289    -0.651215       0.97
 O      -2.037757    -0.179953    -0.248604     132.98
 C       0.306956     0.775630    -0.502779      49.71
 H      -0.306402     1.779192    -0.247471      21.19
 C       2.299835    -0.627177    -0.656041      -3.91
 C       3.812039    -0.802999    -0.663308     107.19
 H       4.109705    -1.727718    -1.163242      26.97
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 O       4.437190     0.336142    -1.180413     144.33
 H       4.332039     1.072464    -0.453302      29.86
 C       4.260385    -1.354424     0.841327      84.91
 H       3.681132    -2.171911     1.069641      28.71
 O       5.609006    -1.924532     0.879108     249.98
 H       6.211128    -1.480329     0.352872      27.78
 C       4.395205    -0.098424     1.930684     120.33
 O       5.492247     0.805841     1.601030     206.80
 H       5.208395     1.576994     2.026619      30.47
 H       4.467788    -0.529809     2.929666      29.90
 H       3.458720     0.419176     1.985195      28.63
55
name = lig-Water-frame_548
 C      -1.982505     3.544736     1.893813     -22.81
 H      -2.626748     4.095032     1.265126      21.22
 C      -1.503232     1.118697     2.707795      57.54
 H      -1.810366     0.109706     2.421275      24.67
 C      -0.269048     1.453818     3.176688      24.25
 O       0.578698     0.685020     3.893547     193.64
 C       0.567037    -0.666644     3.408607     122.97
 H       1.436848    -0.970846     3.961424      28.21
 H       0.824608    -0.684391     2.207090      26.76
 H      -0.213089    -1.116556     3.877081      27.63
 C       0.094006     3.048000     3.361273       4.93
 O       1.261433     3.185586     3.961757     239.28
 H       1.485684     4.008151     4.418913      23.27
 C      -0.853256     3.901054     2.734099      54.44
 H      -0.459804     4.902019     2.719642      27.95
 C      -2.319011     2.129199     1.918417      42.44
 C      -3.347114     1.514108     1.019894      94.16
 H      -3.837045     2.445119     0.586460      23.95
 O      -4.148910     0.482927     1.568371     301.37
 H      -4.988333     0.593329     1.074650      27.21
 C      -2.733330     1.121793    -0.459051      91.13
 H      -2.131251     1.969109    -0.809121      22.46
 C      -3.809050     1.062866    -1.544823      76.47
 O      -4.952717     0.116268    -1.247412     180.55
 H      -4.653719    -0.647648    -0.595019      22.77
 H      -3.381860     0.704624    -2.678413      24.22
 H      -4.512885     2.004168    -1.675624      24.45
 C       1.738416     0.692916    -0.571360      34.75
 H       2.179906     1.716398    -0.184105      21.98
 C       1.369067    -1.729137    -0.579149      29.54
 H       1.933872    -2.778584    -0.867486      22.77
 C      -0.079132    -1.645195    -0.742812      30.32
 O      -0.780641    -2.879842    -0.877458     189.03
 C      -0.816996    -3.408362    -2.204286     103.67
 H      -1.130936    -4.517835    -2.133139      25.45
 H      -1.518427    -3.028800    -3.162539      23.28
 H       0.380970    -3.430638    -2.529213      23.44
 C      -0.640710    -0.409606    -0.648917      -3.36
 O      -2.011507    -0.088638    -0.276253     119.14
 C       0.240171     0.817102    -0.457035      42.89
 H      -0.114389     1.768377    -0.563310      21.80
 C       2.303464    -0.617220    -0.610784       6.20
 C       3.808631    -0.834544    -0.629539      99.12
 H       4.038747    -1.685132    -1.497984      22.81
 O       4.393183     0.294886    -1.157517     184.94
 H       4.254500     0.928079    -0.471979      30.26
 C       4.225266    -1.219725     0.848561      78.61
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 H       3.372460    -2.014683     1.132110      24.28
 O       5.610033    -1.909121     0.901648     141.62
 H       6.333970    -1.291311     0.297421      21.27
 C       4.339525    -0.124023     1.876103      98.78
 O       5.476363     0.775971     1.617132     242.79
 H       5.261571     1.730673     2.003919      26.98
 H       4.721443    -0.600508     2.881490      24.29
 H       3.404399     0.553836     1.907499      23.97
55
name = lig-Water-frame_549
 C      -1.949763     3.483243     1.893499      29.26
 H      -2.714736     4.241549     1.404839      25.86
 C      -1.491892     1.135256     2.671166      55.93
 H      -1.709165     0.039264     2.515906      23.36
 C      -0.263926     1.512662     3.198066      14.93
 O       0.573244     0.650428     3.867706     213.79
 C       0.556982    -0.606803     3.427443     130.08
 H       1.536510    -0.850702     3.977521      25.23
 H       0.941139    -0.829806     2.518352      30.58
 H      -0.313552    -1.367456     3.876945      24.15
 C       0.100848     3.001393     3.363501       2.50
 O       1.301100     3.197050     3.996130     198.91
 H       1.464562     4.184062     4.352254      23.15
 C      -0.882993     3.869691     2.787713      46.98
 H      -0.636415     5.055182     2.875318      20.36
 C      -2.330663     2.110319     1.889195      48.85
 C      -3.356073     1.553009     0.942760      93.39
 H      -4.169227     2.334418     0.529502      22.20
 O      -4.144617     0.511174     1.594234     285.06
 H      -5.101339     0.539624     1.252178      24.96
 C      -2.775068     1.159203    -0.427004      94.09
 H      -2.213322     2.072125    -0.743359      22.17
 C      -3.794372     1.025894    -1.562274     101.95
 O      -4.985130     0.121986    -1.238882     221.32
 H      -4.489686    -0.706570    -0.958900      24.88
 H      -3.466904     0.800535    -2.521309      28.76
 H      -4.158798     2.002992    -1.694882      29.19
 C       1.745571     0.666515    -0.504195      40.08
 H       2.344368     1.516824    -0.391568      23.50
 C       1.344533    -1.703468    -0.638212      71.50
 H       1.756691    -2.659117    -0.748861      24.35
 C      -0.033560    -1.689447    -0.737542      24.23
 O      -0.750573    -2.852011    -0.926493     237.53
 C      -0.766366    -3.423470    -2.201937     124.77
 H      -1.121362    -4.584726    -2.164686      25.49
 H      -1.634037    -3.047939    -2.615439      26.64
 H       0.223199    -3.289062    -2.552481      26.17
 C      -0.668536    -0.320682    -0.602445      -4.28
 O      -1.971983    -0.058340    -0.323345     130.68
 C       0.234041     0.778770    -0.460706      64.62
 H      -0.078907     1.890349    -0.738557      21.43
 C       2.247986    -0.618032    -0.556721      29.60
 C       3.772222    -0.923085    -0.591060     107.14
 H       3.955017    -1.555267    -1.469745      23.78
 O       4.385020     0.284423    -1.133866     187.65
 H       4.289021     1.033071    -0.525867      28.85
 C       4.238530    -1.135924     0.826385      97.49
 H       3.479403    -1.697034     1.263401      28.70
 O       5.580028    -1.879428     0.920915     190.45
 H       6.233484    -1.410689     0.393414      25.72
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 C       4.294092    -0.120878     1.853025     113.29
 O       5.465557     0.765406     1.614583     283.95
 H       5.151382     1.667380     2.035491      27.07
 H       4.550664    -0.660268     2.698620      27.09
 H       3.370188     0.496432     1.995952      24.45
55
name = lig-Water-frame_550
 C      -1.938067     3.402654     1.931671      93.94
 H      -2.453696     4.242508     1.659678      24.82
 C      -1.502631     1.173522     2.577660      54.29
 H      -1.593128     0.125522     2.664518      24.60
 C      -0.271837     1.645346     3.253448      18.71
 O       0.556504     0.692763     3.845136     184.56
 C       0.608337    -0.679744     3.511728     125.38
 H       1.429775    -1.188823     4.014353      28.63
 H       0.825755    -0.925711     2.300891      29.44
 H      -0.191315    -1.284419     3.615521      29.46
 C       0.045966     2.895418     3.329584      17.94
 O       1.345968     3.232909     4.040311     193.15
 H       1.359470     4.211358     4.195592      25.40
 C      -0.871913     3.885997     2.830594      39.29
 H      -0.875685     4.883587     3.017750      16.41
 C      -2.294682     2.077081     1.882311      53.31
 C      -3.422820     1.599239     0.864620     102.15
 H      -4.264558     2.330102     0.702022      24.69
 O      -4.134907     0.533965     1.617828     317.03
 H      -5.133673     0.422956     1.562696      24.12
 C      -2.791551     1.195024    -0.421929      83.55
 H      -2.106576     2.106090    -0.639257      22.62
 C      -3.835526     0.983462    -1.551074      83.59
 O      -4.972825     0.140426    -1.246560     216.60
 H      -4.635634    -0.764921    -1.203247      27.69
 H      -3.257117     0.661604    -2.617676      25.60
 H      -4.001968     2.160899    -1.687323      26.25
 C       1.657293     0.634976    -0.424885      58.16
 H       2.509627     1.433376    -0.705751      23.21
 C       1.335815    -1.697964    -0.709462      65.03
 H       1.752045    -2.804391    -0.671812      23.36
 C      -0.020056    -1.652905    -0.722086       3.28
 O      -0.734360    -2.827139    -0.909535     198.66
 C      -0.745408    -3.471238    -2.207749      97.74
 H      -0.876099    -4.533905    -2.099415      27.07
 H      -1.748018    -2.880547    -2.477794      23.28
 H       0.176187    -3.150057    -3.080172      22.69
 C      -0.643412    -0.207874    -0.537946       3.04
 O      -1.961517    -0.072808    -0.374794     131.09
 C       0.303183     0.768357    -0.510487      71.47
 H      -0.149936     1.701412    -0.612317      26.92
 C       2.195512    -0.641382    -0.503424      31.64
 C       3.703213    -0.933501    -0.560825      89.59
 H       3.978260    -1.852838    -1.293649      22.50
 O       4.400547     0.281079    -1.118221     158.65
 H       4.344131     1.145778    -0.550183      28.83
 C       4.292012    -1.144289     0.786637      91.81
 H       3.554109    -1.874673     1.390403      26.68
 O       5.507404    -1.854048     0.951810     197.24
 H       6.245573    -1.489067     0.374411      24.05
 C       4.284454    -0.050643     1.848350     107.16
 O       5.436721     0.777940     1.615642     295.41
 H       5.118962     1.536509     2.068947      29.29
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 H       4.275695    -0.777204     2.841845      25.48
 H       3.299178     0.418897     2.061186      26.42
55
name = lig-Water-frame_551
 C      -1.887245     3.386459     2.036769      76.56
 H      -2.510426     4.294286     1.611437      23.09
 C      -1.457016     1.214382     2.514394      53.70
 H      -1.632469     0.100205     2.682857      24.63
 C      -0.348509     1.616182     3.278953      13.93
 O       0.554874     0.750178     3.842782     136.93
 C       0.686141    -0.794958     3.517137     108.41
 H       1.359796    -1.393602     4.175646      27.68
 H       0.707376    -0.756629     2.513072      32.72
 H      -0.478504    -1.244494     3.612178      26.18
 C       0.063193     2.950726     3.340446       5.96
 O       1.342144     3.255752     4.054649     177.09
 H       1.360987     4.226000     4.181396      24.94
 C      -0.865331     3.843274     2.833089      64.64
 H      -0.972572     5.003020     3.248066      19.86
 C      -2.289109     2.029134     1.833826      42.20
 C      -3.506790     1.613014     0.876975      88.54
 H      -4.201338     2.616877     0.821465      24.61
 O      -4.112735     0.535456     1.649410     278.70
 H      -5.112231     0.541096     1.582448      26.06
 C      -2.781856     1.209651    -0.455896      96.71
 H      -2.101515     1.976349    -0.707241      27.65
 C      -3.843007     0.981822    -1.574259     103.79
 O      -4.939435     0.176108    -1.271298     244.72
 H      -4.784904    -0.840568    -1.220788      28.83
 H      -3.219776     0.532759    -2.300992      30.88
 H      -4.267390     1.903408    -1.790449      29.73
 C       1.648461     0.610199    -0.383566      74.73
 H       2.196122     1.371652    -0.749370      28.41
 C       1.347916    -1.757009    -0.761570      43.17
 H       1.777544    -2.782515    -0.719957      25.51
 C      -0.063400    -1.532783    -0.703451      15.89
 O      -0.710084    -2.809863    -0.851023     173.53
 C      -0.766638    -3.437835    -2.269705      90.21
 H      -0.542050    -4.659719    -2.023926      23.91
 H      -1.651087    -3.200448    -2.782216      27.37
 H      -0.140436    -3.186375    -3.047971      27.35
 C      -0.582882    -0.212051    -0.483888      21.95
 O      -1.989149    -0.096461    -0.417972     172.28
 C       0.333523     0.824321    -0.557735      58.67
 H      -0.171599     1.836931    -0.452000      23.34
 C       2.178285    -0.679383    -0.464373      24.54
 C       3.649615    -0.889313    -0.556794      98.22
 H       3.941063    -1.908200    -0.917613      24.34
 O       4.425282     0.264657    -1.120692     210.05
 H       4.314204     0.980241    -0.500730      31.63
 C       4.287097    -1.212862     0.828534      99.33
 H       3.673417    -2.012225     1.147132      28.78
 O       5.457839    -1.839470     0.974049     203.76
 H       6.319184    -1.630867     0.301671      20.78
 C       4.270409    -0.024088     1.877144     117.10
 O       5.391106     0.803278     1.629309     235.79
 H       5.189773     1.721476     2.224347      23.88
 H       4.297624    -0.475684     2.809681      30.30
 H       3.248923     0.545525     1.885752      27.05
55
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name = lig-Water-frame_552
 C      -1.913278     3.416133     2.100237      64.52
 H      -2.553038     4.043054     1.584746      26.12
 C      -1.403984     1.162228     2.491632      73.71
 H      -1.718268     0.160493     2.475545      28.58
 C      -0.386755     1.536933     3.288886     -20.35
 O       0.582683     0.762413     3.870303     103.24
 C       0.653474    -0.873692     3.528318      96.20
 H       1.356658    -1.298993     4.271328      28.93
 H       0.959026    -0.738791     2.350705      29.88
 H      -0.282064    -1.101363     3.772886      30.27
 C       0.134336     3.040159     3.398727     -15.11
 O       1.290074     3.265408     4.040034     135.61
 H       1.496372     4.268672     4.325073      18.68
 C      -0.844041     3.859274     2.865433      80.58
 H      -0.833811     4.789135     3.182106      28.55
 C      -2.300890     2.053729     1.765058      16.13
 C      -3.514577     1.631650     0.963205      91.57
 H      -4.068328     2.565644     0.768632      27.76
 O      -4.108210     0.534127     1.674019     263.80
 H      -5.064267     0.689715     1.403898      26.03
 C      -2.799133     1.191527    -0.491180      83.59
 H      -2.063304     2.045269    -0.902675      26.25
 C      -3.815109     0.984237    -1.588038      87.37
 O      -4.931615     0.182445    -1.293774     249.18
 H      -4.640812    -0.728116    -1.025886      29.81
 H      -3.147786     0.417908    -2.452409      27.04
 H      -4.512626     1.846652    -2.062970      24.59
 C       1.679988     0.593711    -0.381961      54.54
 H       2.251475     1.638059    -0.598233      26.57
 C       1.339002    -1.790462    -0.771955      41.77
 H       1.756444    -2.816609    -0.911514      25.57
 C      -0.074010    -1.468255    -0.700921      22.18
 O      -0.705480    -2.789098    -0.816976     126.22
 C      -0.800892    -3.435603    -2.282306      73.17
 H      -0.481447    -4.350455    -2.119827      28.24
 H      -1.844650    -3.631995    -2.899562      24.28
 H       0.147491    -2.932497    -3.057471      24.07
 C      -0.581652    -0.251504    -0.454745      27.22
 O      -2.024989    -0.118839    -0.449485     174.98
 C       0.279123     0.916009    -0.564666      50.69
 H       0.035247     1.994626    -0.401443      24.66
 C       2.188544    -0.725442    -0.461105      33.27
 C       3.662304    -0.841323    -0.512750      97.31
 H       3.884401    -1.806471    -1.112764      26.04
 O       4.439678     0.219564    -1.129758     177.78
 H       4.312347     0.870940    -0.419958      32.53
 C       4.203036    -1.233485     0.913627      93.43
 H       3.423871    -2.097468     1.127295      28.02
 O       5.503127    -1.864943     0.977455     219.12
 H       6.119332    -1.663963     0.372318      27.33
 C       4.209745    -0.018004     1.888368     112.75
 O       5.354608     0.868747     1.653807     215.92
 H       5.222385     1.637597     2.171003      30.84
 H       4.403269    -0.254654     3.059918      26.50
 H       3.359020     0.616207     1.673771      28.62
55
name = lig-Water-frame_553
 C      -2.008791     3.406736     2.102215      55.80
 H      -2.680434     4.206167     1.595793      24.56
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 C      -1.420119     1.082475     2.442941       8.77
 H      -1.687179    -0.005826     2.245596      29.13
 C      -0.310104     1.531865     3.312463     -48.20
 O       0.624729     0.718255     3.912099      75.79
 C       0.632901    -0.847920     3.520094     108.49
 H       1.415007    -1.127239     4.222897      31.98
 H       1.101562    -1.064318     2.626292      33.36
 H      -0.460481    -1.272443     3.849446      26.56
 C       0.127912     3.021158     3.436835      -1.17
 O       1.260270     3.292260     4.042012     164.00
 H       1.534785     4.124057     4.426716      22.62
 C      -0.801438     3.894098     2.910976      43.11
 H      -0.652499     5.126631     3.072508      22.03
 C      -2.244718     2.128298     1.778030      26.74
 C      -3.405906     1.630407     1.033739      85.06
 H      -4.225935     2.463291     0.627013      27.08
 O      -4.137503     0.551229     1.681189     239.89
 H      -5.087625     0.566769     1.330517      25.78
 C      -2.809436     1.187785    -0.523096      87.11
 H      -2.226899     1.953213    -0.818395      32.25
 C      -3.797116     0.981776    -1.669409     110.01
 O      -4.932139     0.145982    -1.295972     259.95
 H      -4.482701    -0.586482    -0.791202      30.43
 H      -3.307226     0.561315    -2.532506      30.81
 H      -4.131827     1.858353    -2.126224      29.75
 C       1.670086     0.644104    -0.427335      43.37
 H       2.394982     1.386161    -0.172463      32.21
 C       1.318928    -1.768853    -0.744944      59.33
 H       1.623034    -2.816877    -1.203459      26.31
 C      -0.027334    -1.549050    -0.722462      23.77
 O      -0.738899    -2.764656    -0.824778     159.71
 C      -0.811873    -3.380571    -2.303203      83.99
 H      -0.204332    -4.521503    -2.081304      25.34
 H      -1.780220    -3.707567    -2.568371      26.62
 H      -0.112895    -2.830135    -2.743820      30.02
 C      -0.665180    -0.187875    -0.457820      23.95
 O      -2.056893    -0.141307    -0.468462     153.08
 C       0.263055     0.956772    -0.516046      60.65
 H       0.052317     2.005677    -0.470192      28.58
 C       2.205698    -0.722254    -0.492474      33.98
 C       3.728991    -0.870510    -0.467531     106.14
 H       3.846281    -1.537913    -1.395718      27.41
 O       4.443771     0.173603    -1.115661      90.13
 H       4.513346     1.015910    -0.480233      30.86
 C       4.122428    -1.248885     0.993763      97.83
 H       3.341810    -1.903751     1.370943      28.69
 O       5.535440    -1.912613     1.005981     131.71
 H       6.133018    -1.524114     0.182999      18.90
 C       4.159797    -0.011164     1.937320     109.87
 O       5.343224     0.919778     1.648597     176.15
 H       5.018693     1.756943     2.234805      24.97
 H       4.139066    -0.192972     2.935639      31.95
 H       3.225507     0.639381     1.619300      30.92
55
name = lig-Water-frame_554
 C      -2.062076     3.492486     2.115514      43.83
 H      -2.651567     4.319820     1.795054      20.21
 C      -1.409712     1.047534     2.420600      35.23
 H      -1.477035     0.018920     2.120456      28.38
 C      -0.228580     1.542113     3.293897     -15.68
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 O       0.663180     0.631014     3.938599     102.68
 C       0.602632    -0.772964     3.579960     126.65
 H       1.396424    -1.101892     4.309698      28.53
 H       1.027140    -1.272883     2.560977      28.57
 H      -0.253041    -1.414726     3.659814      27.94
 C       0.030012     2.941851     3.444862       4.82
 O       1.282219     3.298949     4.066527     136.54
 H       1.396431     4.266374     4.497902      19.86
 C      -0.810772     3.966860     2.922150      30.73
 H      -0.530948     4.939157     2.844287      21.55
 C      -2.164551     2.125524     1.861377      16.24
 C      -3.328632     1.613163     0.995516     101.38
 H      -4.091958     2.298156     0.767480      28.58
 O      -4.170490     0.572317     1.684383     257.43
 H      -5.095301     0.517058     1.353961      26.60
 C      -2.825864     1.155750    -0.525369      83.88
 H      -2.074087     2.088866    -0.754351      25.67
 C      -3.797358     0.975889    -1.744892      83.30
 O      -4.916118     0.102514    -1.295952     203.67
 H      -4.474481    -0.555117    -0.626438      27.40
 H      -3.239385     0.482535    -2.693364      26.85
 H      -3.963782     2.124475    -2.020249      26.25
 C       1.650143     0.651851    -0.461031      62.22
 H       2.443274     1.288941     0.073793      29.62
 C       1.334146    -1.744403    -0.737882      61.51
 H       1.603403    -2.638358    -1.189594      27.95
 C      -0.038981    -1.618394    -0.728065      -4.41
 O      -0.805291    -2.744002    -0.863113     208.82
 C      -0.774922    -3.397672    -2.211325      80.05
 H      -0.207570    -4.179776    -2.217797      29.10
 H      -1.897300    -3.525256    -2.392368      25.67
 H      -0.291097    -2.362957    -3.000930      24.41
 C      -0.718491    -0.125392    -0.505647       5.99
 O      -2.082300    -0.150925    -0.478763     147.94
 C       0.265776     0.935053    -0.442556      73.52
 H      -0.154632     2.023445    -0.555719      27.24
 C       2.211452    -0.636346    -0.537535      27.00
 C       3.757478    -0.932101    -0.458200     102.24
 H       3.947136    -1.707151    -1.225095      27.70
 O       4.471635     0.171215    -1.076984     164.97
 H       4.691156     0.966250    -0.656205      31.47
 C       4.126059    -1.251438     1.051836      87.06
 H       3.379516    -1.914346     1.615698      27.54
 O       5.531429    -1.953906     1.041805     145.50
 H       6.008871    -1.475777     0.246986      22.84
 C       4.105448     0.030075     1.932372     104.86
 O       5.317517     0.966076     1.654779     195.47
 H       4.841800     1.782102     2.102040      25.68
 H       3.885955    -0.309556     3.088623      27.22
 H       3.181403     0.501412     1.785019      30.60
55
name = lig-Water-frame_555
 C      -2.007868     3.611301     2.188400      39.60
 H      -2.742040     4.356577     1.814051      19.89
 C      -1.303787     1.095534     2.457701     106.30
 H      -1.343482     0.068204     2.070539      26.97
 C      -0.196854     1.501978     3.238221     -12.15
 O       0.674007     0.565444     3.937118     164.01
 C       0.640664    -0.750656     3.637359     143.50
 H       1.238562    -1.271481     4.370947      27.94
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 H       0.841270    -0.910365     2.606924      28.92
 H      -0.389155    -1.361053     3.721352      26.07
 C      -0.039511     2.900366     3.465831     -13.29
 O       1.297749     3.295918     4.093948      91.94
 H       1.168233     4.221912     4.369897      25.13
 C      -0.884864     3.951883     2.879886      50.33
 H      -0.384780     5.054087     2.796388      21.56
 C      -2.141916     2.071882     1.938375     -44.13
 C      -3.290961     1.555426     0.904201      93.31
 H      -4.009115     2.613319     0.897341      23.17
 O      -4.179403     0.581373     1.690537     240.01
 H      -5.153359     0.742751     1.374423      24.57
 C      -2.801076     1.141206    -0.520091     105.53
 H      -2.121085     1.852227    -0.745871      28.20
 C      -3.787303     0.986270    -1.783775      92.65
 O      -4.883828     0.081747    -1.308246     259.79
 H      -4.574834    -0.624636    -0.749206      28.48
 H      -3.232041     0.487550    -2.600118      27.91
 H      -4.201371     1.975218    -1.843622      27.04
 C       1.664042     0.649377    -0.449725      63.41
 H       2.229478     1.517895    -0.004920      27.72
 C       1.346119    -1.695702    -0.748800      34.29
 H       1.897285    -2.759548    -1.073916      23.43
 C      -0.091519    -1.590343    -0.702263      -1.30
 O      -0.880292    -2.728519    -0.904597     225.93
 C      -0.771377    -3.300595    -2.138494     115.67
 H       0.073736    -4.265256    -2.419506      25.28
 H      -1.846031    -3.472410    -2.385755      26.80
 H      -0.672805    -2.644272    -2.928851      28.58
 C      -0.689420    -0.152412    -0.577139       2.56
 O      -2.099025    -0.142117    -0.481917     180.32
 C       0.214762     0.900146    -0.386293      75.32
 H      -0.167522     1.839736    -0.468862      28.59
 C       2.214901    -0.569600    -0.597523      30.79
 C       3.728851    -0.967496    -0.445773      78.51
 H       4.098681    -2.056856    -0.790138      24.75
 O       4.525206     0.160767    -1.058696     160.30
 H       4.726464     0.925887    -0.447377      27.55
 C       4.188237    -1.248555     1.091530      87.31
 H       3.550011    -2.036309     1.595746      27.05
 O       5.479042    -1.971432     1.086412     219.09
 H       5.998155    -1.591066     0.458687      28.66
 C       4.076636     0.046754     1.945369     100.59
 O       5.245633     0.994053     1.674255     199.37
 H       4.916668     1.887243     2.044267      25.67
 H       4.091573    -0.283436     2.935256      29.25
 H       3.012173     0.578150     1.789603      26.65
55
name = lig-Water-frame_556
 C      -1.979649     3.622433     2.233685      35.03
 H      -2.740366     4.255431     1.714361      16.94
 C      -1.189541     1.151978     2.483678      95.95
 H      -1.333440     0.118552     2.125032      26.47
 C      -0.151426     1.460664     3.229980      12.90
 O       0.668292     0.588076     3.939979     172.61
 C       0.634006    -0.815658     3.672395     129.61
 H       1.260291    -1.496003     4.341677      27.41
 H       0.918427    -0.729938     2.534800      26.24
 H      -0.438402    -0.958015     3.886535      25.88
 C      -0.027170     2.892676     3.494858      -8.89
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 O       1.253366     3.271000     4.097144     125.45
 H       1.170005     4.219226     4.332144      25.22
 C      -0.877914     3.929329     2.862105      62.17
 H      -0.474136     4.916834     3.016674      31.63
 C      -2.174843     2.063322     1.972815     -33.05
 C      -3.297181     1.551966     0.875106      93.75
 H      -3.716622     2.474780     0.751085      25.53
 O      -4.177390     0.599884     1.669116     262.37
 H      -5.101421     0.911240     1.521002      25.47
 C      -2.775098     1.113036    -0.529750      93.15
 H      -1.973605     1.933233    -0.895478      22.92
 C      -3.796248     0.973757    -1.711927      86.13
 O      -4.855729     0.083148    -1.349085     222.38
 H      -4.583320    -0.840104    -0.925749      23.54
 H      -3.186789     0.597895    -2.657012      26.19
 H      -4.502273     1.879038    -1.968940      23.62
 C       1.632219     0.719989    -0.402675      33.69
 H       2.117723     1.704901    -0.303050      25.20
 C       1.336220    -1.672797    -0.779558      43.16
 H       1.848170    -2.528808    -0.776788      25.76
 C      -0.104176    -1.505166    -0.678159      15.48
 O      -0.940623    -2.682850    -0.900712     216.74
 C      -0.781099    -3.270741    -2.134027     124.50
 H      -0.093954    -3.928351    -2.276563      30.22
 H      -1.781698    -3.857904    -2.372296      26.37
 H      -0.783421    -2.494241    -3.202329      23.51
 C      -0.652481    -0.266032    -0.637009      19.41
 O      -2.088891    -0.141490    -0.481078     183.06
 C       0.188822     0.828312    -0.363384      50.80
 H      -0.169454     1.954039    -0.238723      24.38
 C       2.244005    -0.593408    -0.656474       2.47
 C       3.708603    -0.984875    -0.397949      83.27
 H       3.998285    -1.935005    -0.718134      25.94
 O       4.586948     0.130050    -1.044808     207.91
 H       4.653761     0.635713    -0.132592      25.85
 C       4.244959    -1.230042     1.104094      91.04
 H       3.559615    -2.016910     1.464808      26.56
 O       5.404933    -1.976015     1.144000     200.44
 H       6.291356    -1.651150     0.522384      21.46
 C       4.067151     0.065480     1.953273     107.44
 O       5.158392     1.001763     1.683979     198.04
 H       4.937063     1.945798     2.159791      23.19
 H       4.351036    -0.214573     3.078984      25.41
 H       3.189397     0.535215     1.758136      28.87
55
name = lig-Water-frame_557
 C      -2.044118     3.487372     2.197706      52.43
 H      -2.622732     4.233912     1.702002      20.57
 C      -1.186647     1.171344     2.433298      60.76
 H      -1.350851     0.131201     2.238028      28.20
 C      -0.062813     1.494061     3.301904      26.88
 O       0.695451     0.654228     3.972720     143.24
 C       0.588987    -0.867228     3.666762     121.51
 H       1.309634    -1.424914     4.225679      29.39
 H       0.944591    -1.079285     2.635129      29.21
 H      -0.478278    -1.026010     3.870726      26.45
 C       0.046286     2.895929     3.508147      18.78
 O       1.171864     3.239495     4.091529     183.93
 H       1.382517     4.223405     4.388025      22.57
 C      -0.765254     3.886416     2.928040      59.43
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 H      -0.576540     4.999983     3.230627      28.31
 C      -2.200618     2.105270     1.975163       0.49
 C      -3.272683     1.553588     0.924776      70.11
 H      -3.861084     2.601240     0.416523      24.38
 O      -4.158905     0.637296     1.622117     251.23
 H      -5.131897     0.898552     1.653781      25.04
 C      -2.721032     1.120982    -0.557466      92.54
 H      -2.126659     1.912114    -0.906654      26.89
 C      -3.823423     0.959055    -1.621326     108.27
 O      -4.845047     0.055750    -1.397674     278.24
 H      -4.549772    -0.857562    -1.123570      27.01
 H      -3.238703     0.830092    -2.583675      27.36
 H      -4.373120     1.809048    -2.064373      26.29
 C       1.573759     0.776279    -0.366193      35.60
 H       2.175308     1.744519    -0.649188      22.57
 C       1.306653    -1.618427    -0.796345      46.82
 H       1.718399    -2.775155    -0.546255      23.42
 C      -0.069210    -1.508344    -0.698671      29.84
 O      -0.983417    -2.598799    -0.862074     169.90
 C      -0.874772    -3.234770    -2.229838     105.29
 H       0.305296    -3.922028    -2.110432      23.75
 H      -1.471463    -4.181751    -2.199247      25.38
 H      -0.751889    -2.521778    -2.894428      27.19
 C      -0.685306    -0.311290    -0.649239      23.59
 O      -2.048912    -0.174847    -0.484498     150.93
 C       0.214324     0.797019    -0.360863      51.71
 H      -0.189202     1.685425    -0.028119      28.51
 C       2.252544    -0.606409    -0.672661       4.64
 C       3.717668    -0.958702    -0.361507      77.79
 H       3.853209    -1.930651    -1.110528      22.07
 O       4.632335     0.073104    -0.994697     237.58
 H       4.834964     0.562724    -0.222532      30.35
 C       4.233925    -1.188404     1.092337      97.11
 H       3.340638    -1.852245     1.453311      26.45
 O       5.390673    -1.980811     1.189562     225.69
 H       6.194084    -1.737108     0.714766      26.98
 C       4.125193     0.048619     2.008388     110.93
 O       5.099850     1.019606     1.673639     211.38
 H       4.677006     1.769156     2.188441      25.12
 H       4.204649    -0.155930     3.083540      28.37
 H       3.033271     0.517860     1.810559      26.01
55
name = lig-Water-frame_558
 C      -2.035677     3.369216     2.185707      54.49
 H      -2.583431     4.255015     1.738537      21.57
 C      -1.196478     1.180850     2.411377      37.77
 H      -1.390610     0.078484     2.289818      27.59
 C      -0.083513     1.551575     3.318044      13.57
 O       0.764050     0.673081     4.018094      57.95
 C       0.540239    -0.871473     3.650983     104.12
 H       1.316792    -1.253797     4.383736      27.74
 H       0.790324    -1.304482     2.627435      29.12
 H      -0.500692    -1.417271     3.822630      26.21
 C       0.110648     2.924260     3.486522      30.42
 O       1.169169     3.228500     4.138286     226.31
 H       1.428909     4.110547     4.365227      26.85
 C      -0.725307     3.833910     2.976291      59.60
 H      -0.758287     4.901829     3.353394      23.95
 C      -2.212107     2.111376     1.931465      19.84
 C      -3.263237     1.621598     0.949884      95.80
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 H      -3.893021     2.326342     0.586742      28.64
 O      -4.130003     0.672656     1.573633     269.57
 H      -5.121565     0.869217     1.598040      26.96
 C      -2.701217     1.124170    -0.535732      74.87
 H      -2.059425     2.009806    -0.936680      25.28
 C      -3.827941     0.970193    -1.571449      95.86
 O      -4.861314     0.000875    -1.457113     273.09
 H      -4.479802    -0.807682    -1.101986      29.05
 H      -3.195773     0.726925    -2.545448      26.84
 H      -4.209154     2.025769    -1.783581      27.08
 C       1.596019     0.764035    -0.400803      54.83
 H       2.152412     1.601700    -0.590896      25.40
 C       1.328773    -1.642256    -0.773326      60.80
 H       1.482689    -2.608125    -0.636100      27.06
 C      -0.069910    -1.563801    -0.762015       3.87
 O      -1.016584    -2.529332    -0.838780     193.04
 C      -0.869300    -3.292060    -2.225602      88.15
 H       0.083775    -3.431658    -2.202482      29.24
 H      -1.473398    -4.165280    -2.226671      27.66
 H      -0.835284    -2.251636    -3.065403      23.39
 C      -0.709467    -0.258005    -0.609768      22.02
 O      -2.010065    -0.221368    -0.496765     146.18
 C       0.204722     0.779144    -0.361213      59.17
 H      -0.354663     1.680933     0.070850      26.80
 C       2.219390    -0.549214    -0.631141      17.17
 C       3.748617    -0.927862    -0.411197      97.00
 H       3.830753    -1.701062    -1.040181      25.69
 O       4.669337     0.007431    -0.942986     240.08
 H       5.127729     0.722777    -0.365408      27.41
 C       4.151567    -1.167735     1.081703      94.12
 H       3.346367    -1.715799     1.533352      28.51
 O       5.387094    -1.998687     1.245443     170.68
 H       6.108887    -1.667423     0.649103      26.14
 C       4.136329     0.013510     2.045420     123.19
 O       5.066767     1.048832     1.661685     224.56
 H       4.503004     1.897014     2.061095      22.88
 H       4.071980    -0.294532     3.186925      26.93
 H       3.159114     0.333719     1.969164      29.33
55
name = lig-Water-frame_559
 C      -1.927312     3.408331     2.229383      43.30
 H      -2.622958     4.115658     1.839737      24.48
 C      -1.190253     1.164496     2.449393      42.99
 H      -1.364600     0.134031     2.284878      30.90
 C      -0.183417     1.558161     3.275086      16.24
 O       0.800083     0.648081     4.019769      79.74
 C       0.513848    -0.875672     3.671861     116.89
 H       1.166437    -1.192549     4.447018      30.03
 H       0.719622    -1.146748     2.571626      30.66
 H      -0.380272    -1.351488     3.924353      30.11
 C       0.152918     2.941434     3.447811      -0.37
 O       1.262958     3.221748     4.242294      62.27
 H       1.388780     4.245238     4.384383      24.47
 C      -0.835686     3.802675     2.964482      75.71
 H      -0.787483     4.803829     3.344247      24.78
 C      -2.194088     2.017511     1.860387     -13.08
 C      -3.250206     1.661583     0.934075      78.79
 H      -4.116926     2.626373     0.768406      23.10
 O      -4.099601     0.677069     1.546874     257.39
 H      -5.029548     0.933190     1.379298      26.21
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 C      -2.704736     1.122699    -0.469770      81.04
 H      -1.991774     1.842575    -0.914110      27.60
 C      -3.798200     1.006685    -1.570469      88.28
 O      -4.885402    -0.050211    -1.523394     211.75
 H      -4.466479    -0.779421    -0.851745      24.95
 H      -3.239547     0.639509    -2.466174      27.18
 H      -4.166276     2.059708    -1.373376      26.73
 C       1.637671     0.689618    -0.473719      73.63
 H       2.275705     1.716472    -0.281669      26.69
 C       1.329941    -1.673910    -0.736580      26.42
 H       1.753862    -2.851060    -0.797011      23.59
 C      -0.102384    -1.526191    -0.824572       9.78
 O      -1.051982    -2.521366    -0.850744     215.20
 C      -0.861480    -3.254655    -2.198449      78.63
 H       0.421004    -3.286467    -2.418348      23.83
 H      -1.668965    -4.078534    -2.376590      24.95
 H      -1.219841    -2.671700    -2.936704      27.87
 C      -0.634463    -0.237926    -0.559615      27.14
 O      -2.020502    -0.240134    -0.505350     145.35
 C       0.153869     0.818914    -0.344722      68.06
 H      -0.280971     1.782125    -0.057312      28.84
 C       2.188473    -0.484562    -0.560864      11.12
 C       3.757091    -0.849949    -0.438360      97.86
 H       3.976442    -1.954466    -1.005528      22.48
 O       4.732562    -0.028692    -0.933579     241.25
 H       5.150360     0.706048    -0.326165      25.74
 C       4.074470    -1.183616     1.089260      60.33
 H       3.300447    -1.908062     1.622366      27.83
 O       5.373990    -2.006333     1.293335      96.26
 H       5.975194    -1.620240     0.428865      21.06
 C       4.123255    -0.031766     2.074472     105.28
 O       5.027398     1.093683     1.664768     215.65
 H       4.700305     1.986436     1.902812      27.65
 H       4.314614    -0.481055     3.098287      28.24
 H       3.012874     0.401968     2.039193      27.04
55
name = lig-Water-frame_560
 C      -1.877945     3.412476     2.222010      52.65
 H      -2.689800     4.121173     1.943929      22.29
 C      -1.240070     1.105768     2.468552      63.83
 H      -1.272517     0.001015     2.282575      28.86
 C      -0.192887     1.553053     3.278602       8.17
 O       0.761005     0.608691     3.959866     115.93
 C       0.525241    -0.837546     3.712893     115.86
 H       1.245310    -1.440938     4.390129      28.56
 H       0.779066    -0.925930     2.675491      31.97
 H      -0.624462    -1.036217     4.111043      24.66
 C       0.192720     2.921544     3.434661      -8.14
 O       1.350151     3.224869     4.334775     155.32
 H       1.429805     4.233088     4.480161      25.50
 C      -0.913709     3.815540     2.986425      54.97
 H      -0.753713     4.966357     3.260822      21.67
 C      -2.095109     1.991414     1.843803      36.24
 C      -3.277651     1.702909     0.886795      96.67
 H      -3.725372     2.621733     0.832539      29.86
 O      -4.078665     0.662877     1.534341     261.35
 H      -5.015432     0.910912     1.242532      24.24
 C      -2.721691     1.088218    -0.419969      94.56
 H      -1.967844     1.766374    -0.861709      29.04
 C      -3.773042     1.032674    -1.549305      91.92
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 O      -4.881977    -0.093426    -1.564783     175.47
 H      -4.742016    -0.634557    -0.778020      29.46
 H      -3.255892     0.900606    -2.550686      27.14
 H      -4.351980     1.974137    -1.482248      27.28
 C       1.613580     0.740393    -0.510922      64.86
 H       2.192025     1.439487    -0.077633      30.95
 C       1.314111    -1.733279    -0.703179      50.37
 H       1.957779    -2.477975    -0.958188      27.66
 C      -0.081873    -1.472839    -0.849223      27.54
 O      -1.071177    -2.552455    -0.909591     197.72
 C      -0.835873    -3.207318    -2.166740     119.19
 H       0.027909    -3.461550    -2.526686      30.74
 H      -1.415431    -4.107294    -2.166823      28.93
 H      -1.682385    -2.695100    -3.022189      24.88
 C      -0.592865    -0.246038    -0.517251      20.55
 O      -2.050258    -0.228890    -0.492653     115.40
 C       0.190233     0.914640    -0.336216      50.06
 H      -0.134760     1.932016    -0.212332      29.46
 C       2.215017    -0.557116    -0.516947     -21.92
 C       3.739621    -0.847912    -0.423869     103.48
 H       3.908131    -1.740485    -0.798668      29.80
 O       4.824777    -0.023258    -0.958429     275.43
 H       4.927351     0.507714    -0.167092      28.74
 C       4.019252    -1.241979     1.125469      70.66
 H       3.316441    -1.949731     1.420352      29.36
 O       5.347490    -1.976555     1.288524     151.40
 H       5.871306    -1.858325     0.573713      28.11
 C       4.071263    -0.033036     2.086157     116.60
 O       5.004787     1.099688     1.654147     170.43
 H       4.637229     2.035633     2.099027      24.20
 H       4.593673    -0.469528     3.028436      29.41
 H       3.134938     0.420284     2.266043      28.28
55
name = lig-Water-frame_561
 C      -1.941416     3.354345     2.141190      40.07
 H      -2.666485     4.155846     1.962392      21.81
 C      -1.286537     1.010575     2.479074      54.98
 H      -1.267435    -0.042018     2.283263      26.64
 C      -0.110749     1.522185     3.324824       5.87
 O       0.696680     0.593370     3.883910     127.93
 C       0.512528    -0.776924     3.794423     136.18
 H       1.202068    -1.504200     4.180881      28.90
 H       0.694737    -1.002835     2.619909      30.35
 H      -0.451630    -0.861784     3.996867      29.54
 C       0.213947     2.910749     3.469867       0.75
 O       1.381759     3.210978     4.377277     195.03
 H       1.626054     4.166821     4.612469      26.60
 C      -0.830806     3.881752     3.088909      28.57
 H      -0.803106     4.899418     3.148684      18.05
 C      -2.002890     2.035113     1.846772      43.44
 C      -3.228051     1.665596     0.880355      73.55
 H      -3.599031     2.875015     0.624540      23.99
 O      -4.079060     0.666836     1.520498     249.46
 H      -5.067602     0.742933     1.374903      21.87
 C      -2.740909     1.058795    -0.437476      96.30
 H      -2.004460     1.883949    -0.796620      27.62
 C      -3.791523     1.033838    -1.535608      99.06
 O      -4.853196    -0.106067    -1.601739     145.46
 H      -4.872148    -0.671761    -0.742161      27.59
 H      -3.309954     1.259463    -2.580482      25.41
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 H      -4.557998     1.871050    -1.721198      24.06
 C       1.580088     0.772619    -0.494562      45.23
 H       2.331602     1.571222     0.005144      25.73
 C       1.333062    -1.710610    -0.686757      57.27
 H       1.965449    -2.618656    -1.141365      24.47
 C      -0.046991    -1.486276    -0.827114      17.33
 O      -1.035920    -2.559609    -0.979916     208.77
 C      -0.955279    -3.184398    -2.184488     114.03
 H       0.188900    -3.526768    -2.720127      24.65
 H      -1.107846    -4.322608    -1.764592      23.88
 H      -1.471066    -2.704247    -2.834066      29.95
 C      -0.627637    -0.196551    -0.479836       2.13
 O      -2.063200    -0.209124    -0.452254     118.96
 C       0.271685     0.990271    -0.356720      50.31
 H      -0.108839     2.089744    -0.322585      26.77
 C       2.209717    -0.645290    -0.511344      -5.49
 C       3.716133    -0.875870    -0.363303      61.92
 H       3.834937    -1.971005    -0.986458      24.19
 O       4.891151    -0.005422    -0.969506     201.68
 H       4.910704     0.570057    -0.071914      22.86
 C       4.021459    -1.268288     1.137130      78.15
 H       3.115690    -2.050573     1.297117      26.85
 O       5.290167    -1.939329     1.285943     114.10
 H       5.994241    -1.979571     0.464392      21.46
 C       4.048954    -0.023831     2.117010     102.45
 O       4.968616     1.096767     1.643112     250.53
 H       4.546362     1.742992     2.205530      27.63
 H       4.728541    -0.336929     2.999517      27.56
 H       3.073007     0.402080     2.566055      25.84
55
name = lig-Water-frame_562
 C      -1.925262     3.373237     2.146107      44.66
 H      -2.654176     4.094699     1.779084      23.60
 C      -1.238571     0.976950     2.533455      57.95
 H      -1.407617    -0.074357     2.225461      27.21
 C      -0.091734     1.461036     3.316820      11.20
 O       0.697014     0.615437     3.852151     165.24
 C       0.486301    -0.749050     3.778274     119.20
 H       1.260744    -1.333228     4.356333      26.99
 H       0.446588    -1.153426     2.784474      30.15
 H      -0.689166    -1.120356     4.047678      25.17
 C       0.227565     2.957962     3.565135       6.53
 O       1.370322     3.163106     4.378472     240.27
 H       1.738344     4.133825     4.608884      25.98
 C      -0.745559     3.862812     3.132585      63.30
 H      -0.735630     5.071395     3.204733      15.98
 C      -1.995628     2.025253     1.822908      20.19
 C      -3.144677     1.639611     0.890028      91.37
 H      -3.658300     2.443891     0.509014      27.82
 O      -4.086401     0.681488     1.518693     281.45
 H      -5.092186     0.804364     1.559938      21.40
 C      -2.750938     1.086621    -0.493041      89.73
 H      -2.123977     1.882037    -0.816282      28.18
 C      -3.882171     1.038975    -1.571678     111.98
 O      -4.804919    -0.107539    -1.639337     224.27
 H      -4.687120    -0.748625    -0.846089      25.06
 H      -3.343906     1.072011    -2.491543      26.72
 H      -4.518420     1.898730    -1.492904      27.33
 C       1.673484     0.745428    -0.413056      49.11
 H       2.282179     1.607529    -0.342107      23.64
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 C       1.388522    -1.705422    -0.723768      59.74
 H       1.496418    -2.732935    -1.050949      23.98
 C      -0.063756    -1.483899    -0.760224       3.89
 O      -0.953501    -2.507934    -1.002897     232.55
 C      -1.001305    -3.297552    -2.221845     112.02
 H      -0.075572    -3.119658    -2.568977      29.13
 H      -1.161753    -4.241248    -1.869269      27.42
 H      -1.668582    -2.666301    -3.148571      23.34
 C      -0.657544    -0.137584    -0.467562       5.49
 O      -2.050785    -0.185968    -0.397979     150.72
 C       0.266686     1.033254    -0.401531      46.99
 H      -0.088892     1.986913    -0.327934      26.62
 C       2.181131    -0.612960    -0.520825      36.76
 C       3.724802    -0.970377    -0.344518      70.45
 H       3.846056    -1.740518    -0.949007      28.24
 O       4.896136     0.008798    -0.932138     238.16
 H       5.180001     0.749209    -0.376282      26.98
 C       4.013753    -1.269902     1.117841     102.91
 H       3.246035    -1.891090     1.401034      29.58
 O       5.246194    -1.916337     1.283686     159.36
 H       5.865268    -1.879725     0.420259      25.72
 C       4.064158    -0.028444     2.168649      95.55
 O       4.902981     1.066634     1.626487     290.49
 H       4.571686     1.916411     2.244705      23.77
 H       4.602140    -0.403469     3.077374      26.92
 H       3.106315     0.253592     2.642282      26.69
55
name = lig-Water-frame_563
 C      -1.820755     3.416144     2.218682      33.07
 H      -2.509598     4.060069     1.603625      21.46
 C      -1.165851     1.020502     2.567961      76.26
 H      -1.463597     0.006065     2.299378      28.18
 C      -0.155873     1.472220     3.254526       3.14
 O       0.766460     0.620784     3.870062     128.63
 C       0.406261    -0.804832     3.768427     123.22
 H       1.172406    -1.010478     4.516877      25.51
 H       0.388291    -1.299588     2.676106      27.13
 H      -0.409962    -1.114719     4.275659      30.42
 C       0.215760     2.973332     3.666680      -8.25
 O       1.348468     3.105570     4.366415     195.24
 H       1.557326     4.059052     4.466121      25.24
 C      -0.717913     3.849897     3.101774      63.84
 H      -0.549617     4.813317     3.377379      32.04
 C      -2.018077     1.993448     1.826950      -0.93
 C      -3.088803     1.584524     0.892695      74.61
 H      -3.976866     2.421250     0.545661      21.77
 O      -4.082623     0.684207     1.535246     226.19
 H      -5.010471     1.117302     1.581562      20.99
 C      -2.760136     1.114939    -0.537636      70.77
 H      -2.060202     1.932583    -1.068727      25.42
 C      -3.977440     1.032263    -1.597849      95.77
 O      -4.755246    -0.118040    -1.671874     268.90
 H      -4.490590    -0.758324    -1.023755      26.27
 H      -3.349719     0.827843    -2.604130      22.94
 H      -4.428324     2.047537    -1.232036      24.46
 C       1.743320     0.703432    -0.336398      58.42
 H       2.422545     1.604062    -0.604880      23.03
 C       1.326836    -1.706145    -0.780894      39.59
 H       1.469320    -2.819311    -0.865007      23.66
 C      -0.068237    -1.423129    -0.685960       8.10
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 O      -0.897048    -2.453467    -0.989070     166.36
 C      -1.038888    -3.331667    -2.299079      76.40
 H       0.050166    -2.954596    -2.724625      24.04
 H      -1.425408    -4.464607    -2.132457      24.85
 H      -1.798825    -3.120481    -2.909216      27.99
 C      -0.632696    -0.104630    -0.481701      20.76
 O      -2.028951    -0.149842    -0.350401     132.53
 C       0.245546     0.985349    -0.450042      50.02
 H      -0.129933     2.099325    -0.284557      26.12
 C       2.226957    -0.528590    -0.529841      25.63
 C       3.740873    -0.972476    -0.335569      59.22
 H       4.033999    -1.916752    -1.106272      22.68
 O       4.862766     0.000276    -0.901873     236.06
 H       5.215814     0.792853    -0.459395      26.99
 C       4.006573    -1.216563     1.118873      91.47
 H       3.202915    -1.933145     1.686586      25.89
 O       5.238308    -1.921310     1.272638     179.81
 H       5.695864    -1.686634     0.527194      30.57
 C       4.097221    -0.051560     2.205856      83.59
 O       4.810086     1.050378     1.638611     317.55
 H       4.748096     1.912298     1.975271      30.19
 H       4.494041    -0.640735     3.157261      24.84
 H       3.044438     0.253668     2.470102      26.49
55
name = lig-Water-frame_564
 C      -1.712704     3.399818     2.259706      67.03
 H      -2.191427     4.178382     1.689078      24.05
 C      -1.196690     1.088189     2.505174      66.02
 H      -1.311126     0.002650     2.508100      27.85
 C      -0.115114     1.561705     3.285526       0.71
 O       0.814606     0.618343     3.875615      65.06
 C       0.378749    -0.868304     3.781624     114.13
 H       1.224527    -1.229479     4.423309      25.44
 H       0.504703    -1.255288     2.843329      28.79
 H      -0.570806    -0.985790     4.578856      24.46
 C       0.129112     2.874904     3.688560      14.32
 O       1.325085     3.056358     4.358447     119.98
 H       1.454371     4.093117     4.466896      24.90
 C      -0.696888     3.832291     3.063483      69.43
 H      -0.481056     4.922783     3.484141      29.52
 C      -2.002453     2.027775     1.898574      13.92
 C      -3.140993     1.580763     0.868025      90.89
 H      -3.661124     2.487459     0.839609      26.87
 O      -4.057570     0.679499     1.560420     274.23
 H      -4.899790     1.152530     1.495840      23.23
 C      -2.742420     1.137827    -0.582186      90.77
 H      -2.148724     1.786061    -1.103192      28.62
 C      -3.978331     1.029680    -1.609901     113.72
 O      -4.739502    -0.144618    -1.698458     278.57
 H      -4.408336    -0.882017    -1.029452      24.46
 H      -3.533628     1.183160    -2.551835      26.85
 H      -4.509525     1.940654    -1.456947      28.24
 C       1.735191     0.735729    -0.307784      44.70
 H       2.514042     1.487215    -0.596225      23.47
 C       1.244710    -1.652225    -0.807484      48.11
 H       1.779251    -2.646914    -0.682668      23.76
 C      -0.034129    -1.368180    -0.662457      30.18
 O      -0.911928    -2.451805    -0.964349     115.52
 C      -1.014774    -3.331495    -2.345219      76.51
 H      -0.205696    -3.312200    -3.028720      27.16
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 H      -1.170639    -4.368422    -2.170822      27.85
 H      -2.189695    -3.071916    -2.844837      24.28
 C      -0.599003    -0.090909    -0.503609      29.22
 O      -2.002213    -0.103748    -0.323332     154.10
 C       0.274496     0.940530    -0.469030      65.27
 H      -0.050261     1.897913    -0.330076      29.82
 C       2.310521    -0.558717    -0.552376      -7.32
 C       3.764648    -0.921704    -0.374853      88.19
 H       4.010769    -1.804220    -0.822275      26.88
 O       4.808072    -0.027370    -0.898073     260.24
 H       4.935312     0.704912    -0.130166      22.98
 C       3.986143    -1.182054     1.199000      96.52
 H       3.284016    -1.807253     1.597775      29.62
 O       5.249267    -1.952440     1.256701     132.30
 H       5.908577    -1.434246     0.491400      21.99
 C       4.079230    -0.077204     2.226244      95.80
 O       4.750036     1.020607     1.639233     303.02
 H       4.614213     1.955833     2.085053      26.40
 H       4.499232    -0.566854     3.081922      26.05
 H       3.011464     0.304376     2.286990      25.88
55
name = lig-Water-frame_565
 C      -1.650595     3.388472     2.235363      44.26
 H      -2.078461     4.328825     1.799553      23.18
 C      -1.204657     1.138042     2.463164      41.09
 H      -1.240427     0.056901     2.527924      25.80
 C      -0.047450     1.557393     3.351403      -0.99
 O       0.829752     0.600800     3.860130     119.35
 C       0.392687    -0.884166     3.898294     110.62
 H       1.190080    -1.603833     4.212682      25.95
 H       0.389675    -1.292853     2.743514      26.80
 H      -0.554379    -0.899163     4.288698      27.30
 C       0.063874     2.791771     3.680633      34.15
 O       1.289479     3.034748     4.357935     114.87
 H       1.482345     3.954138     4.602264      25.16
 C      -0.636337     3.836506     3.086187      61.58
 H      -0.608147     4.882152     3.270898      28.97
 C      -1.995032     2.077149     1.949906      38.50
 C      -3.185969     1.635144     0.873996      81.40
 H      -3.487381     2.820621     0.924939      23.08
 O      -4.015328     0.682177     1.572098     255.22
 H      -5.054288     0.873433     1.441882      19.80
 C      -2.744428     1.136509    -0.588294      83.99
 H      -2.009268     1.964118    -1.098825      25.29
 C      -3.922911     1.034645    -1.608939      96.77
 O      -4.734834    -0.195021    -1.715809     281.23
 H      -4.488964    -0.866301    -1.047912      28.05
 H      -3.591208     1.535947    -2.626408      24.13
 H      -4.825521     1.829228    -1.569046      22.97
 C       1.726568     0.742167    -0.347157      38.98
 H       2.416186     1.618213    -0.331815      22.97
 C       1.340938    -1.557371    -0.782147      56.69
 H       1.775328    -2.511355    -0.765706      25.45
 C      -0.063502    -1.379988    -0.705478      20.16
 O      -0.956870    -2.490607    -0.951610     127.99
 C      -1.045432    -3.295981    -2.372472      81.01
 H      -0.306395    -3.357212    -3.334862      25.34
 H      -0.880657    -4.365771    -1.880053      25.07
 H      -1.925363    -2.883349    -2.590012      27.47
 C      -0.598923    -0.103902    -0.523058      24.85
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 O      -1.970388    -0.057106    -0.321848     184.92
 C       0.373162     0.928447    -0.457209      58.99
 H      -0.058167     2.003458    -0.388038      26.54
 C       2.305036    -0.604555    -0.581210      17.09
 C       3.773513    -0.853826    -0.371199      80.66
 H       3.947061    -2.028460    -0.732183      22.94
 O       4.739949    -0.025643    -0.875064     303.49
 H       4.672026     0.455941    -0.060796      27.18
 C       4.013845    -1.178222     1.254183      75.66
 H       3.121278    -1.953615     1.490653      26.08
 O       5.281466    -1.971860     1.214177     164.33
 H       6.008696    -1.514823     0.805772      26.51
 C       3.995242    -0.078569     2.208536     100.52
 O       4.732611     1.027645     1.635010     276.43
 H       4.309808     1.700754     2.280977      24.06
 H       4.575988    -0.332772     3.256692      23.76
 H       2.995550     0.233661     2.448325      26.17
55
name = lig-Water-frame_566
 C      -1.617885     3.458787     2.184060      52.14
 H      -2.262295     4.249043     1.783300      30.78
 C      -1.108928     1.139774     2.514862      67.59
 H      -1.415405     0.101537     2.216539      26.02
 C      -0.075813     1.378984     3.349060      23.07
 O       0.851241     0.546431     3.854074     190.98
 C       0.440026    -0.877684     3.928207     124.64
 H       1.102701    -1.650179     4.338188      26.99
 H       0.115496    -1.120479     2.976268      28.93
 H      -0.728070    -0.970796     4.257682      25.65
 C       0.119469     2.848788     3.725103      -9.64
 O       1.252959     3.010202     4.376206     117.49
 H       1.445505     3.952588     4.685105      26.84
 C      -0.612826     3.816765     3.098108      62.92
 H      -0.526294     4.926828     3.190102      24.93
 C      -2.029532     2.105967     1.926164      27.29
 C      -3.191721     1.768696     0.919730      89.67
 H      -3.741282     2.636721     0.672165      29.15
 O      -4.001448     0.705011     1.570752     284.41
 H      -4.957536     0.635891     1.371312      27.93
 C      -2.729304     1.191060    -0.559710      87.41
 H      -2.126708     1.945726    -0.853999      29.42
 C      -3.916525     1.068523    -1.615927     104.46
 O      -4.712377    -0.241933    -1.739207     285.21
 H      -4.526889    -0.847377    -0.982442      27.50
 H      -3.473406     1.232430    -2.553964      27.89
 H      -4.726320     1.622651    -1.256644      27.64
 C       1.772008     0.727979    -0.429868      65.14
 H       2.198917     1.698082     0.072285      26.03
 C       1.440846    -1.524552    -0.746880      12.55
 H       1.650299    -2.644892    -1.038117      23.42
 C      -0.105744    -1.431534    -0.787635      -7.38
 O      -0.973826    -2.523675    -0.950628     184.76
 C      -1.031647    -3.281160    -2.355152      86.37
 H      -0.422110    -2.954889    -3.212857      25.66
 H      -0.883429    -4.212890    -1.763973      23.30
 H      -2.143833    -2.833416    -2.598173      22.66
 C      -0.588610    -0.128598    -0.546189      14.17
 O      -1.950248    -0.014138    -0.340457     184.57
 C       0.421088     0.964916    -0.427058      46.97
 H       0.056797     1.985705    -0.436000      26.48
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 C       2.279948    -0.535982    -0.590055      60.73
 C       3.737706    -0.913799    -0.327894      97.11
 H       3.880931    -1.887501    -0.703588      23.27
 O       4.672670     0.009633    -0.851616     237.34
 H       4.830372     0.756239    -0.096166      21.76
 C       4.044974    -1.247154     1.241860      90.42
 H       3.302301    -1.972720     1.392955      28.46
 O       5.299307    -1.998287     1.201426     196.18
 H       6.095948    -1.506538     0.897842      25.33
 C       3.934941    -0.075675     2.233774     100.48
 O       4.705096     1.059439     1.651963     299.51
 H       4.321024     1.784981     2.153455      28.36
 H       4.390671    -0.228137     3.139145      28.30
 H       2.867541     0.156369     2.656126      25.32
55
name = lig-Water-frame_567
 C      -1.648655     3.512523     2.118895      53.34
 H      -2.400530     4.212239     1.728639      28.33
 C      -1.098322     1.079126     2.510523      62.53
 H      -1.432869     0.221494     1.988860      26.07
 C      -0.103561     1.299070     3.367417      21.44
 O       0.886603     0.455464     3.871607     197.40
 C       0.413396    -0.866871     3.932585     120.42
 H       1.127254    -1.430856     4.557918      27.14
 H       0.079013    -1.158580     2.817463      26.74
 H      -0.450292    -0.954146     4.594222      28.16
 C       0.184099     2.839560     3.728497      -9.29
 O       1.256543     2.999230     4.441457     132.91
 H       1.413694     3.995748     4.648750      25.63
 C      -0.619514     3.823639     3.087249      64.86
 H      -0.218458     4.887400     3.288658      22.52
 C      -2.026651     2.166909     1.896063      18.06
 C      -3.186421     1.857492     0.959121      81.23
 H      -4.100612     2.509666     0.518857      23.75
 O      -3.976126     0.732993     1.575464     231.27
 H      -4.933668     0.857292     1.214183      25.25
 C      -2.719718     1.250626    -0.480227      66.60
 H      -2.035570     2.179785    -0.884543      24.98
 C      -3.917134     1.043579    -1.572679      85.43
 O      -4.664482    -0.277652    -1.753106     222.79
 H      -4.551739    -0.824396    -0.857135      23.99
 H      -3.428631     1.020559    -2.601802      24.37
 H      -4.618198     1.856819    -1.074441      24.36
 C       1.802923     0.799071    -0.471650      74.77
 H       2.309078     1.491212     0.104509      29.14
 C       1.373380    -1.626982    -0.760036      21.52
 H       1.750571    -2.510254    -1.189106      26.43
 C      -0.075716    -1.460542    -0.864299       7.17
 O      -0.959002    -2.538664    -0.958035     198.11
 C      -1.072150    -3.205617    -2.286811     100.82
 H      -0.305344    -2.617389    -2.965847      24.70
 H      -0.987544    -4.326379    -2.090201      25.07
 H      -2.114079    -3.312809    -2.674611      25.22
 C      -0.550233    -0.128151    -0.577309       9.41
 O      -1.945555     0.023026    -0.369205     159.56
 C       0.387784     0.968575    -0.415972      46.82
 H       0.107957     2.032401    -0.342346      25.99
 C       2.337814    -0.451294    -0.569742       4.69
 C       3.691517    -0.962121    -0.245575      80.53
 H       3.958370    -1.968045    -0.923821      21.75
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 O       4.622416     0.078192    -0.829304     252.38
 H       4.926758     0.818042    -0.325745      26.56
 C       4.081165    -1.311587     1.184194      75.59
 H       3.339325    -2.172955     1.529606      25.79
 O       5.309990    -2.032865     1.216650     170.63
 H       6.127292    -1.378791     0.825764      21.04
 C       3.880977    -0.074210     2.254586      77.79
 O       4.658231     1.099108     1.680930     256.06
 H       4.447196     2.097187     1.976119      25.80
 H       4.440326    -0.439485     3.307519      24.58
 H       2.876232     0.145298     2.447153      28.00
55
name = lig-Water-frame_568
 C      -1.700915     3.543321     2.086042      56.07
 H      -2.349071     4.369589     1.696550      25.39
 C      -1.200362     1.041879     2.421960       8.40
 H      -1.290321    -0.006660     1.963477      23.48
 C      -0.074192     1.350700     3.421750      -2.58
 O       0.905338     0.393668     3.885711     115.93
 C       0.372580    -0.898407     3.940794     124.72
 H       1.270363    -1.325522     4.448522      27.85
 H       0.297927    -1.405120     3.033120      29.11
 H      -0.398528    -0.871995     4.851652      25.28
 C       0.174112     2.744754     3.652282       2.26
 O       1.290512     3.008654     4.540673     205.07
 H       1.517479     3.960326     4.584387      27.33
 C      -0.595115     3.834924     3.077276      32.47
 H      -0.151026     4.762108     3.321517      17.57
 C      -1.975476     2.239369     1.889677      34.25
 C      -3.205309     1.860242     0.955274      94.89
 H      -3.896102     2.642922     0.803088      28.42
 O      -3.953330     0.772785     1.577839     274.75
 H      -4.860157     1.085442     1.328897      24.77
 C      -2.680620     1.330955    -0.419192      85.12
 H      -2.178915     2.043538    -0.956316      27.15
 C      -3.910364     1.001175    -1.486789      95.64
 O      -4.600491    -0.293674    -1.714697     285.06
 H      -4.631459    -0.794344    -0.913364      29.20
 H      -3.506006     1.204315    -2.506242      26.42
 H      -4.486596     1.929846    -1.500077      27.49
 C       1.800325     0.876985    -0.471382      39.27
 H       2.680447     1.590331    -0.034300      25.67
 C       1.293442    -1.683308    -0.808902      51.07
 H       1.927736    -2.554613    -1.215096      24.95
 C      -0.006752    -1.461276    -0.910841      24.57
 O      -0.947989    -2.553735    -0.963499     189.02
 C      -1.106760    -3.158370    -2.211477     117.71
 H      -0.342147    -2.533539    -2.769075      25.76
 H      -0.730162    -4.209900    -2.589009      26.03
 H      -2.177458    -3.317944    -2.711153      25.17
 C      -0.520833    -0.089781    -0.608555      15.07
 O      -1.933513     0.050255    -0.400208     150.02
 C       0.341330     0.956820    -0.433323      56.23
 H      -0.036317     1.996281    -0.113897      26.42
 C       2.327990    -0.492697    -0.547408     -35.84
 C       3.697064    -0.979264    -0.210332      91.62
 H       3.965156    -1.689503    -0.966693      25.04
 O       4.586148     0.133298    -0.838833     225.72
 H       4.832604     0.767843    -0.112859      24.77
 C       4.075927    -1.375433     1.166312      83.85
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 H       3.432970    -2.092068     1.665061      27.28
 O       5.345108    -2.044396     1.236987     232.42
 H       5.926734    -1.552154     0.756806      27.59
 C       3.895957    -0.087469     2.267874      86.26
 O       4.612753     1.136649     1.709478     254.81
 H       4.321974     2.003966     2.114402      27.58
 H       4.259717    -0.479135     3.105851      29.89
 H       2.754682     0.187673     2.195317      27.17
55
name = lig-Water-frame_569
 C      -1.687415     3.621183     2.136049      34.40
 H      -2.191571     4.455512     1.695561      22.65
 C      -1.260372     1.067427     2.367889      -1.93
 H      -1.251108     0.037944     2.143400      23.17
 C      -0.081632     1.392663     3.402106      -0.93
 O       0.886923     0.401651     3.869675      80.31
 C       0.382842    -0.967276     4.027112     114.64
 H       1.301967    -1.503920     4.309275      27.38
 H       0.211569    -1.690753     3.109243      26.29
 H      -0.503899    -0.972724     4.725314      25.58
 C       0.182256     2.687845     3.596844      20.17
 O       1.294924     3.000083     4.620369     175.46
 H       1.643106     3.996569     4.516400      23.32
 C      -0.574029     3.789521     3.038618      49.72
 H      -0.228070     4.895525     3.338800      18.58
 C      -1.946726     2.203241     1.864911      29.59
 C      -3.165969     1.825684     0.962645     100.58
 H      -3.624213     2.947597     1.004210      24.50
 O      -3.935827     0.828504     1.580060     259.79
 H      -4.961065     1.028783     1.629319      21.30
 C      -2.684898     1.361999    -0.408827      72.32
 H      -2.111521     2.146290    -1.090278      24.27
 C      -3.882485     0.991040    -1.426181      95.46
 O      -4.530141    -0.283982    -1.647061     261.23
 H      -4.688317    -0.860842    -0.796005      26.74
 H      -3.353043     1.230560    -2.372932      27.33
 H      -4.678597     1.810838    -1.676903      26.31
 C       1.822512     0.866770    -0.437824      30.75
 H       2.470735     1.668200    -0.439079      26.44
 C       1.358872    -1.674730    -0.872182      62.49
 H       1.789113    -2.681119    -1.042442      25.28
 C      -0.023954    -1.436214    -0.925342       5.37
 O      -0.939555    -2.566814    -0.933213     210.96
 C      -1.112601    -3.138850    -2.234734     119.49
 H      -0.589177    -2.458207    -3.030465      26.44
 H      -0.434843    -4.004876    -2.430513      25.82
 H      -2.200452    -2.861936    -2.507453      24.28
 C      -0.531973    -0.074619    -0.643999      15.93
 O      -1.903652     0.067740    -0.426112     156.27
 C       0.348734     1.002320    -0.442096      49.48
 H      -0.190332     1.794430    -0.030780      26.40
 C       2.207503    -0.563170    -0.524052     -19.17
 C       3.718418    -0.933219    -0.261080      88.96
 H       3.984910    -1.830345    -1.004888      22.44
 O       4.563556     0.189229    -0.826969     258.84
 H       4.643027     0.596115     0.137932      24.01
 C       4.075247    -1.389922     1.217666      77.62
 H       3.280055    -2.100374     1.662675      26.78
 O       5.370933    -2.056421     1.266218     162.23
 H       6.040913    -1.665221     0.484889      20.58
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 C       3.897700    -0.090075     2.177713      87.90
 O       4.570483     1.149174     1.751708     285.81
 H       4.075696     1.828738     2.389636      23.66
 H       4.190535    -0.468969     3.351308      24.83
 H       2.870626     0.094330     2.177584      28.18
55
name = lig-Water-frame_570
 C      -1.616764     3.636228     2.226607      56.44
 H      -2.116699     4.505375     1.696189      19.24
 C      -1.215145     1.151858     2.409422      77.11
 H      -1.481306     0.066089     2.179950      25.83
 C      -0.133155     1.349003     3.302571      11.57
 O       0.827782     0.426650     3.832568     110.48
 C       0.420263    -1.065868     4.090856     114.68
 H       1.261162    -1.664298     4.520125      27.15
 H      -0.058129    -1.474131     3.212630      26.96
 H      -0.557205    -1.150073     4.705826      26.71
 C       0.249863     2.734754     3.612300     -11.24
 O       1.259773     2.978286     4.655138     199.24
 H       1.604023     3.882493     4.555318      26.66
 C      -0.548882     3.765319     2.998661      61.05
 H      -0.397256     4.717626     3.287089      31.18
 C      -1.943881     2.139677     1.831264       1.94
 C      -3.089947     1.848790     0.987193     102.22
 H      -3.514066     2.810113     0.846852      27.06
 O      -3.937767     0.872512     1.599532     286.94
 H      -4.906589     1.042388     1.737342      25.43
 C      -2.712698     1.370313    -0.465289      86.06
 H      -2.126343     2.168854    -0.861563      26.62
 C      -3.857034     1.030112    -1.422548      94.25
 O      -4.458165    -0.288944    -1.556982     284.42
 H      -4.620597    -0.761247    -0.670408      27.05
 H      -3.129175     0.957844    -2.319065      26.06
 H      -4.779967     1.602728    -1.338539      26.03
 C       1.764927     0.767291    -0.414809      54.95
 H       2.324489     1.773738    -0.703031      22.10
 C       1.418530    -1.634136    -0.917774      51.82
 H       1.644601    -2.719571    -0.880168      23.38
 C      -0.079638    -1.402318    -0.912155       5.48
 O      -0.907360    -2.552799    -0.892091     203.67
 C      -1.091103    -3.062813    -2.312379     103.84
 H      -0.969252    -2.375101    -3.200300      25.47
 H      -0.493363    -4.059045    -2.092418      23.29
 H      -2.245656    -2.944438    -2.351955      24.07
 C      -0.543080    -0.087055    -0.679208      17.73
 O      -1.881782     0.081526    -0.443812     172.21
 C       0.400266     1.038446    -0.448690      29.73
 H      -0.224195     1.948088    -0.026925      22.11
 C       2.137460    -0.602017    -0.505307      28.34
 C       3.721499    -0.899529    -0.382321      82.40
 H       3.938486    -1.919717    -0.795759      23.53
 O       4.535753     0.228943    -0.760635     257.88
 H       4.664634     0.781290     0.005290      24.73
 C       4.085569    -1.348980     1.267230      77.58
 H       3.250212    -2.071522     1.443759      26.38
 O       5.400082    -2.050765     1.287439     170.80
 H       5.933865    -1.998457     0.397851      25.46
 C       3.919131    -0.137629     2.118528     115.87
 O       4.521029     1.141358     1.814387     316.52
 H       4.007112     1.818214     2.425053      24.53
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 H       4.095722    -0.233463     3.090167      29.24
 H       2.753535     0.012812     2.203122      26.00
55
name = lig-Water-frame_571
 C      -1.602913     3.527129     2.232810      48.05
 H      -2.075010     4.397332     1.851873      21.42
 C      -1.152711     1.168501     2.469634      78.58
 H      -1.658889     0.276477     2.207055      23.11
 C      -0.117604     1.346468     3.235081      20.26
 O       0.745379     0.415852     3.800673     104.32
 C       0.417220    -1.127080     4.133469     107.60
 H       1.220982    -1.632690     4.650713      26.68
 H      -0.041293    -1.317624     3.122637      23.34
 H      -0.426735    -1.148703     4.959480      26.41
 C       0.312960     2.763021     3.649181      -2.00
 O       1.190211     2.934359     4.650265     170.23
 H       1.528488     3.931596     4.688898      24.45
 C      -0.457663     3.757960     3.024248      56.72
 H      -0.332168     4.905582     3.394609      26.58
 C      -1.917837     2.195090     1.839452      30.57
 C      -3.042195     1.859320     0.967761     101.40
 H      -3.727070     2.802777     0.618796      23.45
 O      -3.932839     0.892062     1.639236     281.76
 H      -4.893001     1.297333     1.588227      26.37
 C      -2.718065     1.349856    -0.481894      90.50
 H      -2.098438     2.257851    -0.830202      22.66
 C      -3.820575     1.046162    -1.451656      95.30
 O      -4.386785    -0.317168    -1.451913     306.69
 H      -4.514618    -0.627434    -0.550950      27.40
 H      -3.360678     1.012211    -2.421987      26.68
 H      -4.642287     1.779367    -1.135536      25.65
 C       1.674516     0.703473    -0.421285      53.27
 H       2.393009     1.467968    -0.587839      25.29
 C       1.334436    -1.618400    -0.943187      40.36
 H       1.677421    -2.720885    -0.782146      22.15
 C      -0.078126    -1.374415    -0.883936      23.67
 O      -0.861204    -2.502881    -0.878146     207.13
 C      -1.123795    -2.989304    -2.349089     108.82
 H      -0.892862    -2.298322    -3.166170      26.18
 H      -0.782694    -3.990638    -2.323036      26.26
 H      -2.152940    -3.574113    -2.201771      24.56
 C      -0.537336    -0.065298    -0.693907       9.98
 O      -1.891493     0.095036    -0.457308     161.40
 C       0.380793     1.032386    -0.448198      57.77
 H       0.171534     2.049145    -0.311202      23.81
 C       2.222118    -0.597098    -0.507737      25.39
 C       3.698521    -0.866260    -0.421167      88.46
 H       4.012352    -1.844385    -0.950494      23.67
 O       4.511981     0.254986    -0.711845     238.10
 H       4.673427     0.981139    -0.010673      23.72
 C       4.113239    -1.298361     1.211392      79.42
 H       3.340286    -2.060879     1.403702      26.55
 O       5.411215    -2.046499     1.313945     199.24
 H       5.815642    -2.046741     0.468369      29.21
 C       3.878753    -0.164798     2.103593     106.48
 O       4.479758     1.129663     1.860320     297.82
 H       4.092609     1.934917     2.261393      26.69
 H       4.219408    -0.337307     3.299242      24.52
 H       2.813081    -0.096082     2.068879      27.05
55
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name = lig-Water-frame_572
 C      -1.574249     3.428136     2.216063      79.54
 H      -2.193133     4.311217     1.943606      20.97
 C      -1.181880     1.159541     2.457636      42.87
 H      -1.585612     0.129022     2.286662      20.28
 C       0.000921     1.398440     3.260953      15.11
 O       0.686921     0.365446     3.801327     150.07
 C       0.360015    -1.105886     4.162392     107.31
 H       1.377328    -1.506500     4.476046      26.16
 H       0.171126    -1.603985     3.171695      23.97
 H      -0.322620    -1.079825     5.032322      26.50
 C       0.311392     2.743405     3.638230      20.11
 O       1.146138     2.899993     4.656219     180.56
 H       1.367776     3.846725     4.846165      24.74
 C      -0.354916     3.800770     3.092560      29.41
 H      -0.187963     4.750364     3.391321      24.78
 C      -1.875406     2.277594     1.874912      39.69
 C      -3.067352     1.862907     0.905713     111.92
 H      -3.734603     2.673236     0.669265      24.37
 O      -3.926375     0.917461     1.678405     312.26
 H      -4.824893     1.333241     1.529081      28.09
 C      -2.643030     1.327446    -0.474188     107.13
 H      -2.120109     2.160508    -0.994879      23.32
 C      -3.814979     1.043816    -1.471276      89.69
 O      -4.315980    -0.331955    -1.355279     252.92
 H      -4.469182    -0.560859    -0.322441      23.55
 H      -3.742645     1.378232    -2.613365      25.41
 H      -4.430536     1.959130    -1.272533      26.93
 C       1.677193     0.641565    -0.439105      35.49
 H       2.546993     1.391347    -0.262607      26.09
 C       1.259539    -1.611255    -0.907710      58.57
 H       1.626123    -2.587947    -0.933258      21.53
 C      -0.030195    -1.346403    -0.855710      27.01
 O      -0.836940    -2.457949    -0.910935     208.10
 C      -1.205497    -2.988837    -2.302543      90.56
 H      -0.845130    -2.154208    -3.064387      24.67
 H      -0.468559    -3.897023    -2.816241      25.18
 H      -2.144253    -3.515173    -2.286859      26.55
 C      -0.564794     0.006453    -0.676363      22.82
 O      -1.915491     0.099263    -0.471559     180.50
 C       0.310807     1.004206    -0.466153      77.68
 H       0.346519     2.153199    -0.655561      21.16
 C       2.291211    -0.608925    -0.558837      31.96
 C       3.704134    -0.852125    -0.362903      98.92
 H       4.086063    -1.472306    -1.269633      22.91
 O       4.510802     0.300567    -0.707530     233.90
 H       4.507446     0.822406     0.207677      23.88
 C       4.147539    -1.287798     1.077129      75.61
 H       3.406713    -2.066451     1.530653      24.46
 O       5.398364    -2.030093     1.350756     173.06
 H       5.975280    -1.912055     0.368744      20.59
 C       3.832641    -0.157069     2.193648      97.00
 O       4.467367     1.111457     1.869686     277.01
 H       4.002654     2.039495     2.212126      22.57
 H       4.135520    -0.648737     3.029960      28.59
 H       2.696190    -0.087699     2.064028      25.50
55
name = lig-Water-frame_573
 C      -1.457435     3.560163     2.267917      61.49
 H      -2.271945     4.239737     1.945023      18.48
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 C      -1.180149     1.146111     2.449218      41.49
 H      -1.303738     0.069943     2.366425      21.81
 C       0.029436     1.407974     3.259054      14.35
 O       0.676191     0.296089     3.834452     191.41
 C       0.342493    -1.039820     4.147632     114.50
 H       1.371984    -1.271403     4.321868      26.84
 H       0.106255    -1.888134     3.440348      26.81
 H      -0.443135    -1.142358     5.093924      25.55
 C       0.298428     2.709151     3.618648      17.48
 O       1.144754     2.859709     4.706066     161.05
 H       1.296261     3.813110     4.876860      27.65
 C      -0.346396     3.813269     3.095558      12.64
 H      -0.030398     4.894755     3.469967      22.93
 C      -1.893603     2.166526     1.853435      27.08
 C      -3.086936     1.854787     0.885458     102.15
 H      -3.717360     2.839601     0.720714      22.41
 O      -3.904648     0.947090     1.697214     299.87
 H      -4.908883     1.147997     1.740258      25.92
 C      -2.560297     1.314034    -0.516253     112.84
 H      -1.981301     2.071307    -1.076628      25.04
 C      -3.832361     1.067603    -1.483268     100.25
 O      -4.257268    -0.308549    -1.271954     301.71
 H      -4.423714    -0.510602    -0.358423      27.86
 H      -3.730471     1.285269    -2.466950      29.70
 H      -4.611597     1.884976    -1.241458      27.78
 C       1.764726     0.613498    -0.448160      47.02
 H       2.294303     1.440249     0.090014      29.94
 C       1.320114    -1.596219    -0.834654      43.96
 H       1.534201    -2.721969    -1.260666      24.02
 C      -0.042911    -1.293203    -0.835294      19.24
 O      -0.854217    -2.450213    -0.970232     226.26
 C      -1.200032    -2.994577    -2.269593     116.95
 H      -1.233623    -2.110966    -2.850644      27.56
 H      -0.350635    -3.479278    -2.742308      27.47
 H      -2.422286    -3.171995    -2.404649      23.69
 C      -0.628720     0.034830    -0.644337      29.40
 O      -1.937429     0.082371    -0.483932     205.25
 C       0.325367     1.034246    -0.512887      69.77
 H       0.044095     2.035505    -0.793105      21.95
 C       2.245992    -0.634205    -0.626624      40.95
 C       3.775459    -0.855561    -0.341058     140.18
 H       3.981894    -1.458283    -1.175641      26.21
 O       4.520327     0.376918    -0.685315     211.76
 H       4.505127     0.737340     0.194893      26.26
 C       4.142799    -1.311939     1.002526      96.81
 H       3.426575    -1.998612     1.384643      28.34
 O       5.400733    -1.989814     1.329151     215.13
 H       6.110546    -1.793097     0.780494      27.43
 C       3.771983    -0.158949     2.221774      84.10
 O       4.462135     1.103708     1.876721     230.04
 H       3.968737     1.781562     2.311571      27.58
 H       4.119500    -0.862334     3.141707      26.58
 H       2.663166     0.013880     2.290845      26.77
55
name = lig-Water-frame_574
 C      -1.394880     3.667259     2.282668      51.67
 H      -2.083793     4.411816     1.957331      24.24
 C      -1.110639     1.116315     2.459318      57.82
 H      -1.214804     0.034299     2.283374      26.17
 C      -0.040119     1.352572     3.228010      27.87
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 O       0.688974     0.280316     3.856521     220.24
 C       0.331002    -1.010267     4.150276     123.45
 H       1.357109    -1.357070     4.558271      26.52
 H      -0.180108    -1.799132     3.531091      28.02
 H      -0.344953    -1.119232     4.986716      28.52
 C       0.328368     2.670870     3.646723       3.52
 O       1.159119     2.816540     4.767300     165.68
 H       1.379899     3.835986     4.830330      25.89
 C      -0.373549     3.851063     3.079011      35.66
 H      -0.012883     4.780556     3.455397      25.80
 C      -1.898763     2.089789     1.839891      13.63
 C      -3.086858     1.872911     0.909252     105.62
 H      -3.517508     2.892317     0.715468      24.38
 O      -3.886635     0.957489     1.703178     294.84
 H      -4.873232     1.102556     1.877061      26.47
 C      -2.559237     1.342152    -0.592305      96.94
 H      -1.760846     2.075681    -0.989326      24.58
 C      -3.862036     1.100876    -1.429378      90.32
 O      -4.214017    -0.259236    -1.239486     272.70
 H      -4.394801    -0.507722    -0.276505      26.47
 H      -3.445352     1.010438    -2.593967      25.22
 H      -4.797191     1.584625    -1.094833      26.58
 C       1.778888     0.692323    -0.427690      47.41
 H       2.251314     1.464272     0.138043      26.63
 C       1.353476    -1.657576    -0.808317      60.19
 H       1.513303    -2.503865    -1.282082      29.04
 C      -0.079380    -1.269071    -0.825344       5.68
 O      -0.892959    -2.452875    -0.998628     208.95
 C      -1.231774    -2.907925    -2.261086     105.78
 H      -1.608083    -1.937304    -2.864014      24.46
 H      -0.210989    -3.480339    -2.676701      24.02
 H      -2.190469    -3.259127    -2.287584      26.72
 C      -0.620086    -0.001364    -0.612548      24.46
 O      -1.970966     0.046349    -0.489499     196.63
 C       0.391345     1.050064    -0.587107      38.61
 H      -0.138582     2.058781    -0.642634      21.86
 C       2.256499    -0.634359    -0.647596      26.98
 C       3.833965    -0.838912    -0.399136      94.95
 H       4.065356    -1.878274    -1.056409      24.80
 O       4.534438     0.444218    -0.660449      78.95
 H       4.660835     1.015340     0.287217      18.69
 C       4.113414    -1.326805     1.033093      82.38
 H       3.263343    -2.188485     1.098282      25.50
 O       5.391299    -1.946630     1.313274     165.21
 H       6.287103    -1.583804     0.883892      22.27
 C       3.739217    -0.215812     2.210934      99.92
 O       4.458801     1.068153     1.898464     181.46
 H       3.979754     1.808835     2.512440      22.82
 H       4.119817    -0.531428     3.150527      30.21
 H       2.693669     0.056103     2.449506      27.02
55
name = lig-Water-frame_575
 C      -1.449135     3.650729     2.211821      78.27
 H      -1.854063     4.698980     1.901912      19.54
 C      -1.090969     1.056911     2.406611      55.41
 H      -1.342814     0.037958     2.092862      26.46
 C      -0.054573     1.311430     3.279006      23.73
 O       0.719435     0.327538     3.851527     209.68
 C       0.327464    -1.045648     4.194151     101.60
 H       1.086960    -1.652036     4.667222      27.45
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 H      -0.220243    -1.452684     3.296661      27.48
 H      -0.418731    -0.887263     5.186485      24.55
 C       0.346373     2.640130     3.683177      -5.59
 O       1.176913     2.786353     4.814215     213.77
 H       1.553306     3.676454     4.791827      28.02
 C      -0.326694     3.836049     3.120632      60.06
 H      -0.035951     4.879558     3.471406      21.69
 C      -1.848459     2.137243     1.864273       9.92
 C      -3.030309     1.898208     0.944103     103.68
 H      -3.519129     2.902646     0.718478      26.12
 O      -3.876465     0.943411     1.702730     277.51
 H      -4.801783     1.352223     1.733400      25.08
 C      -2.607827     1.396216    -0.611472      90.62
 H      -1.891849     2.089307    -0.918552      27.97
 C      -3.859841     1.101072    -1.399893     117.97
 O      -4.195764    -0.234510    -1.230034     273.54
 H      -4.339637    -0.544893    -0.252482      25.73
 H      -3.537621     1.086762    -2.363717      29.40
 H      -4.761344     1.711475    -1.192543      28.01
 C       1.737403     0.794469    -0.407614       1.08
 H       2.557510     1.573424    -0.024746      24.37
 C       1.306234    -1.668555    -0.807979      43.84
 H       1.697434    -2.742605    -1.313508      25.20
 C      -0.071182    -1.336363    -0.825410      25.58
 O      -0.935059    -2.432855    -0.966836     221.31
 C      -1.266070    -2.762122    -2.307220     108.10
 H      -1.535580    -2.018540    -2.961339      27.89
 H      -0.525675    -3.403145    -2.761482      27.14
 H      -1.976917    -3.884975    -2.039292      22.49
 C      -0.545482    -0.046101    -0.597924      18.75
 O      -1.996099     0.019913    -0.494608     134.63
 C       0.417519     1.038620    -0.658016      59.29
 H       0.120646     2.058342    -0.241862      24.79
 C       2.328290    -0.588955    -0.623689       8.05
 C       3.858768    -0.833954    -0.464889      89.29
 H       4.317280    -1.655992    -0.906592      27.75
 O       4.564927     0.501780    -0.634435     161.68
 H       4.609787     0.871328     0.202962      27.53
 C       4.041160    -1.336182     1.102436      86.82
 H       3.441987    -2.171209     1.020573      27.32
 O       5.376065    -1.910974     1.323158     194.24
 H       6.053468    -1.367766     0.723071      22.07
 C       3.734212    -0.274369     2.179992     100.95
 O       4.447900     1.031977     1.932894     238.69
 H       4.210550     1.833034     2.454593      24.57
 H       4.217252    -0.418007     3.232179      26.45
 H       2.614753    -0.030549     2.390861      26.37
55
name = lig-Water-frame_576
 C      -1.479358     3.566997     2.158789      76.62
 H      -1.811246     4.473890     1.802544      22.54
 C      -1.108643     1.032044     2.325106      45.69
 H      -1.474019     0.077581     1.950928      23.54
 C      -0.037508     1.286457     3.368406      19.87
 O       0.795153     0.364603     3.860082     156.38
 C       0.253121    -1.048307     4.265134      98.21
 H       1.028574    -1.834563     4.518495      27.04
 H      -0.133825    -1.223619     3.244361      26.75
 H      -0.430593    -0.824023     5.005112      28.26
 C       0.328549     2.650368     3.722139      14.86
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 O       1.197750     2.746864     4.843863     211.02
 H       1.719091     3.620572     4.761792      27.35
 C      -0.284706     3.759797     3.158851     103.11
 H      -0.106651     4.836084     3.450532      21.91
 C      -1.772331     2.281959     1.894156      29.39
 C      -2.940158     1.920539     0.964645      98.99
 H      -3.668369     2.822661     0.824213      25.49
 O      -3.877395     0.941378     1.682033     261.95
 H      -4.726494     1.462274     1.605690      25.99
 C      -2.663269     1.421674    -0.520759      68.86
 H      -2.008576     2.271892    -1.074346      23.22
 C      -3.862876     1.109269    -1.369769      95.79
 O      -4.217378    -0.247846    -1.232502     291.53
 H      -4.271384    -0.552890    -0.343656      28.23
 H      -3.676603     1.351847    -2.578501      24.46
 H      -4.554512     2.046817    -1.352781      26.08
 C       1.792475     0.823706    -0.408919       6.43
 H       2.464011     1.589021    -0.389562      26.76
 C       1.329461    -1.644620    -0.843447      50.21
 H       1.674741    -2.578760    -0.968970      26.05
 C      -0.029094    -1.436479    -0.821481      20.34
 O      -0.980166    -2.399300    -0.919296     220.41
 C      -1.335206    -2.738283    -2.324383     101.70
 H      -1.721915    -1.914528    -3.109089      23.85
 H      -0.420378    -3.246165    -3.024291      26.17
 H      -1.705589    -3.610178    -2.110679      27.52
 C      -0.497167    -0.068356    -0.610410       6.42
 O      -1.966946     0.023764    -0.504287      79.91
 C       0.395771     1.040928    -0.656607      59.35
 H       0.270888     1.962837    -0.118438      24.54
 C       2.340218    -0.534805    -0.603071      17.38
 C       3.843479    -0.777869    -0.446192      71.31
 H       4.607953    -1.450151    -1.134595      23.00
 O       4.601094     0.519191    -0.630191     189.74
 H       4.524638     0.808771     0.473424      21.08
 C       4.004803    -1.316439     1.142404      71.13
 H       3.326101    -2.336477     1.239916      24.77
 O       5.347038    -1.859747     1.341034     208.84
 H       5.820124    -1.494636     0.644694      23.97
 C       3.723707    -0.294557     2.203572     104.17
 O       4.454315     0.988179     1.934382     244.61
 H       4.170393     1.806579     2.471231      23.88
 H       4.127400    -0.735161     3.147130      27.60
 H       2.675377    -0.210597     2.202608      28.94
55
name = lig-Water-frame_577
 C      -1.386000     3.523644     2.203720      20.56
 H      -2.061901     4.285616     1.623804      19.25
 C      -1.075327     1.095688     2.317973      42.82
 H      -1.498057     0.157137     1.917425      22.32
 C      -0.074764     1.263376     3.386274      34.77
 O       0.905139     0.360033     3.906407     131.67
 C       0.195711    -1.006654     4.266049      93.78
 H       1.021247    -1.692266     4.386197      27.17
 H      -0.281789    -1.365076     3.352872      27.13
 H      -0.767124    -0.837310     5.089247      25.17
 C       0.300829     2.653230     3.786539      11.06
 O       1.225957     2.711524     4.856738     237.42
 H       1.715896     3.592835     4.766907      24.68
 C      -0.317262     3.686524     3.141486      66.28
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 H      -0.077633     4.658939     3.476182      29.23
 C      -1.735834     2.306437     1.870720      37.85
 C      -2.895940     1.944401     0.978039      91.25
 H      -3.573551     2.789563     0.882611      23.94
 O      -3.860494     0.959511     1.641589     271.72
 H      -4.812545     1.294175     1.662427      26.88
 C      -2.658596     1.440997    -0.418370      81.64
 H      -2.210034     2.151603    -1.003084      24.78
 C      -3.866275     1.158641    -1.389811      93.40
 O      -4.279957    -0.250289    -1.271798     266.63
 H      -4.247237    -0.590220    -0.280991      23.27
 H      -3.636367     1.269783    -2.402232      28.38
 H      -4.551304     2.008288    -1.166242      27.35
 C       1.858609     0.765325    -0.471215      38.78
 H       2.426407     1.813899    -0.665161      23.33
 C       1.420477    -1.568533    -0.856382      57.94
 H       1.800899    -2.725054    -0.737488      21.74
 C       0.010844    -1.449203    -0.802972       9.26
 O      -1.026433    -2.382116    -0.899820     204.83
 C      -1.345609    -2.712742    -2.378386      75.20
 H      -2.030790    -1.984433    -2.743353      25.56
 H      -0.349954    -2.824168    -2.907252      25.96
 H      -2.182344    -3.764309    -2.279873      22.62
 C      -0.496137    -0.072368    -0.643427       5.55
 O      -1.883890     0.058380    -0.513378     114.13
 C       0.394157     1.024693    -0.585299      37.94
 H      -0.026531     2.085254    -0.213594      21.91
 C       2.297088    -0.488402    -0.607123      41.19
 C       3.844387    -0.711343    -0.389561     104.19
 H       4.151464    -1.325979    -1.121522      25.84
 O       4.627107     0.521260    -0.569966     265.60
 H       4.591912     0.966836     0.250591      24.78
 C       3.994729    -1.336347     1.128540      83.90
 H       3.265903    -2.017284     1.436875      27.09
 O       5.302554    -1.803966     1.375861     166.81
 H       5.966380    -1.801386     0.430452      20.22
 C       3.714300    -0.310104     2.244396      79.37
 O       4.463081     0.933932     1.932091     297.47
 H       3.955390     1.656196     2.468229      25.02
 H       3.951820    -0.936769     3.154248      25.58
 H       2.520563    -0.165392     2.156347      25.45
55
name = lig-Water-frame_578
 C      -1.294023     3.562210     2.246998      25.54
 H      -1.988962     4.202218     1.821240      19.78
 C      -1.004246     1.178833     2.376193      54.99
 H      -1.312396     0.210731     2.020421      21.26
 C      -0.086558     1.275448     3.375576      27.96
 O       0.956093     0.315044     3.959600     157.64
 C       0.131628    -0.926339     4.237885     119.57
 H       0.998993    -1.556130     4.577247      25.95
 H      -0.478274    -1.469667     3.451997      25.32
 H      -0.521507    -0.906356     5.000714      29.41
 C       0.265609     2.574290     3.855111      -9.73
 O       1.247264     2.692194     4.848131     199.45
 H       1.609059     3.600480     4.849427      30.07
 C      -0.358085     3.669762     3.134301      86.74
 H       0.030323     4.710199     3.533683      27.42
 C      -1.723172     2.172328     1.820743      46.63
 C      -2.924588     1.958238     0.998857      87.16
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 H      -3.424366     3.054032     0.815945      20.70
 O      -3.831002     0.978581     1.602680     289.49
 H      -4.793554     1.178489     1.708191      28.41
 C      -2.620507     1.411107    -0.375453      81.45
 H      -1.997602     2.276984    -0.951755      19.73
 C      -3.869077     1.178286    -1.348079      77.39
 O      -4.366949    -0.228429    -1.323053     284.41
 H      -4.288815    -0.578290    -0.393924      25.33
 H      -3.431281     1.200576    -2.472527      23.78
 H      -4.772213     1.743956    -0.927303      24.84
 C       1.823114     0.812164    -0.582300      53.41
 H       2.434327     1.625242    -0.654224      27.59
 C       1.492824    -1.559520    -0.836256      61.76
 H       1.925065    -2.514570    -0.679299      21.97
 C       0.033157    -1.382170    -0.788941       6.35
 O      -1.053277    -2.390613    -0.902835     217.93
 C      -1.415153    -2.735544    -2.380760      78.42
 H      -2.209724    -1.902639    -2.468472      23.72
 H      -0.341890    -2.369835    -2.847904      23.72
 H      -1.989363    -3.469438    -2.559143      27.24
 C      -0.491950    -0.054536    -0.674929       7.05
 O      -1.802750     0.114610    -0.515259     179.16
 C       0.414825     1.008589    -0.477330      54.80
 H      -0.125557     1.899849    -0.540779      20.96
 C       2.313338    -0.475041    -0.617489      25.35
 C       3.801907    -0.642501    -0.291590      96.06
 H       3.862131    -1.519594    -1.193013      19.82
 O       4.648412     0.503918    -0.523287     238.10
 H       4.639935     1.129064     0.353262      21.71
 C       4.002851    -1.310565     1.087815      88.27
 H       3.059159    -2.042575     1.349929      23.33
 O       5.298475    -1.768590     1.383950     242.59
 H       5.852219    -2.053872     0.733506      30.72
 C       3.673839    -0.324293     2.240112      85.77
 O       4.451190     0.876142     1.966485     334.23
 H       3.984254     1.578840     2.412396      29.81
 H       3.826877    -0.797195     3.290133      22.91
 H       2.710080     0.000455     2.294626      26.00
55
name = lig-Water-frame_579
 C      -1.312545     3.509780     2.206090     111.99
 H      -1.840391     4.570387     2.004436      21.94
 C      -0.943882     1.159587     2.425921      42.53
 H      -1.040280     0.087837     2.156641      17.98
 C       0.013351     1.321695     3.426703      16.23
 O       0.907199     0.259848     3.979896     191.35
 C       0.138553    -0.879325     4.205503     111.72
 H       0.815621    -1.591805     4.736886      24.85
 H      -0.420884    -1.323356     3.406750      24.68
 H      -0.491646    -0.688883     5.324811      22.64
 C       0.233780     2.507187     3.902424      -8.59
 O       1.251404     2.678921     4.824918     114.61
 H       1.470456     3.691432     4.937689      26.07
 C      -0.298030     3.704109     3.243166      77.19
 H      -0.006647     4.654671     3.463006      18.50
 C      -1.691585     2.137684     1.812583      73.39
 C      -2.979902     1.975315     1.000647     124.86
 H      -3.308503     2.958646     0.801716      25.94
 O      -3.804530     0.990736     1.578318     327.06
 H      -4.755596     1.339259     1.638547      27.46
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 C      -2.541247     1.398343    -0.426848      95.91
 H      -1.932718     2.157422    -0.729853      23.35
 C      -3.867427     1.141034    -1.276704      99.71
 O      -4.453130    -0.196164    -1.381246     336.72
 H      -4.393902    -0.634054    -0.526613      28.24
 H      -3.515022     1.418139    -2.306481      25.44
 H      -4.739761     1.677137    -1.027925      26.72
 C       1.731844     0.889157    -0.689077      48.25
 H       2.596081     1.702101    -0.558746      25.75
 C       1.486088    -1.566411    -0.790433      28.66
 H       2.026950    -2.601588    -0.758421      19.88
 C       0.034504    -1.329389    -0.796959       3.27
 O      -1.039232    -2.416654    -0.901191     201.70
 C      -1.459923    -2.623216    -2.339076      71.03
 H      -2.203671    -1.830628    -2.483416      24.37
 H      -0.719345    -2.357429    -2.989852      27.97
 H      -1.774396    -3.907209    -2.832528      21.00
 C      -0.440113    -0.034257    -0.674666      19.06
 O      -1.782144     0.176048    -0.505950     223.83
 C       0.439471     0.993619    -0.403819      86.90
 H      -0.030845     2.017882    -0.832352      19.47
 C       2.353597    -0.435503    -0.615503       9.04
 C       3.748782    -0.633539    -0.247906     108.12
 H       4.126722    -1.371936    -0.854423      25.37
 O       4.663190     0.485079    -0.489107     247.97
 H       4.628962     0.878457     0.483568      19.81
 C       3.955828    -1.278196     1.083565     100.48
 H       3.323443    -2.120925     0.956467      25.69
 O       5.293082    -1.753090     1.428706     182.61
 H       5.836276    -2.155482     0.610018      24.43
 C       3.643940    -0.329545     2.233556      90.95
 O       4.449676     0.833827     2.021796     271.69
 H       4.109179     1.713502     2.464777      24.75
 H       3.895210    -0.624448     3.255735      23.42
 H       2.529262     0.118320     2.328608      21.55
55
name = lig-Water-frame_580
 C      -1.327860     3.469603     2.205384      68.60
 H      -1.620331     4.443292     2.019154      25.20
 C      -0.881637     1.059647     2.465118      48.97
 H      -0.946024     0.021534     2.180514      17.12
 C       0.125536     1.277338     3.461198      25.35
 O       0.830830     0.246550     3.962393     258.41
 C       0.136999    -0.875902     4.291746     112.18
 H       0.737632    -1.742324     4.592996      27.06
 H      -0.400712    -1.175124     3.338535      25.26
 H      -0.516564    -0.529843     4.980056      28.65
 C       0.260492     2.606008     3.967557       0.06
 O       1.254134     2.678608     4.820121     182.49
 H       1.409647     3.621301     4.978685      23.23
 C      -0.276089     3.680227     3.325210     117.09
 H       0.041888     4.806181     3.536754      22.58
 C      -1.668904     2.199982     1.841233      42.99
 C      -2.945598     1.933457     0.971825     126.83
 H      -3.524832     3.018134     0.789778      22.86
 O      -3.816720     1.012060     1.568928     309.81
 H      -4.695055     1.447245     1.562665      26.39
 C      -2.495280     1.393528    -0.473555      79.57
 H      -1.833159     2.305971    -0.909581      19.77
 C      -3.860624     1.101221    -1.222006      92.01
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 O      -4.523666    -0.167482    -1.441831     273.71
 H      -4.514652    -0.783421    -0.575855      24.98
 H      -3.696038     1.557595    -2.299338      24.65
 H      -4.618136     1.991552    -1.011668      25.82
 C       1.775774     0.925454    -0.752541      56.58
 H       2.383572     1.810523    -0.534921      28.81
 C       1.450570    -1.558749    -0.727038      35.80
 H       1.839242    -2.606430    -0.968647      20.92
 C       0.033715    -1.352950    -0.820137      -1.37
 O      -0.978202    -2.436030    -0.912098     221.89
 C      -1.517360    -2.545967    -2.307571     101.35
 H      -2.423155    -1.922156    -2.564701      24.55
 H      -0.766720    -2.323581    -3.291347      24.27
 H      -1.488085    -3.500108    -2.461555      25.96
 C      -0.419346    -0.012647    -0.630962      11.05
 O      -1.793129     0.204593    -0.490321     206.56
 C       0.414719     1.075158    -0.421779      82.35
 H       0.169152     2.031308    -0.635131      22.66
 C       2.317843    -0.379931    -0.629988      11.26
 C       3.769394    -0.629232    -0.254427      77.45
 H       4.496719    -1.473771    -0.863677      21.32
 O       4.662888     0.468893    -0.452946     205.14
 H       4.743401     0.789427     0.552588      21.00
 C       3.905118    -1.264983     1.127078      92.76
 H       3.454897    -2.310992     0.841224      23.21
 O       5.297628    -1.752795     1.468338     114.69
 H       5.698626    -1.905785     0.497487      22.31
 C       3.559299    -0.300925     2.258848      98.84
 O       4.473783     0.835557     2.072438     254.93
 H       4.175257     1.665370     2.535135      24.94
 H       3.977713    -0.773002     3.259800      24.23
 H       2.558680    -0.125382     2.221063      26.49
55
name = lig-Water-frame_581
 C      -1.259053     3.463468     2.302029      13.56
 H      -1.810463     4.362791     1.747405      22.41
 C      -0.824025     1.000182     2.497688      50.93
 H      -1.071822     0.013820     2.055872      19.50
 C       0.134690     1.243999     3.427955      70.27
 O       0.832738     0.267168     3.951430     242.93
 C       0.092663    -0.930445     4.354908      81.72
 H       0.791581    -1.796181     4.510723      26.97
 H      -0.441915    -1.230992     3.455726      27.97
 H      -0.934452    -0.561886     4.974857      25.17
 C       0.312454     2.687460     3.993631       8.98
 O       1.289171     2.694058     4.872014     201.23
 H       1.616386     3.638591     5.088832      19.96
 C      -0.322561     3.684788     3.332741      71.61
 H       0.002587     4.620761     3.631407      34.00
 C      -1.653076     2.205437     1.892450      60.30
 C      -2.852346     1.921931     0.921214     116.47
 H      -3.458451     2.736135     0.811244      25.26
 O      -3.847773     1.035195     1.566018     285.16
 H      -4.776412     1.412827     1.557408      28.27
 C      -2.483007     1.434254    -0.509129      90.30
 H      -2.081016     2.150741    -1.151126      23.65
 C      -3.873946     1.136695    -1.228742     101.67
 O      -4.580686    -0.148812    -1.479105     290.46
 H      -4.590455    -0.702962    -0.703640      29.13
 H      -3.815536     1.418437    -2.347987      26.18
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 H      -4.395645     1.928998    -0.732852      26.72
 C       1.841095     0.936574    -0.749582      48.29
 H       2.367781     1.933981    -0.653255      27.81
 C       1.388404    -1.526962    -0.690167      65.34
 H       1.702769    -2.515426    -0.989148      25.47
 C       0.027919    -1.385326    -0.823465      10.89
 O      -0.880590    -2.417589    -0.944140     232.11
 C      -1.540100    -2.437804    -2.318888      82.21
 H      -2.669840    -2.200655    -2.418608      23.34
 H      -0.883624    -2.163769    -2.980414      27.78
 H      -1.576023    -3.778186    -2.096047      19.86
 C      -0.452160     0.024655    -0.565878      12.74
 O      -1.797794     0.177388    -0.472607     190.26
 C       0.420869     1.162790    -0.515981      53.02
 H       0.039660     2.301341    -0.230882      18.50
 C       2.279849    -0.371124    -0.663078      14.62
 C       3.860917    -0.665907    -0.309951     108.15
 H       4.184181    -1.417281    -0.927084      29.85
 O       4.657892     0.476044    -0.414425     186.92
 H       4.947802     0.904928     0.515472      20.45
 C       3.883485    -1.302020     1.173860      95.79
 H       3.265278    -2.171429     1.237844      28.61
 O       5.296718    -1.736491     1.473901     176.58
 H       5.761636    -1.706755     0.689706      28.81
 C       3.514880    -0.312251     2.308828      95.14
 O       4.495409     0.850800     2.121017     220.14
 H       4.094095     1.629985     2.593193      24.78
 H       3.727779    -0.891903     3.162627      28.83
 H       2.335735    -0.139734     2.239115      24.30
55
name = lig-Water-frame_582
 C      -1.237323     3.487667     2.365060      -3.85
 H      -1.879353     4.061005     1.770724      23.59
 C      -0.849299     1.013109     2.461657      65.45
 H      -1.139732     0.060236     2.040119      22.46
 C       0.093027     1.303493     3.401440      55.75
 O       0.887063     0.253011     3.982468     180.46
 C      -0.006362    -0.978115     4.379967      99.48
 H       0.767755    -1.645513     4.754395      28.26
 H      -0.480201    -1.441952     3.477406      27.26
 H      -0.691077    -0.904659     5.114872      29.10
 C       0.357650     2.642296     3.948052      16.24
 O       1.353173     2.730269     4.968085     264.36
 H       1.834902     3.626426     5.098316      21.29
 C      -0.361950     3.722610     3.345810      88.74
 H      -0.086258     4.774578     3.707031      29.67
 C      -1.608694     2.126004     1.963884      84.62
 C      -2.739318     1.915465     0.898838      98.91
 H      -3.360017     3.001868     0.750467      22.93
 O      -3.868568     1.047273     1.559876     264.63
 H      -4.807951     1.412574     1.541082      29.52
 C      -2.519882     1.421582    -0.539930      75.06
 H      -2.080623     2.152826    -1.350310      21.67
 C      -3.899676     1.186044    -1.276530     102.49
 O      -4.623861    -0.120577    -1.497235     252.44
 H      -4.625446    -0.636537    -0.623091      26.55
 H      -3.785616     1.425522    -2.336061      26.56
 H      -4.607595     1.756661    -0.544676      24.94
 C       1.845361     0.971211    -0.700004       6.56
 H       2.627016     1.846426    -0.874124      19.73
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 C       1.347144    -1.480288    -0.686439      53.86
 H       1.824449    -2.582351    -0.863786      24.28
 C      -0.001252    -1.316249    -0.787057      22.84
 O      -0.787795    -2.378140    -0.979418     224.67
 C      -1.596072    -2.472118    -2.254548     102.09
 H      -2.616704    -2.181641    -2.154563      25.52
 H      -0.802541    -1.897065    -3.018942      23.79
 H      -1.758319    -3.424007    -2.378554      28.17
 C      -0.465844     0.075603    -0.521300      -1.68
 O      -1.811266     0.126344    -0.453901     141.47
 C       0.430769     1.244087    -0.627099      60.14
 H       0.041401     1.972769    -0.037231      21.63
 C       2.301655    -0.396883    -0.688641      -0.59
 C       3.869692    -0.711999    -0.325725      90.49
 H       4.051472    -1.570323    -1.223051      26.75
 O       4.680446     0.499824    -0.399354     132.98
 H       4.818300     0.847285     0.456412      27.31
 C       3.892594    -1.323354     1.207095      88.91
 H       3.028727    -2.064514     1.562330      26.07
 O       5.274270    -1.716680     1.485391     105.00
 H       6.042301    -1.615039     0.700522      20.27
 C       3.484131    -0.331191     2.313132      86.19
 O       4.487123     0.850553     2.192996     202.66
 H       4.007638     1.718002     2.569543      23.60
 H       3.492508    -0.929227     3.367813      26.00
 H       2.507877     0.098356     2.300264      25.58
55
name = lig-Water-frame_583
 C      -1.296606     3.435680     2.363316     113.01
 H      -1.943220     4.283827     1.917622      25.92
 C      -0.916656     1.051631     2.399376      65.31
 H      -1.070434     0.005080     2.151464      19.50
 C       0.098522     1.358692     3.440202       5.10
 O       0.900279     0.220216     4.025451     128.63
 C      -0.044367    -1.023914     4.374311      90.12
 H       0.770575    -1.550818     4.974245      25.81
 H      -0.427550    -1.596966     3.503053      24.95
 H      -0.642153    -0.908993     5.444410      23.13
 C       0.416180     2.583286     3.891980      16.47
 O       1.402190     2.753202     5.049627     172.16
 H       1.751728     3.696956     4.934838      33.45
 C      -0.331520     3.781816     3.417636      52.47
 H      -0.275018     4.848752     3.706760      12.80
 C      -1.564069     2.064869     2.005453      43.48
 C      -2.694901     1.970105     0.910766      97.01
 H      -2.937704     2.938117     0.777396      24.42
 O      -3.861492     1.063294     1.539176     258.78
 H      -4.729001     1.547761     1.511523      26.74
 C      -2.561122     1.367629    -0.583785      80.89
 H      -1.898516     2.044544    -1.102052      23.20
 C      -3.970227     1.213216    -1.292692     101.87
 O      -4.644074    -0.095856    -1.495131     237.43
 H      -4.637710    -0.537261    -0.547899      24.89
 H      -3.796792     1.760913    -2.379925      24.84
 H      -4.804695     1.684401    -0.850464      26.76
 C       1.849604     0.982311    -0.662343       2.78
 H       2.650123     1.638504    -0.841015      21.33
 C       1.387254    -1.453195    -0.704805      42.29
 H       1.761492    -2.389864    -0.657392      24.28
 C      -0.019508    -1.164114    -0.736974      15.70
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 O      -0.734704    -2.372860    -1.006094     190.86
 C      -1.615440    -2.475875    -2.169385     101.88
 H      -2.522053    -1.769016    -1.860706      22.29
 H      -1.252561    -1.934447    -3.004541      26.88
 H      -1.783310    -3.616301    -2.883192      22.88
 C      -0.439696     0.117948    -0.530126      17.59
 O      -1.847925     0.087809    -0.439570     169.42
 C       0.434739     1.242625    -0.711694      59.75
 H       0.058317     2.114451    -0.000146      19.35
 C       2.339619    -0.394919    -0.686695      12.37
 C       3.790652    -0.772281    -0.335845      88.04
 H       4.237163    -1.394467    -1.055609      27.78
 O       4.707524     0.492715    -0.421088     139.31
 H       4.536419     0.791952     0.680361      19.30
 C       3.897929    -1.320712     1.220353      99.93
 H       3.219242    -2.134739     1.366544      27.78
 O       5.261610    -1.704611     1.503554     167.62
 H       5.872942    -1.692127     0.730404      25.63
 C       3.501167    -0.310863     2.327543     102.06
 O       4.454012     0.837347     2.283504     264.64
 H       4.072533     1.706095     2.485528      28.34
 H       3.481348    -0.694849     3.278754      28.67
 H       2.529483     0.262650     2.190987      23.91
55
name = lig-Water-frame_584
 C      -1.341729     3.412284     2.401916      59.19
 H      -1.857161     4.349349     2.224291      25.21
 C      -0.864196     1.009140     2.449275      62.82
 H      -1.033845    -0.066171     2.216817      17.82
 C       0.120000     1.296211     3.476058      14.57
 O       0.844549     0.190928     4.056871     195.92
 C      -0.002714    -1.049963     4.439810      97.88
 H       0.773204    -1.663921     4.846151      25.92
 H      -0.397876    -1.597081     3.599379      26.37
 H      -0.760643    -0.627351     5.054988      26.47
 C       0.496194     2.633133     3.902161       5.06
 O       1.416212     2.761183     5.077585     202.96
 H       1.611301     3.755670     4.908688      31.62
 C      -0.322640     3.766462     3.439869      64.13
 H      -0.292077     4.802703     3.787288      19.60
 C      -1.621387     2.126753     1.932628      30.63
 C      -2.700179     1.973664     0.933608      91.40
 H      -2.897762     3.209322     0.766430      19.46
 O      -3.827631     1.112310     1.501490     224.95
 H      -4.654489     1.682684     1.545757      25.14
 C      -2.584063     1.307653    -0.563079      78.01
 H      -1.799475     1.984762    -1.020062      21.75
 C      -4.050597     1.247884    -1.333574     106.54
 O      -4.637716    -0.076997    -1.482076     306.59
 H      -4.646508    -0.478957    -0.638159      29.76
 H      -3.921567     1.760479    -2.192131      28.55
 H      -4.868799     2.002279    -0.954293      26.42
 C       1.846617     0.932145    -0.654752      13.57
 H       2.699300     1.846243    -0.626557      18.31
 C       1.426824    -1.379474    -0.723661      57.49
 H       1.672918    -2.577736    -0.504042      17.86
 C       0.043631    -1.099241    -0.721986       6.67
 O      -0.690797    -2.387171    -1.017444     174.70
 C      -1.675737    -2.454356    -2.111064     116.09
 H      -2.439650    -1.873092    -1.766927      24.94
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 H      -1.410966    -1.795804    -3.123886      24.56
 H      -1.722955    -3.304262    -2.514208      28.88
 C      -0.461564     0.173354    -0.581848      25.65
 O      -1.892326     0.067750    -0.434588     186.07
 C       0.443098     1.238745    -0.712692      59.30
 H       0.242744     2.284839    -0.518167      19.05
 C       2.351866    -0.375670    -0.661288      44.32
 C       3.724516    -0.767451    -0.306636      83.64
 H       4.419257    -1.526076    -0.973487      23.49
 O       4.701907     0.457130    -0.407339     269.63
 H       4.565647     0.828524     0.388490      32.03
 C       3.907364    -1.300432     1.198075      83.76
 H       3.386814    -2.368770     1.081383      23.39
 O       5.253119    -1.697331     1.525564     156.19
 H       5.684784    -1.805583     0.646306      28.70
 C       3.510223    -0.224382     2.315838      93.32
 O       4.442245     0.805766     2.356610     251.83
 H       4.015866     1.765946     2.547189      22.79
 H       3.520740    -0.682584     3.433290      23.75
 H       2.460647     0.080861     1.972396      23.08
55
name = lig-Water-frame_585
 C      -1.337819     3.436193     2.504380       3.50
 H      -1.985518     4.304217     2.264373      22.72
 C      -0.783182     0.990992     2.541565      41.41
 H      -1.040191     0.007011     2.219253      19.74
 C       0.149723     1.193253     3.502939      36.03
 O       0.765770     0.167644     4.083148     242.07
 C       0.073461    -1.029459     4.483150      87.12
 H       0.759126    -1.841445     4.919146      24.46
 H      -0.412996    -1.521178     3.546340      24.76
 H      -0.914871    -0.548116     4.868814      25.54
 C       0.547747     2.699323     3.953531       1.04
 O       1.396248     2.770848     5.043642     241.62
 H       1.720389     3.734511     5.247681      20.96
 C      -0.318286     3.659666     3.423592      56.77
 H      -0.196223     4.699522     3.913025      26.00
 C      -1.650816     2.174704     1.862060      23.98
 C      -2.770744     1.994960     0.911651     119.16
 H      -3.193921     2.889801     0.718379      24.51
 O      -3.789283     1.190547     1.467359     265.71
 H      -4.634018     1.677137     1.632656      26.74
 C      -2.593844     1.308471    -0.496508      86.79
 H      -2.027943     1.971873    -1.205894      22.77
 C      -4.127926     1.291568    -1.324042      80.70
 O      -4.621483    -0.042468    -1.480715     265.71
 H      -4.646245    -0.561449    -0.556615      24.40
 H      -3.883438     1.620351    -2.549711      24.47
 H      -4.623185     2.099461    -0.803676      27.43
 C       1.861267     0.929355    -0.661130      56.62
 H       2.353681     1.761179    -0.446399      28.02
 C       1.432179    -1.372048    -0.719009      43.20
 H       1.605845    -2.328702    -0.640854      20.55
 C       0.124085    -1.138564    -0.753924      11.48
 O      -0.634663    -2.380131    -1.012815     164.30
 C      -1.709204    -2.331552    -2.058363      71.57
 H      -2.860029    -2.125797    -1.638934      20.67
 H      -1.409216    -1.777815    -2.961335      24.64
 H      -1.805230    -3.715044    -2.116318      21.50
 C      -0.537507     0.206108    -0.653877      23.78
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 O      -1.922555     0.055266    -0.440964     192.00
 C       0.481160     1.253648    -0.687541      70.17
 H       0.298024     2.351913    -1.059500      19.84
 C       2.364392    -0.355429    -0.625067      45.72
 C       3.775604    -0.720429    -0.256571     100.70
 H       4.106161    -1.601654    -0.850715      24.32
 O       4.674990     0.395339    -0.421871     268.75
 H       4.692844     1.082055     0.438503      22.40
 C       3.900729    -1.295630     1.173727      96.68
 H       3.357705    -2.218932     1.097972      24.26
 O       5.264235    -1.675374     1.524086     134.42
 H       5.686542    -2.054909     0.563121      26.81
 C       3.471730    -0.206030     2.308975     105.46
 O       4.452495     0.807169     2.408663     296.32
 H       4.008159     1.640757     2.682604      26.90
 H       3.398217    -0.711099     3.189325      26.57
 H       2.456245    -0.001114     1.993777      25.36
55
name = lig-Water-frame_586
 C      -1.371880     3.437140     2.555391      36.29
 H      -2.086948     4.235476     2.242843      21.75
 C      -0.785664     1.044469     2.561089      40.65
 H      -1.037230    -0.000805     2.198379      17.42
 C       0.192713     1.183302     3.541971      31.94
 O       0.743725     0.136414     4.135978     258.29
 C       0.095643    -1.008970     4.468564     118.09
 H       0.599394    -1.660712     5.146119      25.83
 H      -0.208461    -1.474521     3.568851      27.36
 H      -0.867659    -0.891533     5.082024      26.77
 C       0.543141     2.656890     3.985417      11.07
 O       1.383042     2.784087     5.005854     228.58
 H       1.756698     3.611241     5.381042      23.17
 C      -0.276862     3.576051     3.449594      60.77
 H      -0.161425     4.515365     3.876695      28.10
 C      -1.578461     2.200891     1.891192       4.11
 C      -2.845609     2.004549     0.852573      87.93
 H      -3.548603     2.996192     0.563427      20.14
 O      -3.788570     1.235598     1.475400     258.06
 H      -4.656858     1.645402     1.698101      26.10
 C      -2.625145     1.366943    -0.479127     100.18
 H      -2.206832     2.002731    -1.249321      23.79
 C      -4.108715     1.315967    -1.329782     110.94
 O      -4.623949    -0.010511    -1.459605     290.76
 H      -4.609843    -0.532558    -0.624294      26.34
 H      -3.927811     1.421250    -2.263988      29.07
 H      -4.694058     2.066394    -0.709984      26.93
 C       1.849470     0.941730    -0.665693      41.49
 H       2.445009     2.005431    -0.293848      22.42
 C       1.459237    -1.375981    -0.710754      21.68
 H       1.839695    -2.554684    -0.865498      17.39
 C       0.086983    -1.164280    -0.811320      12.14
 O      -0.591386    -2.338805    -0.998971     209.43
 C      -1.777060    -2.317186    -1.946274     113.42
 H      -2.731015    -2.227694    -1.642665      26.63
 H      -1.412880    -1.755898    -2.902810      25.03
 H      -1.815363    -3.253612    -2.014549      28.05
 C      -0.555917     0.164092    -0.731025      12.27
 O      -1.933127     0.062133    -0.457100     184.97
 C       0.464929     1.274626    -0.689462      86.40
 H       0.221819     2.118197    -1.344945      23.11
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 C       2.393689    -0.337545    -0.568964      35.21
 C       3.840470    -0.657144    -0.188619      95.72
 H       3.991532    -1.611433    -0.983080      21.42
 O       4.656981     0.356746    -0.451060     290.91
 H       4.807840     0.955207     0.384173      24.69
 C       3.898772    -1.258251     1.184795      86.93
 H       3.071116    -2.114308     1.333811      22.57
 O       5.286959    -1.659699     1.481614     214.92
 H       5.743353    -2.077174     0.834615      35.40
 C       3.425636    -0.268453     2.263206      78.79
 O       4.469250     0.809158     2.445112     211.61
 H       4.048363     1.689675     2.800238      24.42
 H       3.246154    -0.915513     3.269932      22.79
 H       2.361399     0.274065     2.064325      20.60
55
name = lig-Water-frame_587
 C      -1.413760     3.409489     2.559738      55.82
 H      -1.999200     4.272434     2.328266      20.78
 C      -0.838227     1.120013     2.518527      52.01
 H      -0.996497     0.121788     2.225533      15.40
 C       0.204062     1.263421     3.565202       1.06
 O       0.787944     0.133526     4.219425     211.20
 C       0.052367    -1.043112     4.466228     106.40
 H       0.737067    -1.485031     5.279985      23.44
 H      -0.022249    -1.737613     3.511367      22.22
 H      -0.862965    -1.016330     5.182589      25.11
 C       0.503646     2.498202     3.988697      16.49
 O       1.402456     2.762279     5.000752     104.00
 H       1.614375     3.810606     5.138017      22.70
 C      -0.266073     3.562318     3.478145      55.34
 H      -0.106050     4.648425     3.906321      19.76
 C      -1.497077     2.201303     1.957522       9.86
 C      -2.900811     2.075062     0.806879      93.82
 H      -3.220072     3.013346     0.593579      25.72
 O      -3.833777     1.221462     1.536106     275.93
 H      -4.717151     1.689473     1.691788      24.80
 C      -2.677891     1.426700    -0.541014      93.71
 H      -2.023557     2.181440    -1.159077      21.34
 C      -4.042192     1.298221    -1.252457      90.59
 O      -4.647325     0.005448    -1.431195     288.66
 H      -4.583411    -0.504809    -0.598503      27.33
 H      -3.842184     1.702647    -2.485172      23.96
 H      -4.922667     1.926726    -0.919599      26.74
 C       1.845865     1.021834    -0.630223      45.42
 H       2.499805     1.740349    -0.515515      26.18
 C       1.512458    -1.416677    -0.717478      28.29
 H       1.937627    -2.297051    -1.022870      18.66
 C       0.037564    -1.154382    -0.866240      11.51
 O      -0.596638    -2.301274    -0.981548     214.03
 C      -1.795246    -2.310990    -1.827237      63.14
 H      -2.821509    -1.843228    -1.357196      18.63
 H      -1.578898    -1.714091    -2.864914      22.94
 H      -1.776659    -3.583179    -2.336791      20.53
 C      -0.504142     0.089425    -0.789844      32.91
 O      -1.934557     0.103736    -0.484723     199.39
 C       0.392184     1.239259    -0.743298      81.49
 H       0.053083     2.159239    -1.269639      21.28
 C       2.396765    -0.317042    -0.494956      11.88
 C       3.829720    -0.676768    -0.171213     104.24
 H       4.117160    -1.369367    -0.974144      21.07
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 O       4.693708     0.374333    -0.493723     337.72
 H       4.858824     0.740558     0.350875      28.57
 C       3.896215    -1.231983     1.216673      99.81
 H       3.091711    -1.935532     1.401781      24.91
 O       5.285232    -1.636310     1.472505     201.10
 H       5.825672    -2.102562     0.687148      29.47
 C       3.382472    -0.310658     2.267204     105.89
 O       4.476609     0.785021     2.478755     237.23
 H       4.088682     1.698334     2.719768      25.21
 H       3.252073    -0.816993     3.144942      25.93
 H       2.581890     0.268593     2.046379      23.93
55
name = lig-Water-frame_588
 C      -1.373696     3.430742     2.606835      55.73
 H      -1.930415     4.394262     2.354487      19.88
 C      -0.837112     1.157957     2.504590      59.02
 H      -1.033955     0.111077     2.126417      18.76
 C       0.148308     1.242119     3.540364      12.27
 O       0.831693     0.175238     4.289946     150.51
 C       0.039008    -1.135265     4.495609     106.56
 H       0.834540    -1.486205     5.117211      25.82
 H       0.037729    -1.835968     3.743635      27.28
 H      -1.015593    -0.897537     4.928370      25.64
 C       0.471748     2.444025     4.018045      -0.66
 O       1.439723     2.744995     5.003803     105.86
 H       1.467990     3.680583     4.873341      24.76
 C      -0.308993     3.600122     3.493078      66.09
 H      -0.063320     4.522264     3.878344      23.04
 C      -1.517523     2.178306     1.956527      15.31
 C      -2.886003     2.098592     0.836856      63.74
 H      -3.007447     3.329208     0.739448      24.11
 O      -3.893510     1.213566     1.605099     259.96
 H      -4.769710     1.671280     1.653859      25.90
 C      -2.676390     1.492919    -0.612953     100.63
 H      -2.001056     2.178342    -1.008770      25.78
 C      -3.999735     1.292058    -1.264887     129.03
 O      -4.667222     0.005342    -1.403551     275.46
 H      -4.586963    -0.543932    -0.500870      24.43
 H      -3.858823     1.764237    -2.085005      31.09
 H      -4.830908     1.928669    -0.965587      28.93
 C       1.792811     1.054568    -0.584935      28.09
 H       2.726364     1.902241    -0.778041      18.63
 C       1.519732    -1.379223    -0.738641      53.03
 H       1.997252    -2.404291    -1.095413      20.35
 C       0.115012    -1.167752    -0.904305      21.72
 O      -0.655099    -2.310793    -0.970667     220.58
 C      -1.833015    -2.360170    -1.762543     114.73
 H      -2.472549    -1.793830    -1.194868      23.95
 H      -1.701924    -1.642215    -2.682915      25.78
 H      -1.951226    -3.168773    -2.185815      28.45
 C      -0.476631     0.081687    -0.818215      22.33
 O      -1.927694     0.171583    -0.526162     176.03
 C       0.355519     1.182744    -0.835421      56.74
 H      -0.111666     2.245358    -0.829493      20.69
 C       2.335770    -0.294148    -0.435131      18.85
 C       3.778650    -0.701134    -0.211416      72.05
 H       4.222861    -1.556995    -0.977151      21.27
 O       4.751332     0.428482    -0.532044     216.67
 H       5.088962     0.723331     0.516236      22.40
 C       3.920624    -1.220304     1.235170      90.57
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 H       3.194910    -2.195346     1.227966      22.61
 O       5.279390    -1.627464     1.484383     164.27
 H       5.612804    -1.836562     0.494927      25.99
 C       3.420316    -0.279696     2.307052      85.38
 O       4.480082     0.738110     2.508248     223.09
 H       4.026546     1.631890     2.602695      24.70
 H       3.237200    -0.802816     3.347034      22.39
 H       2.391926     0.260979     1.830346      20.34
55
name = lig-Water-frame_589
 C      -1.319472     3.487451     2.632770      30.79
 H      -1.862097     4.327628     2.326057      21.57
 C      -0.807755     1.088703     2.494189      54.64
 H      -1.052962     0.155228     2.034964      22.71
 C       0.091963     1.132780     3.531389      29.29
 O       0.827748     0.214590     4.318494     154.89
 C       0.070012    -1.180522     4.539810      91.27
 H       0.735327    -1.733345     5.291842      25.95
 H       0.001042    -1.910372     3.572648      24.84
 H      -0.960096    -0.900275     4.744980      26.70
 C       0.431672     2.527979     4.055269      -8.97
 O       1.456234     2.703069     4.982986     137.05
 H       1.651855     3.781158     5.004698      24.22
 C      -0.326932     3.595513     3.535240      38.54
 H      -0.037385     4.643337     3.957235      25.28
 C      -1.629498     2.201718     1.912954      21.69
 C      -2.816162     2.107946     0.937338      94.23
 H      -3.126384     3.078023     0.930103      24.92
 O      -3.932520     1.238164     1.652616     234.30
 H      -4.877386     1.629804     1.651724      28.25
 C      -2.622911     1.532274    -0.588931      72.06
 H      -1.991430     2.350252    -1.223730      21.70
 C      -4.016957     1.292029    -1.287347      91.21
 O      -4.670979    -0.006363    -1.373617     275.61
 H      -4.628594    -0.500036    -0.560635      27.95
 H      -3.867145     1.762392    -2.495194      24.08
 H      -4.597128     2.085502    -0.626547      26.22
 C       1.761379     1.066575    -0.564411      46.07
 H       2.316860     1.849195    -0.797196      23.45
 C       1.497529    -1.345951    -0.780537      63.20
 H       1.884298    -2.384611    -0.903483      23.84
 C       0.193962    -1.222505    -0.933278      15.16
 O      -0.682638    -2.357202    -0.953138     175.49
 C      -1.858724    -2.320678    -1.716984      76.18
 H      -2.692538    -1.924701    -0.978762      21.73
 H      -1.784430    -1.480690    -2.575344      23.44
 H      -2.358818    -3.553916    -2.127659      21.40
 C      -0.502975     0.113700    -0.826530       1.11
 O      -1.901111     0.242158    -0.580373     150.98
 C       0.372277     1.188623    -0.900012      56.90
 H      -0.071193     2.065354    -0.504735      22.95
 C       2.275201    -0.251310    -0.423003      32.21
 C       3.766094    -0.684923    -0.278170      78.31
 H       4.022600    -1.649771    -0.777036      25.19
 O       4.795757     0.475822    -0.528160     232.16
 H       5.211550     0.695129     0.252757      30.79
 C       3.923885    -1.255814     1.246040      97.79
 H       3.497528    -2.224832     1.090670      27.00
 O       5.276051    -1.618913     1.476353     201.69
 H       5.643726    -1.611319     0.646250      30.95
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 C       3.445955    -0.228573     2.356982     127.87
 O       4.475977     0.690357     2.531577     267.71
 H       4.007412     1.617668     2.585702      25.22
 H       3.186990    -0.678692     3.281940      28.34
 H       2.579251     0.046609     1.984088      29.59
55
name = lig-Water-frame_590
 C      -1.325497     3.483220     2.568278      18.72
 H      -1.894056     4.437731     2.265123      23.83
 C      -0.830774     1.002549     2.439077      42.23
 H      -1.038261     0.008861     1.980429      23.25
 C       0.081530     1.110989     3.590175      38.59
 O       0.783720     0.203292     4.322649     166.64
 C       0.147395    -1.213688     4.544103      97.61
 H       0.376995    -1.788540     5.440348      27.11
 H       0.122979    -1.614325     3.603659      28.20
 H      -1.004689    -0.934533     4.791745      26.01
 C       0.380437     2.569237     4.066997      15.26
 O       1.465417     2.686732     4.950906     272.58
 H       1.821152     3.505250     5.300806      25.58
 C      -0.290214     3.623395     3.629498      14.59
 H      -0.133715     4.611604     3.958309      21.88
 C      -1.679950     2.249580     1.949438      41.87
 C      -2.764601     2.068135     1.050960      94.86
 H      -3.438893     3.087636     0.958541      21.41
 O      -3.942235     1.267794     1.685417     235.73
 H      -4.859783     1.676703     1.645225      29.30
 C      -2.540114     1.570497    -0.543205      76.10
 H      -2.204615     2.273293    -1.211981      25.06
 C      -4.034709     1.345591    -1.324619     111.12
 O      -4.664681     0.004566    -1.360755     250.04
 H      -4.652986    -0.516521    -0.439258      23.34
 H      -4.044078     1.413558    -2.300799      28.30
 H      -4.505194     2.005019    -0.674741      28.82
 C       1.714129     1.029384    -0.574330      26.92
 H       2.275842     2.152419    -0.617646      19.49
 C       1.493962    -1.346339    -0.804740      52.66
 H       1.881368    -2.373249    -0.734797      25.89
 C       0.102352    -1.242165    -0.960408       9.93
 O      -0.660382    -2.419855    -0.936951     187.21
 C      -1.972535    -2.295480    -1.682623     113.75
 H      -2.832971    -2.197015    -1.062498      26.15
 H      -1.881340    -1.570336    -2.520501      26.26
 H      -2.203188    -3.173691    -1.886597      30.19
 C      -0.516704     0.121669    -0.839741       1.79
 O      -1.851771     0.300090    -0.640834     148.62
 C       0.382267     1.213478    -0.911025      48.03
 H      -0.038609     2.173161    -0.389869      21.75
 C       2.288189    -0.198295    -0.464262      41.16
 C       3.770506    -0.609833    -0.268909      82.75
 H       3.926583    -1.587914    -0.962746      24.11
 O       4.796867     0.482575    -0.548115     196.17
 H       5.306407     0.654365     0.334652      27.44
 C       3.925714    -1.271318     1.236503      86.30
 H       3.330562    -2.284529     1.217792      26.74
 O       5.295446    -1.612050     1.478561     135.13
 H       6.043084    -1.463429     0.653868      22.52
 C       3.473753    -0.261194     2.385752     105.71
 O       4.480762     0.688030     2.554873     213.73
 H       4.130612     1.579365     2.681481      27.71
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 H       3.188120    -0.758175     3.388670      27.52
 H       2.367922     0.257579     2.031073      25.95
55
name = lig-Water-frame_591
 C      -1.337197     3.481494     2.512641      55.28
 H      -1.844533     4.363288     2.254658      28.02
 C      -0.864684     0.959898     2.418344      37.28
 H      -1.026688    -0.057807     2.028534      22.65
 C       0.044572     1.169503     3.624963      -2.25
 O       0.736902     0.152689     4.339460     160.12
 C       0.162763    -1.174727     4.540843     111.09
 H       0.429320    -1.710779     5.482595      26.24
 H       0.365794    -1.672455     3.477266      25.31
 H      -0.852075    -1.029435     4.759253      28.57
 C       0.372820     2.528373     4.093348       3.55
 O       1.477515     2.632310     4.930029     189.20
 H       1.704838     3.561559     5.336492      23.59
 C      -0.326064     3.683142     3.648984      51.24
 H      -0.119241     4.710451     4.057932      21.76
 C      -1.619803     2.247260     2.067243      33.62
 C      -2.832779     2.055520     1.092845     102.74
 H      -3.286143     2.973070     0.866337      24.74
 O      -3.916289     1.272856     1.716781     267.91
 H      -4.755011     1.803847     1.641071      28.63
 C      -2.510644     1.569846    -0.487653      68.33
 H      -2.091501     2.487005    -1.172702      20.74
 C      -4.021215     1.349554    -1.286521      76.63
 O      -4.654501     0.020635    -1.338422     237.29
 H      -4.680804    -0.428931    -0.437571      25.36
 H      -4.026445     1.533148    -2.529309      24.74
 H      -4.880907     2.148967    -0.864727      26.08
 C       1.712771     1.076018    -0.617677      58.60
 H       2.239005     1.872752    -0.160613      29.42
 C       1.465953    -1.337102    -0.813214      33.04
 H       1.967333    -2.406369    -0.601915      24.04
 C      -0.024036    -1.217591    -0.966668      10.74
 O      -0.648001    -2.465873    -0.943897     166.86
 C      -2.074314    -2.272954    -1.614294      60.64
 H      -2.940942    -2.037657    -0.963729      22.62
 H      -1.997785    -1.576089    -2.688933      22.00
 H      -1.998907    -3.543587    -2.133926      20.98
 C      -0.492668     0.118580    -0.871830      22.94
 O      -1.813491     0.337372    -0.700019     184.67
 C       0.342424     1.248224    -0.858990      55.35
 H       0.009483     2.215046    -0.690524      22.68
 C       2.343965    -0.198057    -0.545469     -18.04
 C       3.782901    -0.546156    -0.220830      98.59
 H       3.972062    -1.146724    -1.160479      22.54
 O       4.769786     0.462941    -0.560702     216.19
 H       5.244193     0.555771     0.427560      25.27
 C       3.927580    -1.265887     1.199894      95.07
 H       3.167490    -2.037457     1.422252      26.69
 O       5.350073    -1.613548     1.480881     182.33
 H       5.992641    -1.442957     0.776921      27.09
 C       3.428364    -0.318990     2.392558     110.34
 O       4.515450     0.708543     2.583189     150.61
 H       4.085513     1.649052     2.812918      25.19
 H       3.348826    -0.890108     3.332378      28.00
 H       2.672142     0.263933     2.198725      29.25
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name = lig-Water-frame_592
 C      -1.288103     3.518463     2.557263      57.52
 H      -1.947120     4.348965     2.130175      25.06
 C      -0.872727     1.000334     2.493841      63.59
 H      -1.103656     0.016393     2.105921      21.59
 C      -0.019486     1.211943     3.617305       7.08
 O       0.700095     0.128187     4.362435     160.56
 C       0.168574    -1.131691     4.492231     118.32
 H       0.822446    -1.495515     5.337560      24.94
 H       0.482865    -1.895765     3.802395      27.09
 H      -1.057024    -1.163349     4.590553      25.01
 C       0.363816     2.496763     4.107364     -10.51
 O       1.492845     2.573455     4.934710     174.40
 H       1.412808     3.569476     5.014189      24.81
 C      -0.396573     3.711328     3.607467      57.43
 H      -0.074436     4.659981     4.089507      22.34
 C      -1.566916     2.133737     2.134271      23.46
 C      -2.886890     2.032914     1.090499      66.97
 H      -3.165210     3.191748     0.806429      21.48
 O      -3.870001     1.269574     1.745052     288.59
 H      -4.734013     1.800303     1.708713      27.77
 C      -2.540975     1.585681    -0.457881      84.11
 H      -1.999799     2.399173    -0.771574      20.62
 C      -4.034569     1.366673    -1.267582     112.54
 O      -4.635471     0.053538    -1.324910     331.70
 H      -4.689931    -0.403778    -0.424281      25.53
 H      -3.713015     1.776231    -2.177293      26.73
 H      -4.803725     2.029510    -1.110499      29.49
 C       1.743965     1.112431    -0.639560      42.07
 H       2.354614     1.849844     0.091511      27.19
 C       1.418311    -1.312930    -0.804114      37.36
 H       1.820700    -2.248146    -0.696104      24.30
 C      -0.021662    -1.195633    -0.944967      11.71
 O      -0.683151    -2.461324    -0.978471     194.06
 C      -2.127890    -2.357697    -1.616133      96.81
 H      -2.839321    -1.883341    -0.893022      21.45
 H      -2.091205    -1.666997    -2.428881      26.15
 H      -2.171270    -3.158195    -2.054911      27.15
 C      -0.477535     0.138332    -0.913025      22.95
 O      -1.823462     0.356559    -0.752737     224.96
 C       0.338164     1.266779    -0.790739      67.97
 H      -0.116506     2.325231    -1.047310      19.66
 C       2.333753    -0.220693    -0.638597     -12.75
 C       3.782208    -0.510275    -0.209385     107.29
 H       4.069057    -1.223524    -1.128358      23.78
 O       4.747849     0.451541    -0.522358     284.03
 H       5.114342     0.695279     0.240053      32.67
 C       3.939210    -1.207845     1.175318      94.91
 H       3.226291    -2.079313     1.276886      26.50
 O       5.377637    -1.627481     1.502129     148.08
 H       5.865718    -1.517975     0.639171      26.09
 C       3.468123    -0.363524     2.392738      91.96
 O       4.550678     0.738416     2.623268     127.16
 H       4.024093     1.544346     2.801548      28.19
 H       3.440794    -1.034637     3.271567      27.16
 H       2.420034     0.307120     2.216661      23.56
55
name = lig-Water-frame_593
 C      -1.269481     3.518810     2.604866      61.03
 H      -1.906881     4.212198     2.100938      23.41
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 C      -0.877550     1.045692     2.617800      69.90
 H      -1.187247     0.055529     2.210037      19.48
 C      -0.037030     1.211489     3.641061      32.14
 O       0.662983     0.178002     4.350873     184.13
 C       0.163652    -1.149848     4.467340     127.32
 H       0.818576    -1.347306     5.327178      23.86
 H       0.504092    -2.033342     3.765691      24.14
 H      -0.827617    -1.255685     4.550012      28.73
 C       0.318433     2.479772     4.080533      -6.49
 O       1.471146     2.546848     4.935236     197.45
 H       1.604980     3.540510     4.962355      29.16
 C      -0.400119     3.681089     3.597686      68.73
 H      -0.124769     4.637460     3.991350      23.60
 C      -1.585056     2.082439     2.115920      29.71
 C      -2.858103     2.025036     1.072342      88.15
 H      -3.103991     3.071699     1.014011      22.23
 O      -3.840690     1.271639     1.775076     290.94
 H      -4.776498     1.604243     1.791083      31.02
 C      -2.631669     1.579211    -0.399161      88.83
 H      -1.909376     2.510012    -0.643189      15.72
 C      -3.994150     1.394155    -1.235324      84.62
 O      -4.604309     0.101823    -1.339193     317.94
 H      -4.648748    -0.424251    -0.414999      22.55
 H      -3.447122     1.741108    -2.264134      21.97
 H      -4.854387     2.228475    -0.930736      25.36
 C       1.798814     1.123485    -0.617427      42.17
 H       2.407693     1.935470    -0.124473      24.49
 C       1.367923    -1.268185    -0.800340      47.08
 H       1.738237    -2.448888    -0.884325      18.17
 C       0.048218    -1.190286    -0.916327       8.76
 O      -0.743751    -2.412919    -1.033323     178.70
 C      -2.127214    -2.397180    -1.588396      45.61
 H      -2.766219    -2.038243    -0.807724      20.74
 H      -2.103152    -1.389639    -2.412742      18.29
 H      -2.615136    -3.588657    -2.121065      18.96
 C      -0.498495     0.187229    -0.938359      12.69
 O      -1.876005     0.355247    -0.801347     207.55
 C       0.377345     1.305033    -0.752052     103.61
 H      -0.114011     2.139538    -1.127493      20.88
 C       2.268430    -0.211410    -0.706020      31.45
 C       3.768724    -0.546360    -0.262199      84.57
 H       4.078644    -1.562653    -0.687017      23.27
 O       4.733907     0.470112    -0.488132     219.51
 H       5.079823     1.055552     0.348864      24.52
 C       3.947500    -1.147038     1.181195      85.92
 H       3.496184    -2.164045     0.917121      21.99
 O       5.377376    -1.630720     1.512643     108.55
 H       5.754621    -1.842599     0.473217      23.31
 C       3.530134    -0.346410     2.383597     115.59
 O       4.561620     0.741459     2.665441     177.20
 H       4.012702     1.608939     2.753532      23.48
 H       3.490525    -1.079409     3.251583      25.43
 H       2.545480    -0.123025     2.298221      25.90
55
name = lig-Water-frame_594
 C      -1.326710     3.415742     2.581379      89.55
 H      -1.842326     4.325036     2.159938      18.08
 C      -0.943724     1.030497     2.694430      61.51
 H      -1.149112     0.025603     2.403241      19.84
 C       0.004192     1.190733     3.725372      55.90
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 O       0.630723     0.254140     4.313619     237.50
 C       0.221326    -1.212735     4.454162     102.04
 H       0.505352    -1.499087     5.522161      24.70
 H       0.493122    -1.752719     3.542607      25.27
 H      -1.007044    -1.274167     4.688571      25.64
 C       0.296766     2.509244     4.069156      12.93
 O       1.416665     2.550466     4.923506     271.67
 H       1.939729     3.392166     5.145101      26.97
 C      -0.331726     3.618968     3.636304      16.59
 H      -0.135857     4.710282     3.927040       9.96
 C      -1.639616     2.157933     2.056216      26.67
 C      -2.780638     1.985848     1.107202     107.51
 H      -3.220855     3.108942     1.090666      21.08
 O      -3.829910     1.254876     1.821618     240.81
 H      -4.794711     1.534449     1.695000      31.30
 C      -2.694508     1.591553    -0.342128     109.70
 H      -2.232369     2.388520    -0.824747      23.16
 C      -3.929457     1.484507    -1.211947     113.23
 O      -4.567636     0.154741    -1.359869     348.23
 H      -4.560107    -0.359877    -0.552501      27.90
 H      -3.681136     1.460995    -2.279547      25.94
 H      -4.532359     2.184050    -0.830224      29.25
 C       1.824947     1.122117    -0.594350      44.24
 H       2.520519     2.052155    -0.474411      18.29
 C       1.384256    -1.311603    -0.819943      58.54
 H       1.689895    -2.219455    -0.992628      23.07
 C       0.002906    -1.150485    -0.910303      17.94
 O      -0.784886    -2.357997    -1.090021     227.23
 C      -2.134192    -2.410468    -1.604775     108.24
 H      -2.821706    -2.288126    -0.701980      23.54
 H      -2.224547    -1.682747    -2.293846      27.46
 H      -2.473554    -3.254277    -1.802096      27.15
 C      -0.519977     0.234785    -0.918864      36.58
 O      -1.940132     0.339991    -0.843908     184.33
 C       0.424102     1.306497    -0.751385      85.53
 H      -0.044594     2.344191    -0.970617      18.46
 C       2.257072    -0.183560    -0.720517      44.06
 C       3.759424    -0.608014    -0.283559      79.57
 H       4.122604    -1.611801    -0.751712      24.35
 O       4.733711     0.510172    -0.478602     198.81
 H       4.677728     1.123198     0.381860      25.92
 C       3.976204    -1.131166     1.178214      91.18
 H       3.473753    -2.072333     1.051269      25.58
 O       5.363456    -1.627331     1.475603     201.13
 H       5.765281    -2.076501     0.815590      31.36
 C       3.625368    -0.354899     2.403492     120.58
 O       4.532974     0.732740     2.703070     205.03
 H       4.120838     1.671489     2.711129      22.11
 H       3.674843    -0.995018     3.267544      27.38
 H       2.418759    -0.139803     2.321000      24.00
55
name = lig-Water-frame_595
 C      -1.380730     3.351984     2.567417      73.93
 H      -1.734937     4.344879     2.305264      23.12
 C      -1.034193     1.018847     2.745022      56.76
 H      -1.171102    -0.070993     2.502845      17.95
 C      -0.045015     1.214835     3.729911      19.85
 O       0.654587     0.241357     4.333027     206.94
 C       0.216767    -1.230944     4.468423     110.23
 H       0.494675    -1.706042     5.394258      25.83
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 H       0.533349    -1.596365     3.466672      24.44
 H      -0.779190    -1.195218     4.514013      28.92
 C       0.365004     2.563615     4.123312      -4.28
 O       1.374969     2.545022     4.930151     218.42
 H       1.829181     3.387898     5.197104      17.62
 C      -0.321879     3.597468     3.611467      39.11
 H      -0.051691     4.548392     3.918511      23.80
 C      -1.652622     2.195552     2.030187      45.94
 C      -2.767879     1.980793     1.166182     112.17
 H      -3.272418     2.934375     0.959482      25.74
 O      -3.827962     1.215259     1.883463     219.04
 H      -4.666904     1.590050     1.493364      29.38
 C      -2.695089     1.577992    -0.347304     102.28
 H      -2.328255     2.490320    -1.042789      21.87
 C      -3.883182     1.518048    -1.201401      89.53
 O      -4.542621     0.216845    -1.381912     277.97
 H      -4.499349    -0.397275    -0.498000      23.37
 H      -3.757856     1.711431    -2.319324      26.07
 H      -4.639094     2.450162    -0.777575      25.84
 C       1.822465     1.135609    -0.578700      83.62
 H       2.541193     1.985676    -0.985500      21.61
 C       1.389625    -1.320697    -0.854282      31.36
 H       1.914411    -2.438881    -1.089874      20.93
 C      -0.099098    -1.086703    -0.930665       6.71
 O      -0.784001    -2.299119    -1.137367     186.21
 C      -2.143538    -2.369103    -1.540009      69.28
 H      -2.861051    -2.265600    -0.759988      22.86
 H      -2.610636    -1.705049    -2.646578      19.87
 H      -2.239813    -3.727427    -1.898755      21.14
 C      -0.544267     0.265392    -0.857306      16.80
 O      -1.982085     0.330793    -0.871847     195.68
 C       0.429977     1.325450    -0.779303      54.67
 H       0.219783     2.378336    -0.572266      20.36
 C       2.316395    -0.214322    -0.679675      18.38
 C       3.768921    -0.641806    -0.287184      89.05
 H       4.155325    -1.256424    -1.204951      23.04
 O       4.709591     0.544423    -0.479539     240.61
 H       4.388295     0.998827     0.224310      34.20
 C       4.020453    -1.175556     1.156695      86.07
 H       3.139232    -1.965040     1.511210      25.47
 O       5.342228    -1.606561     1.454927     168.27
 H       5.854961    -2.335497     0.857773      22.87
 C       3.665594    -0.358225     2.441133     109.88
 O       4.505044     0.737669     2.734724     219.48
 H       4.061656     1.627506     2.696679      25.36
 H       3.882384    -1.037987     3.350795      25.18
 H       2.697945     0.057739     2.380311      22.81
55
name = lig-Water-frame_596
 C      -1.359740     3.418289     2.625182      49.51
 H      -1.887277     4.308811     2.247861      21.98
 C      -1.108112     1.016695     2.778698      60.87
 H      -1.303837     0.016040     2.451808      22.16
 C      -0.136654     1.262256     3.697497       0.54
 O       0.711612     0.177903     4.401068     132.96
 C       0.211256    -1.194271     4.445994     100.13
 H       0.801568    -1.813660     5.217706      24.14
 H       0.623161    -1.753205     3.502518      25.66
 H      -0.991870    -1.161999     4.279020      22.87
 C       0.397156     2.556188     4.140715     -10.06
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 O       1.399933     2.544298     4.996482     141.45
 H       1.458865     3.562706     5.153772      25.22
 C      -0.362762     3.594943     3.535886      65.30
 H      -0.005950     4.629661     3.909140      26.69
 C      -1.629447     2.108466     2.052161      12.89
 C      -2.839545     1.967893     1.165713      74.89
 H      -3.291491     3.030251     0.922969      25.79
 O      -3.820322     1.178518     1.933265     250.13
 H      -4.656768     1.492082     1.505815      28.46
 C      -2.619018     1.570827    -0.420805     112.99
 H      -2.100413     2.445984    -0.732435      27.51
 C      -3.945112     1.555105    -1.209931     124.56
 O      -4.529388     0.272637    -1.384172     312.83
 H      -4.514343    -0.247050    -0.590496      29.61
 H      -3.634149     2.197436    -2.129221      26.54
 H      -4.599614     2.248316    -0.905097      31.45
 C       1.823075     1.108791    -0.627054      81.03
 H       2.430044     1.899841    -1.003051      25.61
 C       1.378855    -1.310762    -0.900021      44.99
 H       1.760624    -2.230013    -0.988812      25.85
 C      -0.103244    -1.036903    -0.965060       9.25
 O      -0.774373    -2.219335    -1.179235     188.95
 C      -2.204648    -2.406088    -1.556468     123.54
 H      -2.930259    -2.141750    -0.738390      24.15
 H      -2.543847    -1.960096    -2.379897      28.18
 H      -1.970035    -3.259566    -1.816942      28.74
 C      -0.585560     0.285608    -0.782164      27.40
 O      -1.991732     0.346213    -0.876226     220.54
 C       0.425266     1.354990    -0.778228      52.31
 H       0.199493     2.357631    -0.391344      22.07
 C       2.356462    -0.287082    -0.603170       6.78
 C       3.804921    -0.631975    -0.338977      90.40
 H       4.125535    -1.119904    -1.265321      24.62
 O       4.668388     0.557851    -0.484365     128.43
 H       4.164117     1.271437     0.230538      27.74
 C       4.009616    -1.267539     1.168625      87.75
 H       3.212037    -1.860866     1.477974      30.38
 O       5.343487    -1.599829     1.442160     174.51
 H       5.623513    -2.375625     0.789096      23.64
 C       3.716010    -0.346345     2.480673     104.64
 O       4.512541     0.766239     2.766604     235.16
 H       3.897220     1.602011     2.709454      24.03
 H       3.801859    -1.085083     3.240302      28.08
 H       2.621966     0.097770     2.462817      22.27
55
name = lig-Water-frame_597
 C      -1.355442     3.472286     2.630373      35.79
 H      -2.059260     4.194985     2.183117      16.45
 C      -1.164979     1.007222     2.775813      48.04
 H      -1.401152     0.009126     2.364967      21.71
 C      -0.132453     1.262340     3.743612       7.95
 O       0.743101     0.138796     4.461654     143.62
 C       0.216690    -1.168108     4.370635     127.85
 H       0.741427    -1.649924     5.145439      26.97
 H       0.568773    -1.805105     3.511559      27.92
 H      -0.811357    -1.323870     4.399950      27.19
 C       0.334186     2.476533     4.078711       7.97
 O       1.447289     2.595516     5.087742     115.75
 H       1.337917     3.571113     5.280377      30.32
 C      -0.336708     3.638313     3.523114      57.69
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 H      -0.159029     4.658086     3.771075      25.07
 C      -1.635972     2.066113     2.108154     -51.22
 C      -2.916862     1.945749     1.131178      84.07
 H      -3.224808     3.026655     1.077259      26.56
 O      -3.814406     1.156298     1.953970     247.49
 H      -4.813709     1.250546     1.766908      25.45
 C      -2.555621     1.575565    -0.462593     111.09
 H      -1.737310     2.432108    -0.536846      25.08
 C      -3.984113     1.627408    -1.230467      94.70
 O      -4.527771     0.327967    -1.413679     269.19
 H      -4.511497    -0.162779    -0.512973      26.20
 H      -3.662173     2.134071    -2.130114      27.22
 H      -4.908395     2.251916    -0.625148      26.99
 C       1.814708     1.013439    -0.704408      56.31
 H       2.506947     2.073218    -0.693193      23.52
 C       1.340535    -1.234559    -0.919094      57.31
 H       1.585309    -2.445802    -0.936071      24.31
 C      -0.019967    -0.991546    -1.000247      21.91
 O      -0.772911    -2.129834    -1.212712     161.75
 C      -2.243863    -2.416949    -1.532811      61.08
 H      -2.919960    -2.197768    -0.671359      22.36
 H      -2.519857    -1.727724    -2.680774      20.90
 H      -2.026939    -3.700347    -1.851750      22.38
 C      -0.594882     0.297349    -0.725739      23.28
 O      -1.977840     0.378703    -0.858849     236.22
 C       0.403923     1.360860    -0.732809      54.82
 H      -0.001897     2.396012    -0.505770      19.02
 C       2.322283    -0.327142    -0.543988      29.07
 C       3.840756    -0.591998    -0.371570      89.99
 H       4.221156    -1.428092    -1.170459      24.12
 O       4.603706     0.586499    -0.464673     191.85
 H       4.294135     1.421210    -0.085876      29.88
 C       3.982331    -1.286387     1.186821      57.93
 H       3.239799    -2.316806     1.157410      26.94
 O       5.357409    -1.629332     1.422159     176.40
 H       5.501640    -2.246627     0.793625      30.12
 C       3.713537    -0.319885     2.481406     127.44
 O       4.538301     0.803417     2.795269     242.56
 H       3.985756     1.623096     2.802451      26.50
 H       3.681761    -1.152707     3.298768      27.92
 H       2.599574    -0.189787     2.516806      26.02
55
name = lig-Water-frame_598
 C      -1.383491     3.439205     2.570012      57.41
 H      -2.043604     4.244067     2.239861      16.78
 C      -1.157109     0.962553     2.781991      13.10
 H      -1.355324    -0.042637     2.381999      19.04
 C      -0.078599     1.143767     3.814989      13.48
 O       0.729271     0.156038     4.485936     152.79
 C       0.260198    -1.182667     4.299019     108.94
 H       0.594805    -1.637456     5.324670      24.19
 H       0.506103    -1.707246     3.283256      25.56
 H      -0.889877    -1.367293     4.618153      22.56
 C       0.312049     2.466728     4.063112      40.65
 O       1.442184     2.655038     5.139992     189.91
 H       1.529847     3.605268     5.468555      29.72
 C      -0.296484     3.682225     3.531464      37.44
 H      -0.125312     4.746686     3.831462      14.08
 C      -1.714328     2.130201     2.151279     -12.21
 C      -2.934066     1.918281     1.124058     109.23
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 H      -3.336784     2.981526     1.086844      24.56
 O      -3.825474     1.126326     1.959966     266.25
 H      -4.801479     1.203115     1.932992      26.76
 C      -2.546222     1.635069    -0.438037     103.21
 H      -1.788239     2.370176    -0.658835      26.08
 C      -4.013728     1.743115    -1.208590      98.67
 O      -4.530231     0.367816    -1.447924     276.33
 H      -4.523667    -0.121358    -0.533845      25.89
 H      -3.983116     1.975779    -2.390778      24.36
 H      -4.639018     2.181540    -0.602677      31.26
 C       1.799023     0.980783    -0.747689      72.15
 H       2.391256     1.749001    -0.417905      28.80
 C       1.329488    -1.242089    -0.913563      63.70
 H       1.362335    -2.295573    -0.928182      24.62
 C       0.008734    -0.930031    -1.026864      14.16
 O      -0.789786    -2.073822    -1.240977     215.65
 C      -2.222140    -2.428989    -1.578864     115.01
 H      -2.878225    -2.299461    -0.715348      25.12
 H      -2.477107    -1.892876    -2.347250      27.68
 H      -2.454984    -3.370737    -1.707940      28.59
 C      -0.543498     0.306079    -0.711074      13.18
 O      -1.948029     0.396951    -0.826556     236.66
 C       0.370943     1.337591    -0.665206      90.30
 H       0.066866     2.350166    -0.767084      22.13
 C       2.280843    -0.306069    -0.538929      27.46
 C       3.830302    -0.579099    -0.337499      92.24
 H       4.279263    -1.383878    -0.887758      26.93
 O       4.575918     0.614070    -0.473146     209.90
 H       4.209106     1.456181    -0.226807      29.83
 C       3.949020    -1.273915     1.184344      81.52
 H       3.544577    -2.208112     1.001294      29.09
 O       5.371488    -1.667800     1.411191      59.61
 H       5.659574    -2.332441     0.564429      24.12
 C       3.656097    -0.360767     2.476855     113.78
 O       4.564049     0.808765     2.809998     206.36
 H       4.060310     1.741200     2.855280      25.07
 H       3.807344    -0.957036     3.343382      28.97
 H       2.553835    -0.139746     2.460987      25.87
55
name = lig-Water-frame_599
 C      -1.383817     3.409548     2.533252      53.60
 H      -1.911382     4.350095     2.281429      28.59
 C      -1.081469     0.935738     2.813270      44.96
 H      -1.275965    -0.059611     2.421853      18.82
 C      -0.043200     1.024094     3.839584      67.62
 O       0.687372     0.192746     4.483620     164.99
 C       0.273648    -1.238188     4.290979     116.12
 H       0.703156    -1.792240     5.100833      26.03
 H       0.479480    -1.543933     3.298609      26.70
 H      -0.783536    -1.137917     4.514434      23.67
 C       0.356566     2.556598     4.129262       7.39
 O       1.392957     2.685873     5.152873     269.02
 H       1.608246     3.673387     5.340702      22.69
 C      -0.298231     3.667754     3.512257      36.74
 H       0.034827     4.636047     3.962034      20.55
 C      -1.809569     2.169762     2.184026      41.06
 C      -2.911043     1.928275     1.159440     104.38
 H      -3.548759     2.878933     0.964271      22.83
 O      -3.835506     1.071737     1.959109     250.86
 H      -4.777966     1.439795     1.780471      26.17
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 C      -2.596898     1.698271    -0.400934      89.10
 H      -1.999829     2.605785    -0.827902      21.02
 C      -3.985947     1.791619    -1.239669      90.19
 O      -4.538011     0.403559    -1.456616     255.29
 H      -4.537948    -0.135579    -0.695332      28.61
 H      -4.184004     2.177626    -2.174090      28.14
 H      -4.681068     2.531686    -0.452577      24.37
 C       1.742145     0.996047    -0.736231      65.12
 H       2.520094     1.806881    -0.140523      23.79
 C       1.329003    -1.293784    -0.890828      38.58
 H       1.483286    -2.450988    -0.957519      21.26
 C      -0.048311    -0.913246    -1.048601       6.18
 O      -0.811510    -2.067810    -1.268450     209.04
 C      -2.170193    -2.387837    -1.562741      66.78
 H      -2.855125    -2.108717    -0.664187      20.76
 H      -2.760272    -1.652134    -2.584399      18.85
 H      -2.492653    -3.611324    -1.798318      21.35
 C      -0.523824     0.328384    -0.733341      18.95
 O      -1.911373     0.406789    -0.779345     221.18
 C       0.390526     1.317453    -0.614788     105.14
 H       0.214531     2.397297    -0.940590      22.11
 C       2.274261    -0.288818    -0.589655      30.81
 C       3.756920    -0.550458    -0.218424      83.78
 H       4.373553    -1.329224    -0.941689      23.53
 O       4.589042     0.633975    -0.501446     111.12
 H       3.886109     1.472276    -0.235801      26.78
 C       3.978775    -1.196467     1.165261      78.29
 H       3.339459    -2.282959     1.086464      25.10
 O       5.394695    -1.722150     1.387846      66.54
 H       5.781229    -2.142943     0.584035      27.57
 C       3.590468    -0.409301     2.472099      95.72
 O       4.574168     0.788934     2.799320     190.21
 H       4.047067     1.632681     2.764675      27.66
 H       3.887693    -0.924191     3.427463      25.24
 H       2.558409     0.143240     2.382505      21.71
55
name = lig-Water-frame_600
 C      -1.351448     3.438875     2.546508      25.30
 H      -1.821152     4.349035     2.167260      25.95
 C      -0.995916     0.942756     2.846040      49.58
 H      -1.246242    -0.054176     2.410241      17.40
 C      -0.053878     1.093451     3.796552      67.78
 O       0.674972     0.172665     4.499934     206.74
 C       0.275248    -1.261810     4.314924      91.33
 H       0.979644    -2.002667     4.851804      23.71
 H       0.509697    -1.506096     3.133610      22.98
 H      -0.833922    -1.167420     4.348691      23.32
 C       0.401502     2.611142     4.213274     -18.36
 O       1.319366     2.705494     5.136203     187.28
 H       1.507263     3.708555     5.098672      28.69
 C      -0.296298     3.588527     3.504282      45.24
 H      -0.001619     4.551815     3.849208      28.00
 C      -1.843643     2.135383     2.223500      38.84
 C      -2.906001     1.962736     1.207074      96.71
 H      -3.509214     2.864381     1.047251      22.10
 O      -3.859935     1.017367     1.928625     261.73
 H      -4.663835     1.516714     1.650381      25.86
 C      -2.651832     1.751656    -0.394016      84.66
 H      -2.253566     2.725431    -0.774782      18.47
 C      -3.988058     1.798265    -1.195614     105.81
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 O      -4.554335     0.466347    -1.465566     297.55
 H      -4.477932    -0.200874    -0.646904      24.06
 H      -4.014194     2.572649    -2.163137      24.70
 H      -4.565739     2.445053    -0.705069      27.79
 C       1.759035     1.050989    -0.633150      68.32
 H       2.300035     1.833871    -0.334909      24.59
 C       1.313494    -1.354245    -0.866064      52.82
 H       1.755319    -2.405320    -0.989397      22.67
 C      -0.089816    -0.992457    -1.060391      25.37
 O      -0.825137    -2.095737    -1.302267     236.91
 C      -2.207153    -2.306111    -1.571133     111.37
 H      -2.726452    -1.985221    -0.728525      24.93
 H      -2.585311    -1.832115    -2.346161      27.05
 H      -1.993641    -3.281714    -1.835273      22.74
 C      -0.568862     0.351764    -0.777726      28.74
 O      -1.894255     0.445783    -0.720246     217.16
 C       0.438636     1.366071    -0.609802      71.74
 H       0.175183     2.375123    -0.774283      21.38
 C       2.266728    -0.304021    -0.659330      35.62
 C       3.718670    -0.525007    -0.142348      95.91
 H       4.083291    -1.176252    -0.895353      26.63
 O       4.577417     0.665629    -0.516864     194.60
 H       4.005091     1.330420    -0.298254      33.49
 C       4.005714    -1.165796     1.174441     106.98
 H       3.239685    -1.880449     1.276046      28.65
 O       5.407269    -1.757387     1.374896      88.28
 H       5.744827    -2.035256     0.486939      27.42
 C       3.575012    -0.397942     2.471609     108.54
 O       4.569380     0.737560     2.762656     216.48
 H       4.002616     1.560409     2.667417      26.94
 H       3.585791    -1.101724     3.329586      26.44
 H       2.652449     0.073059     2.382350      24.17
55
name = lig-Water-frame_601
 C      -1.325426     3.429677     2.573210      69.00
 H      -1.758831     4.291341     2.040910      17.73
 C      -0.990588     0.984488     2.813233      48.84
 H      -1.170289    -0.007501     2.471735      20.82
 C      -0.018883     1.270701     3.795133      18.41
 O       0.678317     0.125210     4.525908     190.39
 C       0.294595    -1.256151     4.273658     100.79
 H       0.989432    -1.951155     4.713224      25.02
 H       0.446256    -1.474477     3.272946      29.23
 H      -0.824840    -1.612875     4.423219      24.81
 C       0.347675     2.537318     4.208800      14.62
 O       1.273005     2.740900     5.133163     104.25
 H       1.493798     3.752220     5.204490      33.16
 C      -0.278211     3.532839     3.515427     101.62
 H      -0.111593     4.674408     3.625066      22.41
 C      -1.770243     2.098221     2.284482      25.93
 C      -2.920947     1.975732     1.246270      84.94
 H      -3.383427     3.076431     1.344479      23.07
 O      -3.877676     0.980835     1.862878     271.75
 H      -4.859711     1.269296     1.734028      27.65
 C      -2.697101     1.783612    -0.373173      84.15
 H      -2.127858     2.722089    -0.629768      20.27
 C      -3.984586     1.792180    -1.176151      90.15
 O      -4.577505     0.539425    -1.469049     333.66
 H      -4.383154    -0.020715    -0.682458      28.97
 H      -3.621148     2.261911    -2.015464      27.08
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 H      -4.863532     2.429975    -0.521799      24.11
 C       1.809434     1.060426    -0.506391      61.60
 H       2.453063     2.184069    -0.583012      20.03
 C       1.312987    -1.362600    -0.852896      62.05
 H       1.737684    -2.348435    -0.966164      23.88
 C      -0.084142    -1.070222    -1.045631      13.78
 O      -0.810047    -2.132147    -1.336026     191.47
 C      -2.222507    -2.226060    -1.556194      61.69
 H      -2.886216    -2.053879    -0.557858      21.45
 H      -2.567480    -1.623679    -2.749320      20.45
 H      -2.031653    -3.372384    -1.847525      21.18
 C      -0.559752     0.354946    -0.831341      10.39
 O      -1.929806     0.523766    -0.658266     222.65
 C       0.419837     1.406379    -0.639257      32.98
 H       0.026506     2.470543    -0.443337      16.98
 C       2.233900    -0.295405    -0.684363      35.61
 C       3.713040    -0.484233    -0.151634      76.49
 H       3.935007    -1.374778    -0.985140      24.87
 O       4.562406     0.674158    -0.523498     143.23
 H       4.104765     1.557929    -0.253546      25.64
 C       4.024275    -1.136993     1.239621      81.16
 H       3.068109    -1.919505     1.335590      26.40
 O       5.390296    -1.778427     1.362911      69.40
 H       5.591995    -2.015800     0.297543      23.10
 C       3.633255    -0.357975     2.470733     115.07
 O       4.542250     0.665194     2.719423     226.72
 H       4.057800     1.576126     2.679334      24.76
 H       3.328344    -1.174819     3.199967      25.65
 H       2.451671    -0.028343     2.279901      23.15
55
name = lig-Water-frame_602
 C      -1.302193     3.365454     2.603705      77.36
 H      -1.696839     4.218035     2.043216      17.68
 C      -1.005096     1.057226     2.778829      57.22
 H      -1.121658    -0.029554     2.554385      21.08
 C       0.022723     1.293924     3.809088      -1.56
 O       0.668013     0.108414     4.546256     159.25
 C       0.298946    -1.253284     4.213039     103.00
 H       1.046002    -1.833555     4.851703      24.23
 H       0.381081    -1.495942     3.008464      24.32
 H      -0.591903    -1.759239     4.630021      26.22
 C       0.281224     2.492150     4.185087      19.72
 O       1.262937     2.773094     5.162859      34.19
 H       1.394892     3.750072     5.375702      27.72
 C      -0.293016     3.587825     3.493207      40.73
 H       0.011142     4.571689     3.634543      21.52
 C      -1.675920     2.064222     2.302335      37.60
 C      -2.952749     1.995471     1.304307      94.51
 H      -3.318312     2.969522     1.474510      26.96
 O      -3.893993     0.952965     1.785323     324.44
 H      -4.864100     1.100883     1.829486      27.36
 C      -2.697726     1.808012    -0.279615      90.47
 H      -1.928665     2.618691    -0.542752      23.61
 C      -4.006716     1.817801    -1.127504     101.99
 O      -4.600744     0.595566    -1.467112     334.48
 H      -4.395775     0.011098    -0.754062      31.76
 H      -3.489382     2.031133    -2.197602      24.11
 H      -4.726355     2.354245    -0.686930      28.03
 C       1.826218     1.122156    -0.422884      54.16
 H       2.480926     1.803440    -0.633029      25.28
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 C       1.312479    -1.313091    -0.851966      56.19
 H       1.606212    -2.491342    -0.901880      22.83
 C      -0.047337    -1.067412    -1.009556       6.92
 O      -0.791175    -2.180403    -1.362747     195.42
 C      -2.246016    -2.185295    -1.597804     121.23
 H      -2.857279    -2.088236    -0.791284      28.65
 H      -2.476696    -1.638226    -2.381563      29.60
 H      -2.710690    -3.191855    -1.786131      24.90
 C      -0.518343     0.351353    -0.869668       1.44
 O      -1.983120     0.599280    -0.603900     210.70
 C       0.378451     1.415044    -0.665451      46.74
 H       0.009467     2.303992    -0.180736      22.77
 C       2.221839    -0.236180    -0.632662      18.49
 C       3.721972    -0.481002    -0.236663      84.17
 H       4.103532    -1.287074    -0.818575      29.77
 O       4.543510     0.667628    -0.533707     147.86
 H       4.320350     1.635555    -0.094776      23.69
 C       3.986229    -1.148428     1.291082      94.40
 H       3.362504    -1.996450     1.219838      30.11
 O       5.339519    -1.782753     1.321499     155.22
 H       5.499429    -2.092272     0.497332      31.78
 C       3.625593    -0.342647     2.447886     149.58
 O       4.524663     0.627771     2.694623     216.08
 H       4.128948     1.495876     2.801655      28.66
 H       3.462411    -1.007044     3.335869      28.19
 H       2.705075    -0.017928     2.156466      28.65
55
name = lig-Water-frame_603
 C      -1.288083     3.335834     2.612934      64.62
 H      -1.740507     4.173329     2.095815      24.42
 C      -0.941744     1.027808     2.818716      77.37
 H      -1.227495     0.017907     2.551694      26.19
 C       0.019758     1.113851     3.795466       1.83
 O       0.634169     0.136802     4.545163     182.37
 C       0.334222    -1.278876     4.137489     115.81
 H       1.202669    -1.656293     4.721587      26.25
 H       0.319337    -1.489352     3.176759      30.27
 H      -0.596811    -1.575278     4.813426      26.00
 C       0.291004     2.594208     4.220027     -33.76
 O       1.249841     2.771591     5.201344     140.62
 H       1.249549     3.804232     5.341702      23.64
 C      -0.300075     3.659006     3.483074      42.79
 H       0.234939     4.632710     3.774229      20.61
 C      -1.680837     2.069924     2.224702      41.28
 C      -2.964497     1.980158     1.366400      86.49
 H      -3.558639     3.042919     1.489962      24.32
 O      -3.886468     0.911783     1.722493     276.13
 H      -4.816524     1.391662     1.762794      24.32
 C      -2.650711     1.837595    -0.149372      93.29
 H      -2.054890     2.664406    -0.512560      24.74
 C      -3.953598     1.855719    -1.138898      85.06
 O      -4.635704     0.611398    -1.451090     236.89
 H      -4.495474    -0.198721    -0.795124      27.09
 H      -3.771275     2.210226    -2.102050      26.80
 H      -4.777809     2.772044    -0.781673      24.08
 C       1.752374     1.136946    -0.400858      29.19
 H       2.791167     1.873528    -0.530951      22.75
 C       1.326343    -1.266970    -0.846190      56.69
 H       1.522705    -2.247162    -0.838766      27.48
 C      -0.052926    -1.021814    -0.989490       0.87
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 O      -0.781618    -2.237707    -1.378924     137.54
 C      -2.273981    -2.194674    -1.619679      68.64
 H      -2.838033    -1.712070    -0.619992      23.77
 H      -2.556037    -1.130927    -2.472970      21.85
 H      -2.770340    -3.069341    -1.845913      25.13
 C      -0.523838     0.358763    -0.871843      -0.35
 O      -2.008134     0.621944    -0.562684     152.83
 C       0.381315     1.388201    -0.652156      59.59
 H      -0.036696     2.259082    -0.127264      24.91
 C       2.239995    -0.175603    -0.533997       6.85
 C       3.719972    -0.477686    -0.288383      73.54
 H       4.432868    -1.267808    -0.888573      23.94
 O       4.547208     0.671021    -0.552750     205.71
 H       4.430231     1.300765     0.071321      34.68
 C       3.954743    -1.200655     1.247833      82.99
 H       3.367914    -2.255985     1.141636      26.90
 O       5.282557    -1.760395     1.309064      99.76
 H       5.504464    -2.314835     0.442847      24.36
 C       3.577904    -0.378574     2.447258     115.77
 O       4.562097     0.651881     2.685698     181.46
 H       4.047340     1.512315     2.939846      28.00
 H       3.605956    -0.855856     3.453037      28.05
 H       2.566789     0.238850     2.059962      25.91
55
name = lig-Water-frame_604
 C      -1.311735     3.368249     2.569596      45.08
 H      -1.893677     4.221375     2.145986      22.65
 C      -0.906405     0.919904     2.839449      69.00
 H      -1.338982    -0.022570     2.492595      26.70
 C       0.017631     1.048212     3.817882       6.10
 O       0.599390     0.165269     4.523289     203.95
 C       0.383847    -1.283949     4.167659     106.11
 H       1.337246    -1.782183     4.413365      26.81
 H       0.211289    -1.546020     2.939969      24.89
 H      -0.525820    -1.421321     4.633068      28.17
 C       0.311245     2.625848     4.229500     -38.71
 O       1.223116     2.768049     5.242292     183.87
 H       1.404449     3.760623     5.337545      26.93
 C      -0.236549     3.701690     3.542250      17.83
 H       0.108253     4.727137     3.697417      22.76
 C      -1.702306     2.086871     2.163557      16.01
 C      -2.969796     1.972406     1.404522     104.24
 H      -3.546661     2.818310     1.445301      26.93
 O      -3.883931     0.889105     1.684201     298.34
 H      -4.665088     1.459098     1.620601      26.12
 C      -2.617904     1.873856    -0.080121      78.69
 H      -2.197980     2.909492    -0.455810      22.00
 C      -3.930586     1.930872    -1.120442      83.08
 O      -4.676912     0.614025    -1.422925     236.44
 H      -4.545959    -0.148635    -0.836114      30.19
 H      -3.737867     2.477138    -2.170032      23.79
 H      -4.517201     2.698705    -0.831710      27.64
 C       1.742704     1.150824    -0.429857      73.64
 H       2.309602     1.936601    -0.169719      30.93
 C       1.329539    -1.168008    -0.821645      41.32
 H       1.720660    -2.358040    -0.825267      24.77
 C      -0.099268    -0.992213    -1.003359       5.52
 O      -0.780625    -2.270557    -1.384065     127.88
 C      -2.307467    -2.064745    -1.610883      95.31
 H      -2.551536    -1.649542    -0.754274      28.98
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 H      -2.458839    -1.377176    -2.291670      30.06
 H      -2.495837    -3.228986    -2.002342      23.98
 C      -0.594870     0.365751    -0.832885      10.98
 O      -1.987428     0.598768    -0.529852     149.05
 C       0.389954     1.373001    -0.595998      58.14
 H      -0.079836     2.351940    -0.307952      24.70
 C       2.250666    -0.168786    -0.449858      -3.11
 C       3.756498    -0.505365    -0.300237     103.56
 H       4.126450    -1.161786    -1.019409      25.09
 O       4.565417     0.676240    -0.575717     170.84
 H       4.544096     1.121285     0.420741      28.38
 C       3.909483    -1.308484     1.133879      96.11
 H       3.169424    -2.052310     1.165287      29.15
 O       5.249376    -1.724733     1.306699     187.48
 H       5.457257    -2.486452     0.585672      24.52
 C       3.506768    -0.378173     2.436148      98.89
 O       4.614096     0.714870     2.674823     162.10
 H       4.048874     1.476868     2.951060      30.30
 H       3.438047    -0.975076     3.409633      28.14
 H       2.645230     0.089482     2.321221      29.29
55
name = lig-Water-frame_605
 C      -1.327470     3.428125     2.530375      90.15
 H      -1.961041     4.258101     2.249156      21.33
 C      -0.963451     0.844047     2.784768      43.82
 H      -1.292356    -0.193645     2.492070      22.42
 C      -0.018723     1.166606     3.825642       1.92
 O       0.618022     0.135713     4.527178     164.88
 C       0.442413    -1.269750     4.149490     106.35
 H       1.302214    -1.989573     4.276678      27.02
 H       0.186096    -1.325608     3.196010      32.30
 H      -0.599874    -1.656132     4.640915      25.52
 C       0.328273     2.577441     4.209121      17.98
 O       1.203309     2.757947     5.294576      97.06
 H       1.603332     3.706461     5.394556      32.71
 C      -0.207771     3.699746     3.567814      73.71
 H      -0.076880     4.793090     3.672170      12.81
 C      -1.657802     2.087041     2.207928       9.15
 C      -2.943531     1.929971     1.383838      93.62
 H      -3.573676     2.989655     1.505263      21.21
 O      -3.872541     0.877716     1.673515     300.78
 H      -4.899435     1.182607     1.572287      24.00
 C      -2.625892     1.920837    -0.124655      79.98
 H      -2.126368     2.822456    -0.292862      23.01
 C      -3.889438     1.973166    -1.106592      70.28
 O      -4.712540     0.655865    -1.401368     237.13
 H      -4.435363     0.022200    -0.743675      30.38
 H      -3.467387     2.294785    -2.028626      25.80
 H      -4.725461     2.734360    -0.502219      23.07
 C       1.742461     1.159069    -0.451102      46.31
 H       2.064058     2.213421     0.193413      26.33
 C       1.315877    -1.122675    -0.790344      60.00
 H       1.735231    -1.997904    -0.910002      27.87
 C      -0.131783    -0.996812    -1.033009       4.13
 O      -0.777032    -2.238503    -1.377645     156.11
 C      -2.259698    -2.008114    -1.593910      78.43
 H      -2.699039    -1.709935    -0.478281      22.31
 H      -2.442321    -1.280820    -2.768065      22.17
 H      -2.438255    -2.930426    -1.877521      26.64
 C      -0.665699     0.363017    -0.761473      17.60
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 O      -1.950692     0.576239    -0.497095     162.41
 C       0.343002     1.367418    -0.535117      36.18
 H       0.027634     2.387350    -0.548442      21.82
 C       2.253615    -0.171114    -0.400492       4.18
 C       3.768235    -0.545328    -0.288351     104.29
 H       3.678755    -1.254144    -1.305828      23.10
 O       4.580858     0.686417    -0.549879     153.51
 H       4.873034     0.936188     0.421342      27.70
 C       3.862989    -1.339363     1.030822      87.66
 H       2.881989    -2.037520     1.114623      26.79
 O       5.224021    -1.712977     1.311952     225.38
 H       5.428445    -2.439029     0.845570      30.76
 C       3.510695    -0.385566     2.410453      78.48
 O       4.630610     0.754488     2.656167     104.01
 H       4.133012     1.598499     2.857513      28.44
 H       3.367381    -1.134615     3.200527      28.38
 H       2.359271     0.121419     2.445290      24.89
55
name = lig-Water-frame_606
 C      -1.283818     3.454944     2.554980      85.92
 H      -1.971226     4.290566     2.284869      24.80
 C      -1.033996     0.872079     2.735815      60.97
 H      -1.176070    -0.158304     2.538408      22.43
 C      -0.075440     1.274799     3.805477      -5.99
 O       0.668445     0.105605     4.549998     108.65
 C       0.440750    -1.258936     4.144688     102.28
 H       1.280665    -1.899997     4.362550      26.54
 H       0.163290    -1.166407     2.942405      25.36
 H      -0.254335    -1.820710     4.673662      27.42
 C       0.351537     2.532350     4.189119      22.04
 O       1.194987     2.724199     5.352548     155.96
 H       1.471480     3.699624     5.367612      26.37
 C      -0.262611     3.664635     3.510723     130.65
 H      -0.092264     4.739287     3.914890      18.83
 C      -1.617777     2.048915     2.288281      26.03
 C      -2.940959     1.935807     1.331870     112.61
 H      -3.349782     2.831050     1.542765      23.37
 O      -3.870282     0.858053     1.686892     369.02
 H      -4.819134     1.023936     1.633063      30.01
 C      -2.659190     1.920661    -0.197989      74.35
 H      -1.802848     2.741790    -0.317511      18.33
 C      -3.880570     1.994720    -1.045599      96.47
 O      -4.724145     0.736316    -1.373411     265.35
 H      -4.237516     0.126018    -0.667611      26.71
 H      -3.435394     2.232207    -2.013079      25.50
 H      -4.607661     2.543685    -0.589849      26.82
 C       1.723923     1.215445    -0.407923      61.09
 H       2.148978     1.973907     0.142065      29.91
 C       1.257663    -1.086992    -0.771325      50.72
 H       1.759212    -2.182159    -1.122628      23.50
 C      -0.118623    -0.992691    -1.040461       8.91
 O      -0.779081    -2.145982    -1.361069     229.07
 C      -2.181470    -1.933065    -1.592046     118.41
 H      -2.852737    -1.802603    -0.823534      26.78
 H      -2.378510    -1.409352    -2.406867      28.86
 H      -2.716968    -3.066105    -1.829242      23.85
 C      -0.658706     0.337204    -0.685597      20.27
 O      -1.963703     0.574198    -0.460698     188.19
 C       0.281891     1.348660    -0.503302      49.37
 H       0.058659     2.455427    -0.683054      20.55
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 C       2.237022    -0.115917    -0.374562      15.48
 C       3.708023    -0.583909    -0.328678     105.36
 H       3.761907    -1.160495    -1.145320      28.99
 O       4.603990     0.658044    -0.495365     173.79
 H       5.057595     0.843413     0.275865      30.45
 C       3.804694    -1.290439     0.985945     107.13
 H       3.135602    -2.082362     0.962397      29.45
 O       5.184722    -1.710469     1.336327     160.76
 H       5.522333    -2.636229     0.882672      23.97
 C       3.509632    -0.362616     2.348865      89.90
 O       4.601409     0.752489     2.634455     148.22
 H       4.139278     1.692391     2.628829      28.07
 H       3.641352    -1.222002     3.112900      26.98
 H       2.621314     0.079126     2.342777      27.47
55
name = lig-Water-frame_607
 C      -1.240660     3.422431     2.603963      45.65
 H      -1.861420     4.214778     2.234312      27.19
 C      -1.037591     0.978594     2.770832      64.80
 H      -1.233284    -0.111270     2.488756      21.97
 C      -0.098166     1.243572     3.791551      -2.94
 O       0.706809     0.121171     4.569565      97.34
 C       0.430357    -1.236683     4.091470     103.19
 H       1.508597    -1.612495     4.312855      25.21
 H       0.315449    -1.375754     3.060392      29.96
 H      -0.291029    -1.866945     4.801312      24.67
 C       0.364372     2.531938     4.178338       6.09
 O       1.176044     2.684509     5.383868     213.87
 H       1.252833     3.692973     5.446099      22.62
 C      -0.308904     3.631759     3.486085      94.82
 H      -0.070543     4.491395     4.023945      20.12
 C      -1.666870     2.033805     2.291561      40.88
 C      -2.920433     1.937313     1.290460      91.36
 H      -3.455180     3.012881     1.582241      21.53
 O      -3.835856     0.824785     1.714717     301.28
 H      -4.809060     1.302387     1.706286      25.87
 C      -2.618978     1.883726    -0.213750      92.23
 H      -1.921600     2.550953    -0.542967      24.28
 C      -3.879202     1.982967    -1.042510      80.18
 O      -4.693797     0.821497    -1.315823     291.35
 H      -4.284542     0.074344    -0.851870      29.77
 H      -3.717158     2.467716    -2.118081      25.12
 H      -4.673299     2.857642    -0.621662      25.29
 C       1.672567     1.229629    -0.337063      57.49
 H       2.521335     2.096452     0.053903      24.08
 C       1.252203    -1.116851    -0.784252      70.87
 H       1.511082    -2.018062    -1.144133      27.18
 C      -0.088173    -0.939959    -0.999053      23.47
 O      -0.793021    -2.045038    -1.337243     226.16
 C      -2.143213    -1.981561    -1.592812      88.81
 H      -2.914870    -1.555456    -0.764219      22.41
 H      -2.434464    -1.013761    -2.567142      21.55
 H      -2.542770    -2.855215    -1.857440      26.19
 C      -0.619074     0.308765    -0.621210      17.36
 O      -2.025338     0.567079    -0.432587     218.37
 C       0.272237     1.370900    -0.498355      69.95
 H      -0.121321     2.337695    -0.570002      20.57
 C       2.173769    -0.052534    -0.398274      33.68
 C       3.630678    -0.540728    -0.350786      84.12
 H       4.131469    -1.301815    -1.241706      25.14
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 O       4.608591     0.598149    -0.459397     105.09
 H       5.257854     0.658493     0.451361      25.04
 C       3.798580    -1.207182     1.004116     103.96
 H       3.276140    -2.278028     0.906518      26.45
 O       5.153166    -1.728024     1.358262     128.86
 H       5.427870    -2.587207     0.861645      24.99
 C       3.578574    -0.358101     2.264532     111.71
 O       4.540166     0.728531     2.595825     194.14
 H       4.042061     1.542343     2.460922      33.08
 H       3.810110    -0.954672     3.086083      29.28
 H       2.486366     0.199337     2.254864      24.47
55
name = lig-Water-frame_608
 C      -1.289124     3.333639     2.589531     101.83
 H      -1.757545     4.226823     2.113246      24.85
 C      -0.999482     1.023276     2.854571      72.25
 H      -1.342254     0.108839     2.482458      25.18
 C      -0.032247     1.153718     3.838321      14.74
 O       0.695423     0.180356     4.549036     164.01
 C       0.479997    -1.237543     4.099330     114.72
 H       1.481060    -1.523403     4.186235      29.62
 H       0.276891    -1.547896     2.931775      27.46
 H      -0.292380    -1.639861     4.662368      29.73
 C       0.345166     2.511837     4.174148      28.88
 O       1.136041     2.657655     5.377267     303.35
 H       1.196821     3.644392     5.679693      17.13
 C      -0.255070     3.582672     3.572341      60.28
 H      -0.072343     4.692626     4.024886      19.99
 C      -1.774782     2.110505     2.218051      22.99
 C      -2.902880     1.979902     1.308593     137.91
 H      -3.499114     2.787161     1.368683      25.44
 O      -3.802587     0.823654     1.740906     306.64
 H      -4.611216     1.359895     1.784389      28.87
 C      -2.571526     1.815498    -0.207451      69.05
 H      -2.001118     2.716774    -0.758325      18.91
 C      -3.939920     2.034851    -1.091709      91.75
 O      -4.661113     0.888513    -1.257877     346.08
 H      -4.368041     0.041126    -0.966095      32.16
 H      -3.829825     2.546133    -2.027380      29.42
 H      -4.357717     2.887782    -0.602795      28.31
 C       1.650860     1.269379    -0.235268      79.04
 H       2.414627     2.000929    -0.421515      25.58
 C       1.285554    -1.118902    -0.803174      52.64
 H       1.606518    -2.224087    -1.174757      23.87
 C      -0.089243    -0.874181    -0.920965      17.77
 O      -0.797164    -1.970760    -1.310297     225.93
 C      -2.186979    -1.933725    -1.623881      87.17
 H      -2.541499    -1.472128    -0.750583      22.92
 H      -2.313946    -1.208011    -2.397812      26.18
 H      -2.390688    -3.098158    -2.074570      22.38
 C      -0.619897     0.335999    -0.562221      16.20
 O      -2.071552     0.525244    -0.421661     274.47
 C       0.287408     1.425936    -0.484953      64.02
 H      -0.329974     2.364926    -0.306329      16.76
 C       2.107099    -0.065306    -0.479759      27.74
 C       3.618314    -0.480864    -0.374972     109.75
 H       3.947795    -1.164496    -1.006677      33.36
 O       4.622856     0.545276    -0.412880     203.21
 H       5.068977     0.329069     0.402990      33.52
 C       3.823747    -1.189670     1.037494     107.13
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 H       3.155122    -1.991522     1.072818      32.37
 O       5.145993    -1.743825     1.366556     166.31
 H       5.257964    -2.429193     0.784522      30.93
 C       3.608199    -0.324609     2.200071     144.17
 O       4.484868     0.704780     2.528026     202.22
 H       3.933221     1.585880     2.436940      28.10
 H       3.658557    -0.917535     3.216796      29.72
 H       2.591698     0.000660     2.244729      29.53
55
name = lig-Water-frame_609
 C      -1.337499     3.328030     2.574657     131.45
 H      -1.634400     4.239497     2.077105      11.00
 C      -1.006704     1.046648     2.909820      60.20
 H      -1.381811     0.026581     2.555920      21.70
 C       0.047149     1.110007     3.882385      38.59
 O       0.667443     0.224405     4.501719     248.54
 C       0.553058    -1.225722     4.079241     102.25
 H       1.536265    -1.828028     4.295204      26.59
 H       0.143841    -1.340845     3.069291      28.05
 H      -0.344713    -1.606012     4.712318      26.83
 C       0.331485     2.473599     4.226085      34.32
 O       1.094386     2.634452     5.368531     129.45
 H       1.212326     3.538597     5.657646      30.62
 C      -0.221653     3.570291     3.649759      -4.28
 H      -0.104981     4.543641     3.815196      29.54
 C      -1.800791     2.160282     2.203881      46.67
 C      -2.907425     1.982895     1.301221     152.50
 H      -3.664228     2.926444     1.225128      26.21
 O      -3.748178     0.845754     1.767013     311.53
 H      -4.716464     1.155533     1.858787      30.40
 C      -2.567810     1.798669    -0.241005     106.62
 H      -2.024351     2.629582    -0.575857      23.02
 C      -3.934044     2.095163    -1.106752      63.58
 O      -4.685704     0.931234    -1.227772     280.34
 H      -4.230089     0.058761    -0.818118      27.04
 H      -3.659841     2.512500    -2.184855      26.21
 H      -4.455640     2.936840    -0.322856      24.09
 C       1.632830     1.270468    -0.193250      61.97
 H       2.328779     2.185138    -0.584333      22.58
 C       1.307404    -1.140496    -0.843999      56.54
 H       1.756662    -2.112575    -1.034295      25.91
 C      -0.109439    -0.856887    -0.843326      11.80
 O      -0.775263    -1.929282    -1.287587     185.26
 C      -2.221034    -1.917524    -1.650272      82.48
 H      -2.701982    -1.652826    -0.663059      22.55
 H      -2.335023    -1.133309    -2.734090      21.82
 H      -2.311223    -2.924462    -1.962697      25.62
 C      -0.649373     0.423296    -0.507543      12.89
 O      -2.069689     0.463071    -0.428835     260.99
 C       0.254504     1.509856    -0.429719      57.13
 H      -0.181158     2.429355    -0.075960      16.95
 C       2.113715    -0.085467    -0.560065      14.37
 C       3.607961    -0.426086    -0.338874      78.08
 H       3.674823    -1.372850    -1.257433      26.89
 O       4.639553     0.511767    -0.378124     161.30
 H       5.120669     0.267112     0.432913      30.44
 C       3.840336    -1.188297     1.067499      91.39
 H       2.846573    -1.848399     1.258278      29.47
 O       5.152229    -1.756210     1.354392     107.54
 H       5.241142    -2.474507     0.518913      23.69
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 C       3.577389    -0.322322     2.239563     136.59
 O       4.453738     0.732251     2.440747     208.13
 H       4.022182     1.628884     2.581133      25.24
 H       3.440976    -1.032830     3.010704      31.64
 H       2.434516     0.000599     2.143162      27.71
55
name = lig-Water-frame_610
 C      -1.297775     3.442787     2.619156      31.40
 H      -1.646542     4.340056     2.080474      13.55
 C      -1.062245     1.032508     2.926852      60.90
 H      -1.281104     0.007473     2.750984      24.14
 C       0.013038     1.189281     3.818776       5.07
 O       0.704187     0.168726     4.493739     208.90
 C       0.592232    -1.214017     4.095100     121.56
 H       1.361579    -1.876233     4.370091      27.25
 H       0.194560    -1.149415     3.016171      25.58
 H      -0.164743    -1.633599     4.735488      26.22
 C       0.320922     2.455791     4.307518      36.09
 O       1.084070     2.599801     5.394266     145.61
 H       1.245886     3.631908     5.448314      32.10
 C      -0.286335     3.533360     3.621362      34.71
 H       0.058463     4.697935     3.838308      27.81
 C      -1.742565     2.118062     2.268322      26.82
 C      -2.987564     1.982560     1.246227     143.45
 H      -3.451479     2.909887     1.329069      29.98
 O      -3.698278     0.868002     1.800141     317.09
 H      -4.730824     0.943492     1.792829      29.33
 C      -2.629446     1.806495    -0.260330     109.70
 H      -1.746573     2.561682    -0.431586      23.59
 C      -3.872499     2.162435    -1.078413     109.72
 O      -4.739729     0.933918    -1.213387     314.63
 H      -4.172995     0.401441    -0.662405      32.35
 H      -3.656018     2.472982    -1.995446      31.36
 H      -4.557499     2.756046    -0.524197      29.16
 C       1.628841     1.248255    -0.241305      50.81
 H       2.172094     2.251961    -0.301498      21.28
 C       1.286088    -1.127309    -0.871492      59.01
 H       1.772885    -2.143479    -1.026127      25.35
 C      -0.101016    -0.848100    -0.778563      17.11
 O      -0.779628    -1.918757    -1.271856     192.35
 C      -2.217400    -1.863344    -1.679679     102.58
 H      -3.107676    -1.900777    -0.945136      25.50
 H      -2.448423    -1.268420    -2.541663      27.20
 H      -2.430470    -3.062278    -1.961449      25.39
 C      -0.673792     0.487594    -0.473902      16.85
 O      -2.040869     0.424246    -0.447625     227.08
 C       0.210466     1.582976    -0.320909      54.22
 H       0.030247     2.612598     0.014319      19.64
 C       2.182500    -0.027061    -0.588821      24.42
 C       3.595806    -0.483331    -0.316505     107.66
 H       3.649609    -1.094734    -1.074394      31.86
 O       4.661059     0.498054    -0.366190     160.08
 H       5.386922     0.453833     0.464004      22.47
 C       3.785949    -1.193577     1.092810      96.42
 H       2.996455    -1.901782     1.198085      31.05
 O       5.145594    -1.787259     1.291595     162.64
 H       5.417358    -2.398800     0.572249      26.14
 C       3.465471    -0.313497     2.302567     121.24
 O       4.454966     0.781684     2.367309     155.40
 H       3.995761     1.642817     2.694651      24.47
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 H       3.436905    -1.128768     3.146840      27.96
 H       2.498039     0.148773     1.962527      27.57
55
name = lig-Water-frame_611
 C      -1.246353     3.525337     2.660199      39.60
 H      -1.693648     4.389536     2.166997      20.14
 C      -1.127277     1.007852     2.925066      67.97
 H      -1.331528    -0.072765     2.768538      24.07
 C      -0.037748     1.252342     3.766363     -35.99
 O       0.768901     0.114836     4.502448     122.30
 C       0.569259    -1.198445     4.111451     115.82
 H       1.558486    -1.770293     4.302137      25.74
 H       0.464945    -1.290781     2.924730      26.98
 H      -0.255940    -1.721269     4.703539      24.80
 C       0.261334     2.462239     4.327419      25.39
 O       1.113640     2.602735     5.453542     119.02
 H       1.366248     3.554678     5.357969      31.10
 C      -0.339539     3.566606     3.594134      37.24
 H       0.122242     4.386057     3.938696      30.69
 C      -1.681275     2.091873     2.328863       6.72
 C      -3.011543     1.967158     1.240241     120.46
 H      -3.471253     3.037236     1.469510      25.19
 O      -3.677657     0.866462     1.835357     334.71
 H      -4.600099     1.051340     1.653798      29.57
 C      -2.667552     1.836735    -0.239902      92.70
 H      -1.751660     2.398328    -0.392306      24.94
 C      -3.835091     2.172659    -1.053123      86.37
 O      -4.779085     0.937502    -1.203348     255.56
 H      -4.352888     0.355283    -0.554284      30.46
 H      -3.630748     2.655646    -2.153404      25.55
 H      -4.584836     3.004964    -0.607145      25.46
 C       1.604899     1.249048    -0.322062      59.87
 H       2.292807     2.163524     0.039703      28.11
 C       1.278503    -1.051302    -0.867831      43.65
 H       1.558590    -2.165412    -1.128994      23.57
 C      -0.071613    -0.819707    -0.742363      14.44
 O      -0.841758    -1.921433    -1.251093     178.78
 C      -2.225632    -1.911815    -1.685855     100.74
 H      -3.121964    -1.800249    -1.090669      26.86
 H      -2.582436    -1.058983    -2.646857      23.61
 H      -2.341305    -2.907377    -2.143762      27.31
 C      -0.662956     0.503797    -0.457959       5.10
 O      -2.033243     0.431320    -0.469733     156.60
 C       0.207888     1.605358    -0.192738      62.88
 H       0.091429     2.693657     0.036279      22.54
 C       2.226173     0.044676    -0.575385      -2.65
 C       3.619076    -0.526197    -0.243587      76.29
 H       3.984426    -1.318044    -1.222969      22.55
 O       4.694047     0.505281    -0.378249     230.63
 H       5.278313     0.531099     0.327496      29.54
 C       3.723402    -1.216614     1.101090      94.45
 H       3.101792    -2.240141     1.059852      26.03
 O       5.127202    -1.802525     1.231266     160.94
 H       5.458292    -2.369942     0.570523      27.13
 C       3.381202    -0.300824     2.335806     111.79
 O       4.457284     0.812745     2.322108     169.11
 H       3.927033     1.634917     2.633360      27.35
 H       3.443444    -0.741597     3.309738      29.47
 H       2.427814     0.231462     2.073256      28.39
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name = lig-Water-frame_612
 C      -1.268216     3.502495     2.630446      32.22
 H      -1.721158     4.413125     2.236459      22.74
 C      -1.164139     0.962713     2.925754      45.18
 H      -1.485889    -0.044100     2.593638      21.83
 C      -0.042698     1.211383     3.803142     -31.45
 O       0.811644     0.129987     4.497664     107.19
 C       0.565487    -1.236697     4.107835     120.56
 H       1.556647    -1.574954     4.279808      26.58
 H       0.538565    -1.483554     2.987634      27.61
 H      -0.330104    -1.763568     4.485993      25.05
 C       0.183752     2.482443     4.306681       7.22
 O       1.147303     2.627311     5.488283      74.49
 H       1.547718     3.539096     5.525690      29.64
 C      -0.296510     3.615062     3.671850      45.98
 H       0.163912     4.631112     4.103094      21.28
 C      -1.685605     2.154526     2.320125       7.86
 C      -2.946450     1.982649     1.332354     126.51
 H      -3.592648     2.852146     1.453212      24.31
 O      -3.690553     0.855352     1.859228     302.01
 H      -4.667141     1.155941     1.639740      25.72
 C      -2.655986     1.844516    -0.181100      84.15
 H      -1.904822     2.616224    -0.498744      21.99
 C      -3.882683     2.180376    -1.091702      88.07
 O      -4.790660     0.965234    -1.192713     222.98
 H      -4.715984     0.128406    -0.544882      26.39
 H      -3.623811     2.500885    -2.024853      28.77
 H      -4.251931     3.145368    -0.627650      26.15
 C       1.615301     1.328728    -0.372357      61.12
 H       2.384286     1.791476     0.359812      28.08
 C       1.293120    -0.961067    -0.852819      50.24
 H       1.458667    -1.947735    -1.203318      23.94
 C      -0.086258    -0.779674    -0.749953       6.83
 O      -0.914193    -1.915511    -1.209033     170.18
 C      -2.253784    -1.935053    -1.748164      85.23
 H      -2.936630    -1.626186    -0.844719      22.34
 H      -2.367839    -1.132416    -2.512943      24.93
 H      -2.246853    -2.978915    -2.390113      23.50
 C      -0.635685     0.494625    -0.444749       5.30
 O      -2.051485     0.480789    -0.487388     176.85
 C       0.246138     1.571664    -0.097100      46.93
 H      -0.068540     2.546590     0.130887      22.46
 C       2.228521     0.034375    -0.560294     -31.64
 C       3.699229    -0.542856    -0.236244      95.82
 H       3.973816    -1.289966    -0.797831      31.07
 O       4.699488     0.514195    -0.421062     231.91
 H       5.229958     0.524223     0.434169      25.33
 C       3.674226    -1.300845     1.116529     101.54
 H       3.132194    -2.247751     0.996133      27.04
 O       5.102324    -1.783916     1.208383      98.29
 H       5.323836    -2.446557     0.339362      24.72
 C       3.358361    -0.263149     2.324886      98.06
 O       4.439888     0.810294     2.294600     206.95
 H       3.971018     1.719948     2.420076      27.35
 H       3.373137    -0.500736     3.423085      26.78
 H       2.257543     0.207462     2.330971      26.45
55
name = lig-Water-frame_613
 C      -1.282882     3.446756     2.620519      59.36
 H      -1.754574     4.358985     2.226980      21.90
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 C      -1.158084     0.957768     2.930202      33.90
 H      -1.538554     0.069509     2.447704      19.19
 C      -0.047314     1.081930     3.884924     -11.13
 O       0.805383     0.192219     4.462117     149.59
 C       0.585876    -1.283075     4.079758      95.88
 H       1.519129    -1.770668     4.541167      25.01
 H       0.491474    -1.480657     2.899881      24.90
 H      -0.328071    -1.742479     4.495793      25.72
 C       0.174581     2.523250     4.325345     -10.30
 O       1.164040     2.645978     5.486391      61.57
 H       1.564206     3.588871     5.596160      29.74
 C      -0.241557     3.700880     3.762008      35.67
 H      -0.119155     4.706647     4.062946      20.92
 C      -1.732857     2.225488     2.287411      23.52
 C      -2.860003     1.994892     1.451275     136.61
 H      -3.636329     2.842941     1.457722      22.49
 O      -3.732748     0.842814     1.870247     281.19
 H      -4.689107     1.102672     1.843700      28.91
 C      -2.618996     1.851218    -0.139254      78.25
 H      -2.164597     2.829172    -0.545214      19.81
 C      -3.920499     2.125121    -1.078621      67.76
 O      -4.817475     1.009141    -1.195771     290.33
 H      -4.793450     0.297791    -0.573512      30.66
 H      -3.564596     2.232527    -2.203152      24.11
 H      -4.285563     3.125015    -0.565956      24.34
 C       1.700819     1.387186    -0.333263      59.56
 H       2.373884     1.923543     0.353841      28.30
 C       1.281207    -0.905227    -0.847726      49.54
 H       1.654855    -1.972784    -1.332251      21.92
 C      -0.153738    -0.753088    -0.804497      10.54
 O      -0.934063    -1.902338    -1.141670     191.12
 C      -2.276777    -1.941584    -1.792136      77.33
 H      -2.829038    -1.817689    -0.958985      25.01
 H      -2.151803    -0.952895    -2.586725      21.58
 H      -2.348823    -2.944072    -2.346302      23.78
 C      -0.630558     0.482708    -0.428158      14.16
 O      -2.066836     0.575744    -0.494314     194.51
 C       0.289642     1.497581    -0.056234      33.73
 H      -0.260435     2.413608     0.377460      17.56
 C       2.217232     0.002001    -0.553035     -19.09
 C       3.728415    -0.494302    -0.234162      73.64
 H       3.912489    -1.580981    -0.951948      25.91
 O       4.699223     0.508610    -0.463314     167.56
 H       5.147441     0.594354     0.544379      22.47
 C       3.669962    -1.341285     1.154942      93.61
 H       2.879755    -2.156682     1.079706      27.42
 O       5.080342    -1.770219     1.193167     155.47
 H       5.039989    -2.327548     0.431960      31.73
 C       3.356451    -0.217356     2.325679     103.72
 O       4.406479     0.786631     2.264614     226.49
 H       4.008564     1.728336     2.251985      28.18
 H       3.396450    -0.717648     3.313559      27.38
 H       2.356404     0.136088     2.252638      28.20
55
name = lig-Water-frame_614
 C      -1.246218     3.460433     2.679900      59.31
 H      -1.769304     4.283667     2.190850      21.38
 C      -1.114110     1.004810     2.944267      54.08
 H      -1.457219     0.063882     2.409971      22.44
 C      -0.109079     1.028469     3.936268      -9.17
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 O       0.783866     0.214779     4.416367     158.25
 C       0.626710    -1.318717     4.055820      97.08
 H       1.275768    -1.939032     4.675819      27.01
 H       0.560478    -1.366048     2.988659      29.45
 H      -0.345950    -1.556519     4.607494      26.10
 C       0.242410     2.551387     4.394303     -46.85
 O       1.167891     2.656816     5.459896     173.50
 H       1.355090     3.615663     5.461256      28.83
 C      -0.275815     3.735805     3.762666      64.53
 H      -0.252627     4.806406     4.141969      17.91
 C      -1.727967     2.207583     2.332716      32.00
 C      -2.889541     2.000456     1.485659     108.96
 H      -3.475666     2.977515     1.531413      23.22
 O      -3.761201     0.822798     1.887070     288.52
 H      -4.691784     1.154525     1.982227      28.85
 C      -2.625967     1.891265    -0.115824      86.29
 H      -2.065684     2.776704    -0.419971      22.22
 C      -3.912941     2.041567    -1.032322      91.94
 O      -4.875117     1.052549    -1.213192     327.80
 H      -4.663774     0.490589    -0.424281      29.11
 H      -3.545018     2.121493    -2.053670      26.01
 H      -4.564619     2.949152    -0.741254      23.90
 C       1.789309     1.378820    -0.221975      43.97
 H       2.363415     2.433797     0.118394      29.33
 C       1.230740    -0.953108    -0.891729      57.44
 H       1.687051    -1.786385    -1.203165      26.91
 C      -0.207691    -0.772058    -0.890899      21.61
 O      -0.914196    -1.896177    -1.063492     202.83
 C      -2.241349    -1.889431    -1.844369      84.06
 H      -3.235069    -1.968546    -1.076384      22.51
 H      -2.311676    -1.090709    -2.518881      26.51
 H      -2.422413    -2.966368    -2.317071      23.83
 C      -0.656693     0.480798    -0.418614      12.40
 O      -2.051536     0.690703    -0.492986     185.14
 C       0.324724     1.442888    -0.045162      40.86
 H      -0.085865     2.207112     0.541623      21.11
 C       2.239051     0.041041    -0.532749     -50.84
 C       3.669189    -0.513163    -0.284638     110.48
 H       3.793475    -1.166381    -1.013072      29.33
 O       4.704634     0.489773    -0.478111     242.73
 H       4.996268     0.710299     0.320903      33.75
 C       3.688831    -1.272126     1.191707      98.56
 H       2.722912    -1.926975     1.243402      28.56
 O       5.039752    -1.769790     1.204605     173.48
 H       5.011079    -2.398427     0.439453      28.24
 C       3.396283    -0.240718     2.322469     105.68
 O       4.378343     0.760427     2.229922     240.37
 H       3.893443     1.632199     2.329175      29.28
 H       3.479231    -0.928617     3.183080      28.74
 H       2.303236     0.222175     1.977155      26.62
55
name = lig-Water-frame_615
 C      -1.214920     3.499233     2.757163      58.38
 H      -1.716237     4.322719     2.236251      25.20
 C      -1.074384     1.038685     2.945064      68.88
 H      -1.263616     0.071955     2.572913      27.64
 C      -0.180032     1.140135     3.965408     -14.76
 O       0.790851     0.164351     4.386956     145.34
 C       0.614468    -1.305368     4.098671     102.12
 H       1.348252    -1.933850     4.610081      28.29
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 H       0.717964    -1.421440     2.843604      28.79
 H      -0.385825    -1.423061     4.424683      28.13
 C       0.287392     2.547779     4.432056     -28.70
 O       1.170165     2.674800     5.421051     205.03
 H       1.272105     3.704322     5.467712      23.71
 C      -0.342050     3.705892     3.743057      83.96
 H      -0.173390     4.705296     4.235768      21.02
 C      -1.668709     2.146590     2.443231      48.72
 C      -2.981318     2.008063     1.456576      93.98
 H      -3.457681     3.012278     1.622068      24.46
 O      -3.771262     0.816825     1.903965     289.20
 H      -4.717571     1.233803     2.008138      26.82
 C      -2.680223     1.958043    -0.071004      78.92
 H      -1.836475     2.737585    -0.260076      22.39
 C      -3.894160     2.022345    -1.002181      98.84
 O      -4.944429     1.037205    -1.204997     289.85
 H      -4.749695     0.486281    -0.324126      27.81
 H      -3.380770     2.270553    -1.989707      26.03
 H      -4.539263     2.929039    -0.839748      24.76
 C       1.818879     1.362024    -0.093316      66.51
 H       2.285236     2.299462    -0.149374      22.95
 C       1.187404    -0.957262    -0.930221      33.84
 H       1.690750    -2.078654    -1.164964      25.36
 C      -0.193335    -0.785666    -0.962652      15.88
 O      -0.939904    -1.917773    -1.010628     208.59
 C      -2.229496    -1.880302    -1.826805      89.50
 H      -3.145714    -1.860309    -1.414267      28.19
 H      -2.519496    -0.977014    -2.690325      24.29
 H      -2.181180    -2.932587    -2.402008      24.56
 C      -0.671510     0.493216    -0.426593      10.57
 O      -2.006559     0.771969    -0.490564     160.99
 C       0.372301     1.407903    -0.046661      53.33
 H       0.134491     2.287182     0.640897      25.93
 C       2.240114     0.100203    -0.510828      -0.65
 C       3.560300    -0.507816    -0.311261      80.90
 H       3.817178    -1.185594    -1.362375      24.54
 O       4.703627     0.458969    -0.516328     112.50
 H       4.907806     0.924848     0.442652      26.42
 C       3.693206    -1.144432     1.166690     112.73
 H       2.903478    -1.908618     1.292255      31.64
 O       4.989656    -1.788834     1.231831      92.75
 H       5.165409    -2.579479     0.486299      23.78
 C       3.425048    -0.307220     2.270933     137.80
 O       4.365538     0.761640     2.210782     161.27
 H       3.839218     1.592480     2.525079      27.38
 H       3.448516    -0.868268     3.263581      30.72
 H       2.533161     0.098735     2.073405      33.10
55
name = lig-Water-frame_616
 C      -1.259361     3.490802     2.782750      75.45
 H      -1.658548     4.407877     2.339615      27.38
 C      -1.037770     1.028548     2.959704      39.96
 H      -1.176607    -0.057762     2.662478      26.16
 C      -0.134916     1.302996     4.038746       9.95
 O       0.803358     0.112842     4.369788     128.60
 C       0.578138    -1.246550     4.101443     123.66
 H       1.451957    -1.772836     4.570898      28.65
 H       0.774429    -1.546728     3.107105      34.26
 H      -0.528972    -1.629476     4.202597      27.56
 C       0.240145     2.511249     4.385402      32.60
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 O       1.193372     2.719464     5.398724     216.14
 H       1.403637     3.670679     5.631211      21.98
 C      -0.335753     3.640025     3.813234      49.43
 H      -0.028716     4.588350     4.170350      13.24
 C      -1.670001     2.153430     2.491533      39.63
 C      -3.026550     2.007771     1.456658      84.46
 H      -3.662846     2.955702     1.737723      24.25
 O      -3.782547     0.841695     1.915970     296.04
 H      -4.715077     1.088338     1.915931      29.85
 C      -2.708901     2.018123    -0.000698      78.31
 H      -2.049608     2.828293    -0.160574      23.96
 C      -3.885810     2.081408    -1.020810      71.99
 O      -4.984108     0.988673    -1.163785     271.56
 H      -5.057577     0.358062    -0.483684      32.29
 H      -3.318658     2.282188    -2.007006      25.64
 H      -4.366354     3.154457    -0.746951      24.29
 C       1.772089     1.292467    -0.000801      68.80
 H       2.523945     2.281731    -0.222383      20.50
 C       1.225422    -0.953359    -0.956050      51.67
 H       1.399841    -1.913814    -1.088963      29.26
 C      -0.159655    -0.768370    -0.986813       0.33
 O      -1.014620    -1.939731    -0.986074     197.32
 C      -2.201328    -1.878075    -1.867412      83.67
 H      -3.217710    -1.781602    -1.178586      23.83
 H      -2.206052    -1.103178    -2.556196      28.40
 H      -1.992373    -2.836611    -2.484428      23.71
 C      -0.625594     0.527178    -0.447466       5.64
 O      -1.963794     0.804269    -0.485725     140.60
 C       0.391488     1.430525    -0.019964      61.06
 H       0.131878     2.370790     0.450720      26.49
 C       2.179864     0.092609    -0.516720      24.18
 C       3.516445    -0.493247    -0.370167     110.95
 H       3.681591    -1.217378    -1.012756      31.21
 O       4.703039     0.431308    -0.543782     136.89
 H       4.590574     1.006960     0.315293      27.14
 C       3.696012    -1.119253     1.033228     108.58
 H       3.040787    -2.083532     1.165276      31.17
 O       4.969438    -1.821456     1.263338     119.83
 H       5.061715    -2.494799     0.664836      30.69
 C       3.470595    -0.343033     2.262048     134.30
 O       4.369167     0.800319     2.219104     109.93
 H       3.936529     1.614825     2.561342      26.74
 H       3.458330    -0.772212     3.234188      33.91
 H       2.273444     0.078834     2.277501      31.01
55
name = lig-Water-frame_617
 C      -1.320517     3.465348     2.816334      94.09
 H      -1.704010     4.396002     2.399446      34.69
 C      -0.993984     1.017288     3.020452      34.36
 H      -1.188446     0.022177     2.707691      26.45
 C      -0.053862     1.264736     4.048856      22.03
 O       0.808218     0.131162     4.375144     130.23
 C       0.514927    -1.211196     4.087475     127.93
 H       1.260932    -1.653581     4.766683      28.81
 H       0.882161    -1.627757     2.958311      30.54
 H      -0.354117    -1.784315     4.265837      29.95
 C       0.238991     2.563191     4.405163      41.65
 O       1.230623     2.748313     5.391155     222.99
 H       1.460764     3.728895     5.566264      27.34
 C      -0.333694     3.597436     3.870026      55.43
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 H       0.173323     4.635758     4.067627      12.16
 C      -1.757797     2.185884     2.451366      19.23
 C      -3.045808     2.007425     1.539613     106.70
 H      -3.727359     2.834291     1.702908      25.52
 O      -3.784233     0.863072     1.926523     269.15
 H      -4.803677     0.973022     1.731476      27.04
 C      -2.723269     2.035761     0.038566      65.91
 H      -2.306444     3.133700    -0.176170      21.52
 C      -3.891771     2.162198    -1.026481      72.23
 O      -4.994080     0.972226    -1.139728     229.56
 H      -5.078678     0.236101    -0.449861      28.96
 H      -3.515984     2.094481    -2.035217      26.24
 H      -4.335855     3.090018    -0.747657      26.39
 C       1.738097     1.243547     0.026267      63.25
 H       2.447882     1.930977     0.167000      24.26
 C       1.246872    -0.912414    -0.965446      43.46
 H       1.473261    -2.108799    -1.141532      25.53
 C      -0.159749    -0.735375    -0.954104      -3.06
 O      -1.066841    -1.923839    -0.966380     163.90
 C      -2.188482    -1.893823    -1.884867      79.94
 H      -2.956441    -1.876516    -1.216633      26.46
 H      -1.779702    -0.900573    -2.541747      22.53
 H      -2.109676    -2.888548    -2.608859      23.32
 C      -0.548215     0.565760    -0.478060       5.96
 O      -1.933235     0.817657    -0.472570     124.77
 C       0.360628     1.511936     0.018148      58.79
 H      -0.087007     2.500209     0.222742      23.45
 C       2.108189     0.001673    -0.550895      33.53
 C       3.546530    -0.458095    -0.394828      96.11
 H       3.631777    -1.565530    -1.041518      24.00
 O       4.673954     0.412062    -0.573295     191.97
 H       4.503496     0.998478     0.129368      32.64
 C       3.684966    -1.206563     0.920980      97.74
 H       2.946181    -1.963315     0.887142      33.74
 O       4.977617    -1.835135     1.291151      99.31
 H       4.969407    -2.609127     0.621578      27.55
 C       3.442404    -0.298520     2.269697     120.86
 O       4.389544     0.848597     2.238105     115.42
 H       3.884300     1.707658     2.475625      25.72
 H       3.707232    -0.996559     3.195795      31.24
 H       2.510210    -0.050077     2.349057      32.27
55
name = lig-Water-frame_618
 C      -1.374577     3.444262     2.876250      15.33
 H      -1.839802     4.337034     2.421960      24.37
 C      -0.997979     1.068952     3.077080      57.56
 H      -1.249079     0.046401     2.699285      23.44
 C       0.012611     1.111649     3.985968      28.65
 O       0.803727     0.201716     4.403909     208.14
 C       0.509998    -1.237672     4.047179     121.61
 H       1.049317    -1.711566     4.917579      27.08
 H       0.814940    -1.414794     3.109241      30.42
 H      -0.531599    -1.657897     4.434718      25.58
 C       0.319999     2.590126     4.512429     -35.51
 O       1.280604     2.766825     5.395520     255.78
 H       1.446056     3.790432     5.402515      29.68
 C      -0.372940     3.658460     3.838832       8.60
 H       0.101977     4.551157     3.969300      24.85
 C      -1.841394     2.178143     2.426669      32.24
 C      -3.048867     2.006256     1.630468      92.41
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 H      -3.746828     2.992475     1.656740      24.31
 O      -3.796444     0.850193     1.947667     296.14
 H      -4.706919     1.021758     1.571656      26.77
 C      -2.728127     2.054713     0.015345      78.04
 H      -2.351481     3.012047    -0.149789      23.02
 C      -3.907499     2.164281    -0.993258      73.86
 O      -4.993873     0.980718    -1.122036     233.81
 H      -4.729721     0.344462    -0.336621      25.53
 H      -3.663525     1.973228    -2.137187      22.76
 H      -4.648055     3.153894    -0.832403      23.98
 C       1.679461     1.186955     0.009896      49.93
 H       2.501110     1.796059     0.815220      26.62
 C       1.178845    -0.987227    -1.000643      60.98
 H       1.683330    -1.854634    -1.262071      28.43
 C      -0.183628    -0.719375    -0.885956      25.28
 O      -1.056924    -1.877520    -0.928768     217.85
 C      -2.109754    -1.877601    -1.948078      96.72
 H      -3.206450    -1.865033    -1.332751      23.60
 H      -2.038946    -1.036704    -2.473215      28.77
 H      -2.268686    -2.836430    -2.586681      24.61
 C      -0.524513     0.606303    -0.504715       5.94
 O      -1.912787     0.839236    -0.452261     167.94
 C       0.326030     1.613145     0.036864      67.34
 H      -0.193847     2.595858     0.130506      19.72
 C       2.120898    -0.048050    -0.557055     -23.28
 C       3.609853    -0.521223    -0.434392     106.41
 H       3.716821    -1.183891    -1.183414      29.35
 O       4.630971     0.396800    -0.626786     143.76
 H       4.627818     1.180579     0.164983      26.68
 C       3.668111    -1.266658     0.924467      85.87
 H       2.688134    -1.937713     0.738857      28.98
 O       4.981366    -1.852676     1.273116      49.04
 H       5.086623    -2.779491     0.695001      20.02
 C       3.472278    -0.294469     2.260981      92.91
 O       4.400356     0.898180     2.262111      54.74
 H       3.776492     1.702312     2.321389      28.51
 H       3.894444    -0.998272     2.894048      33.99
 H       2.280735     0.081012     2.441493      25.32
55
name = lig-Water-frame_619
 C      -1.456652     3.430579     2.914272      29.10
 H      -1.965385     4.289590     2.491607      20.40
 C      -1.084150     1.102586     3.065546      64.75
 H      -1.317226     0.103455     2.694669      18.47
 C       0.042736     1.148285     3.927104      17.02
 O       0.833082     0.201660     4.460377     176.06
 C       0.484448    -1.264388     4.109940      99.76
 H       1.084476    -1.886545     4.762590      26.28
 H       0.804769    -1.377057     2.881314      24.04
 H      -0.579215    -1.189134     4.205913      25.20
 C       0.333012     2.543187     4.528629     -44.11
 O       1.355846     2.789474     5.417154     203.98
 H       1.579700     3.790522     5.553772      26.93
 C      -0.381122     3.675287     3.811976      56.10
 H      -0.048492     4.810033     3.944129      28.09
 C      -1.834151     2.157358     2.506389      43.29
 C      -3.074019     2.029507     1.642565      98.08
 H      -3.590373     2.946600     1.766445      26.17
 O      -3.812195     0.821253     1.972944     312.14
 H      -4.729364     1.039287     1.656739      28.50
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 C      -2.735528     2.043846    -0.019293      69.76
 H      -2.021387     2.983194    -0.164033      20.25
 C      -3.984683     2.121768    -0.998267     106.83
 O      -4.966430     0.995299    -1.068367     343.02
 H      -4.529038     0.486528    -0.440916      30.31
 H      -3.538896     2.220707    -1.943965      28.39
 H      -4.543679     2.917014    -0.947401      27.49
 C       1.666822     1.167787     0.042673      61.74
 H       2.141217     1.490310     0.795967      28.72
 C       1.128298    -1.048923    -1.035999      32.01
 H       1.657945    -1.976791    -1.520974      24.00
 C      -0.212191    -0.737041    -0.817603      21.20
 O      -1.035151    -1.816180    -0.895418     240.90
 C      -2.085448    -1.857538    -1.957176      98.54
 H      -3.101627    -1.770838    -1.686520      25.99
 H      -2.343064    -0.905347    -2.740511      22.91
 H      -2.142465    -2.924852    -2.592000      23.65
 C      -0.575370     0.677202    -0.503224      -2.37
 O      -1.918338     0.864675    -0.435196     203.45
 C       0.308935     1.663209    -0.002452      72.62
 H      -0.016329     2.624730     0.329589      19.94
 C       2.148941    -0.051380    -0.539129      -8.47
 C       3.634801    -0.587574    -0.446951      90.64
 H       3.884518    -1.130825    -1.590889      23.12
 O       4.613069     0.427711    -0.677992     158.80
 H       4.755910     1.029164     0.040204      33.29
 C       3.627717    -1.280997     0.959394     103.37
 H       2.877045    -1.982532     1.002866      30.03
 O       4.978057    -1.895274     1.223315     112.44
 H       5.178795    -2.689318     0.907434      24.57
 C       3.495072    -0.290503     2.202002     123.57
 O       4.389726     0.933185     2.279899      89.43
 H       3.779074     1.721768     2.282893      29.26
 H       3.972041    -0.989017     3.026937      29.90
 H       2.598796     0.014962     2.516471      24.13
55
name = lig-Water-frame_620
 C      -1.517638     3.447479     2.961723      62.91
 H      -2.085138     4.309158     2.568317      18.59
 C      -1.156126     1.070109     3.043587      54.17
 H      -1.426650     0.097965     2.668239      13.96
 C       0.048031     1.315938     3.905256       5.67
 O       0.885382     0.146053     4.522931     142.94
 C       0.464715    -1.227091     4.127463     111.05
 H       1.046138    -2.064410     4.610482      24.23
 H       0.660806    -1.442866     3.184917      29.43
 H      -0.653633    -1.097971     4.018079      22.80
 C       0.302071     2.530072     4.449511      -9.99
 O       1.429735     2.781549     5.436452     122.31
 H       1.636407     3.805221     5.728198      28.06
 C      -0.357259     3.657796     3.811953      61.04
 H      -0.279101     4.666868     4.048802      28.51
 C      -1.822604     2.144080     2.611918      27.34
 C      -3.069045     2.019437     1.597326      89.87
 H      -3.683858     3.018301     1.929739      23.75
 O      -3.829177     0.801655     1.991710     301.31
 H      -4.887566     0.948573     1.964224      26.07
 C      -2.719820     2.045226    -0.021080      85.17
 H      -2.042205     2.801331    -0.214192      23.32
 C      -4.026679     2.059972    -1.029061      74.75
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 O      -4.915753     1.014158    -1.002158     284.97
 H      -4.472635     0.244102    -0.458547      25.40
 H      -3.315683     2.413756    -1.940165      23.37
 H      -4.627906     3.182900    -0.820972      24.17
 C       1.645517     1.126614     0.055390      52.26
 H       2.297350     1.663682     1.011715      18.03
 C       1.161921    -1.046703    -1.051771      42.98
 H       1.168209    -2.010815    -1.657783      22.33
 C      -0.203891    -0.719876    -0.767913       3.36
 O      -1.066377    -1.763265    -0.885249     217.96
 C      -2.091146    -1.813808    -2.010736      84.70
 H      -3.192314    -1.798642    -1.488875      22.76
 H      -1.997875    -1.119100    -2.739069      27.68
 H      -1.805841    -2.837138    -2.511856      23.71
 C      -0.649118     0.741061    -0.475523       0.64
 O      -1.978025     0.875811    -0.425678     196.75
 C       0.325662     1.648787    -0.079180      49.52
 H       0.238824     2.551513     0.638764      15.90
 C       2.128303    -0.079204    -0.538483      19.58
 C       3.609216    -0.632161    -0.488799     101.18
 H       3.796678    -1.261662    -1.267537      28.25
 O       4.623272     0.466529    -0.728097     108.71
 H       4.764140     0.947816     0.132593      30.83
 C       3.648271    -1.272444     0.980271      90.09
 H       2.934756    -2.179077     1.322849      26.20
 O       4.982132    -1.910086     1.183790      70.84
 H       5.110279    -2.919105     0.882693      21.52
 C       3.590551    -0.306241     2.167866     118.67
 O       4.373508     0.947259     2.276456     135.76
 H       3.792714     1.794226     2.375428      25.15
 H       3.818775    -0.790113     3.066898      29.12
 H       2.459536    -0.012295     2.564166      21.22
55
name = lig-Water-frame_621
 C      -1.520201     3.484515     3.038359      34.36
 H      -2.125412     4.309093     2.679262      18.76
 C      -1.135642     1.004418     3.070504      36.38
 H      -1.472695     0.002795     2.675551      14.78
 C       0.034326     1.354383     3.898515     -10.91
 O       0.923825     0.111171     4.565858     107.33
 C       0.419120    -1.149553     4.134684     101.08
 H       0.760082    -2.012193     4.741323      26.22
 H       0.756727    -1.480150     2.929882      24.43
 H      -0.661360    -1.436448     4.214625      25.62
 C       0.337455     2.624917     4.392380      -6.34
 O       1.464967     2.739824     5.425873     161.08
 H       1.507365     3.743665     5.582340      26.03
 C      -0.383198     3.624718     3.811504      82.08
 H      -0.225221     4.649966     4.302097      32.03
 C      -1.895380     2.156696     2.644507       6.82
 C      -3.067530     2.009368     1.576012     125.28
 H      -3.702889     2.783828     1.757305      26.85
 O      -3.850241     0.785285     2.007007     294.25
 H      -4.772079     0.974050     2.126211      29.78
 C      -2.739592     2.037122     0.017558      90.19
 H      -2.148645     3.018852    -0.283427      23.57
 C      -3.982458     2.117863    -1.034738     101.38
 O      -4.864742     1.001212    -0.935346     265.39
 H      -4.545626     0.101905    -0.606392      28.19
 H      -3.588558     2.154551    -2.003178      29.29
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 H      -4.478311     2.887610    -0.757766      30.14
 C       1.666467     1.082213     0.087344      59.77
 H       2.327583     1.736360     0.533061      27.20
 C       1.149152    -0.990277    -1.048010      56.97
 H       1.061335    -1.927814    -1.584612      25.46
 C      -0.182332    -0.631318    -0.744942      -2.85
 O      -1.131230    -1.714084    -0.882158     199.94
 C      -2.103986    -1.795339    -2.034937      74.11
 H      -3.014764    -1.920065    -1.463823      23.80
 H      -1.612843    -1.002839    -2.822488      23.59
 H      -1.556477    -2.814423    -2.387300      22.66
 C      -0.695087     0.727090    -0.444216      -6.71
 O      -2.074229     0.858930    -0.421018     195.76
 C       0.379079     1.625145    -0.112472      49.46
 H       0.229235     2.360165     0.615964      19.92
 C       2.108605    -0.134091    -0.558792      44.43
 C       3.535376    -0.622388    -0.464517      75.28
 H       3.718692    -1.689460    -1.163654      26.14
 O       4.636459     0.484312    -0.761265       0.37
 H       4.668305     0.851852     0.286851      27.66
 C       3.720294    -1.284361     1.007661      82.21
 H       2.962711    -1.947762     1.256621      32.86
 O       5.023823    -1.931928     1.137998      71.21
 H       4.730147    -2.920830     0.852363      25.70
 C       3.627876    -0.278529     2.197384     120.15
 O       4.369521     0.958231     2.245679     135.34
 H       3.760742     1.701212     2.510218      27.07
 H       3.871291    -0.873334     3.174412      28.16
 H       2.563091    -0.122474     2.187202      27.71
55
name = lig-Water-frame_622
 C      -1.535864     3.476088     3.087027     -15.40
 H      -2.104734     4.381327     2.821090      24.13
 C      -1.085682     0.992449     3.113815      44.98
 H      -1.322458     0.004387     2.831594      20.34
 C       0.021383     1.259068     3.915095       6.11
 O       0.917022     0.120212     4.580579     136.40
 C       0.374724    -1.128723     4.099842     124.83
 H       0.768296    -1.788941     4.933742      26.31
 H       0.708938    -1.284482     3.209025      31.29
 H      -0.667103    -1.425283     4.359392      27.66
 C       0.445117     2.669781     4.373288     -24.47
 O       1.440479     2.691902     5.359211     301.22
 H       1.578513     3.712857     5.504782      22.13
 C      -0.410322     3.681021     3.860528      44.74
 H      -0.084118     4.604548     4.355282      26.11
 C      -1.972160     2.168347     2.634585      42.68
 C      -3.076510     1.966165     1.587686     111.29
 H      -3.905606     2.895047     1.554806      24.24
 O      -3.833621     0.764316     2.018004     263.24
 H      -4.828796     1.119483     2.057719      25.09
 C      -2.767990     2.061395     0.037282     102.10
 H      -2.315174     3.007486    -0.132595      24.43
 C      -3.883554     2.128122    -0.989529      74.70
 O      -4.849695     0.967907    -0.879887     230.29
 H      -4.399148     0.182435    -0.679980      30.45
 H      -3.768967     1.972382    -2.173448      23.72
 H      -4.642736     3.080664    -0.698894      25.66
 C       1.701760     1.030730     0.051509      29.90
 H       2.582385     1.883613     0.249342      22.98
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 C       1.065722    -0.920201    -1.032001      50.79
 H       1.384691    -2.006543    -1.479059      24.11
 C      -0.243780    -0.540394    -0.759732      25.73
 O      -1.176917    -1.642433    -0.854280     212.51
 C      -2.002378    -1.792364    -2.057152      98.17
 H      -3.161387    -1.893242    -1.742931      24.20
 H      -1.864008    -0.951726    -2.712607      26.94
 H      -1.787886    -2.834415    -2.493593      25.29
 C      -0.702208     0.664275    -0.414915       2.93
 O      -2.141314     0.822327    -0.419008     174.48
 C       0.408328     1.572312    -0.096350      47.33
 H       0.042922     2.517878     0.464424      19.50
 C       2.123103    -0.164792    -0.568347      39.46
 C       3.489621    -0.643710    -0.423969      79.34
 H       3.643427    -1.534295    -0.925773      29.87
 O       4.622923     0.459656    -0.747098     120.61
 H       4.649050     0.848448     0.049408      30.47
 C       3.835698    -1.222797     1.039831      75.83
 H       2.827414    -1.890604     1.080311      29.37
 O       5.058624    -1.982451     1.073392     153.58
 H       4.713642    -2.762733     0.889287      32.49
 C       3.644624    -0.275423     2.251192     116.00
 O       4.377691     0.966147     2.195216     117.19
 H       3.724945     1.633570     2.587458      26.43
 H       3.887405    -0.888612     3.079568      30.14
 H       2.499423    -0.029332     2.037948      26.06
55
name = lig-Water-frame_623
 C      -1.584343     3.439985     3.097537      68.13
 H      -2.111569     4.383208     2.916934      30.47
 C      -1.063807     1.050220     3.141452      54.43
 H      -1.236206    -0.050990     2.934203      19.86
 C       0.068960     1.181232     3.991594      19.21
 O       0.848921     0.187415     4.558767     185.13
 C       0.345396    -1.145990     4.166471     105.72
 H       1.027246    -1.709293     4.834110      26.49
 H       0.733237    -1.355372     2.969810      25.24
 H      -0.791986    -1.088372     4.259777      25.20
 C       0.497646     2.595623     4.320531       6.04
 O       1.405999     2.674803     5.271007     294.83
 H       1.743881     3.560931     5.564099      24.54
 C      -0.369114     3.736587     3.964880      74.66
 H      -0.133495     4.791238     4.215095      17.45
 C      -1.976236     2.171996     2.634829      32.45
 C      -3.148148     1.953106     1.611432     126.99
 H      -3.726154     2.779483     1.645925      26.39
 O      -3.816158     0.757035     2.025423     315.62
 H      -4.781797     0.956767     1.837886      28.09
 C      -2.783105     2.061727     0.050057      92.62
 H      -2.099802     3.007249     0.009161      22.45
 C      -3.879748     2.115570    -0.942199      97.04
 O      -4.851067     0.942046    -0.824149     223.47
 H      -4.125035     0.218332    -0.674642      25.18
 H      -3.521391     2.174052    -1.937119      28.23
 H      -4.462548     3.012278    -0.948250      26.65
 C       1.759083     1.063870    -0.015935      29.56
 H       2.592933     1.776830     0.047852      22.25
 C       1.017388    -0.908909    -1.021117      49.01
 H       1.371813    -1.814713    -1.281351      25.01
 C      -0.345464    -0.570594    -0.828974      31.02
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 O      -1.223323    -1.572414    -0.822008     274.07
 C      -1.924485    -1.807728    -2.047237     122.28
 H      -3.042769    -1.671348    -2.125741      25.08
 H      -2.046373    -0.876968    -2.775942      24.19
 H      -1.995988    -2.786184    -2.754738      24.91
 C      -0.716598     0.672063    -0.368202      14.70
 O      -2.140935     0.786144    -0.413641     180.01
 C       0.375926     1.522921    -0.029433      55.93
 H       0.127753     2.578813     0.057027      19.18
 C       2.116069    -0.160856    -0.556276      -8.26
 C       3.527365    -0.634408    -0.343440      74.76
 H       3.747519    -1.581334    -1.172905      27.61
 O       4.581101     0.391121    -0.742833      82.49
 H       4.663957     1.071936     0.114150      27.79
 C       3.888107    -1.138897     1.059032     110.36
 H       3.124680    -1.859924     1.083664      31.50
 O       5.097981    -2.016793     1.005027      44.43
 H       4.783693    -3.045972     0.885682      25.68
 C       3.639339    -0.286178     2.259018     118.07
 O       4.391427     0.972616     2.146681     102.82
 H       3.824033     1.702707     2.541306      26.27
 H       3.810794    -0.849952     3.238030      28.62
 H       2.557828     0.083729     2.273656      26.42
55
name = lig-Water-frame_624
 C      -1.581370     3.434297     3.134214     103.28
 H      -2.237698     4.281952     2.875824      27.07
 C      -1.060879     1.106915     3.158369      46.73
 H      -1.345797     0.127050     2.844684      19.66
 C       0.094384     1.214822     4.045137      26.50
 O       0.770969     0.250493     4.527109     220.12
 C       0.364493    -1.150256     4.205351     127.57
 H       0.999404    -1.893571     4.704179      27.44
 H       0.460601    -1.406823     3.247406      30.60
 H      -0.680997    -1.092675     4.255348      26.60
 C       0.441820     2.531514     4.246845      52.11
 O       1.432402     2.651052     5.222068     130.73
 H       1.653970     3.623964     5.471383      31.85
 C      -0.340990     3.705407     4.020948      80.54
 H      -0.193043     4.829030     4.051539      15.25
 C      -1.912681     2.148967     2.652617       9.59
 C      -3.182659     1.940322     1.646552      94.77
 H      -3.833615     2.961590     1.958058      22.72
 O      -3.807993     0.743620     2.023877     331.33
 H      -4.777232     0.686103     1.764736      28.97
 C      -2.757930     2.041525     0.096239      97.74
 H      -1.948425     2.765345     0.019497      23.97
 C      -3.927189     2.106337    -0.912647      71.67
 O      -4.821449     0.930750    -0.774267     240.29
 H      -4.132693     0.194328    -0.678348      25.67
 H      -3.143139     2.206727    -1.848544      24.16
 H      -4.518513     3.124448    -0.956421      24.09
 C       1.760773     1.147289    -0.107909      39.28
 H       2.614708     1.919812     0.101001      28.00
 C       0.998086    -0.915330    -0.994478      39.88
 H       1.164198    -2.137349    -1.280407      21.93
 C      -0.367388    -0.625173    -0.897384      23.97
 O      -1.315330    -1.561004    -0.810557     259.04
 C      -1.930374    -1.787309    -2.117499      92.76
 H      -3.080539    -1.620962    -1.867072      22.44
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 H      -1.627311    -0.936177    -2.801481      24.73
 H      -1.664699    -2.695781    -2.662552      24.67
 C      -0.739796     0.694682    -0.327194      17.20
 O      -2.096561     0.777218    -0.390591     181.50
 C       0.346457     1.502740     0.029852      90.86
 H       0.311950     2.596362    -0.107354      19.27
 C       2.083103    -0.140812    -0.522289      14.20
 C       3.623133    -0.629824    -0.315175     112.21
 H       3.804732    -1.294875    -1.112311      26.23
 O       4.533716     0.329623    -0.723332     199.95
 H       4.598528     1.099424    -0.045884      29.83
 C       3.898626    -1.133756     1.052947     102.51
 H       3.147464    -2.012128     1.309809      27.54
 O       5.149031    -2.040279     0.941705      61.53
 H       4.854133    -3.042493     0.985563      25.92
 C       3.644115    -0.269299     2.282503     114.05
 O       4.418393     0.983533     2.107907     133.89
 H       3.906232     1.769772     2.398123      29.22
 H       3.800756    -0.703283     3.268015      28.60
 H       2.544057     0.015243     2.431843      26.00
55
name = lig-Water-frame_625
 C      -1.530371     3.451972     3.191326      66.06
 H      -2.273292     4.182637     2.850802      14.99
 C      -1.070675     1.130186     3.162927      61.13
 H      -1.436021     0.184313     2.709276      16.29
 C      -0.008860     1.306442     3.986175      27.81
 O       0.753412     0.236357     4.529255     188.09
 C       0.378536    -1.124552     4.244179     113.39
 H       0.853507    -1.983238     4.817121      25.84
 H       0.390480    -1.393639     3.027823      23.47
 H      -0.742596    -1.418729     4.590418      25.41
 C       0.393775     2.561056     4.253957      34.71
 O       1.500573     2.639428     5.193385     201.32
 H       1.417018     3.606010     5.311963      34.21
 C      -0.404594     3.627027     3.960974      75.63
 H      -0.026017     4.598525     4.160282      22.98
 C      -1.835249     2.136606     2.681324      40.18
 C      -3.177581     1.977882     1.719532     111.67
 H      -3.788614     2.714485     1.992510      23.23
 O      -3.795179     0.704574     2.026526     329.96
 H      -4.824702     0.641238     1.805383      27.31
 C      -2.738186     2.001517     0.181895      94.65
 H      -1.983140     2.797137    -0.036049      23.89
 C      -3.932545     2.123740    -0.904820      79.52
 O      -4.772233     0.938371    -0.742173     265.80
 H      -4.293544     0.153393    -0.680942      30.79
 H      -3.324544     1.958846    -1.752423      28.77
 H      -4.629340     3.061946    -0.818879      23.87
 C       1.717061     1.227287    -0.201456      41.50
 H       2.415841     2.048107     0.292131      25.43
 C       0.995208    -1.015144    -0.967086      43.64
 H       1.020102    -1.958206    -1.196732      21.78
 C      -0.331074    -0.606208    -0.888920       4.01
 O      -1.418965    -1.593695    -0.820237     259.17
 C      -1.972294    -1.740202    -2.205785      65.61
 H      -3.002000    -1.846277    -1.787847      21.82
 H      -1.351911    -0.983173    -2.844304      22.76
 H      -1.294247    -2.732052    -2.373991      20.59
 C      -0.719265     0.647484    -0.331674       3.34
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 O      -2.062258     0.796974    -0.339656     204.56
 C       0.348776     1.541018     0.048718      93.46
 H       0.251332     2.672683     0.116212      19.07
 C       2.077703    -0.120972    -0.480680      10.00
 C       3.640064    -0.611922    -0.316623      94.18
 H       3.835548    -1.545771    -1.133875      22.69
 O       4.524450     0.323123    -0.715834     249.60
 H       4.507264     1.005855    -0.106427      31.97
 C       3.871194    -1.247965     1.075709      82.59
 H       3.097547    -1.944433     1.388414      26.91
 O       5.208004    -2.040489     0.898919     172.48
 H       4.860684    -2.847285     1.061496      30.81
 C       3.672987    -0.210638     2.303580      90.72
 O       4.452308     0.999408     2.076465     156.40
 H       3.823471     1.793184     2.285555      27.55
 H       4.035083    -0.711464     3.240957      25.83
 H       2.485572    -0.111404     2.343516      23.18
55
name = lig-Water-frame_626
 C      -1.535726     3.446922     3.184293      43.85
 H      -2.154626     4.304212     2.930314      28.22
 C      -1.131246     1.076335     3.111546      64.65
 H      -1.324654     0.056604     2.739028      15.99
 C      -0.089075     1.313682     3.928557      15.90
 O       0.750696     0.210393     4.544539     181.27
 C       0.324483    -1.138101     4.256855     126.17
 H       1.021280    -1.723048     4.864729      26.35
 H       0.412492    -1.268867     3.233824      25.73
 H      -0.534843    -1.458100     4.739775      28.14
 C       0.398899     2.585506     4.340078      -3.27
 O       1.549240     2.654519     5.144246     192.73
 H       1.502806     3.641897     5.497544      24.11
 C      -0.444047     3.601898     3.889765     103.86
 H       0.077689     4.494859     4.387344      15.26
 C      -1.824226     2.194625     2.698385      47.29
 C      -3.099262     1.965883     1.797791     110.74
 H      -3.958879     2.848471     1.980656      24.95
 O      -3.777271     0.647965     2.038027     311.02
 H      -4.710688     0.895259     1.958543      28.34
 C      -2.725185     1.995749     0.251748      97.66
 H      -2.202201     2.981877     0.014149      23.55
 C      -3.905519     2.097941    -0.847861      82.36
 O      -4.759092     0.961695    -0.719537     227.52
 H      -4.247722     0.063285    -0.685096      24.94
 H      -3.535336     1.922145    -2.021879      23.87
 H      -4.576424     2.923069    -0.785629      25.23
 C       1.656389     1.274639    -0.247635      28.62
 H       2.299589     2.005536     0.233069      22.35
 C       1.019518    -1.063140    -0.902781      42.09
 H       1.216882    -2.281310    -1.219538      18.37
 C      -0.321958    -0.607963    -0.813991      14.13
 O      -1.476813    -1.594829    -0.832956     234.81
 C      -1.943170    -1.759144    -2.245579      95.71
 H      -3.086355    -1.984980    -2.331381      23.36
 H      -1.583527    -0.915019    -3.013820      23.94
 H      -1.531179    -2.676776    -2.461458      25.62
 C      -0.651473     0.617292    -0.348016      -7.64
 O      -2.052849     0.825266    -0.263019     219.35
 C       0.332627     1.615280     0.019645      90.04
 H      -0.008484     2.534870     0.512916      17.92
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 C       2.085089    -0.125095    -0.468491      37.92
 C       3.556192    -0.666841    -0.349220      79.14
 H       3.691335    -1.608091    -0.871854      26.30
 O       4.557219     0.352977    -0.730159     144.84
 H       4.454623     1.111168     0.082186      26.30
 C       3.858562    -1.340567     1.112230      66.77
 H       2.988039    -2.073176     1.283281      24.97
 O       5.243064    -2.006708     0.878409     113.55
 H       4.881881    -3.011182     1.205421      24.71
 C       3.732568    -0.194060     2.293539      98.08
 O       4.465871     1.032242     2.049809     179.42
 H       3.810476     1.741832     2.232709      29.07
 H       4.224465    -0.701358     3.153538      24.81
 H       2.670243    -0.044881     2.304091      23.60
55
name = lig-Water-frame_627
 C      -1.603496     3.473879     3.117662      55.06
 H      -2.080200     4.445855     2.955841      24.38
 C      -1.197544     0.997610     3.041222      43.78
 H      -1.288223    -0.032436     2.763805      13.74
 C      -0.053895     1.251060     3.952814       1.20
 O       0.721419     0.222168     4.549101     157.68
 C       0.308649    -1.152856     4.307877      97.63
 H       1.336118    -1.517888     4.691377      22.97
 H       0.360332    -1.416667     3.138992      21.52
 H      -0.758195    -1.408764     4.825469      22.90
 C       0.382062     2.545541     4.411114      -5.40
 O       1.576902     2.707118     5.099682     157.11
 H       1.764578     3.468373     5.687243      23.48
 C      -0.341079     3.640826     3.922962     106.11
 H      -0.230912     4.630409     4.346807      24.74
 C      -1.909649     2.222570     2.672983      24.16
 C      -3.046567     1.951335     1.851268     138.19
 H      -3.702381     2.711693     1.910694      26.39
 O      -3.739873     0.611828     2.061219     274.61
 H      -4.705108     1.000277     2.165285      24.70
 C      -2.723635     2.039555     0.270555      89.38
 H      -2.229235     2.994794     0.168986      25.25
 C      -3.848366     2.019988    -0.803761     101.21
 O      -4.785238     0.959352    -0.695854     252.11
 H      -4.142647     0.179434    -0.678060      26.43
 H      -3.617203     2.246254    -1.824818      26.36
 H      -4.552162     3.052564    -0.690461      24.51
 C       1.616245     1.272487    -0.246063      49.06
 H       2.545686     2.042697     0.075509      22.22
 C       1.068196    -1.112021    -0.821248      31.28
 H       1.407621    -1.996279    -1.072257      20.87
 C      -0.328502    -0.705182    -0.731931       2.89
 O      -1.503532    -1.561378    -0.865252     255.29
 C      -1.937384    -1.801137    -2.275211     100.72
 H      -2.939084    -1.830478    -2.811248      23.90
 H      -1.817347    -0.929306    -3.001584      24.24
 H      -1.600032    -2.849769    -2.876745      23.33
 C      -0.622486     0.667663    -0.339742      21.82
 O      -2.029433     0.847350    -0.172936     189.51
 C       0.277111     1.665671    -0.040829      57.50
 H      -0.139399     2.307327     0.808617      11.92
 C       2.058589    -0.140254    -0.495845      25.77
 C       3.451468    -0.707754    -0.340804      56.87
 H       3.584515    -1.687106    -1.066127      23.53
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 O       4.578513     0.384500    -0.729385     135.23
 H       4.528631     0.962478     0.028175      29.95
 C       3.856809    -1.352314     1.120220      81.90
 H       3.104718    -2.197464     1.196087      24.66
 O       5.221038    -1.990222     0.895140     147.66
 H       5.263666    -2.934277     1.185528      27.98
 C       3.840494    -0.248861     2.246995     106.01
 O       4.470997     1.068414     2.016455     171.88
 H       3.826692     1.817507     2.264492      26.29
 H       4.208266    -0.634895     3.191584      25.99
 H       2.670696     0.125783     2.494261      21.48
55
name = lig-Water-frame_628
 C      -1.580066     3.533493     3.097181      57.70
 H      -2.166140     4.437857     2.813937      21.01
 C      -1.182611     0.989356     3.040848      39.24
 H      -1.444854    -0.057304     2.637515      19.35
 C      -0.023081     1.165771     3.981972      14.94
 O       0.675098     0.249581     4.540959     188.75
 C       0.332054    -1.168152     4.346667     126.32
 H       1.215320    -1.706527     4.589046      27.38
 H       0.115820    -1.529501     3.329038      26.85
 H      -0.543306    -1.377610     4.796030      28.22
 C       0.341040     2.527485     4.447685       4.90
 O       1.619832     2.731633     5.070187      82.75
 H       1.699796     3.556089     5.684977      27.70
 C      -0.296910     3.690257     3.954508      84.30
 H      -0.343132     4.758203     4.232466      23.76
 C      -1.974950     2.165759     2.663121       2.99
 C      -3.063806     1.899564     1.805522     120.82
 H      -3.829205     2.845913     1.991838      21.78
 O      -3.697263     0.616402     2.099142     292.47
 H      -4.668171     0.696539     2.278032      24.91
 C      -2.719499     2.071781     0.271231      77.49
 H      -1.992596     2.987855     0.224636      23.57
 C      -3.849496     2.041686    -0.725342     105.19
 O      -4.804522     0.933471    -0.683804     220.90
 H      -4.238521     0.199141    -0.594303      30.03
 H      -3.321652     2.332872    -1.765731      25.59
 H      -4.365062     2.878537    -0.478108      28.58
 C       1.652168     1.245202    -0.212955      48.69
 H       2.414678     1.865507    -0.121645      25.16
 C       1.060463    -1.105352    -0.722397      49.75
 H       1.562245    -2.205767    -1.033230      22.22
 C      -0.330917    -0.800351    -0.662137       9.43
 O      -1.522689    -1.535494    -0.922284     223.52
 C      -1.928184    -1.865725    -2.385927      86.88
 H      -3.100458    -1.763031    -2.435324      23.98
 H      -1.536727    -0.811708    -2.865722      25.03
 H      -1.432720    -2.593101    -2.843711      27.90
 C      -0.669760     0.677578    -0.335367      13.79
 O      -1.979211     0.855439    -0.081697     144.77
 C       0.243280     1.685293    -0.079491      77.61
 H       0.033877     2.357987     0.702664      21.29
 C       1.997341    -0.108322    -0.524287      39.27
 C       3.408951    -0.729842    -0.327575      65.84
 H       3.534497    -1.369183    -1.239111      25.77
 O       4.566555     0.370107    -0.734656      79.00
 H       4.628185     0.934410     0.104715      26.37
 C       3.873466    -1.329596     1.075731     104.75
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 H       3.224484    -2.116566     1.366934      28.86
 O       5.194428    -1.957900     0.920775     176.60
 H       5.340921    -2.855116     1.166488      29.44
 C       3.899189    -0.290129     2.222953     121.40
 O       4.483971     1.095002     1.969626     155.69
 H       3.859596     1.824504     2.349080      25.10
 H       4.263613    -0.656815     3.228106      28.20
 H       2.943445    -0.074239     2.524622      29.03
55
name = lig-Water-frame_629
 C      -1.500390     3.529586     3.101186      52.38
 H      -2.162173     4.282159     2.678866      20.86
 C      -1.126989     1.025017     3.086955      60.39
 H      -1.497324     0.179985     2.622521      25.08
 C      -0.078463     1.180347     3.964347      39.93
 O       0.673338     0.210536     4.550831     221.37
 C       0.365515    -1.182544     4.361233     110.45
 H       1.111742    -1.994181     4.724851      26.42
 H      -0.016931    -1.423782     3.316230      27.37
 H      -0.548944    -1.468911     5.153749      24.94
 C       0.308409     2.545299     4.449747      30.58
 O       1.655709     2.738132     5.063708      14.59
 H       1.450284     3.676623     5.381132      21.71
 C      -0.377248     3.720161     3.935050     103.15
 H       0.012743     4.757931     4.243625      28.30
 C      -1.930505     2.124730     2.720381       4.94
 C      -3.192058     1.894695     1.716642     114.08
 H      -3.875944     2.605245     2.025568      24.69
 O      -3.651600     0.613967     2.139467     333.50
 H      -4.622458     0.571585     2.206231      26.26
 C      -2.671528     2.063130     0.297826      94.71
 H      -2.012711     2.860536     0.155770      26.86
 C      -3.848945     2.108189    -0.670359      77.23
 O      -4.803852     0.916053    -0.689000     159.39
 H      -4.325016     0.025150    -0.405235      27.12
 H      -3.240762     2.082960    -1.590522      26.44
 H      -4.576083     3.048865    -0.239333      24.44
 C       1.646716     1.191743    -0.185509      51.12
 H       2.590976     2.061851    -0.162171      23.22
 C       1.000709    -1.146045    -0.650125      60.17
 H       1.313186    -2.113069    -0.846129      27.94
 C      -0.352129    -0.822092    -0.616077       9.95
 O      -1.527490    -1.542290    -0.978149     206.04
 C      -1.920196    -1.819339    -2.469546      74.01
 H      -2.891371    -1.971918    -1.957433      22.94
 H      -1.419439    -0.946966    -2.906019      26.50
 H      -1.155327    -2.735954    -2.837831      24.81
 C      -0.711393     0.628697    -0.327689      10.03
 O      -1.954890     0.841720     0.005516     160.03
 C       0.290520     1.654067    -0.108794      61.56
 H       0.193088     2.725334     0.389533      22.81
 C       1.966074    -0.061401    -0.510261      59.06
 C       3.427868    -0.667694    -0.341703      82.24
 H       3.578968    -1.354312    -1.247203      28.71
 O       4.520045     0.324317    -0.733024      88.94
 H       4.754635     0.910818     0.165782      23.81
 C       3.902795    -1.302453     1.014770      96.19
 H       3.134551    -2.001106     1.626570      30.26
 O       5.190019    -1.898466     0.931276      71.77
 H       5.060779    -2.987447     1.200745      23.51
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 C       3.960457    -0.290687     2.221090     103.40
 O       4.496968     1.092966     1.920320      85.95
 H       3.908827     1.766906     2.375966      25.48
 H       4.543618    -0.781049     3.009064      30.68
 H       2.714248    -0.272719     2.518815      26.98
55
name = lig-Water-frame_630
 C      -1.459194     3.451460     3.082821      81.90
 H      -2.033671     4.277831     2.609922      29.79
 C      -1.113345     1.083266     3.119725      62.71
 H      -1.413689     0.061390     2.679292      22.20
 C      -0.103093     1.264450     3.993542      14.56
 O       0.713133     0.142973     4.570484     186.80
 C       0.333371    -1.236107     4.413191     123.64
 H       1.154712    -1.865113     4.677536      28.90
 H      -0.069857    -1.294981     3.339308      27.42
 H      -0.333563    -1.413144     5.140275      29.26
 C       0.290117     2.557557     4.405869      56.50
 O       1.627554     2.749522     5.058823      86.15
 H       1.592149     3.747188     5.206395      32.01
 C      -0.436175     3.723906     3.931802      42.53
 H       0.191467     4.539357     4.158161       8.16
 C      -1.862575     2.164335     2.773727       9.55
 C      -3.248411     1.908110     1.723866      96.53
 H      -4.151153     2.645455     1.968674      24.81
 O      -3.619248     0.584617     2.164503     301.08
 H      -4.661151     0.641473     2.014574      24.63
 C      -2.647936     2.004938     0.334583      94.44
 H      -2.019542     2.991477     0.122223      24.10
 C      -3.868004     2.161657    -0.610640      89.12
 O      -4.786854     0.905571    -0.695940     193.51
 H      -4.388246     0.144205    -0.199599      28.07
 H      -3.478734     2.100279    -1.718244      25.03
 H      -4.501400     2.886730    -0.489113      29.46
 C       1.651832     1.230619    -0.172506      64.03
 H       2.351609     1.859914    -0.056616      27.16
 C       0.923438    -1.147152    -0.586412      59.94
 H       1.167639    -2.311511    -0.744968      23.70
 C      -0.415391    -0.768882    -0.601310      22.90
 O      -1.499899    -1.564662    -1.005326     235.90
 C      -1.832443    -1.800355    -2.469502      91.82
 H      -2.839019    -2.219271    -2.300618      25.53
 H      -1.685329    -0.854804    -3.340637      23.72
 H      -1.418901    -2.682842    -2.732771      27.60
 C      -0.667052     0.593498    -0.296470      17.73
 O      -1.990512     0.802902     0.086636     173.02
 C       0.355193     1.606585    -0.124734      66.60
 H       0.167215     2.653224    -0.233585      23.40
 C       1.981919    -0.128218    -0.462003      13.69
 C       3.474735    -0.571282    -0.391012     111.69
 H       3.567676    -1.574467    -1.039354      26.20
 O       4.470528     0.280069    -0.717863     247.60
 H       4.661177     0.773899    -0.008532      32.35
 C       3.892440    -1.246622     1.005387      98.39
 H       3.171779    -1.887198     1.358603      33.06
 O       5.201937    -1.885197     0.934343     168.98
 H       4.836638    -2.717841     1.063603      32.29
 C       3.970939    -0.264386     2.208720     133.91
 O       4.501490     1.054760     1.878201     143.14
 H       3.947951     1.799386     2.349793      25.04
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 H       4.770496    -0.784076     2.799551      31.39
 H       3.051326    -0.230428     2.546503      28.24
55
name = lig-Water-frame_631
 C      -1.471849     3.433369     3.039389     100.88
 H      -1.882704     4.313855     2.600328      27.52
 C      -1.137500     1.085674     3.133639      54.20
 H      -1.238707     0.068285     2.918938      20.92
 C      -0.045278     1.290276     4.091409       3.44
 O       0.764818     0.125736     4.583643     126.73
 C       0.291799    -1.261182     4.440864      98.52
 H       1.354989    -1.743708     4.477003      26.06
 H      -0.088583    -1.494272     3.462000      27.16
 H      -0.578134    -1.514799     5.278983      24.71
 C       0.313304     2.588046     4.368204      51.95
 O       1.546842     2.765432     5.040228     188.88
 H       1.891853     3.684334     5.292405      38.10
 C      -0.408775     3.664753     3.963830      21.92
 H       0.116860     4.734594     3.999806      10.37
 C      -1.883203     2.213105     2.754863      29.58
 C      -3.210490     1.948104     1.850164      90.82
 H      -4.087915     2.600110     1.782375      25.86
 O      -3.633229     0.556726     2.159477     325.49
 H      -4.574259     0.594164     1.984095      29.16
 C      -2.674355     1.987479     0.346326     102.10
 H      -2.092658     2.835116     0.289585      25.70
 C      -3.861635     2.119501    -0.629284      88.44
 O      -4.767053     0.911585    -0.687988     264.26
 H      -4.373694     0.327413    -0.074057      29.54
 H      -3.756308     2.381358    -1.741483      23.14
 H      -4.652665     3.129219    -0.570078      22.85
 C       1.676938     1.202717    -0.185441      42.75
 H       2.569989     2.058748     0.089405      21.20
 C       0.895840    -1.140214    -0.542256      72.25
 H       1.022865    -2.244547    -0.663388      22.98
 C      -0.471902    -0.695887    -0.618876      15.49
 O      -1.468611    -1.587937    -1.024996     256.50
 C      -1.777229    -1.780328    -2.452102     102.80
 H      -2.841106    -2.119127    -2.853435      23.67
 H      -1.918696    -1.033207    -3.248102      24.06
 H      -1.221006    -2.824880    -2.842390      23.09
 C      -0.635225     0.599908    -0.237244      28.81
 O      -2.025710     0.744601     0.147119     181.21
 C       0.350705     1.562385    -0.162037      89.94
 H      -0.024881     2.534893    -0.618415      19.94
 C       1.999130    -0.234903    -0.385060      12.85
 C       3.479411    -0.588688    -0.397839     104.46
 H       3.549546    -1.537014    -0.982215      27.20
 O       4.450471     0.269854    -0.755375     200.53
 H       4.602115     0.931998     0.135720      19.92
 C       3.865571    -1.131748     1.003500      90.23
 H       3.056859    -2.041023     1.014919      28.26
 O       5.209308    -1.879398     0.920808     111.45
 H       4.896168    -2.824482     0.948667      29.61
 C       4.020535    -0.240631     2.168765     129.16
 O       4.502011     1.023392     1.835064     177.43
 H       4.005973     1.762315     2.256363      26.07
 H       4.765136    -0.643360     2.849447      30.37
 H       3.005964    -0.051610     2.981857      25.12
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name = lig-Water-frame_632
 C      -1.462070     3.516993     3.033602      84.93
 H      -1.910556     4.436417     2.559744      21.77
 C      -1.113385     1.085672     3.215794      39.68
 H      -1.339979     0.001241     3.001120      19.87
 C      -0.011569     1.224929     4.150205      33.01
 O       0.798354     0.157830     4.585645     171.95
 C       0.258509    -1.271014     4.481308     119.16
 H       1.205586    -1.773935     4.450559      27.67
 H      -0.194290    -1.711259     3.472258      24.44
 H      -0.403485    -1.604044     5.174343      28.30
 C       0.398692     2.626128     4.384487      42.08
 O       1.492280     2.768519     5.031495     203.43
 H       1.764194     3.657859     5.392560      35.23
 C      -0.379222     3.658976     3.939277       9.15
 H      -0.200598     4.651948     3.990538      14.55
 C      -1.978801     2.175692     2.690676      26.20
 C      -3.117460     1.954094     1.960113      89.66
 H      -3.958872     2.714613     1.978685      24.54
 O      -3.660832     0.546708     2.143880     286.46
 H      -4.691284     0.536194     2.093044      28.43
 C      -2.745863     1.974610     0.363308      68.70
 H      -1.940072     2.845192     0.352840      20.65
 C      -3.924199     2.116138    -0.700308     101.73
 O      -4.741873     0.936490    -0.674507     293.25
 H      -4.337081     0.309451     0.066466      22.90
 H      -3.568510     2.422287    -1.730316      24.75
 H      -4.409344     2.880970    -0.260813      26.06
 C       1.747662     1.133630    -0.200748      60.77
 H       2.445691     1.888062    -0.023008      22.60
 C       0.882866    -1.119597    -0.521001      63.78
 H       1.020281    -2.219544    -0.673969      22.57
 C      -0.452718    -0.676894    -0.662503      27.32
 O      -1.463316    -1.608371    -1.043646     263.59
 C      -1.744076    -1.851127    -2.472650      84.02
 H      -2.782702    -2.034199    -2.659563      23.03
 H      -1.628372    -0.685168    -3.071296      21.43
 H      -0.936038    -2.389069    -2.880764      23.84
 C      -0.708602     0.610819    -0.165069      32.70
 O      -2.035966     0.694122     0.183353     198.34
 C       0.321544     1.564119    -0.226350      86.95
 H      -0.089035     2.519423    -0.550633      15.36
 C       1.989266    -0.272789    -0.294975      34.83
 C       3.454681    -0.686095    -0.349697      84.20
 H       3.612761    -1.536725    -1.200093      24.40
 O       4.465433     0.328113    -0.813270     193.50
 H       4.489301     0.953027    -0.047927      24.33
 C       3.816854    -1.112728     0.982158     104.50
 H       3.146274    -1.863761     1.100005      30.41
 O       5.202852    -1.869329     0.904426      43.83
 H       5.138241    -2.966273     0.781960      25.26
 C       4.015542    -0.211091     2.224036     138.83
 O       4.522235     1.027820     1.768237     212.95
 H       3.944074     1.778336     2.224396      22.89
 H       4.746930    -0.628370     2.959479      29.13
 H       3.293257    -0.075923     2.835418      29.30
55
name = lig-Water-frame_633
 C      -1.484473     3.555921     3.021033      56.63
 H      -1.968295     4.434465     2.648656      22.84
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 C      -1.099272     1.079679     3.317895      42.71
 H      -1.549726     0.136855     3.020275      22.93
 C      -0.012403     1.193986     4.151033      47.57
 O       0.805299     0.184070     4.582675     170.65
 C       0.259284    -1.278538     4.468898      93.91
 H       1.153744    -1.970728     4.638409      25.04
 H      -0.232524    -1.475952     3.580123      27.22
 H      -0.394134    -1.595844     5.463369      23.44
 C       0.410151     2.587310     4.378963      28.22
 O       1.538109     2.780577     5.082750      80.04
 H       1.371269     3.752765     5.426343      28.82
 C      -0.390096     3.683085     3.854968      53.57
 H      -0.207181     4.820852     4.269997      19.34
 C      -1.925762     2.156670     2.738239       8.33
 C      -3.133991     1.908801     1.943553      86.37
 H      -3.742737     2.782881     2.427873      22.03
 O      -3.703863     0.550578     2.134815     294.65
 H      -4.707222     0.685469     2.264989      27.33
 C      -2.777561     1.975509     0.386163      77.56
 H      -2.067911     2.711399     0.197766      24.99
 C      -3.948091     2.111769    -0.724492      78.16
 O      -4.722335     0.951704    -0.660122     297.63
 H      -4.385431     0.287065    -0.025897      27.05
 H      -3.299118     2.315313    -1.675681      24.89
 H      -4.493186     2.944260    -0.016491      23.27
 C       1.714205     1.059217    -0.227307      53.63
 H       2.567566     1.850460    -0.177639      19.26
 C       0.879285    -1.115618    -0.524353      52.63
 H       1.121924    -2.258154    -0.781357      21.87
 C      -0.403599    -0.707032    -0.702639      28.75
 O      -1.464398    -1.624798    -1.042198     260.33
 C      -1.677139    -1.823499    -2.493362      56.24
 H      -2.763610    -2.233967    -2.329204      20.90
 H      -1.369499    -0.693051    -2.826271      20.69
 H      -0.716851    -2.279499    -3.035008      21.73
 C      -0.803676     0.599271    -0.126094      13.14
 O      -2.058656     0.670864     0.207918     198.07
 C       0.319492     1.566261    -0.285013      45.56
 H       0.099020     2.674686    -0.227445      17.03
 C       1.977475    -0.256371    -0.221964      42.98
 C       3.449810    -0.756188    -0.359693      79.45
 H       3.600109    -1.483227    -1.094247      27.62
 O       4.457281     0.384796    -0.884647     120.85
 H       4.493450     1.041506    -0.167816      23.87
 C       3.829815    -1.195140     1.013411      83.10
 H       3.003631    -1.965340     1.525442      25.45
 O       5.202050    -1.864707     0.890055     138.88
 H       5.151435    -2.726681     0.644464      29.52
 C       4.043080    -0.196589     2.261703      92.00
 O       4.545059     1.066965     1.705787     182.53
 H       3.976312     1.773152     2.127401      23.87
 H       4.780054    -0.709683     2.887441      27.00
 H       2.852836    -0.038311     2.842531      20.77
55
name = lig-Water-frame_634
 C      -1.529156     3.518004     3.002863      76.82
 H      -2.141277     4.413031     2.714834      22.82
 C      -1.164315     1.082408     3.374527      65.07
 H      -1.598639     0.146369     3.097992      21.71
 C       0.002856     1.221124     4.133738       6.70
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 O       0.806940     0.170960     4.585578     186.76
 C       0.277277    -1.277747     4.516366      93.94
 H       1.108183    -2.001627     4.662902      26.28
 H      -0.347527    -1.218675     3.523780      24.20
 H      -0.323189    -1.248549     5.380642      26.58
 C       0.353414     2.520841     4.336645      19.50
 O       1.606976     2.828136     5.166109     154.33
 H       1.297433     3.703335     5.499968      24.85
 C      -0.366683     3.734434     3.808234      40.12
 H      -0.094692     4.523659     4.373372      15.11
 C      -1.770038     2.166014     2.850131      23.39
 C      -3.180952     1.860453     1.900259      98.76
 H      -3.766776     2.594691     2.411705      27.12
 O      -3.757744     0.575486     2.143581     316.32
 H      -4.702764     0.785421     2.274680      28.31
 C      -2.801628     1.966558     0.405390      89.85
 H      -2.098739     2.826999     0.067502      25.50
 C      -3.906447     2.121047    -0.634141      99.25
 O      -4.737035     0.946185    -0.668605     312.71
 H      -4.359472     0.256753    -0.148121      30.91
 H      -3.466039     2.269660    -1.594423      29.23
 H      -4.583961     2.979575    -0.513472      26.73
 C       1.610868     1.071590    -0.250742      54.59
 H       2.576921     1.736330    -0.403445      22.38
 C       0.926291    -1.160829    -0.552072      47.74
 H       1.152091    -2.126510    -0.846607      25.66
 C      -0.408313    -0.734340    -0.701950      18.29
 O      -1.438479    -1.642155    -1.011316     248.83
 C      -1.575732    -1.767738    -2.480372      91.56
 H      -2.439481    -2.347891    -2.543862      25.34
 H      -1.611317    -0.602510    -2.877918      22.94
 H      -0.913169    -2.482674    -3.030507      25.07
 C      -0.788421     0.579149    -0.164884      12.38
 O      -2.123929     0.668382     0.230725     197.34
 C       0.301840     1.559556    -0.304752      72.49
 H       0.404595     2.573385     0.173029      21.10
 C       1.981339    -0.278749    -0.200770      36.85
 C       3.440680    -0.734852    -0.355265      49.58
 H       3.561838    -1.710733    -1.152381      25.61
 O       4.417893     0.400029    -0.955182       7.33
 H       4.550044     1.130737    -0.101610      19.12
 C       3.877820    -1.333406     1.112491      93.91
 H       3.185826    -1.910690     1.612101      30.55
 O       5.201834    -1.840439     0.892066      82.69
 H       5.037117    -2.747524     0.428902      24.88
 C       4.011255    -0.177898     2.249954     111.37
 O       4.567878     1.088466     1.659400     168.85
 H       3.989212     1.878410     2.092935      22.93
 H       4.743489    -0.622536     2.926450      27.37
 H       3.130943    -0.044620     2.554583      29.08
55
name = lig-Water-frame_635
 C      -1.522703     3.508214     3.028152      76.37
 H      -2.304858     4.188963     2.703508      23.49
 C      -1.221942     1.051220     3.426173      62.79
 H      -1.568400     0.015200     3.172533      19.91
 C       0.027636     1.200277     4.112175       4.82
 O       0.825355     0.152328     4.590691     194.41
 C       0.275886    -1.202528     4.547714      99.95
 H       1.108722    -1.911302     4.524000      28.43
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 H      -0.276265    -1.369266     3.668468      29.74
 H      -0.512216    -1.152734     5.431812      26.01
 C       0.353529     2.555376     4.321668      31.67
 O       1.623479     2.858991     5.216817     143.97
 H       1.543178     3.803520     5.686139      20.71
 C      -0.327163     3.701359     3.792584      39.49
 H       0.031478     4.659182     4.386439      26.22
 C      -1.741967     2.170040     2.874372      16.83
 C      -3.159785     1.834842     1.900812      78.71
 H      -4.081631     2.620347     2.119481      23.41
 O      -3.803488     0.598886     2.166857     287.72
 H      -4.871871     0.722534     2.148513      22.81
 C      -2.798618     1.988101     0.420877     110.42
 H      -2.142043     2.838083     0.260544      26.36
 C      -3.876695     2.114657    -0.551649      90.35
 O      -4.782349     0.931829    -0.678922     243.14
 H      -4.241669     0.113511    -0.267930      24.95
 H      -3.540868     2.204358    -1.702492      22.94
 H      -4.600748     3.051603    -0.784846      24.80
 C       1.556990     1.079122    -0.290371      44.46
 H       2.314692     1.781175    -0.442275      25.96
 C       0.968981    -1.195230    -0.585200      14.01
 H       1.219840    -2.346617    -1.002292      24.02
 C      -0.422576    -0.745508    -0.650919      12.22
 O      -1.392759    -1.665958    -0.982900     212.84
 C      -1.502389    -1.726149    -2.458193      90.37
 H      -2.488950    -2.297908    -2.861186      24.06
 H      -1.816663    -0.643195    -3.055792      22.46
 H      -0.756344    -2.509160    -2.915059      24.59
 C      -0.743555     0.560531    -0.246315      12.89
 O      -2.169641     0.672582     0.229133     162.17
 C       0.258214     1.552539    -0.254486      75.05
 H       0.284746     2.459123     0.308376      22.51
 C       1.978381    -0.303848    -0.244747      27.00
 C       3.435290    -0.711545    -0.331400      67.76
 H       3.480859    -1.496781    -0.970871      29.29
 O       4.355691     0.381372    -0.980004     125.80
 H       4.539990     0.825546    -0.227762      27.86
 C       3.959155    -1.363928     1.184915      86.17
 H       3.167914    -2.230684     1.573012      26.87
 O       5.215257    -1.854475     0.909179      58.53
 H       5.051345    -2.626189     0.148050      23.21
 C       4.040378    -0.173349     2.155550     106.57
 O       4.583088     1.087664     1.624449     163.11
 H       4.017773     1.803121     2.049565      25.21
 H       4.623365    -0.378094     3.125393      27.55
 H       2.821924     0.101365     2.614412      24.76
55
name = lig-Water-frame_636
 C      -1.472772     3.505034     3.084390      61.30
 H      -2.265765     4.142689     2.672221      22.49
 C      -1.213141     0.980899     3.484694      51.65
 H      -1.522575     0.019776     3.205769      24.32
 C       0.040188     1.167380     4.094911       4.44
 O       0.854314     0.156188     4.587439     212.81
 C       0.242686    -1.100281     4.594269     122.18
 H       1.137104    -1.824962     4.582886      28.44
 H      -0.273314    -1.555035     3.625881      26.87
 H      -0.477289    -1.426368     5.385701      28.20
 C       0.441684     2.644771     4.362922       5.49
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 O       1.597242     2.868614     5.231798     180.78
 H       1.632770     3.809971     5.585805      26.50
 C      -0.282537     3.673886     3.824111      16.99
 H      -0.039482     4.707593     3.991676      30.24
 C      -1.883969     2.136373     2.812359     -29.06
 C      -3.157014     1.872299     1.941611      90.99
 H      -3.903827     2.640508     1.880313      25.35
 O      -3.846814     0.602007     2.202576     319.46
 H      -4.795381     0.695250     1.999684      26.52
 C      -2.767894     2.004651     0.463046      97.52
 H      -2.055723     2.869192     0.458121      22.75
 C      -3.908536     2.095174    -0.598504      84.34
 O      -4.825687     0.905435    -0.658363     242.57
 H      -4.245554     0.147085    -0.503334      28.86
 H      -3.316931     2.073205    -1.475790      29.80
 H      -4.505587     3.057126    -0.498411      25.87
 C       1.554991     1.050200    -0.331872      39.97
 H       2.265167     2.097280    -0.294211      27.35
 C       0.966466    -1.253605    -0.639040      52.18
 H       1.176654    -2.164029    -0.933604      30.03
 C      -0.379820    -0.775007    -0.587669      19.44
 O      -1.364499    -1.696047    -0.980794     191.10
 C      -1.485978    -1.734147    -2.466302      96.36
 H      -2.411985    -2.180118    -2.722138      27.34
 H      -1.650965    -0.745181    -3.089614      26.14
 H      -0.434028    -2.078055    -2.723815      27.15
 C      -0.776231     0.553371    -0.308383       8.99
 O      -2.151228     0.673934     0.187001     164.17
 C       0.200477     1.527700    -0.161002      52.71
 H      -0.164571     2.568510     0.217861      19.26
 C       1.969240    -0.283526    -0.339147       6.82
 C       3.427949    -0.665579    -0.271739      68.25
 H       3.480135    -1.656995    -1.094602      26.47
 O       4.272242     0.307864    -0.979522      84.85
 H       4.682382     0.814272    -0.047369      18.02
 C       3.988996    -1.323561     1.207096     112.19
 H       3.360476    -2.155199     1.324233      30.26
 O       5.268858    -1.906963     0.912307     129.16
 H       5.241823    -2.354295     0.159503      29.59
 C       4.018913    -0.154170     2.125110     153.48
 O       4.602710     1.052661     1.576411     184.61
 H       3.962077     1.780747     2.020300      23.25
 H       4.466162    -0.273557     3.062298      30.96
 H       3.114775     0.029529     2.360061      32.65
55
name = lig-Water-frame_637
 C      -1.457931     3.414451     3.115810      21.80
 H      -1.907043     4.403260     2.732443      24.11
 C      -1.193307     0.966460     3.491332      27.29
 H      -1.486254    -0.084178     3.216795      24.62
 C       0.053035     1.221927     4.101850       0.73
 O       0.871733     0.191182     4.580832     227.84
 C       0.227808    -1.102222     4.609023     119.10
 H       1.078211    -1.708450     4.830830      28.92
 H      -0.181595    -1.362072     3.660406      29.05
 H      -0.429173    -1.425697     5.497310      28.07
 C       0.553266     2.659279     4.426260      -3.08
 O       1.562086     2.858358     5.216995      58.96
 H       1.431189     3.888896     5.447412      25.98
 C      -0.257885     3.687948     3.846243      13.65
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 H       0.027296     4.774910     3.792751      24.96
 C      -2.033061     2.084521     2.801796     -43.31
 C      -3.169204     1.901189     1.975134      75.30
 H      -3.811770     2.948198     2.016041      24.40
 O      -3.850684     0.606486     2.247757     263.90
 H      -4.869417     0.805719     1.974346      22.00
 C      -2.734801     1.977520     0.503471      94.67
 H      -2.032260     2.863409     0.421540      22.41
 C      -3.930280     2.058677    -0.642107      69.86
 O      -4.858726     0.894013    -0.626346     238.16
 H      -4.235591     0.136052    -0.640678      28.04
 H      -3.117288     2.056497    -1.516542      25.63
 H      -4.513989     2.958270    -0.318961      26.01
 C       1.555062     1.116746    -0.339113      60.70
 H       2.220753     1.791049    -0.121612      32.56
 C       0.935833    -1.234771    -0.669704      50.26
 H       1.225703    -2.433155    -0.954087      23.70
 C      -0.335856    -0.836525    -0.557095      11.06
 O      -1.357861    -1.720344    -0.989793     184.11
 C      -1.437000    -1.742904    -2.446966      63.50
 H      -2.353177    -2.477771    -2.567193      23.34
 H      -1.456936    -0.431651    -3.005017      23.04
 H      -0.385512    -1.903944    -2.823407      26.02
 C      -0.854682     0.544053    -0.317519       6.19
 O      -2.092840     0.675258     0.114093     176.34
 C       0.144345     1.494010    -0.069706      68.90
 H      -0.278584     2.455093    -0.086624      19.72
 C       1.959930    -0.249860    -0.449154      13.34
 C       3.421621    -0.688011    -0.266165     105.07
 H       3.492465    -1.549274    -0.817834      31.48
 O       4.210561     0.232768    -0.919805     185.96
 H       4.697909     0.801536    -0.315745      23.89
 C       4.015992    -1.249781     1.114539      97.94
 H       3.224914    -2.081221     1.386843      28.18
 O       5.352675    -1.942573     0.940694      79.39
 H       5.393792    -2.299366    -0.073729      23.73
 C       4.023360    -0.146880     2.126007     101.06
 O       4.616951     1.018619     1.523598     175.77
 H       4.053738     1.762584     1.847964      27.50
 H       4.542738    -0.443526     3.125685      26.79
 H       2.706695     0.062825     2.231848      24.85
55
name = lig-Water-frame_638
 C      -1.462988     3.315706     3.125458      62.34
 H      -1.646069     4.302906     2.795773      24.35
 C      -1.199039     1.011247     3.434233      41.08
 H      -1.370054    -0.038480     3.298035      20.87
 C       0.067211     1.327365     4.132939      -7.90
 O       0.872215     0.245978     4.579335     174.25
 C       0.251042    -1.143281     4.639004      91.06
 H       1.160884    -1.788735     4.987805      25.28
 H      -0.175191    -1.295503     3.617006      25.27
 H      -0.527066    -1.015091     5.510669      25.10
 C       0.536275     2.601767     4.406870      43.92
 O       1.571645     2.874330     5.226540     -83.77
 H       1.433437     3.804352     5.594544      40.17
 C      -0.238731     3.676727     3.854820     138.35
 H       0.189883     4.732480     3.829152       7.54
 C      -2.038366     2.050528     2.921235      16.42
 C      -3.226299     1.925831     1.973865      98.99
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 H      -3.754098     2.811159     2.226375      28.16
 O      -3.855694     0.644429     2.286585     292.07
 H      -4.823551     0.774896     2.203421      24.70
 C      -2.730315     1.924029     0.494656     100.09
 H      -2.124996     2.772077     0.270680      27.65
 C      -3.888074     2.004552    -0.644216      88.42
 O      -4.866812     0.896357    -0.597189     211.84
 H      -4.279505     0.020320    -0.725492      26.31
 H      -3.519594     2.180025    -1.613191      29.89
 H      -4.646113     2.937744    -0.393360      26.34
 C       1.502369     1.163405    -0.315049      39.83
 H       2.543052     1.794916     0.106363      25.08
 C       0.969834    -1.229094    -0.697954      48.23
 H       1.158127    -2.168656    -0.870908      24.45
 C      -0.391522    -0.874339    -0.564006       9.80
 O      -1.354714    -1.745308    -0.996670     230.08
 C      -1.385368    -1.704136    -2.426539     103.80
 H      -1.995432    -2.553533    -2.692602      25.94
 H      -1.606183    -0.755446    -2.554174      30.29
 H      -0.458171    -2.092283    -3.060868      26.57
 C      -0.841135     0.491151    -0.280040      16.04
 O      -2.082028     0.676525     0.043565     194.13
 C       0.127384     1.447864    -0.040387      73.19
 H      -0.113337     2.564092    -0.224543      21.15
 C       1.937236    -0.215844    -0.531790       6.65
 C       3.395257    -0.738981    -0.263036     100.98
 H       3.490949    -1.877816    -0.862046      24.31
 O       4.198185     0.184036    -0.902608     198.73
 H       4.665182     0.799832    -0.332051      23.55
 C       4.012088    -1.206532     0.998553      96.78
 H       3.283677    -1.837886     1.548108      27.84
 O       5.420024    -1.959406     0.955195      86.17
 H       5.544151    -2.210282    -0.067876      26.72
 C       3.981042    -0.147525     2.144962     115.36
 O       4.636733     0.989803     1.478559     196.73
 H       4.112539     1.810214     1.792145      27.55
 H       4.461734    -0.524336     2.989078      28.59
 H       3.042298     0.009126     2.249261      31.45
55
name = lig-Water-frame_639
 C      -1.413495     3.296591     3.161755      10.63
 H      -1.990974     4.151759     2.549975      20.18
 C      -1.161245     1.070870     3.393209      54.47
 H      -1.378624     0.016645     3.303674      16.60
 C       0.040630     1.338316     4.150233      -6.29
 O       0.873047     0.302803     4.579935     100.95
 C       0.292424    -1.127718     4.688891     112.39
 H       1.027963    -1.806093     4.936638      28.18
 H      -0.141515    -1.536604     3.704360      25.87
 H      -0.547814    -0.891060     5.310433      25.85
 C       0.460145     2.597494     4.369103      36.42
 O       1.614372     2.880763     5.251913     142.41
 H       1.550768     3.779631     5.773762      26.13
 C      -0.236500     3.608457     3.840771      18.63
 H       0.184416     4.567750     3.954757      14.08
 C      -1.984098     2.034781     3.051938      38.91
 C      -3.241320     1.895541     1.977098      85.83
 H      -4.033376     2.788332     2.267537      27.88
 O      -3.860326     0.691968     2.330388     232.81
 H      -4.902118     0.705367     2.349176      24.14
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 C      -2.767348     1.874540     0.416465      93.61
 H      -2.096278     2.810860     0.180003      26.60
 C      -3.888858     1.974691    -0.598186     108.06
 O      -4.850539     0.885000    -0.579373     250.78
 H      -4.480145     0.040490    -0.707844      30.86
 H      -3.791316     2.256540    -1.753117      26.43
 H      -4.532498     2.821317    -0.470839      28.95
 C       1.517744     1.162016    -0.248490      54.28
 H       2.199892     1.795095     0.022567      28.72
 C       0.971383    -1.164677    -0.713350      41.97
 H       1.290484    -2.355372    -0.934114      20.95
 C      -0.446825    -0.872606    -0.588271      21.20
 O      -1.351214    -1.799970    -0.989176     190.73
 C      -1.328012    -1.745089    -2.421182      76.47
 H      -2.078368    -2.492735    -2.887577      24.73
 H      -1.990094    -0.466430    -2.657444      21.73
 H      -0.418939    -2.062585    -2.935929      26.28
 C      -0.753509     0.408172    -0.211860      22.47
 O      -2.142344     0.665637    -0.008963     210.92
 C       0.174017     1.459963    -0.073593      77.91
 H      -0.002301     2.502533    -0.000414      23.30
 C       1.914535    -0.193526    -0.554661      27.12
 C       3.356514    -0.841081    -0.332246     112.82
 H       3.378993    -1.700884    -0.902124      29.71
 O       4.233444     0.157080    -0.952098     142.89
 H       4.582305     0.746019    -0.041304      18.41
 C       4.000965    -1.195975     0.996201      97.32
 H       3.364476    -2.003947     1.463500      27.87
 O       5.445664    -1.942716     0.944498     113.87
 H       5.655796    -2.160638     0.116288      33.55
 C       4.007357    -0.163424     2.084033      94.93
 O       4.656005     0.985772     1.462661     148.71
 H       4.178683     1.784804     1.873021      26.22
 H       4.510535    -0.545816     3.067138      25.98
 H       2.752412     0.140671     2.470866      23.77
55
name = lig-Water-frame_640
 C      -1.421191     3.373743     3.157617      58.35
 H      -2.117771     3.867753     2.609565      22.44
 C      -1.067514     1.034594     3.409596      57.69
 H      -1.460745     0.009682     3.185746      21.89
 C       0.003418     1.247163     4.152092       7.49
 O       0.884008     0.327504     4.581305     174.10
 C       0.319934    -1.058532     4.698917     108.80
 H       1.103598    -1.818421     5.121614      26.41
 H      -0.010179    -1.611146     3.814896      27.76
 H      -0.723058    -1.077265     5.371878      25.29
 C       0.462913     2.623503     4.420686       2.41
 O       1.644034     2.858673     5.257049      61.20
 H       1.509474     3.798669     5.655587      25.58
 C      -0.262424     3.585901     3.799603      52.61
 H       0.101468     4.679516     4.068962      24.54
 C      -1.980316     2.086069     3.079251     -13.94
 C      -3.232716     1.870888     2.015825      78.67
 H      -3.939313     2.630941     1.992468      28.17
 O      -3.878562     0.704400     2.387851     263.82
 H      -4.886079     0.769946     2.259391      24.87
 C      -2.787370     1.867822     0.321311      96.15
 H      -2.156089     2.683139     0.243426      29.80
 C      -3.950537     1.959402    -0.595122      98.27
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 O      -4.855295     0.872527    -0.556933     282.31
 H      -4.453803    -0.026367    -0.696132      27.81
 H      -3.534462     2.109577    -1.570810      29.16
 H      -4.577267     2.981200    -0.186561      25.19
 C       1.549055     1.105554    -0.184946      55.44
 H       2.243941     2.164281    -0.026469      20.18
 C       0.919722    -1.148811    -0.738259      49.61
 H       1.318554    -2.064274    -0.969467      25.74
 C      -0.419599    -0.876395    -0.617696      17.11
 O      -1.360090    -1.877079    -0.985023     231.61
 C      -1.371397    -1.748414    -2.458097      95.75
 H      -2.195249    -2.375458    -2.844649      25.88
 H      -1.724983    -1.004202    -2.868610      30.86
 H      -0.193143    -1.732528    -2.686384      25.82
 C      -0.735837     0.392608    -0.119790      10.69
 O      -2.191909     0.621064    -0.054954     177.15
 C       0.237286     1.472165    -0.119499      58.28
 H      -0.124114     2.460088     0.342708      21.50
 C       1.930422    -0.197530    -0.510844      44.14
 C       3.333389    -0.865536    -0.437329      86.97
 H       3.269353    -1.848102    -1.248720      25.59
 O       4.297347     0.141894    -0.997932     208.36
 H       4.424093     0.561669    -0.224052      30.90
 C       3.968078    -1.266533     1.050250      89.63
 H       3.481424    -2.277802     1.245602      27.69
 O       5.431135    -1.888687     0.947681      28.49
 H       5.758365    -2.156816    -0.066993      25.03
 C       4.002210    -0.169137     2.039854     148.41
 O       4.671003     1.001227     1.476693     194.95
 H       4.204103     1.746534     1.943552      27.56
 H       4.558839    -0.428388     2.898518      31.58
 H       3.154311     0.084719     2.407633      31.67
55
name = lig-Water-frame_641
 C      -1.517511     3.416915     3.123005      35.52
 H      -2.190412     4.344151     2.636412      19.75
 C      -1.083877     0.957240     3.400275      46.71
 H      -1.378970    -0.001606     3.089372      23.66
 C       0.047465     1.220155     4.188914      13.00
 O       0.906940     0.286191     4.597407     202.00
 C       0.333500    -1.018094     4.737962     124.34
 H       1.096377    -1.455645     5.307924      27.02
 H       0.193566    -1.483393     3.666691      26.15
 H      -0.484535    -1.154746     5.338206      29.52
 C       0.487962     2.593136     4.496624     -11.93
 O       1.636600     2.828726     5.235292     -22.36
 H       1.516543     3.816572     5.477562      24.38
 C      -0.241052     3.673789     3.801714      65.60
 H      -0.058142     4.655751     3.988658      26.99
 C      -1.973892     2.127166     3.021256      -9.44
 C      -3.167659     1.842827     2.046686      59.73
 H      -3.860259     2.838697     1.811134      24.93
 O      -3.909974     0.684367     2.450676     267.97
 H      -4.845686     0.802996     2.166794      27.57
 C      -2.791035     1.835227     0.304378      74.58
 H      -2.053771     2.763486     0.210494      26.27
 C      -4.036701     1.991652    -0.579052     105.28
 O      -4.890366     0.849202    -0.532112     249.46
 H      -4.266144     0.017060    -0.676904      25.25
 H      -3.333756     2.044162    -1.549549      25.66
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 H      -4.552184     2.765491    -0.207604      28.79
 C       1.635814     1.114703    -0.123313      65.95
 H       2.277480     1.927890    -0.164698      24.69
 C       0.904178    -1.127029    -0.758673      52.09
 H       1.276300    -2.195512    -1.130589      24.00
 C      -0.410269    -0.888354    -0.626043       3.10
 O      -1.373703    -1.925689    -0.988898     161.93
 C      -1.389623    -1.806011    -2.474708      72.12
 H      -2.047427    -2.674079    -2.803011      25.34
 H      -1.704900    -0.517222    -3.152408      22.49
 H      -0.410101    -1.761009    -2.719861      27.95
 C      -0.794034     0.434421    -0.060482       3.10
 O      -2.195748     0.557436    -0.095373     146.13
 C       0.224658     1.458808    -0.117010      72.16
 H      -0.109742     2.294346     0.496889      23.41
 C       1.969748    -0.237721    -0.436049      37.07
 C       3.343854    -0.860306    -0.565356      88.47
 H       3.327618    -1.662661    -1.089833      31.17
 O       4.351428     0.098340    -1.065735     147.36
 H       4.523297     0.817420    -0.186401      19.95
 C       3.940701    -1.410503     1.022889      84.95
 H       3.397081    -2.266126     1.309053      29.87
 O       5.405605    -1.816775     0.936136     105.24
 H       5.589438    -1.992989    -0.056493      25.85
 C       4.050109    -0.181035     2.006105      94.47
 O       4.680235     1.022072     1.495725     164.08
 H       4.138433     1.792342     1.953933      24.91
 H       4.736779    -0.494240     2.872025      26.37
 H       2.836220     0.139574     2.445525      23.67
55
name = lig-Water-frame_642
 C      -1.596671     3.503005     3.101724      58.10
 H      -1.917518     4.430115     2.914002      20.74
 C      -1.151408     0.957803     3.388769      34.86
 H      -1.303448    -0.120146     3.036747      21.32
 C       0.093561     1.258509     4.212835       9.65
 O       0.941589     0.237051     4.633643     176.33
 C       0.393852    -1.016216     4.750525     104.04
 H       1.252777    -1.427118     5.378430      24.82
 H       0.380336    -1.391513     3.782966      28.68
 H      -0.688682    -1.047829     5.422978      24.99
 C       0.447738     2.580729     4.502514      18.49
 O       1.618075     2.806447     5.208953      95.02
 H       1.646103     3.822778     5.448573      21.19
 C      -0.241134     3.718662     3.831294      87.79
 H      -0.006276     4.889353     3.974806      26.96
 C      -1.953883     2.092892     2.907191      16.27
 C      -3.110171     1.844088     2.024053      92.13
 H      -3.614050     2.735040     2.072773      27.71
 O      -3.931999     0.675525     2.507113     270.65
 H      -4.930255     0.723290     2.143476      25.14
 C      -2.773663     1.797180     0.375547      95.07
 H      -2.144960     2.567824     0.101799      28.95
 C      -4.048312     1.986181    -0.571401      85.14
 O      -4.925782     0.814956    -0.514337     281.45
 H      -4.304061     0.138113    -0.625220      29.15
 H      -3.708659     2.151384    -1.591862      28.14
 H      -4.826455     3.004513    -0.338852      23.22
 C       1.672974     1.091001    -0.092862      58.30
 H       2.596591     1.889239    -0.128172      21.58
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 C       0.959309    -1.153134    -0.774633      31.96
 H       1.038150    -2.150101    -1.273028      23.62
 C      -0.453791    -0.873202    -0.591005     -12.18
 O      -1.377943    -1.923888    -1.011026     187.54
 C      -1.450158    -1.812772    -2.511505      97.12
 H      -1.773696    -2.867880    -2.838983      24.36
 H      -1.711890    -0.960281    -2.744268      30.20
 H      -0.332911    -2.065171    -3.029445      25.56
 C      -0.851003     0.433857    -0.085779      15.56
 O      -2.184077     0.514895    -0.120074     178.04
 C       0.193325     1.411666    -0.043635      73.19
 H       0.022712     2.404278     0.417232      25.17
 C       2.002956    -0.274419    -0.370845      31.10
 C       3.399572    -0.797066    -0.600701      83.24
 H       3.432263    -1.905566    -1.266892      24.48
 O       4.400256     0.068217    -1.112402     165.44
 H       4.605411     0.748066    -0.503443      30.11
 C       3.946695    -1.490685     0.939779      78.71
 H       3.155634    -2.202765     1.522998      27.38
 O       5.357362    -1.743972     0.904783     144.98
 H       5.492801    -1.863214     0.018739      29.14
 C       4.047850    -0.210094     2.018954     103.49
 O       4.675562     1.048091     1.506195     217.56
 H       4.107736     1.757956     1.875395      29.10
 H       4.661475    -0.586812     2.820950      28.38
 H       3.122497    -0.037246     2.293789      29.01
55
name = lig-Water-frame_643
 C      -1.540036     3.527377     3.154594      52.36
 H      -2.089512     4.618827     2.925528      15.31
 C      -1.166277     1.023529     3.399140      47.29
 H      -1.325376     0.019084     3.106098      22.07
 C       0.069620     1.272219     4.185994      12.80
 O       0.981778     0.264481     4.673885     188.56
 C       0.448435    -1.059588     4.814873     118.04
 H       1.175633    -1.734830     5.286482      27.50
 H       0.388617    -1.657510     3.755165      27.55
 H      -0.457385    -0.979170     5.155768      32.39
 C       0.378265     2.635649     4.453346      17.98
 O       1.612711     2.800225     5.187230     185.91
 H       1.593247     3.714870     5.513122      20.97
 C      -0.310318     3.730374     3.862529      12.24
 H       0.132557     4.644637     4.044964      28.05
 C      -1.890379     2.050743     2.800368       2.31
 C      -3.090978     1.811412     1.955429      83.46
 H      -3.713231     2.804137     2.312193      22.75
 O      -3.942601     0.693115     2.538626     277.65
 H      -4.861092     0.681325     2.283551      26.41
 C      -2.801607     1.749965     0.456231      87.82
 H      -2.049757     2.565095     0.072992      21.47
 C      -4.095973     2.001781    -0.539298      86.05
 O      -4.961837     0.799451    -0.499431     261.85
 H      -4.396782    -0.031990    -0.582454      25.74
 H      -3.950356     2.240346    -1.715078      25.12
 H      -4.652247     2.777412    -0.410723      27.42
 C       1.649605     1.040326    -0.083431      42.63
 H       2.534886     1.727673     0.122490      24.97
 C       0.955773    -1.180739    -0.768382      39.73
 H       1.099420    -2.134403    -1.325743      23.16
 C      -0.444516    -0.871148    -0.554310      12.42
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 O      -1.362777    -1.885700    -1.044180     204.24
 C      -1.419710    -1.945907    -2.529631      76.76
 H      -2.013046    -2.777346    -2.871809      26.15
 H      -2.237919    -0.723165    -2.687768      20.40
 H      -0.555396    -2.023963    -3.017013      29.36
 C      -0.844085     0.383627    -0.168624      13.37
 O      -2.210226     0.510409    -0.116744     190.99
 C       0.218461     1.374229     0.078915      71.44
 H       0.078929     2.511230     0.117555      21.59
 C       2.025141    -0.304388    -0.352281      18.72
 C       3.475757    -0.818416    -0.569968     105.01
 H       3.441939    -1.543223    -1.206223      30.79
 O       4.450049     0.040661    -1.179734     143.99
 H       4.682986     0.761665    -0.454977      28.08
 C       3.934674    -1.430852     0.886267     109.86
 H       3.295382    -2.099428     1.323741      30.82
 O       5.308336    -1.702023     0.862925      75.22
 H       5.656974    -1.887477    -0.194855      19.72
 C       4.059842    -0.266713     1.990360      81.99
 O       4.665275     1.045583     1.507165     175.02
 H       4.024158     1.792827     1.901568      25.91
 H       4.592155    -0.647493     2.911819      28.72
 H       2.837659    -0.015562     2.434008      24.44
55
name = lig-Water-frame_644
 C      -1.476037     3.518559     3.197159      33.90
 H      -2.188243     4.129367     2.837735      19.55
 C      -1.112968     1.091325     3.419629      54.88
 H      -1.462769     0.051078     3.185083      23.98
 C       0.017286     1.278992     4.149078      18.91
 O       1.011433     0.328947     4.704395     133.96
 C       0.526513    -1.145962     4.810202     103.67
 H       1.088060    -1.875165     5.400289      28.25
 H       0.347663    -1.642989     3.926048      29.99
 H      -0.686761    -1.043347     5.213981      25.35
 C       0.346697     2.658645     4.400219      23.23
 O       1.595824     2.807059     5.154395     119.38
 H       1.435942     3.750655     5.663906      24.29
 C      -0.390375     3.707502     3.908108      34.93
 H       0.184866     4.677422     4.154613      24.05
 C      -1.803108     2.090739     2.743374     -33.04
 C      -3.142782     1.792370     1.928994      93.46
 H      -3.724978     2.614571     2.016389      26.53
 O      -3.915987     0.721979     2.554907     242.89
 H      -4.952074     0.803933     2.310172      21.86
 C      -2.848863     1.744711     0.437969     100.14
 H      -2.139913     2.535076     0.356035      24.77
 C      -4.122535     1.950112    -0.524801      73.08
 O      -5.001461     0.797935    -0.485226     239.40
 H      -4.545866    -0.138457    -0.508423      24.81
 H      -3.780942     2.165078    -1.535904      27.15
 H      -4.817463     2.965202    -0.013195      22.95
 C       1.578256     0.958728    -0.049520      50.61
 H       2.328173     1.754538     0.310107      27.03
 C       0.937485    -1.195619    -0.737821      47.68
 H       1.338762    -2.167751    -1.279304      23.92
 C      -0.381445    -0.935190    -0.574639      25.21
 O      -1.333467    -1.845088    -1.071323     253.33
 C      -1.481386    -2.008534    -2.516694      90.16
 H      -2.391230    -2.683570    -2.731006      23.85
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 H      -2.119919    -1.248785    -2.879421      28.22
 H      -0.410274    -1.787230    -3.099227      25.02
 C      -0.802106     0.375104    -0.232153     -11.36
 O      -2.253492     0.519216    -0.089698     168.95
 C       0.272324     1.345725     0.172450      91.65
 H      -0.020674     2.345286     0.001047      24.52
 C       2.020880    -0.338659    -0.386130      32.40
 C       3.514451    -0.834241    -0.476133      88.26
 H       3.380540    -1.711113    -1.322286      28.55
 O       4.503994     0.048954    -1.227366      86.21
 H       4.771078     0.650801    -0.360450      27.39
 C       3.943452    -1.249464     0.838716     114.49
 H       3.328547    -2.307152     1.039679      27.90
 O       5.311510    -1.702465     0.784017     118.72
 H       5.696198    -1.941872    -0.063191      24.20
 C       3.988031    -0.292481     1.976277     130.25
 O       4.637487     1.014442     1.509095     208.00
 H       4.097511     1.687982     1.979587      29.80
 H       4.550636    -0.631370     2.862192      31.08
 H       3.104830    -0.039910     2.385604      30.81
55
name = lig-Water-frame_645
 C      -1.505859     3.413785     3.148516      80.28
 H      -2.341316     4.114035     2.668333      18.78
 C      -1.083338     1.085795     3.389666      44.93
 H      -1.541974     0.097850     3.318855      27.75
 C       0.037828     1.302907     4.160432      20.08
 O       1.009751     0.369558     4.722698      77.82
 C       0.522042    -1.190388     4.813644      97.57
 H       1.171435    -1.679620     5.592712      27.61
 H       0.426653    -1.588688     3.684840      27.45
 H      -0.332927    -1.225846     5.285473      30.73
 C       0.381153     2.608659     4.378648      31.24
 O       1.550298     2.850539     5.122694      51.21
 H       1.433761     3.663570     5.620678      42.37
 C      -0.379008     3.733222     4.006190      52.10
 H      -0.131095     4.788600     4.206048      19.40
 C      -1.749540     2.184134     2.740325     -19.21
 C      -3.174536     1.771947     1.941511      66.81
 H      -3.868118     2.801301     1.755373      25.62
 O      -3.896586     0.754998     2.556373     261.43
 H      -4.841489     0.920544     2.344866      25.55
 C      -2.906853     1.738296     0.376102      95.91
 H      -2.240454     2.679963     0.412933      20.95
 C      -4.152250     1.921576    -0.445871     106.57
 O      -5.057451     0.794246    -0.476812     296.23
 H      -4.581748     0.006099    -0.403451      30.41
 H      -3.610658     2.149506    -1.472379      25.41
 H      -4.648918     2.582785    -0.000509      29.30
 C       1.554898     0.889383     0.016536      53.20
 H       2.199881     1.831456     0.392946      25.53
 C       1.013229    -1.251198    -0.721551      52.07
 H       1.295218    -2.157029    -1.103044      26.40
 C      -0.363992    -0.984137    -0.641297      18.50
 O      -1.314177    -1.821291    -1.083280     248.28
 C      -1.547875    -2.046048    -2.499689      83.63
 H      -2.157612    -2.943584    -2.509885      25.30
 H      -2.127967    -1.080923    -3.285123      23.83
 H      -0.664196    -2.037629    -3.018697      29.56
 C      -0.768740     0.390864    -0.240752      -0.69
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 O      -2.254880     0.519090    -0.063109     169.46
 C       0.239266     1.277212     0.198196      83.96
 H      -0.110013     2.395135     0.194024      21.82
 C       2.000440    -0.353843    -0.432487      49.22
 C       3.480390    -0.820703    -0.489399      97.23
 H       3.475950    -1.848736    -0.908674      31.82
 O       4.542230     0.076335    -1.222018     138.72
 H       4.885492     0.563898    -0.548800      32.07
 C       3.974756    -1.161009     0.816855     121.32
 H       3.430795    -1.998169     0.892519      33.54
 O       5.358704    -1.717915     0.726769     122.28
 H       5.614981    -1.989273    -0.154356      26.17
 C       3.945394    -0.265631     1.973754     129.91
 O       4.607978     0.952602     1.509913     175.16
 H       4.141188     1.721777     2.060238      26.45
 H       4.591882    -0.718018     2.743646      32.01
 H       2.779622     0.028084     2.431076      27.05
55
name = lig-Water-frame_646
 C      -1.551151     3.419780     3.093162      70.89
 H      -2.058120     4.278792     2.779399      22.27
 C      -1.075264     1.052071     3.335177      57.32
 H      -1.510838     0.064608     3.341495      29.84
 C       0.094091     1.275881     4.179547      -8.94
 O       0.971902     0.369748     4.736869      67.06
 C       0.545042    -1.175948     4.787035     100.79
 H       1.412523    -1.416581     5.372324      30.03
 H       0.658946    -1.521736     3.827158      31.63
 H      -0.516592    -1.315220     5.457863      26.40
 C       0.441816     2.634806     4.391696      12.97
 O       1.522744     2.884308     5.100451     103.75
 H       1.487314     3.865826     5.556395      26.93
 C      -0.400840     3.744492     4.065140      75.57
 H      -0.362251     4.812386     4.327456      18.38
 C      -1.784464     2.136536     2.742447      41.63
 C      -3.169577     1.840206     1.932646      86.70
 H      -3.717329     2.688087     1.970388      29.09
 O      -3.881012     0.787032     2.557484     275.86
 H      -4.883030     0.857388     2.373026      26.01
 C      -2.920416     1.720608     0.374097      93.59
 H      -2.444412     2.690362     0.084149      25.39
 C      -4.140418     1.857965    -0.405410      87.52
 O      -5.119325     0.790997    -0.477946     246.32
 H      -4.527768    -0.023252    -0.283951      28.31
 H      -3.839071     2.222792    -1.444200      27.09
 H      -4.846486     2.874591     0.055447      24.12
 C       1.568288     0.884942     0.105486      59.85
 H       2.282196     1.621927     0.325904      26.27
 C       1.063581    -1.333256    -0.727444      95.91
 H       1.255856    -2.503015    -1.033701      26.37
 C      -0.348829    -0.943922    -0.711642      24.07
 O      -1.328053    -1.820160    -1.092049     231.84
 C      -1.636372    -2.059026    -2.509767      84.67
 H      -1.860198    -3.198276    -2.417291      23.43
 H      -2.109956    -1.178306    -3.062312      25.33
 H      -0.576603    -2.465234    -3.072840      25.22
 C      -0.787391     0.350524    -0.222744      20.33
 O      -2.204842     0.510424    -0.052207     200.51
 C       0.145817     1.233781     0.179260      51.47
 H       0.009774     2.181523     0.617478      27.42
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 C       2.015846    -0.335245    -0.467121      50.69
 C       3.444493    -0.754732    -0.558657      82.82
 H       3.559211    -1.897894    -0.971202      31.10
 O       4.537710     0.086151    -1.221272      97.33
 H       5.101546     0.670293    -0.453922      25.34
 C       4.031527    -1.147537     0.819845      89.12
 H       3.229738    -2.038115     1.209758      31.84
 O       5.422428    -1.727476     0.695059      32.50
 H       5.412607    -2.030683    -0.389870      24.11
 C       3.900483    -0.196792     2.002486     143.40
 O       4.579351     0.909765     1.523466     212.83
 H       4.210825     1.715627     1.985763      28.29
 H       4.489821    -0.776112     2.763680      32.09
 H       2.866609    -0.144415     2.253372      32.71
55
name = lig-Water-frame_647
 C      -1.510208     3.503396     3.113929      25.61
 H      -1.970411     4.504125     2.780901      18.30
 C      -1.038143     1.012448     3.311460      79.50
 H      -1.413468    -0.055338     3.207745      30.05
 C       0.106350     1.257490     4.147179     -14.80
 O       0.914709     0.334412     4.753738     144.62
 C       0.581269    -1.090549     4.803246     129.11
 H       1.587181    -1.423018     5.192024      28.32
 H       0.688610    -1.613958     3.744385      28.74
 H      -0.307072    -1.380484     5.235171      31.27
 C       0.434742     2.712335     4.396848       1.80
 O       1.564151     2.934659     5.128378     230.45
 H       1.618015     3.873842     5.413354      22.04
 C      -0.490837     3.700754     4.040405      60.57
 H      -0.388681     4.745175     4.549311      24.35
 C      -1.883404     2.016099     2.736791     -29.03
 C      -3.101573     1.908268     1.924423      76.54
 H      -3.723474     2.919046     2.244526      22.85
 O      -3.875940     0.809876     2.556176     263.70
 H      -4.899864     0.767168     2.334031      24.64
 C      -2.890783     1.710529     0.405506      86.98
 H      -2.423083     2.576716    -0.130733      25.64
 C      -4.220261     1.864443    -0.395060     107.17
 O      -5.158921     0.767851    -0.482325     252.18
 H      -4.701040    -0.104705    -0.178754      28.67
 H      -4.077688     2.202872    -1.497782      27.11
 H      -4.621831     2.683576    -0.117178      31.15
 C       1.542928     0.881395     0.157499      41.74
 H       2.571763     1.589032     0.354056      24.57
 C       1.036912    -1.417428    -0.755723      42.51
 H       1.254682    -2.357641    -0.965226      26.72
 C      -0.304755    -0.894757    -0.783215      23.49
 O      -1.360526    -1.831911    -1.096492     207.04
 C      -1.616919    -2.165960    -2.509067      96.40
 H      -2.183707    -3.090264    -2.482552      27.47
 H      -2.407138    -1.202352    -2.891437      24.03
 H      -0.754256    -2.352754    -3.025027      29.56
 C      -0.849532     0.274953    -0.203607      20.28
 O      -2.149177     0.490220    -0.050237     191.43
 C       0.145629     1.225303     0.180661      52.38
 H      -0.043202     1.988213     1.041234      29.27
 C       2.028304    -0.317812    -0.491396      26.79
 C       3.482609    -0.715702    -0.596487      92.75
 H       3.478869    -1.547490    -1.370174      32.44
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 O       4.515524     0.109434    -1.218757     157.05
 H       4.980336     0.523186    -0.458751      30.22
 C       4.030266    -1.222622     0.862977     105.55
 H       3.463222    -1.904293     1.325321      34.64
 O       5.454842    -1.728234     0.650671     106.82
 H       5.398524    -2.051201    -0.210188      30.93
 C       3.916138    -0.200966     2.000355     119.52
 O       4.575046     0.923593     1.540499     199.05
 H       4.153354     1.733835     1.955424      29.26
 H       4.287829    -0.631953     2.965392      31.17
 H       2.666257    -0.100341     2.221659      30.54
55
name = lig-Water-frame_648
 C      -1.494644     3.518398     3.124154      31.12
 H      -2.059490     4.367964     2.717243      18.45
 C      -1.018619     0.960788     3.294884      60.52
 H      -1.195085    -0.049975     3.045721      27.68
 C       0.088962     1.316511     4.088097       3.54
 O       0.858634     0.306324     4.774684     191.46
 C       0.695687    -1.023821     4.754530     139.25
 H       1.456741    -1.611831     5.300132      28.06
 H       0.475412    -1.472530     3.802396      29.59
 H      -0.348538    -1.432212     5.308697      26.96
 C       0.387581     2.706171     4.397227      -0.52
 O       1.633637     2.966750     5.153094     190.36
 H       1.688648     3.972401     5.555218      18.43
 C      -0.552775     3.676737     4.029392      57.21
 H      -0.356889     4.551046     4.541143      26.37
 C      -1.902160     2.006398     2.787977     -26.04
 C      -3.075079     1.954574     1.939397      88.71
 H      -3.536110     2.881049     2.073193      26.14
 O      -3.874583     0.825682     2.539906     280.28
 H      -4.821859     0.884123     2.241808      26.94
 C      -2.859789     1.724397     0.389762      63.97
 H      -2.151492     2.514253    -0.063581      23.75
 C      -4.283158     1.836357    -0.433404      69.92
 O      -5.197710     0.723161    -0.481047     264.94
 H      -4.889666    -0.068285    -0.113939      30.87
 H      -4.046586     2.031607    -1.548442      25.65
 H      -4.807994     2.930452     0.127191      23.67
 C       1.556777     0.869061     0.146561      55.46
 H       2.222217     1.522744     0.463560      27.70
 C       1.001840    -1.361059    -0.778928      47.45
 H       1.331514    -2.487480    -1.097982      23.69
 C      -0.305528    -0.924088    -0.860611      25.57
 O      -1.386864    -1.856474    -1.098498     210.09
 C      -1.644437    -2.249994    -2.465882      93.23
 H      -2.572886    -2.982195    -2.533420      23.79
 H      -2.401072    -1.443562    -2.924123      24.89
 H      -0.613658    -2.142462    -3.231635      24.33
 C      -0.821164     0.254803    -0.179459       1.01
 O      -2.155762     0.453252    -0.040764     157.90
 C       0.191258     1.225061     0.247685      47.89
 H      -0.215850     1.782462     1.032653      26.62
 C       1.994466    -0.328319    -0.497363      34.90
 C       3.530924    -0.709010    -0.602597      96.12
 H       3.411843    -1.411842    -1.390317      32.26
 O       4.482118     0.148276    -1.214219     181.94
 H       4.892352     0.561813    -0.422914      28.70
 C       4.039528    -1.300601     0.889557      89.22
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 H       3.460214    -2.350924     1.266130      28.36
 O       5.460474    -1.717074     0.640213      55.53
 H       5.489418    -2.210497    -0.238890      27.08
 C       3.909710    -0.251786     1.998404     127.19
 O       4.597461     0.980395     1.555987     217.48
 H       3.972389     1.732494     1.979365      27.52
 H       4.164682    -0.423728     3.072505      30.67
 H       2.879794     0.076050     2.009546      29.61
55
name = lig-Water-frame_649
 C      -1.567195     3.415051     3.086376      57.05
 H      -2.222619     4.182956     2.684585      20.42
 C      -1.034824     0.959820     3.264585      60.80
 H      -1.042243    -0.123556     2.898957      24.75
 C       0.083037     1.358791     4.055010       3.12
 O       0.832253     0.361304     4.796836     179.06
 C       0.723611    -1.059716     4.711165     131.01
 H       1.442462    -1.608437     5.351491      27.71
 H       0.459857    -1.361004     3.645009      28.21
 H      -0.105745    -1.226236     5.349547      29.49
 C       0.374781     2.644621     4.430014       4.53
 O       1.671421     2.980127     5.142780      26.99
 H       1.556638     3.805154     5.781967      27.88
 C      -0.524015     3.677697     4.070831      88.90
 H      -0.304888     4.788417     4.486910      19.59
 C      -1.818606     2.089249     2.876369      28.78
 C      -3.066810     1.917475     1.933794      63.02
 H      -3.620088     3.028048     1.822480      25.93
 O      -3.864759     0.855323     2.504597     256.66
 H      -4.879196     1.011732     2.211256      22.99
 C      -2.824094     1.739702     0.337379      76.02
 H      -2.118857     2.524815     0.123068      27.65
 C      -4.314153     1.841967    -0.450338     101.44
 O      -5.241281     0.680587    -0.485399     241.91
 H      -4.861896    -0.127778     0.064790      27.05
 H      -3.978290     2.030953    -1.481970      27.16
 H      -4.840941     2.499457     0.017416      29.88
 C       1.551313     0.844052     0.095834      50.44
 H       2.170155     1.760983     0.728380      24.26
 C       1.009369    -1.278663    -0.829858      59.41
 H       1.278635    -2.201397    -1.226614      26.31
 C      -0.389744    -0.978450    -0.903432      19.80
 O      -1.401491    -1.895975    -1.102967     237.45
 C      -1.697911    -2.289006    -2.445603     115.09
 H      -2.376814    -3.149822    -2.480620      27.00
 H      -2.230496    -1.372820    -3.071847      25.69
 H      -0.904926    -2.282448    -3.114128      28.79
 C      -0.719776     0.276120    -0.175486      -2.53
 O      -2.203112     0.403918    -0.020619     129.66
 C       0.198998     1.162902     0.324563      53.99
 H      -0.221877     1.977637     0.997626      26.20
 C       1.968533    -0.343215    -0.479911      39.39
 C       3.521235    -0.732459    -0.561176      74.79
 H       3.459644    -1.804356    -1.263145      28.29
 O       4.451756     0.203939    -1.197957     119.45
 H       4.863991     0.864589    -0.380574      22.47
 C       4.051019    -1.417654     0.884440     105.39
 H       3.567350    -2.309672     0.900471      32.76
 O       5.458414    -1.699575     0.651460      33.70
 H       5.562500    -2.451773    -0.175288      22.72
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 C       3.919137    -0.278870     1.979078     105.81
 O       4.625556     1.039526     1.572013     163.17
 H       3.985837     1.682034     1.963158      30.57
 H       4.200359    -0.490577     3.004669      31.17
 H       2.753548     0.062394     1.879402      26.94
55
name = lig-Water-frame_650
 C      -1.597368     3.351408     3.129680      48.74
 H      -2.365817     4.093978     2.714479      20.12
 C      -1.024578     0.999337     3.246817      86.22
 H      -1.145029     0.036227     2.839672      27.36
 C       0.081743     1.292505     4.057564       0.77
 O       0.846769     0.462678     4.813326     153.33
 C       0.694780    -1.102870     4.671737     102.80
 H       1.681752    -1.431674     5.097209      27.53
 H       0.681956    -1.417676     3.595630      28.48
 H      -0.248637    -1.267574     5.363830      25.67
 C       0.395867     2.661838     4.494746     -17.21
 O       1.655860     2.953619     5.108161     -70.83
 H       1.457262     3.726082     5.733974      33.66
 C      -0.473747     3.719443     4.096882      52.67
 H      -0.320105     4.702059     4.249767      15.99
 C      -1.788979     2.101642     2.877092      53.37
 C      -3.057988     1.883086     1.902794      72.57
 H      -3.632511     2.750357     1.792758      29.02
 O      -3.864995     0.896124     2.459377     297.56
 H      -4.845600     0.941059     2.319807      25.56
 C      -2.812266     1.701155     0.311444      69.03
 H      -2.177408     2.684708     0.079098      24.52
 C      -4.277471     1.791942    -0.460796      71.57
 O      -5.257314     0.622306    -0.490909     224.22
 H      -4.785501    -0.044676     0.096608      27.81
 H      -4.024112     2.212401    -1.589535      24.59
 H      -5.085595     2.667485     0.049721      23.09
 C       1.552540     0.900331     0.101660      50.60
 H       2.203262     1.498392     0.504374      31.58
 C       0.974273    -1.205824    -0.924639      37.30
 H       1.344789    -2.183265    -1.424239      25.85
 C      -0.451335    -0.982816    -0.875019      16.12
 O      -1.414782    -1.945230    -1.104568     221.29
 C      -1.775899    -2.291671    -2.447697      80.81
 H      -2.160677    -3.391575    -2.370252      24.20
 H      -2.287219    -1.311362    -2.996267      24.21
 H      -0.684237    -2.678900    -3.135059      23.88
 C      -0.718740     0.254571    -0.210720       9.42
 O      -2.230992     0.371273     0.001237     130.58
 C       0.189593     1.098712     0.403172      76.45
 H       0.058092     2.134739     0.740641      26.95
 C       2.005930    -0.344404    -0.452929      18.52
 C       3.480282    -0.817684    -0.510438      92.35
 H       3.621046    -1.724814    -1.025793      29.97
 O       4.415074     0.268434    -1.157304     133.50
 H       4.604479     0.859847    -0.528975      34.59
 C       4.086886    -1.439129     0.818538      92.78
 H       3.384597    -2.439846     0.867252      30.51
 O       5.471336    -1.710712     0.668862     119.22
 H       5.527760    -2.396659     0.125714      31.40
 C       3.916755    -0.284778     1.930339     107.01
 O       4.658480     1.050417     1.580419      90.97
 H       4.016693     1.796406     2.048296      27.37
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 H       4.282170    -0.693757     2.907432      32.61
 H       2.774019    -0.223723     1.972383      29.44
55
name = lig-Water-frame_651
 C      -1.569993     3.415460     3.266618      24.16
 H      -2.247851     4.110519     2.896401      24.93
 C      -0.978026     1.036556     3.248443      73.53
 H      -1.353418     0.052356     2.836532      26.93
 C       0.079927     1.254908     4.104721      14.18
 O       0.887469     0.503702     4.821072     177.19
 C       0.678610    -1.086277     4.648443     107.48
 H       1.676721    -1.331272     4.906892      27.44
 H       0.714352    -1.456878     3.624745      29.57
 H      -0.231332    -1.561836     5.145210      26.95
 C       0.390297     2.719470     4.521880     -14.66
 O       1.604057     2.905953     5.073289      14.79
 H       1.601119     3.864427     5.547007      27.61
 C      -0.453096     3.717748     4.065341      44.33
 H      -0.210562     4.890798     4.158721      21.94
 C      -1.854089     2.016143     2.771204     -20.64
 C      -3.025808     1.846963     1.847907      70.95
 H      -3.700167     2.883748     1.931604      23.25
 O      -3.858808     0.893912     2.439588     229.33
 H      -4.922586     0.930595     2.271080      22.15
 C      -2.830652     1.648622     0.312745      90.36
 H      -2.345456     2.462459    -0.117344      26.28
 C      -4.268017     1.782543    -0.465348     100.30
 O      -5.220683     0.572529    -0.500737     262.15
 H      -4.800954    -0.104617    -0.002480      30.02
 H      -4.172112     2.122169    -1.477155      27.52
 H      -4.741388     2.598600    -0.115572      28.38
 C       1.562534     0.904355     0.114600      38.72
 H       2.551004     1.629152     0.416879      28.24
 C       0.938492    -1.174759    -1.044564      38.78
 H       1.309145    -2.116957    -1.536273      26.14
 C      -0.445481    -0.961649    -0.815726      14.82
 O      -1.425269    -1.987844    -1.094065     240.88
 C      -1.770208    -2.333434    -2.490678      99.04
 H      -2.292468    -3.305431    -2.268290      25.94
 H      -2.507608    -1.514306    -2.930047      25.64
 H      -0.942314    -2.694932    -2.850651      30.46
 C      -0.845878     0.213381    -0.232974      13.37
 O      -2.223503     0.362795     0.013826     169.39
 C       0.211789     1.074916     0.434065      68.83
 H       0.057849     2.137719     0.602856      28.17
 C       2.025532    -0.347328    -0.436230      19.22
 C       3.453997    -0.864834    -0.466466      80.23
 H       3.725075    -1.730064    -1.397105      27.36
 O       4.350969     0.291619    -1.125985      23.35
 H       4.400071     1.014875    -0.298253      29.66
 C       4.082485    -1.381136     0.754431     108.30
 H       3.492839    -2.164080     1.187648      33.34
 O       5.490049    -1.728137     0.707221      68.18
 H       5.586667    -2.648390     0.136756      22.25
 C       3.940769    -0.322740     1.884242     105.97
 O       4.660797     1.027141     1.600159      75.77
 H       4.128594     1.671291     2.081690      31.61
 H       4.388626    -0.748745     2.780997      33.71
 H       2.785165    -0.243916     2.113720      29.58
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name = lig-Water-frame_652
 C      -1.572740     3.412751     3.369909       7.11
 H      -2.149489     4.411845     3.070361      21.02
 C      -0.964088     1.020310     3.225624      45.38
 H      -1.284121    -0.016157     3.065433      27.35
 C       0.065810     1.350296     4.179686      17.21
 O       0.934485     0.442711     4.827374     152.40
 C       0.697767    -1.036162     4.609090     108.81
 H       1.639156    -1.511316     5.097087      25.32
 H       0.550204    -1.280904     3.471477      28.69
 H      -0.118157    -1.624669     5.099847      27.73
 C       0.338726     2.714231     4.483425      17.42
 O       1.567246     2.889047     5.066851     144.90
 H       1.760865     3.779148     5.341028      24.19
 C      -0.433655     3.756975     4.022509      57.52
 H      -0.125953     4.723575     4.200455      24.54
 C      -1.878263     2.039325     2.701870     -81.55
 C      -3.035120     1.868565     1.793775      91.03
 H      -3.407543     2.836864     1.954812      25.46
 O      -3.869397     0.841529     2.439556     230.75
 H      -4.801480     0.977431     2.115913      25.48
 C      -2.893958     1.587462     0.303833      88.81
 H      -2.244870     2.373154    -0.343376      23.21
 C      -4.244932     1.723026    -0.463061      66.26
 O      -5.156713     0.550691    -0.513571     193.46
 H      -4.758975    -0.343876    -0.076640      24.18
 H      -4.121940     1.886708    -1.690496      23.55
 H      -4.714871     2.801757     0.087059      22.81
 C       1.635355     0.867359     0.142551      50.08
 H       2.262256     1.686442     0.299942      28.93
 C       0.953563    -1.143216    -1.125266      67.21
 H       1.157982    -2.081336    -1.593938      27.59
 C      -0.433641    -0.982749    -0.791314      10.02
 O      -1.423114    -2.004092    -1.070855     206.26
 C      -1.798849    -2.395132    -2.462175      69.26
 H      -2.623314    -3.210026    -2.298796      24.20
 H      -2.569946    -1.646388    -3.069166      25.29
 H      -0.657993    -2.654800    -3.157812      23.25
 C      -0.947904     0.226372    -0.184531       9.03
 O      -2.217756     0.353648     0.020469     184.42
 C       0.215721     1.076532     0.386083      41.33
 H      -0.220448     2.086189     0.690285      27.11
 C       1.972585    -0.385236    -0.455107      31.74
 C       3.456010    -0.881409    -0.557085     108.06
 H       3.487243    -1.484195    -1.334615      33.34
 O       4.277189     0.310516    -1.064502      85.19
 H       4.264873     0.938603    -0.245536      31.07
 C       4.081471    -1.281803     0.760158     104.50
 H       3.518486    -2.117102     1.383184      31.73
 O       5.505949    -1.767027     0.727923      68.87
 H       5.611684    -2.721523     0.266782      22.98
 C       3.989110    -0.348731     1.853195     119.64
 O       4.649353     0.966539     1.620853      84.82
 H       4.031182     1.639309     2.193140      26.05
 H       4.548487    -0.751379     2.723791      31.97
 H       2.921282    -0.042148     2.258720      27.86
55
name = lig-Water-frame_653
 C      -1.653255     3.400405     3.366899      54.55
 H      -2.097349     4.302449     3.184761      23.55
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 C      -0.980257     1.018366     3.222944      33.79
 H      -1.075874    -0.072023     3.214246      24.38
 C       0.022345     1.420760     4.232730       5.49
 O       0.962148     0.355729     4.827545     117.75
 C       0.745552    -0.996665     4.555396     128.49
 H       1.462818    -1.607000     5.048083      28.00
 H       0.578938    -1.068483     3.536810      32.11
 H      -0.199835    -1.353594     5.209392      26.72
 C       0.319274     2.689110     4.436595      34.93
 O       1.554869     2.873300     5.071615     168.01
 H       1.713249     3.886291     5.331886      22.14
 C      -0.406735     3.772751     4.001674      65.31
 H      -0.079534     4.839203     4.310198      21.65
 C      -1.802045     2.123436     2.727412      -5.63
 C      -3.046190     1.882813     1.776853      60.66
 H      -3.509270     3.017543     1.786765      25.33
 O      -3.862753     0.788158     2.434114     206.03
 H      -4.862647     0.898934     2.115249      24.24
 C      -2.924511     1.565140     0.243993     103.79
 H      -2.301758     2.277848    -0.134609      27.58
 C      -4.234051     1.664688    -0.485119     119.93
 O      -5.091512     0.522500    -0.512510     310.71
 H      -4.677022    -0.279295    -0.171911      28.63
 H      -3.964651     1.817802    -1.454869      29.52
 H      -4.713614     2.441476    -0.032160      28.99
 C       1.611974     0.801813     0.165142      55.53
 H       2.228852     1.807758     0.369112      26.36
 C       0.949762    -1.122922    -1.145118      57.26
 H       1.098407    -2.176023    -1.685786      26.40
 C      -0.450731    -0.997914    -0.797819      10.13
 O      -1.415777    -2.006599    -1.060816     216.21
 C      -1.803251    -2.458444    -2.435595     112.38
 H      -2.619479    -3.247119    -2.382628      26.25
 H      -2.227424    -1.599308    -3.103387      27.49
 H      -1.150174    -2.580123    -3.136274      30.81
 C      -0.875613     0.230555    -0.116411      10.71
 O      -2.270014     0.325169     0.033864     197.34
 C       0.169386     1.093658     0.287702      46.84
 H      -0.196563     1.920751     0.828657      26.72
 C       1.928344    -0.428145    -0.497649      30.45
 C       3.444393    -0.806633    -0.653115      90.80
 H       3.335165    -1.778588    -1.569077      26.43
 O       4.204656     0.321117    -1.000304     152.46
 H       4.266806     0.863248    -0.233306      32.26
 C       4.076488    -1.270508     0.783496      86.63
 H       3.471943    -2.130030     1.117186      34.41
 O       5.512528    -1.802558     0.733932     104.41
 H       5.486129    -2.615332     0.386451      32.64
 C       4.062308    -0.299414     1.900715     149.79
 O       4.627345     0.927860     1.650823     131.90
 H       4.053461     1.564234     2.096180      29.13
 H       4.614931    -0.822162     2.701062      34.61
 H       3.031113    -0.097331     2.226160      28.77
55
name = lig-Water-frame_654
 C      -1.680060     3.416070     3.332707      41.00
 H      -2.489090     4.248311     3.023755      22.75
 C      -0.980504     1.065500     3.284749      58.19
 H      -1.051535    -0.041699     3.036615      23.96
 C      -0.039221     1.321962     4.230238      -8.26
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 O       0.979195     0.346943     4.825539     120.49
 C       0.731243    -0.975756     4.536515     112.45
 H       1.584254    -1.675398     4.859308      26.55
 H       0.653875    -1.184708     3.337021      28.40
 H      -0.249738    -1.108854     5.037295      26.86
 C       0.375939     2.729530     4.428131      15.67
 O       1.561776     2.884879     5.087653     163.66
 H       1.467444     3.786698     5.460697      25.80
 C      -0.423686     3.772328     3.990151      68.63
 H      -0.224300     4.800840     4.330873      22.32
 C      -1.745373     2.169091     2.770396       7.14
 C      -3.066952     1.911076     1.801310      65.83
 H      -3.721599     2.740333     1.625788      26.81
 O      -3.843455     0.759376     2.416580     239.66
 H      -4.837075     0.761482     2.324250      27.61
 C      -2.909310     1.557377     0.241846      82.92
 H      -2.240798     2.520495    -0.062891      23.65
 C      -4.216687     1.574207    -0.518310      84.73
 O      -5.047300     0.479030    -0.510585     279.30
 H      -4.516706    -0.286776    -0.143429      26.17
 H      -3.773435     2.017581    -1.652340      22.98
 H      -4.984459     2.503713    -0.112876      24.02
 C       1.499717     0.757110     0.168992      59.78
 H       2.290435     1.502011     0.520890      26.29
 C       0.874218    -1.183262    -1.146864      54.92
 H       1.170220    -2.002381    -1.640313      26.06
 C      -0.469061    -0.988090    -0.823181      22.12
 O      -1.407072    -2.008672    -1.063389     198.24
 C      -1.837877    -2.469497    -2.390391      77.78
 H      -2.478458    -3.351834    -2.310332      25.07
 H      -2.211222    -1.360612    -2.931175      22.92
 H      -0.875459    -2.938058    -3.286433      23.33
 C      -0.781268     0.172567    -0.083281      24.23
 O      -2.312221     0.272907     0.043706     173.80
 C       0.139091     1.115754     0.199045      54.05
 H      -0.010736     1.959632     0.955473      23.66
 C       1.942445    -0.420781    -0.533942      17.17
 C       3.404695    -0.771807    -0.721451     106.33
 H       3.581037    -1.527576    -1.299234      32.30
 O       4.151042     0.344281    -0.984257     143.55
 H       4.387584     0.872651    -0.014374      23.68
 C       4.062189    -1.324333     0.753417      67.14
 H       3.359996    -2.204438     0.918505      31.45
 O       5.499791    -1.806317     0.728580      54.72
 H       5.320116    -2.818611     0.295438      25.26
 C       4.116348    -0.281525     1.993402     127.81
 O       4.634845     0.945624     1.667943     121.06
 H       4.019980     1.689126     2.063297      24.91
 H       4.605218    -0.829915     2.803391      32.90
 H       2.912310    -0.342714     2.252038      28.83
55
name = lig-Water-frame_655
 C      -1.675510     3.491397     3.279253      51.01
 H      -2.530997     3.966876     2.970937      19.53
 C      -0.999649     1.086509     3.331611      65.77
 H      -1.227326     0.215098     2.766512      25.96
 C      -0.001457     1.236329     4.249035      -7.37
 O       0.981301     0.417003     4.804831     164.40
 C       0.702641    -1.009911     4.474870     111.90
 H       1.541918    -1.554828     4.796802      28.64
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 H       0.687790    -1.263455     3.485319      32.33
 H      -0.417478    -1.287296     4.817664      26.40
 C       0.403290     2.719896     4.418087       0.38
 O       1.575735     2.924582     5.122388     147.64
 H       1.474037     3.754968     5.714802      26.76
 C      -0.486087     3.765617     3.993323      47.68
 H      -0.340493     4.806327     4.296781      24.55
 C      -1.786421     2.164525     2.782339     -19.33
 C      -3.092620     1.874698     1.835724      73.36
 H      -3.909122     2.739609     1.786683      23.68
 O      -3.800557     0.733486     2.410848     246.34
 H      -4.818678     0.883954     2.403563      25.91
 C      -2.844613     1.591987     0.303900      85.73
 H      -2.333655     2.369033    -0.133844      26.79
 C      -4.201101     1.591087    -0.588786     108.23
 O      -5.010928     0.398757    -0.515797     315.45
 H      -4.460298    -0.390389    -0.063766      23.48
 H      -3.963629     1.856631    -1.544814      29.20
 H      -4.854130     2.379235    -0.377861      27.46
 C       1.424210     0.693831     0.139390      57.23
 H       2.235051     1.248602     0.665867      26.40
 C       0.837409    -1.245038    -1.113388      44.48
 H       1.246026    -2.143568    -1.783963      22.28
 C      -0.479073    -1.000337    -0.865297      27.23
 O      -1.403707    -2.022187    -1.059950     257.02
 C      -1.797099    -2.446940    -2.407137     108.41
 H      -2.503468    -3.334215    -2.106046      25.31
 H      -2.374080    -1.537863    -2.733960      24.53
 H      -1.072882    -2.944198    -2.723801      29.85
 C      -0.819708     0.091734    -0.089874      17.06
 O      -2.291347     0.223080     0.046078     158.07
 C       0.144848     1.169504     0.181344      54.96
 H      -0.004268     2.006776     0.800739      24.38
 C       1.906322    -0.398690    -0.578642      36.03
 C       3.372089    -0.739042    -0.667186      76.78
 H       3.919003    -1.626077    -1.503992      25.27
 O       4.140433     0.426160    -0.984321     218.35
 H       4.426091     0.706259    -0.174068      31.71
 C       4.041743    -1.368048     0.729484      75.98
 H       3.343930    -2.248686     0.976843      31.02
 O       5.451583    -1.832896     0.682393      70.09
 H       5.445030    -2.741014     0.243147      27.89
 C       4.080283    -0.370030     2.065452     112.48
 O       4.654134     1.017196     1.681917     106.00
 H       4.044251     1.732957     2.093673      28.41
 H       4.660434    -0.716180     2.963081      30.87
 H       3.086156    -0.304704     2.371935      30.47
55
name = lig-Water-frame_656
 C      -1.654541     3.501068     3.202037      54.47
 H      -2.521070     4.267886     2.966431      22.21
 C      -1.061096     1.087286     3.321017      38.87
 H      -1.356557     0.194444     2.657409      25.63
 C       0.105118     1.286822     4.269771      15.27
 O       0.959956     0.459923     4.762955     115.43
 C       0.653917    -1.048676     4.425300      92.71
 H       1.483940    -1.550160     5.055195      26.55
 H       0.715132    -1.183860     3.212524      28.28
 H      -0.253612    -1.483311     4.751484      29.27
 C       0.358736     2.669883     4.405942      24.17
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 O       1.591660     2.988349     5.170558     229.44
 H       1.595793     3.775207     5.850030      28.57
 C      -0.540712     3.756947     4.022711      61.38
 H      -0.311916     4.862781     4.300593      18.76
 C      -1.880381     2.159360     2.800982       8.06
 C      -3.114995     1.822232     1.875732      98.44
 H      -3.697568     2.726361     2.108120      25.42
 O      -3.765406     0.702267     2.419150     285.72
 H      -4.699385     0.986700     2.343260      26.56
 C      -2.820938     1.604815     0.357224      63.55
 H      -2.114513     2.336230    -0.250170      23.45
 C      -4.165047     1.593744    -0.623228      56.33
 O      -4.974847     0.306353    -0.523479     260.15
 H      -4.571713    -0.393292    -0.018466      26.35
 H      -3.942950     1.563832    -1.888037      23.12
 H      -4.886874     2.606607    -0.343122      23.92
 C       1.427326     0.658373     0.099974      46.07
 H       2.180336     1.199634     0.883806      24.11
 C       0.904330    -1.318498    -1.100823      61.60
 H       1.032637    -2.162026    -1.690512      23.30
 C      -0.492211    -1.052629    -0.901247      25.38
 O      -1.412193    -2.035699    -1.033869     228.40
 C      -1.809827    -2.442344    -2.338628      76.29
 H      -2.592896    -3.103729    -2.085844      25.05
 H      -2.517035    -1.587741    -3.034975      22.66
 H      -0.661921    -3.059911    -2.808647      20.84
 C      -0.924059     0.099018    -0.114624      11.25
 O      -2.225851     0.203297     0.053074     146.02
 C       0.100808     1.158628     0.187874      38.07
 H      -0.191035     2.157153     0.646479      22.32
 C       1.818743    -0.433760    -0.643263      47.44
 C       3.420840    -0.753106    -0.600851      97.85
 H       3.557285    -1.342842    -1.353917      32.28
 O       4.139684     0.511749    -1.003194     164.52
 H       4.577235     0.871861    -0.071055      22.65
 C       4.005035    -1.383318     0.756045      96.66
 H       3.416042    -2.233115     1.096098      31.48
 O       5.396720    -1.864299     0.610896     100.52
 H       5.526078    -2.648957     0.114355      29.41
 C       4.051758    -0.458650     2.086547      87.38
 O       4.667854     1.069157     1.701964      35.53
 H       4.022882     1.707464     2.175997      29.70
 H       4.726511    -0.684111     2.892408      29.45
 H       2.971814    -0.067996     2.606542      26.09
55
name = lig-Water-frame_657
 C      -1.661131     3.505249     3.130374      69.15
 H      -2.073997     4.488170     3.005635      23.49
 C      -1.114783     1.092543     3.293574      40.87
 H      -1.225690     0.070589     3.003296      27.03
 C       0.107729     1.408135     4.188698       7.02
 O       0.944797     0.416409     4.728261      94.56
 C       0.661241    -1.067876     4.361055     104.65
 H       1.339070    -1.497074     5.071199      28.14
 H       0.815892    -1.087771     3.379062      33.03
 H      -0.388187    -1.522150     4.820721      25.88
 C       0.316397     2.699057     4.445023      14.30
 O       1.595505     3.047564     5.209869     192.88
 H       1.506696     3.915285     5.701768      24.79
 C      -0.567737     3.740764     4.053224      57.81
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 H      -0.268599     4.688449     4.329745      17.91
 C      -1.956201     2.137613     2.834281      32.53
 C      -3.076375     1.795864     1.928965      99.52
 H      -3.655762     2.766131     2.111727      25.97
 O      -3.757793     0.659655     2.435822     285.81
 H      -4.760517     0.788873     2.313757      25.51
 C      -2.824342     1.604710     0.331014      73.92
 H      -2.026912     2.248985     0.008301      27.82
 C      -4.131441     1.561764    -0.661583      97.24
 O      -4.956671     0.263027    -0.544291     232.61
 H      -4.534741    -0.473531     0.144304      22.10
 H      -3.791792     1.527943    -1.565953      30.95
 H      -4.665666     2.434426    -0.392201      28.81
 C       1.423915     0.692248     0.100737      46.49
 H       2.095259     1.187906     0.679288      29.16
 C       0.899075    -1.404323    -1.113720      57.98
 H       1.060771    -2.395686    -1.655622      21.44
 C      -0.469629    -1.073199    -0.885469      39.85
 O      -1.446885    -2.049874    -1.004570     282.19
 C      -1.803167    -2.455923    -2.297252     129.80
 H      -2.730996    -3.207861    -2.190487      25.08
 H      -2.024697    -1.879602    -3.170594      27.88
 H      -1.130994    -2.782365    -2.877138      30.45
 C      -0.926858     0.151124    -0.190039      26.91
 O      -2.207274     0.223006     0.082593     171.55
 C       0.023304     1.076948     0.195974      55.59
 H      -0.273487     2.089112     0.472990      25.91
 C       1.827204    -0.472794    -0.655569      20.96
 C       3.445326    -0.713852    -0.513875      84.36
 H       3.346503    -1.514317    -1.549645      25.02
 O       4.149494     0.567492    -0.984823     136.80
 H       4.558480     1.119344    -0.187248      23.84
 C       3.968490    -1.373109     0.807341      93.16
 H       3.324313    -2.315944     1.153788      28.89
 O       5.351552    -1.880110     0.551711      16.60
 H       5.402572    -2.682733    -0.256249      24.42
 C       4.013018    -0.454554     2.078256     104.71
 O       4.673994     1.076945     1.726290      22.77
 H       3.975774     1.679982     2.234297      28.39
 H       4.805985    -0.877595     2.757758      29.59
 H       3.178719    -0.228767     2.507727      31.15
55
name = lig-Water-frame_658
 C      -1.617142     3.514908     3.126975      40.79
 H      -1.992191     4.508906     2.754297      23.96
 C      -1.101623     1.117268     3.316050      74.25
 H      -1.194428    -0.009882     3.375851      22.29
 C       0.030548     1.438482     4.049929     -11.90
 O       0.912032     0.359815     4.684715     128.99
 C       0.648600    -1.048108     4.368636     106.49
 H       1.452851    -1.600000     4.941725      25.44
 H       0.942321    -1.250396     3.176706      27.94
 H      -0.327991    -1.252157     4.585494      27.00
 C       0.330148     2.813065     4.538057      -2.91
 O       1.561424     3.093744     5.223282      50.61
 H       1.402802     4.081673     5.532168      25.31
 C      -0.585152     3.697488     4.054782      61.39
 H      -0.264490     4.799002     4.400278      20.15
 C      -1.982859     2.114011     2.862553      25.75
 C      -3.068373     1.802589     1.944991      91.38
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 H      -3.840044     2.634031     1.807746      26.92
 O      -3.781962     0.601122     2.462363     274.63
 H      -4.764552     0.593892     2.303669      26.62
 C      -2.839339     1.561455     0.309161      81.42
 H      -2.102198     2.419259     0.115957      24.55
 C      -4.070941     1.467989    -0.620834      77.09
 O      -4.942175     0.259957    -0.561616     238.18
 H      -4.485271    -0.392103    -0.015469      26.83
 H      -3.429706     1.628232    -1.773800      22.77
 H      -4.775914     2.461942    -0.445962      24.39
 C       1.364597     0.707590     0.071949      35.26
 H       2.290239     1.497130     0.457214      27.49
 C       0.846809    -1.483965    -1.136235      66.93
 H       1.233823    -2.481571    -1.478603      23.05
 C      -0.442932    -1.082606    -0.839123      18.92
 O      -1.493146    -2.053471    -0.972432     216.62
 C      -1.849999    -2.512569    -2.280544      81.52
 H      -2.575995    -3.214691    -2.278654      27.87
 H      -1.965929    -1.444792    -3.157187      24.27
 H      -0.900550    -3.163080    -3.021018      24.72
 C      -0.861500     0.152206    -0.310846      28.79
 O      -2.240445     0.270479     0.121370     143.85
 C       0.012915     1.001220     0.198272      72.63
 H      -0.265371     1.984236     0.515447      27.81
 C       1.899571    -0.468512    -0.581130       1.85
 C       3.406028    -0.680175    -0.511219      87.63
 H       3.689209    -1.370012    -1.162654      32.55
 O       4.160294     0.584668    -0.946031     173.07
 H       4.398663     1.096291    -0.219641      31.42
 C       3.933743    -1.359244     0.839752      91.35
 H       3.277848    -2.146515     1.056095      31.68
 O       5.313544    -1.908451     0.488715      99.20
 H       5.057315    -2.359251    -0.281009      33.81
 C       4.066690    -0.407077     2.020263     125.10
 O       4.658229     1.031950     1.758932      73.63
 H       4.031999     1.683629     2.241185      27.10
 H       4.722092    -0.977832     2.659604      32.23
 H       2.912402    -0.389944     2.596039      27.11
55
name = lig-Water-frame_659
 C      -1.578048     3.491143     3.140542      33.20
 H      -2.141160     4.173077     2.456672      21.76
 C      -1.078715     1.115086     3.368964      73.35
 H      -1.451938     0.107284     3.431880      24.40
 C       0.026201     1.449296     3.994785       3.78
 O       0.863894     0.343607     4.621018     177.23
 C       0.684746    -1.009464     4.330831     129.45
 H       1.369553    -1.695397     4.866212      25.87
 H       0.831765    -1.389615     3.381152      30.28
 H      -0.520424    -1.209622     4.412895      25.09
 C       0.359212     2.830938     4.598814      -9.06
 O       1.487209     3.142826     5.213069      78.34
 H       1.543032     4.042972     5.637191      30.00
 C      -0.564932     3.752388     4.074242      60.55
 H      -0.490169     4.742976     4.291063      30.11
 C      -1.974761     2.148567     2.870991      11.91
 C      -3.156837     1.785531     1.893128      86.69
 H      -3.928976     2.531366     1.767025      27.31
 O      -3.806501     0.536175     2.494944     247.50
 H      -4.762627     0.670227     2.284985      25.83
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 C      -2.834593     1.515153     0.341642      97.20
 H      -2.438298     2.517357    -0.019999      24.22
 C      -4.003775     1.418071    -0.614293     109.59
 O      -4.922244     0.301955    -0.592766     267.96
 H      -4.405970    -0.537862    -0.188445      23.63
 H      -3.595120     1.547773    -1.480044      29.71
 H      -4.762790     2.212195    -0.637346      25.80
 C       1.394222     0.725383     0.023780      67.72
 H       1.957459     1.501697     0.152400      29.55
 C       0.886494    -1.485761    -1.098752      49.66
 H       1.198799    -2.463865    -1.361036      24.87
 C      -0.462518    -1.155971    -0.821826      15.16
 O      -1.539719    -2.058284    -0.941338     227.78
 C      -1.814344    -2.534837    -2.373240     105.02
 H      -2.780559    -3.259654    -2.268628      25.50
 H      -2.079735    -1.611008    -2.542345      27.29
 H      -1.078059    -3.157873    -2.539163      28.61
 C      -0.874246     0.113689    -0.407667      14.79
 O      -2.233988     0.307224     0.135802     158.03
 C       0.072819     0.992671     0.199748      42.92
 H      -0.278603     1.936184     0.757563      25.31
 C       1.902763    -0.475371    -0.500202      17.45
 C       3.374351    -0.623006    -0.506885      60.20
 H       4.063188    -1.433229    -1.228369      24.68
 O       4.165176     0.559685    -0.906623     138.61
 H       4.240864     1.112752     0.097804      22.79
 C       3.933595    -1.284330     0.821921      83.62
 H       3.110422    -2.144884     1.074627      27.07
 O       5.250262    -1.923729     0.448052       4.59
 H       4.920661    -2.299752    -0.438458      30.17
 C       4.090793    -0.347660     1.990804     153.51
 O       4.626930     0.938010     1.788637     194.71
 H       4.015007     1.642392     2.280342      22.55
 H       4.710336    -0.853271     2.776839      30.01
 H       3.221755    -0.377351     2.412976      31.23
55
name = lig-Water-frame_660
 C      -1.583245     3.424595     3.124507      49.68
 H      -2.181926     4.073056     2.512859      21.38
 C      -1.149803     1.119428     3.390133      31.36
 H      -1.628951     0.133315     3.294127      26.39
 C       0.135936     1.452838     4.068881      18.87
 O       0.837748     0.382886     4.553429     174.71
 C       0.646830    -1.007995     4.281526     128.65
 H       1.185124    -1.599572     5.056506      24.69
 H       0.842897    -1.344571     3.129950      24.89
 H      -0.292775    -1.351543     4.471599      27.97
 C       0.310739     2.788846     4.560969       3.63
 O       1.448346     3.174522     5.216995      16.29
 H       1.539132     3.992998     5.893938      32.06
 C      -0.537175     3.839728     4.089108      45.53
 H      -0.557267     5.003187     4.304056      21.07
 C      -1.954043     2.174032     2.851587      -3.38
 C      -3.243105     1.731531     1.846859      98.23
 H      -4.033880     2.607441     1.986403      25.64
 O      -3.833904     0.495230     2.513376     237.75
 H      -4.799724     0.741285     2.340823      23.21
 C      -2.865116     1.520616     0.402108      99.00
 H      -2.446830     2.417791    -0.092921      24.21
 C      -4.003390     1.387935    -0.603744      73.60
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 O      -4.895206     0.320865    -0.618373     255.67
 H      -4.500116    -0.585417    -0.434437      26.06
 H      -3.472175     1.391606    -1.817382      22.64
 H      -4.742000     2.328040    -0.603624      24.52
 C       1.445461     0.730326    -0.036227      47.27
 H       2.093962     1.819717     0.079674      24.02
 C       0.971758    -1.422047    -0.990633      67.75
 H       1.169498    -2.531084    -1.342088      23.88
 C      -0.510965    -1.255241    -0.834840       5.25
 O      -1.578155    -2.081850    -0.895262     200.14
 C      -1.837912    -2.577264    -2.383754      66.62
 H      -2.758485    -3.029749    -2.273683      26.92
 H      -2.219392    -1.444730    -2.798756      23.32
 H      -0.739706    -3.287550    -2.473146      21.09
 C      -0.905130     0.121811    -0.404690       8.65
 O      -2.162940     0.295593     0.120933     165.22
 C       0.084033     0.997452     0.177640      34.16
 H      -0.205988     1.751417     0.821534      26.52
 C       1.846851    -0.521090    -0.481328      44.12
 C       3.430297    -0.618089    -0.532270     107.53
 H       3.582546    -1.215183    -1.338531      30.17
 O       4.161137     0.551978    -0.820475     230.88
 H       4.220262     0.990462    -0.033677      30.17
 C       3.936298    -1.223142     0.774089     120.26
 H       3.286358    -1.915218     1.122718      31.23
 O       5.164277    -1.931225     0.422478      70.74
 H       5.096426    -2.426070    -0.562915      25.91
 C       4.134949    -0.349126     2.001216     123.16
 O       4.598647     0.880522     1.800086     229.21
 H       4.020435     1.504213     2.292363      26.59
 H       4.724374    -0.753101     2.843595      28.26
 H       2.945055    -0.183734     2.492004      24.00
55
name = lig-Water-frame_661
 C      -1.584486     3.447361     3.124750      38.44
 H      -2.173360     4.362937     2.764869      24.58
 C      -1.209481     1.145907     3.417088      34.81
 H      -1.481853     0.089181     3.169398      27.34
 C       0.137725     1.425874     4.133328      28.08
 O       0.863948     0.428673     4.514681     164.25
 C       0.597997    -1.037390     4.207007     112.38
 H       1.220688    -1.351364     5.089796      25.38
 H       0.973149    -1.131499     3.221730      27.56
 H      -0.489182    -1.456087     4.543750      24.82
 C       0.246693     2.799886     4.496582      10.03
 O       1.455688     3.180242     5.247699     204.43
 H       1.224355     3.901138     5.902036      22.91
 C      -0.565781     3.901397     4.048516      -6.16
 H      -0.373221     4.894216     4.364325      21.06
 C      -1.952724     2.098077     2.801256      12.59
 C      -3.287504     1.698513     1.890140     117.53
 H      -3.941672     2.470861     2.036014      27.51
 O      -3.873667     0.489676     2.506014     275.29
 H      -4.859534     0.604499     2.482438      24.76
 C      -2.912640     1.531320     0.412513      73.86
 H      -2.149288     2.357319     0.073930      23.17
 C      -4.022451     1.398557    -0.682040      94.18
 O      -4.902052     0.310975    -0.645333     352.45
 H      -4.429211    -0.499716    -0.467139      28.53
 H      -3.491792     1.371192    -1.493782      32.04
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 H      -4.503020     2.415998    -0.499725      26.05
 C       1.473430     0.809548    -0.081808      52.99
 H       2.208312     1.440249     0.116456      28.64
 C       0.948695    -1.446009    -0.886205      71.51
 H       1.342437    -2.324590    -1.237750      27.95
 C      -0.521916    -1.243889    -0.825892       9.67
 O      -1.613635    -2.138352    -0.876099     230.98
 C      -1.836703    -2.561571    -2.339041     105.49
 H      -2.840116    -3.187048    -2.302076      25.03
 H      -1.845171    -1.957149    -3.242383      27.59
 H      -1.084550    -3.020646    -2.764044      28.74
 C      -0.881551     0.117534    -0.332894      25.88
 O      -2.101083     0.258225     0.109970     156.82
 C       0.092242     0.979471     0.112844      49.44
 H      -0.213247     1.819513     0.860497      24.66
 C       1.867953    -0.500148    -0.481817      19.62
 C       3.438694    -0.629435    -0.556065     101.06
 H       3.280272    -1.328521    -1.617810      22.38
 O       4.159472     0.560085    -0.764619     155.51
 H       4.330750     1.111855     0.175707      20.94
 C       3.957737    -1.203949     0.712224     110.88
 H       3.180650    -2.026661     1.207299      27.28
 O       5.117467    -1.950293     0.399620     141.44
 H       5.123383    -2.405600    -0.347277      32.78
 C       4.085868    -0.408480     2.067078     129.91
 O       4.607664     0.902328     1.782000     199.37
 H       4.031164     1.613654     2.354777      23.81
 H       4.674657    -0.972256     2.809871      29.28
 H       3.168952    -0.232542     2.357961      28.97
55
name = lig-Water-frame_662
 C      -1.615856     3.553558     3.128681      28.93
 H      -2.202704     4.405694     2.938233      27.72
 C      -1.188736     1.127842     3.454396      50.10
 H      -1.239859     0.102881     3.179334      25.81
 C      -0.029326     1.447619     4.136161      19.28
 O       0.931701     0.441234     4.508154     126.52
 C       0.547135    -1.037644     4.200156     112.74
 H       1.333802    -1.422965     4.833946      26.66
 H       1.024823    -1.207365     3.158253      27.39
 H      -0.453171    -1.280739     4.296125      28.56
 C       0.247368     2.839836     4.464568       1.36
 O       1.443245     3.150120     5.270619     179.12
 H       1.142433     3.942395     5.790040      25.38
 C      -0.606643     3.858325     3.974639      14.78
 H      -0.241561     4.867356     4.350314      16.93
 C      -1.986827     2.055289     2.746803      -7.53
 C      -3.266706     1.656562     1.979210     105.66
 H      -4.043970     2.596466     1.974947      24.62
 O      -3.918134     0.490400     2.491523     269.08
 H      -4.898029     0.538663     2.492508      26.26
 C      -2.911155     1.520575     0.383822      76.77
 H      -2.204336     2.300762     0.311343      24.16
 C      -4.027518     1.450088    -0.704667      71.96
 O      -4.934325     0.296051    -0.673450     287.18
 H      -4.252557    -0.466225    -0.335892      22.48
 H      -3.236026     1.488637    -1.763601      23.03
 H      -4.567390     2.433552    -0.618607      24.94
 C       1.467538     0.836048    -0.127486      47.12
 H       2.437059     1.443589     0.314854      23.35
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 C       0.856873    -1.505094    -0.795171      51.19
 H       1.499062    -2.420240    -1.185832      21.55
 C      -0.491013    -1.164342    -0.784132      17.79
 O      -1.620561    -2.194112    -0.915223     227.24
 C      -1.878204    -2.556722    -2.287739     105.93
 H      -2.660512    -3.312031    -2.355713      25.67
 H      -1.742504    -1.932702    -3.296246      23.74
 H      -0.981763    -3.356299    -2.885167      22.98
 C      -0.810894     0.059299    -0.251076      24.35
 O      -2.115003     0.218365     0.127841     159.91
 C       0.129782     1.027344     0.070254      64.40
 H      -0.221104     1.843729     0.599441      23.82
 C       1.916228    -0.395743    -0.481597       9.41
 C       3.370051    -0.653202    -0.609848      97.04
 H       3.647067    -1.280513    -1.391624      30.16
 O       4.166010     0.600914    -0.735353     157.43
 H       4.433273     0.859886     0.234826      20.98
 C       3.931156    -1.293367     0.700069     114.56
 H       3.212937    -1.964662     0.935441      31.69
 O       5.134778    -1.966984     0.418902     118.16
 H       4.947842    -2.533033    -0.456716      27.88
 C       4.051229    -0.466640     2.069320     105.92
 O       4.626274     0.954794     1.775394     163.23
 H       4.164123     1.654942     2.285955      25.63
 H       4.608034    -1.179574     2.733136      27.95
 H       2.873485    -0.366096     2.496636      24.71
55
name = lig-Water-frame_663
 C      -1.716009     3.591407     3.096736      28.26
 H      -2.467105     4.409020     2.826875      19.97
 C      -1.178781     1.094801     3.435638      49.27
 H      -1.188958     0.001016     3.183975      23.86
 C      -0.147248     1.503736     4.170450      19.48
 O       0.969217     0.449551     4.500950      93.92
 C       0.581730    -0.982915     4.181599     108.04
 H       1.224485    -1.804552     4.728178      26.92
 H       0.761466    -1.342699     3.099231      29.75
 H      -0.559402    -1.186163     4.208290      26.46
 C       0.286249     2.835530     4.454070       6.67
 O       1.388358     3.100824     5.272269     122.29
 H       1.424581     4.076953     5.692951      30.70
 C      -0.582011     3.796693     3.937286      51.77
 H      -0.358456     4.882766     4.142995      21.03
 C      -2.014753     2.103060     2.758438     -20.06
 C      -3.258591     1.653742     2.019461     102.89
 H      -3.881141     2.437513     1.951674      26.82
 O      -3.958124     0.473996     2.490863     255.58
 H      -4.936380     0.717093     2.302821      25.50
 C      -2.888536     1.470424     0.377483      73.29
 H      -2.285843     2.511261     0.269547      21.00
 C      -3.980605     1.515972    -0.747433      86.82
 O      -4.928238     0.290689    -0.693893     291.29
 H      -4.426113    -0.420406    -0.303516      27.47
 H      -3.539618     1.568090    -1.615473      29.48
 H      -4.813480     2.361459    -0.858269      24.32
 C       1.521163     0.878710    -0.136102      60.24
 H       2.111079     1.636161     0.332980      24.31
 C       0.869650    -1.522207    -0.722795      50.68
 H       1.145778    -2.496599    -1.044902      23.78
 C      -0.467065    -1.175276    -0.745150       6.77
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 O      -1.584136    -2.212752    -0.974080     182.87
 C      -1.842740    -2.629419    -2.321142      99.79
 H      -2.766602    -3.275992    -2.314396      24.96
 H      -2.009240    -1.586306    -2.770941      23.82
 H      -1.128922    -3.368683    -2.395656      24.22
 C      -0.778364     0.050074    -0.148797      16.06
 O      -2.167895     0.186468     0.160897     153.75
 C       0.149437     1.104772     0.037122      52.81
 H      -0.265531     2.107084     0.406934      20.54
 C       1.891057    -0.373430    -0.532081      32.84
 C       3.352385    -0.631775    -0.608220      64.58
 H       3.980002    -1.388519    -1.438915      26.48
 O       4.168816     0.629205    -0.734857     114.42
 H       4.496301     0.769194     0.234647      21.55
 C       3.872721    -1.379379     0.707400      79.39
 H       3.019443    -2.245090     0.829576      28.40
 O       5.193007    -1.999624     0.430472      42.25
 H       4.802554    -2.634252    -0.350985      26.65
 C       3.972457    -0.501260     2.018431     132.46
 O       4.646565     0.947131     1.775021     145.76
 H       4.057152     1.711429     2.319627      20.48
 H       4.597492    -1.023354     2.712274      32.07
 H       3.068237    -0.461216     2.535955      29.07
55
name = lig-Water-frame_664
 C      -1.830089     3.523730     3.060694      46.74
 H      -2.526391     4.250874     2.691796      18.44
 C      -1.225718     1.093684     3.348871      39.56
 H      -1.374942     0.065500     3.140183      22.99
 C      -0.123297     1.512407     4.246248      23.49
 O       0.967431     0.447825     4.487168     110.30
 C       0.614063    -0.944926     4.146240     123.02
 H       0.931710    -1.749697     4.742616      29.52
 H       0.627298    -1.182477     3.026349      31.25
 H      -0.437454    -1.063680     4.449953      27.96
 C       0.299411     2.821189     4.452121      22.90
 O       1.340016     3.060959     5.273665     206.71
 H       1.570838     3.953543     5.498571      39.48
 C      -0.570374     3.791542     3.885478     101.73
 H      -0.447817     4.847824     4.001770      18.93
 C      -2.031988     2.177307     2.837170      26.29
 C      -3.234723     1.643369     1.980537      80.01
 H      -4.016919     2.580856     1.981636      23.48
 O      -4.004444     0.466693     2.493668     265.73
 H      -4.870092     0.790534     2.163457      26.32
 C      -2.857156     1.463639     0.392382      85.05
 H      -2.352694     2.307949     0.074099      25.29
 C      -4.002355     1.540230    -0.744012      71.88
 O      -4.904493     0.314086    -0.717757     251.78
 H      -4.529404    -0.524536    -0.305686      25.20
 H      -3.496419     1.552625    -1.956038      23.35
 H      -4.742551     2.311083    -0.761215      25.97
 C       1.521885     0.940811    -0.126502      36.53
 H       2.114359     1.896693     0.185442      23.58
 C       0.934065    -1.481674    -0.677758      61.23
 H       0.967201    -2.616667    -0.940957      23.50
 C      -0.480932    -1.256497    -0.696419      -9.49
 O      -1.510574    -2.186030    -0.966044     192.99
 C      -1.836474    -2.680800    -2.343560      73.73
 H      -2.932487    -2.984915    -2.210156      23.42
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 H      -2.106314    -1.691469    -2.689509      24.87
 H      -0.853925    -3.468859    -2.445915      19.85
 C      -0.811734     0.100086    -0.051947      -4.59
 O      -2.212520     0.176023     0.194183     136.71
 C       0.126441     1.182936     0.019291      50.04
 H      -0.186144     2.215730     0.168990      23.14
 C       1.851711    -0.440450    -0.610613      31.60
 C       3.436920    -0.618336    -0.591435     100.97
 H       3.662915    -1.228212    -1.402188      32.91
 O       4.154273     0.631192    -0.749259     106.43
 H       4.589239     0.953097     0.217436      17.14
 C       3.792875    -1.448552     0.719896      90.89
 H       3.167241    -2.220310     0.909144      31.38
 O       5.226852    -2.044431     0.436590     113.57
 H       5.053142    -2.708156    -0.118605      33.99
 C       3.931756    -0.519368     1.944410     120.60
 O       4.630776     0.895006     1.788458     130.33
 H       3.998476     1.492133     2.166097      29.16
 H       4.724596    -0.818021     2.705872      28.79
 H       2.906979    -0.360210     2.559435      26.85
55
name = lig-Water-frame_665
 C      -1.851901     3.446033     3.078733      54.58
 H      -2.492230     4.206451     2.605125      21.52
 C      -1.229619     1.165865     3.311364      34.12
 H      -1.619032     0.145263     3.050565      25.11
 C      -0.071956     1.403321     4.253706      27.30
 O       0.951007     0.455458     4.478956     128.67
 C       0.585836    -0.891958     4.120507     112.00
 H       1.146291    -1.597212     4.869715      26.73
 H       0.617964    -0.941686     2.953401      30.42
 H      -0.452391    -0.951555     4.573125      27.40
 C       0.248077     2.834596     4.437206      18.90
 O       1.328385     3.011631     5.280352     194.45
 H       1.457847     4.043546     5.385794      25.58
 C      -0.623168     3.810338     3.798094      84.98
 H      -0.355655     4.953019     3.996980      23.90
 C      -2.093259     2.147734     2.897728      55.56
 C      -3.241202     1.685451     1.902358      89.29
 H      -3.937757     2.419663     1.969883      28.36
 O      -4.028674     0.484848     2.482051     259.69
 H      -4.997893     0.644215     2.192540      26.43
 C      -2.864617     1.468819     0.404165      73.33
 H      -2.047811     2.230652    -0.075623      24.32
 C      -4.023868     1.479642    -0.764173      94.31
 O      -4.884681     0.355361    -0.744127     256.28
 H      -4.464140    -0.523861    -0.352168      25.10
 H      -3.512404     1.558035    -1.585162      30.73
 H      -4.616160     2.521542    -0.438122      26.06
 C       1.462481     0.963521    -0.133673      34.68
 H       2.280775     1.774015    -0.300492      25.56
 C       0.940563    -1.476123    -0.679164      58.22
 H       1.273961    -2.538159    -0.831333      26.84
 C      -0.494645    -1.257946    -0.596978       8.18
 O      -1.423620    -2.148395    -0.902721     205.69
 C      -1.821191    -2.707768    -2.318526      88.43
 H      -2.804982    -3.082136    -2.143553      25.77
 H      -1.839571    -1.888647    -3.265168      25.18
 H      -1.168189    -3.263173    -2.902947      26.75
 C      -0.876858     0.113835    -0.013446      -1.77
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 O      -2.235353     0.182548     0.227895     144.23
 C       0.093962     1.232215     0.005390      56.74
 H      -0.203070     2.283745     0.096116      24.12
 C       1.882868    -0.431995    -0.633068      12.36
 C       3.478794    -0.612382    -0.552257      92.20
 H       3.533878    -1.303607    -1.659683      26.28
 O       4.146688     0.624458    -0.763215     134.76
 H       4.452246     0.969637     0.043580      26.52
 C       3.797669    -1.450170     0.704104      80.01
 H       3.082541    -2.296261     1.035956      28.66
 O       5.240285    -2.071516     0.467720      19.52
 H       5.290441    -3.038431    -0.059759      23.44
 C       3.924090    -0.517978     1.922812     121.84
 O       4.595039     0.807172     1.779295     133.37
 H       3.842957     1.507677     2.092697      26.44
 H       4.610402    -0.945209     2.605036      30.32
 H       2.903526    -0.251681     2.303508      28.53
55
name = lig-Water-frame_666
 C      -1.813238     3.450108     3.124477      48.52
 H      -2.400049     4.236855     2.601208      18.45
 C      -1.180736     1.187181     3.345823      61.48
 H      -1.593851     0.232004     3.039713      26.45
 C      -0.054505     1.325213     4.168501      37.19
 O       0.933421     0.488336     4.482226     201.99
 C       0.539923    -0.842903     4.139498     125.29
 H       1.410940    -1.322462     4.539741      28.81
 H       0.620232    -0.965100     3.058750      32.07
 H      -0.536968    -1.062856     4.462754      27.32
 C       0.147830     2.802545     4.405877      -6.38
 O       1.328036     2.999111     5.273656     156.54
 H       1.283381     3.967649     5.502590      21.04
 C      -0.668023     3.839185     3.740980      42.32
 H      -0.369337     4.789984     3.909780      29.77
 C      -2.200349     2.048923     2.898845      21.46
 C      -3.265198     1.717598     1.850132      82.90
 H      -4.067638     2.589720     1.857142      25.47
 O      -4.029919     0.514597     2.448503     269.87
 H      -5.009792     0.578859     2.347884      26.86
 C      -2.861674     1.487174     0.371309      98.79
 H      -2.143385     2.140788     0.135871      29.16
 C      -4.035568     1.454164    -0.671189     102.38
 O      -4.885506     0.382506    -0.770216     303.68
 H      -4.362974    -0.321830    -0.479157      29.96
 H      -3.299066     1.668669    -1.735048      24.90
 H      -4.461555     2.335077    -0.438282      29.67
 C       1.412412     0.917501    -0.217941      54.16
 H       2.182807     1.592057    -0.558719      29.43
 C       0.935889    -1.469873    -0.695770      44.57
 H       1.507175    -2.407475    -0.856353      25.80
 C      -0.444036    -1.157867    -0.471152      19.93
 O      -1.371135    -2.150948    -0.856836     165.80
 C      -1.790816    -2.659394    -2.322533      78.16
 H      -2.718684    -3.350738    -2.064871      24.98
 H      -1.751684    -2.040488    -3.210572      26.31
 H      -1.248092    -3.481163    -3.093834      25.54
 C      -0.914777     0.095947    -0.028135      15.87
 O      -2.247500     0.181604     0.267349     157.78
 C       0.044386     1.237461    -0.000398      60.63
 H      -0.302471     2.310516     0.154236      23.46
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 C       1.920316    -0.342219    -0.571822      -6.58
 C       3.437667    -0.657107    -0.587083      96.82
 H       3.688936    -1.190206    -1.431391      32.93
 O       4.146744     0.599445    -0.805846     102.06
 H       4.364632     1.016639     0.226049      20.47
 C       3.875621    -1.435643     0.664313      94.31
 H       3.023198    -2.105997     0.964512      31.41
 O       5.245200    -2.101696     0.505812      70.76
 H       5.259129    -3.072709     0.162349      24.79
 C       3.937929    -0.513921     1.914099     136.51
 O       4.539668     0.734495     1.754064     105.21
 H       3.982244     1.480209     2.074358      26.23
 H       4.360551    -1.260856     2.707310      29.73
 H       2.843115    -0.319352     2.182266      29.60
55
name = lig-Water-frame_667
 C      -1.834195     3.441988     3.115416      43.39
 H      -2.362067     4.265979     2.681702      19.11
 C      -1.187402     1.110102     3.367758      56.69
 H      -1.277222     0.045736     3.084288      26.39
 C      -0.066561     1.414607     4.053099      30.67
 O       0.908960     0.522557     4.492906     210.16
 C       0.524516    -0.820973     4.160073     124.85
 H       1.498365    -1.419550     4.328098      27.12
 H       0.508815    -1.046784     2.958082      29.16
 H      -0.412649    -1.261073     4.478837      28.73
 C       0.080869     2.730533     4.387187      10.79
 O       1.292605     3.010565     5.236071     126.46
 H       1.241168     3.874070     5.746342      18.68
 C      -0.648561     3.804309     3.759632      86.03
 H      -0.353820     4.981886     3.823034      28.04
 C      -2.250892     2.040170     2.893606     -21.13
 C      -3.348529     1.738286     1.849858      88.00
 H      -3.950280     2.624375     1.697411      27.08
 O      -4.005188     0.543602     2.401422     252.53
 H      -4.984933     0.787330     2.403900      24.14
 C      -2.880802     1.463632     0.366959      92.50
 H      -2.186275     2.458181     0.180448      24.11
 C      -3.947770     1.493913    -0.619423     103.82
 O      -4.901667     0.394501    -0.790628     250.60
 H      -4.315461    -0.434553    -0.599303      26.68
 H      -3.578246     1.640804    -1.509488      29.99
 H      -4.731182     2.499709    -0.546058      24.83
 C       1.360383     0.885347    -0.338368      54.85
 H       2.053503     1.866503    -0.587238      28.12
 C       0.978540    -1.380022    -0.685748      56.12
 H       1.388524    -2.443650    -1.048884      24.58
 C      -0.360138    -1.110626    -0.406663      14.52
 O      -1.344570    -2.178979    -0.830826     174.18
 C      -1.738104    -2.673279    -2.329247      77.42
 H      -2.582677    -3.172239    -2.061706      28.59
 H      -2.013534    -1.594433    -2.945118      24.39
 H      -1.066105    -3.525356    -2.518613      27.21
 C      -0.908346     0.128284    -0.048711      21.92
 O      -2.253988     0.163089     0.307909     164.40
 C      -0.017656     1.191583    -0.004797      69.61
 H      -0.303866     2.164723     0.212377      27.91
 C       1.899305    -0.330880    -0.481897      28.00
 C       3.381161    -0.663801    -0.625385      74.25
 H       3.830321    -1.426882    -1.600153      24.77
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 O       4.165365     0.578406    -0.833947     136.12
 H       4.255295     0.876457     0.020976      32.08
 C       3.972389    -1.406286     0.627553     105.88
 H       3.128484    -2.088468     0.806267      32.07
 O       5.239402    -2.125408     0.549884     136.86
 H       5.021580    -2.977518     0.277637      32.48
 C       3.918349    -0.569835     1.924466     136.53
 O       4.516216     0.696438     1.727406     116.04
 H       3.993395     1.404452     2.226398      26.12
 H       4.106868    -1.165840     2.807037      32.22
 H       2.745500    -0.473123     2.055327      29.55
55
name = lig-Water-frame_668
 C      -1.876764     3.406713     3.080782      43.37
 H      -2.497943     4.288677     2.717870      23.01
 C      -1.293215     0.997091     3.327075      49.78
 H      -1.085313    -0.061641     3.109970      23.00
 C      -0.075981     1.513519     3.956946      -4.85
 O       0.864286     0.545073     4.498214     172.57
 C       0.571615    -0.849168     4.121493     126.42
 H       1.330745    -1.543304     4.394005      28.65
 H       0.338803    -0.913542     3.076005      29.45
 H      -0.264325    -1.385373     4.798816      26.57
 C       0.103540     2.771595     4.414467      27.82
 O       1.230416     3.021839     5.176447     156.11
 H       1.133041     3.791642     5.857836      22.73
 C      -0.618410     3.764750     3.812470      47.02
 H      -0.380937     4.735129     3.836817      26.88
 C      -2.212834     2.080922     2.889037     -16.10
 C      -3.395505     1.726323     1.876409      90.06
 H      -4.028888     2.660286     1.706746      26.93
 O      -3.999664     0.578529     2.349373     270.36
 H      -4.952861     0.925911     2.398341      21.66
 C      -2.873999     1.476411     0.430407     115.39
 H      -2.387118     2.326378     0.133280      28.07
 C      -3.956377     1.589148    -0.608716      86.33
 O      -4.902946     0.390051    -0.794155     209.63
 H      -4.505266    -0.552467    -0.756830      27.88
 H      -3.519203     1.710619    -1.805516      24.32
 H      -4.596200     2.308788    -0.513557      29.09
 C       1.303118     0.977806    -0.444158      47.39
 H       1.800194     1.851088    -0.405040      29.71
 C       1.011159    -1.318658    -0.664542      68.34
 H       1.100913    -2.250423    -1.115021      25.94
 C      -0.330483    -1.161958    -0.431286       8.38
 O      -1.319841    -2.198060    -0.790423     235.01
 C      -1.673291    -2.631015    -2.279921      75.08
 H      -2.791095    -3.031522    -2.056974      24.71
 H      -1.945061    -1.752881    -2.673750      29.37
 H      -0.690876    -3.267363    -2.160566      20.64
 C      -0.908275     0.150812    -0.052265      20.68
 O      -2.245104     0.148427     0.338943     169.45
 C      -0.031009     1.133325    -0.026762      66.09
 H      -0.310732     2.218739     0.285361      26.73
 C       1.906091    -0.383394    -0.426012      34.23
 C       3.403291    -0.654408    -0.694102     104.80
 H       3.463131    -1.385501    -1.433922      29.75
 O       4.181502     0.542154    -0.895995     114.20
 H       4.277810     0.947730     0.108810      22.28
 C       4.026906    -1.383404     0.622981     110.61
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 H       3.304097    -2.310013     0.691445      28.55
 O       5.242727    -2.136843     0.578901      84.15
 H       4.736065    -3.077742     0.246737      26.20
 C       3.833545    -0.649230     1.913380     114.03
 O       4.507594     0.692839     1.719062      71.28
 H       3.999900     1.281080     2.441919      24.57
 H       4.187573    -1.044484     2.913393      29.93
 H       2.736425    -0.468333     1.960918      28.74
55
name = lig-Water-frame_669
 C      -1.864492     3.406746     3.080364      46.99
 H      -2.563323     4.117063     2.751666      24.56
 C      -1.358338     0.968794     3.288047      58.17
 H      -1.458642    -0.070858     2.997500      22.14
 C      -0.125067     1.475012     3.884721      -9.07
 O       0.815935     0.556599     4.489397     176.44
 C       0.609178    -0.895767     4.131128     103.97
 H       1.516137    -1.518888     4.395728      26.84
 H       0.127797    -0.878646     3.007118      24.39
 H      -0.118207    -1.157703     4.846682      28.51
 C       0.156511     2.864502     4.437246      14.39
 O       1.194420     3.038936     5.143772     163.95
 H       1.019582     3.809416     5.686823      24.89
 C      -0.683311     3.728196     3.829161      54.72
 H      -0.316073     4.864699     3.995749      24.07
 C      -2.171131     2.067838     2.842531       8.34
 C      -3.363261     1.742245     1.907374     101.23
 H      -4.170582     2.540962     1.890319      25.20
 O      -4.038783     0.596279     2.317337     279.55
 H      -5.016020     0.760678     2.357187      25.15
 C      -2.889313     1.485525     0.498903      85.08
 H      -2.108114     2.322495     0.109249      22.29
 C      -3.978448     1.595687    -0.696904      76.13
 O      -4.910678     0.393491    -0.795490     265.38
 H      -4.505776    -0.437017    -0.769664      30.50
 H      -3.450497     1.811424    -1.502050      30.67
 H      -4.743531     2.574366    -0.312228      24.69
 C       1.280724     1.026425    -0.499563      38.20
 H       1.945368     2.058542    -0.201551      25.45
 C       0.970163    -1.345405    -0.643871      49.65
 H       1.173841    -2.408447    -1.263314      21.20
 C      -0.415039    -1.203056    -0.490071      16.30
 O      -1.294686    -2.199097    -0.714395     273.35
 C      -1.605505    -2.597315    -2.118412      94.02
 H      -2.502319    -3.123611    -2.205294      25.69
 H      -1.600900    -1.553563    -2.971549      24.43
 H      -0.736343    -3.045000    -2.555078      26.73
 C      -0.936506     0.056083    -0.051814       6.01
 O      -2.227685     0.155417     0.362918     179.02
 C      -0.009826     1.170932    -0.055062      60.95
 H      -0.324328     2.099885     0.245019      24.86
 C       1.964376    -0.312322    -0.417693      20.52
 C       3.442726    -0.620418    -0.684769      89.81
 H       3.307682    -1.473768    -1.690746      23.36
 O       4.202471     0.512039    -0.965810     140.30
 H       4.328213     0.987520    -0.049987      24.01
 C       3.998914    -1.421975     0.625255     121.49
 H       3.319486    -2.176222     0.712643      30.61
 O       5.257689    -2.166179     0.577370     139.64
 H       5.021522    -3.046597     0.230668      30.77
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 C       3.757278    -0.690920     1.892466      97.88
 O       4.488590     0.699677     1.743516      84.12
 H       4.110013     1.246177     2.386506      31.69
 H       4.294924    -1.094423     2.773914      28.70
 H       2.600082    -0.373223     1.977403      24.64
55
name = lig-Water-frame_670
 C      -1.833090     3.395621     3.097620      25.12
 H      -2.591721     4.141439     2.725709      22.79
 C      -1.364938     1.010754     3.256617      64.04
 H      -1.940808     0.078068     2.959494      21.25
 C      -0.169955     1.385760     3.890975      21.54
 O       0.779575     0.559364     4.455905     198.83
 C       0.631532    -0.910213     4.144124     110.34
 H       1.664213    -1.276545     4.168418      27.64
 H       0.268756    -1.099016     3.219843      29.25
 H      -0.241168    -1.134983     4.932299      25.45
 C       0.108303     2.817393     4.334897      -8.68
 O       1.226211     3.077533     5.167388      88.21
 H       1.145254     4.037365     5.582975      22.22
 C      -0.766473     3.801379     3.841564      32.63
 H      -0.553458     4.787868     4.113014      25.33
 C      -2.156902     2.033314     2.778556      18.11
 C      -3.327396     1.772774     1.943144     111.13
 H      -4.060557     2.538804     1.988779      27.40
 O      -4.088977     0.561875     2.319345     282.96
 H      -5.093177     0.715964     2.204594      26.64
 C      -2.888581     1.521435     0.481726      80.71
 H      -2.048769     2.123986     0.316780      27.94
 C      -4.043436     1.587674    -0.691603      98.84
 O      -4.919875     0.431701    -0.805466     255.02
 H      -4.239189    -0.360163    -0.682099      26.74
 H      -3.313836     1.930471    -1.664485      25.02
 H      -4.556793     2.365734    -0.442533      29.34
 C       1.363802     1.066991    -0.473140      53.87
 H       1.946257     1.830548    -0.319372      30.32
 C       0.945829    -1.410540    -0.652190      42.33
 H       1.386036    -2.243272    -1.026273      23.97
 C      -0.488881    -1.194125    -0.537587      16.54
 O      -1.305841    -2.237676    -0.648227     291.08
 C      -1.491855    -2.502134    -2.017581     119.06
 H      -2.325999    -3.302799    -2.214138      25.00
 H      -1.454647    -1.725982    -2.685470      28.78
 H      -0.835664    -3.075464    -2.871060      25.43
 C      -0.930510    -0.004277    -0.050571      12.56
 O      -2.230875     0.163647     0.392031     210.70
 C      -0.029027     1.178206    -0.096546      60.91
 H      -0.415754     2.213904     0.225217      21.90
 C       1.953159    -0.209868    -0.471032       1.57
 C       3.461299    -0.640860    -0.666328     101.68
 H       3.498862    -1.133422    -1.567560      27.77
 O       4.244194     0.500172    -1.044983     202.38
 H       4.382135     0.963772    -0.242214      30.73
 C       3.931898    -1.490008     0.597767     105.36
 H       2.990187    -2.249895     0.742764      27.31
 O       5.291495    -2.176342     0.564123     122.26
 H       5.261087    -3.071776     0.158449      27.63
 C       3.715157    -0.651368     1.871334     106.52
 O       4.471492     0.689687     1.767515      97.14
 H       3.993337     1.414156     2.397712      25.15
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 H       4.150915    -1.290734     2.654317      30.95
 H       2.706449    -0.486184     2.073186      29.30
55
name = lig-Water-frame_671
 C      -1.869474     3.384067     3.074112      88.40
 H      -2.475947     4.197946     2.720718      23.21
 C      -1.369840     1.039508     3.218348      71.66
 H      -1.911641     0.109405     3.174514      25.86
 C      -0.192150     1.339949     3.957773      17.56
 O       0.759824     0.536590     4.402969     161.49
 C       0.632526    -0.885972     4.201824     122.20
 H       1.686825    -1.194779     4.191192      29.82
 H       0.284065    -1.327666     3.072052      27.51
 H       0.023226    -1.416794     4.862875      31.64
 C       0.037927     2.720377     4.201155     -21.00
 O       1.257691     3.119939     5.188832     148.44
 H       1.317312     4.086054     5.446192      29.86
 C      -0.809689     3.860306     3.883714      45.40
 H      -0.809522     4.969097     4.216353      11.82
 C      -2.137245     2.067686     2.748440      47.80
 C      -3.339744     1.755708     1.942969      80.73
 H      -3.939870     2.788296     1.985810      24.64
 O      -4.124712     0.507658     2.340882     281.04
 H      -5.049117     0.883032     2.092520      26.52
 C      -2.895943     1.527704     0.434279      82.21
 H      -2.093145     2.324627     0.268384      24.41
 C      -4.019801     1.579499    -0.680645      95.39
 O      -4.899001     0.463759    -0.817728     257.65
 H      -4.213598    -0.235618    -0.583868      28.95
 H      -3.650656     1.733587    -1.619412      28.59
 H      -4.780052     2.613213    -0.504911      25.38
 C       1.415787     1.070747    -0.395368      43.00
 H       2.202706     2.062299    -0.486791      24.27
 C       0.949501    -1.367021    -0.651223      45.99
 H       1.605937    -2.420058    -0.783122      23.79
 C      -0.444408    -1.194108    -0.553570      18.55
 O      -1.335684    -2.319635    -0.594086     232.75
 C      -1.397655    -2.504485    -2.019266      86.85
 H      -2.312218    -3.126064    -2.019237      24.94
 H      -1.715992    -1.260683    -2.442793      23.03
 H      -0.593439    -3.102558    -2.403870      26.64
 C      -0.910310     0.075802    -0.043638      26.96
 O      -2.254690     0.157159     0.422351     197.14
 C      -0.048829     1.158407    -0.144771      74.67
 H      -0.381802     2.139142     0.105631      22.95
 C       1.876918    -0.210259    -0.570192      11.76
 C       3.457149    -0.637939    -0.638017      70.90
 H       3.638423    -1.307531    -1.745327      25.92
 O       4.303802     0.492985    -1.117596     118.54
 H       4.528082     1.106036    -0.204489      24.64
 C       3.826939    -1.562714     0.557865     106.53
 H       3.122413    -2.260859     0.671989      32.13
 O       5.303599    -2.155213     0.551516      25.01
 H       5.326058    -3.132077    -0.022645      22.47
 C       3.745705    -0.596466     1.847324     108.49
 O       4.440742     0.675162     1.806153     142.75
 H       3.833374     1.353980     2.212709      27.34
 H       3.989566    -1.376085     2.668279      31.00
 H       2.543610    -0.535547     2.168525      28.73
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name = lig-Water-frame_672
 C      -1.913113     3.444883     3.047865      72.93
 H      -2.552956     4.233980     2.632223      21.93
 C      -1.357245     1.032427     3.214809      57.05
 H      -1.605198    -0.052128     3.345845      23.08
 C      -0.242382     1.355618     4.007960       8.07
 O       0.759538     0.479651     4.361752     169.22
 C       0.651632    -0.899437     4.200203     130.56
 H       1.693882    -1.267205     4.399690      27.47
 H       0.325149    -1.128131     3.302745      32.04
 H       0.211284    -1.666951     5.016074      26.66
 C       0.027466     2.735694     4.155817      -0.51
 O       1.268669     3.115679     5.159060     162.58
 H       1.193676     4.073088     5.405178      29.46
 C      -0.844327     3.835894     3.912491      60.76
 H      -0.887054     4.880083     4.302294      16.44
 C      -2.136719     2.109948     2.731354      40.75
 C      -3.381010     1.728472     1.898174      90.41
 H      -3.904389     2.600088     1.881796      26.13
 O      -4.134921     0.493255     2.359873     276.80
 H      -5.100083     0.811023     2.225097      25.90
 C      -2.908643     1.528680     0.397970      88.37
 H      -2.386409     2.473738     0.057208      22.48
 C      -4.023642     1.640483    -0.649358      97.53
 O      -4.868701     0.470109    -0.813041     268.93
 H      -4.434976    -0.322023    -0.541978      30.57
 H      -3.631008     1.698686    -1.828682      23.15
 H      -4.631122     2.418193    -0.550851      28.28
 C       1.430771     1.093058    -0.319147      55.13
 H       1.987033     1.874758    -0.556553      25.31
 C       1.003037    -1.314946    -0.650709      70.15
 H       1.278032    -2.260451    -0.594165      26.30
 C      -0.379676    -1.211063    -0.494997      -7.91
 O      -1.325632    -2.373066    -0.531001     205.22
 C      -1.381464    -2.491959    -2.033920      80.15
 H      -2.382715    -3.020590    -2.131410      24.24
 H      -1.687293    -1.553994    -2.336366      28.46
 H      -0.261993    -2.927450    -2.055865      21.89
 C      -0.911041     0.151279    -0.058170       6.31
 O      -2.265767     0.164332     0.432809     177.23
 C      -0.001293     1.174819    -0.189382      55.63
 H      -0.392455     2.187494     0.014754      21.97
 C       1.840716    -0.279367    -0.676423      23.23
 C       3.431363    -0.648324    -0.714662      86.91
 H       3.548438    -1.401422    -1.419472      28.79
 O       4.369386     0.487470    -1.136678     170.14
 H       4.596089     1.025229    -0.418702      28.66
 C       3.791700    -1.541860     0.538256      72.95
 H       3.126294    -2.513324     0.639822      27.16
 O       5.282361    -2.136708     0.518737     111.90
 H       5.199711    -2.832913    -0.021755      33.18
 C       3.736598    -0.612847     1.846066     127.37
 O       4.402327     0.654265     1.838386     226.41
 H       3.728919     1.284933     2.113080      30.37
 H       4.097182    -1.131799     2.708831      30.25
 H       2.767130    -0.401691     1.972203      30.20
55
name = lig-Water-frame_673
 C      -1.949463     3.531211     3.027696      48.62
 H      -2.688642     4.226615     2.587773      22.67
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 C      -1.338466     1.017324     3.254205      60.41
 H      -1.450067    -0.079935     3.190696      23.22
 C      -0.274461     1.399581     4.023689       1.17
 O       0.766180     0.447913     4.353513     140.78
 C       0.707006    -0.981975     4.243245     115.16
 H       1.733993    -1.306216     4.347137      28.71
 H       0.214623    -1.139487     3.089628      26.25
 H       0.130049    -1.378623     5.034542      29.28
 C       0.089888     2.831289     4.228913       8.07
 O       1.246006     3.073328     5.070705     183.99
 H       0.982284     3.980743     5.544327      24.41
 C      -0.892687     3.756242     3.909642      63.17
 H      -0.713664     4.725441     4.373935      21.93
 C      -2.179795     2.097123     2.711709      17.92
 C      -3.401413     1.678219     1.833562      75.34
 H      -4.269932     2.542927     1.791973      23.50
 O      -4.123814     0.514949     2.374673     258.93
 H      -5.144918     0.607042     2.405892      26.81
 C      -2.954511     1.532184     0.379644      88.64
 H      -2.338671     2.383717     0.044793      23.51
 C      -4.004250     1.629599    -0.690505      82.34
 O      -4.863849     0.465415    -0.802647     244.94
 H      -4.556491    -0.467232    -0.425844      26.27
 H      -3.430317     1.881486    -1.545332      27.53
 H      -4.738991     2.654205    -0.424575      24.19
 C       1.392631     1.018294    -0.295484      52.73
 H       2.032201     2.040505    -0.561853      23.74
 C       0.990206    -1.315466    -0.649354      44.86
 H       1.200661    -2.524532    -0.574067      23.19
 C      -0.390875    -1.181694    -0.359353       5.86
 O      -1.272092    -2.371195    -0.463561     186.99
 C      -1.382910    -2.534551    -1.981074      68.78
 H      -2.140797    -3.266769    -2.486122      24.43
 H      -1.480056    -1.364104    -2.659799      24.61
 H      -0.388822    -2.711319    -2.346463      27.17
 C      -0.921749     0.118982    -0.099476      -0.77
 O      -2.241571     0.208493     0.404615     159.40
 C       0.060184     1.259186    -0.202592      48.65
 H      -0.384261     2.282554    -0.086058      22.15
 C       1.918881    -0.258815    -0.746735      36.88
 C       3.392279    -0.650235    -0.787437      68.50
 H       3.507267    -1.593914    -1.666574      25.08
 O       4.411536     0.441769    -1.154766     118.27
 H       4.626430     0.969948    -0.297246      25.50
 C       3.824706    -1.467142     0.563700      85.79
 H       3.198563    -2.348179     0.609609      29.97
 O       5.227611    -2.085748     0.484171      49.24
 H       5.077615    -2.857778    -0.241934      26.43
 C       3.727036    -0.676150     1.839971     111.08
 O       4.382373     0.647042     1.846388     195.99
 H       3.643145     1.383434     2.097480      27.63
 H       4.218317    -1.068323     2.806917      26.93
 H       2.539617    -0.295154     1.864024      25.77
55
name = lig-Water-frame_674
 C      -2.002613     3.515922     2.996238      49.82
 H      -2.677583     4.294718     2.700741      27.91
 C      -1.357224     1.042862     3.282829      62.94
 H      -1.540094     0.041062     2.893911      24.77
 C      -0.219390     1.446533     4.034043       7.46
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 O       0.781465     0.465282     4.367528     127.07
 C       0.726419    -1.050544     4.234434     113.20
 H       1.797615    -1.398447     4.195200      28.22
 H       0.346643    -1.404578     3.380076      31.41
 H      -0.095346    -1.208463     5.053132      26.51
 C       0.133415     2.841561     4.333552      25.78
 O       1.198089     3.047218     4.973782     207.68
 H       1.130025     3.728558     5.682537      29.27
 C      -0.915326     3.722671     3.912997      60.61
 H      -0.548663     4.755026     4.341521      17.62
 C      -2.243250     2.078080     2.706612       5.64
 C      -3.467421     1.669858     1.792420     105.65
 H      -4.220613     2.333940     1.769519      26.64
 O      -4.089612     0.521627     2.395361     297.78
 H      -5.095745     0.699031     2.342569      26.26
 C      -2.987862     1.523694     0.377375      79.89
 H      -2.088841     2.245012     0.278904      23.51
 C      -4.017734     1.614110    -0.709298     101.67
 O      -4.881528     0.453317    -0.806540     291.86
 H      -4.416356    -0.267436    -0.323930      28.61
 H      -3.328913     1.975730    -1.652094      25.50
 H      -4.565452     2.420985    -0.418125      27.86
 C       1.409683     0.972902    -0.355231      49.67
 H       2.020164     1.845220    -0.297787      27.11
 C       0.953132    -1.380659    -0.635574      17.00
 H       1.298356    -2.341400    -0.795269      27.65
 C      -0.424904    -1.152351    -0.222385      18.00
 O      -1.205525    -2.337195    -0.427939     200.86
 C      -1.374132    -2.533788    -1.973196      77.90
 H      -1.867752    -3.416471    -2.378381      26.43
 H      -1.475013    -1.594171    -2.499929      29.14
 H      -0.365833    -2.788878    -2.631255      28.01
 C      -0.918943     0.111177    -0.131711       8.67
 O      -2.198075     0.262553     0.342077     170.66
 C       0.033478     1.306949    -0.185573      55.31
 H      -0.246094     2.329312    -0.148715      24.63
 C       1.993886    -0.230362    -0.766356      21.05
 C       3.399826    -0.677593    -0.863741      87.49
 H       3.499344    -1.298157    -1.707639      30.89
 O       4.429845     0.374184    -1.166345     130.77
 H       4.537963     0.734620    -0.137513      27.27
 C       3.899513    -1.385334     0.568096      95.57
 H       3.085531    -2.195707     0.647221      31.13
 O       5.154409    -2.033501     0.432035      60.89
 H       5.083597    -2.770112    -0.353316      23.75
 C       3.676685    -0.680946     1.858574     140.85
 O       4.367800     0.664859     1.829934     236.31
 H       3.796148     1.355127     2.131774      31.46
 H       3.992804    -1.305976     2.651427      32.54
 H       2.689949    -0.638243     1.985498      31.85
55
name = lig-Water-frame_675
 C      -2.031602     3.417237     3.001645      55.77
 H      -2.609238     4.367620     2.818981      25.86
 C      -1.402278     1.127527     3.281668      51.74
 H      -1.569448     0.152757     2.740041      28.26
 C      -0.145913     1.436688     4.019431      18.46
 O       0.816619     0.499413     4.378928     114.06
 C       0.710278    -1.066214     4.250427     101.82
 H       1.702492    -1.454653     4.386534      28.33
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 H       0.254632    -1.667035     3.233726      25.75
 H       0.053962    -1.388442     5.045491      28.86
 C       0.003131     2.753996     4.355908      28.06
 O       1.238235     3.047640     4.936038     206.45
 H       1.325358     3.711127     5.697681      23.11
 C      -0.890972     3.750600     3.924025      33.98
 H      -0.726253     4.767782     4.100222      18.45
 C      -2.305761     2.087746     2.724268       0.31
 C      -3.499083     1.658941     1.807109      94.90
 H      -4.282050     2.606246     1.771282      23.97
 O      -4.068170     0.506546     2.413666     296.47
 H      -5.006421     0.765124     2.240321      24.60
 C      -2.940742     1.502781     0.378604     103.73
 H      -2.256542     2.296384     0.382819      27.05
 C      -3.991443     1.592612    -0.744720      87.02
 O      -4.889685     0.444771    -0.815757     286.16
 H      -4.311843    -0.143525    -0.338029      29.63
 H      -3.648165     1.772972    -1.772417      27.14
 H      -4.738144     2.565279    -0.441960      24.71
 C       1.428300     0.975267    -0.434112      46.68
 H       2.210290     1.833509    -0.130632      27.30
 C       0.954486    -1.359717    -0.617250      32.79
 H       1.364361    -2.398536    -1.032883      25.81
 C      -0.383833    -1.194621    -0.158373       9.83
 O      -1.154864    -2.303226    -0.429085     183.92
 C      -1.289517    -2.555760    -1.976762      53.05
 H      -1.990915    -3.548406    -1.857358      24.33
 H      -1.993296    -1.460072    -2.333419      23.80
 H      -0.352161    -2.831613    -2.399768      28.52
 C      -0.902923     0.226164    -0.129821      17.07
 O      -2.181612     0.288574     0.268546     191.73
 C      -0.003726     1.257616    -0.171996      69.85
 H      -0.163509     2.394466    -0.120285      25.93
 C       1.954670    -0.284293    -0.739171      19.01
 C       3.459117    -0.664965    -0.888159      87.95
 H       3.553370    -1.425961    -1.902528      26.67
 O       4.431408     0.305746    -1.148464     226.89
 H       4.569254     0.640842    -0.332106      34.20
 C       3.904444    -1.355709     0.505792     102.12
 H       3.041545    -2.056053     0.683095      30.96
 O       5.111177    -1.994166     0.372641     170.96
 H       5.055456    -2.549817    -0.295962      32.13
 C       3.661922    -0.639954     1.872394     107.68
 O       4.355215     0.663260     1.807709     210.07
 H       3.828112     1.405641     2.267767      28.24
 H       3.954899    -1.540663     2.597336      27.71
 H       2.448496    -0.752011     2.143141      27.10
55
name = lig-Water-frame_676
 C      -2.011295     3.375564     3.082857      44.88
 H      -2.606653     4.203952     2.761450      24.91
 C      -1.415438     1.191218     3.256239      60.36
 H      -1.474484     0.193322     2.902162      29.60
 C      -0.166564     1.351216     3.953146       1.20
 O       0.861336     0.503220     4.379021     128.59
 C       0.664905    -1.068894     4.249733     112.76
 H       1.677375    -1.391099     4.621232      25.15
 H       0.331763    -1.383139     3.338926      27.98
 H       0.129442    -1.548562     5.151043      26.16
 C      -0.122451     2.710925     4.382644       4.79
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 O       1.319794     3.046449     4.922386      79.90
 H       1.213479     3.926489     5.468155      23.38
 C      -0.907023     3.754176     3.886222      55.18
 H      -0.853209     4.936405     3.942563      22.66
 C      -2.359810     2.097624     2.757918      31.71
 C      -3.496991     1.687698     1.857511     106.03
 H      -4.076589     2.522020     1.773740      29.43
 O      -4.076524     0.489502     2.419604     259.91
 H      -5.110901     0.563766     2.271203      23.67
 C      -2.892572     1.500349     0.366567      99.90
 H      -2.416222     2.591378     0.219509      25.39
 C      -4.014596     1.614168    -0.768077      92.56
 O      -4.884804     0.432305    -0.815219     196.27
 H      -4.344656    -0.392942    -0.408025      27.14
 H      -3.696180     1.693617    -1.902976      26.33
 H      -4.641959     2.460345    -0.639781      29.31
 C       1.442581     1.004895    -0.496157      64.17
 H       2.227964     1.732340    -0.151623      29.67
 C       1.000219    -1.330222    -0.609004      64.35
 H       1.176638    -2.304699    -1.058180      27.60
 C      -0.290959    -1.206543    -0.171939       4.89
 O      -1.127703    -2.276670    -0.443720     217.64
 C      -1.293345    -2.579276    -1.897773      91.00
 H      -1.961193    -3.326062    -1.659186      27.52
 H      -2.031284    -1.812328    -2.279332      27.85
 H      -0.181957    -2.753902    -2.298391      26.41
 C      -0.865928     0.280861    -0.098263       6.95
 O      -2.204189     0.292997     0.197740     189.05
 C       0.048631     1.241662    -0.180921      76.59
 H      -0.266266     2.222454    -0.000944      29.25
 C       1.878389    -0.345571    -0.693748      16.27
 C       3.495963    -0.684093    -0.891819     109.83
 H       3.551523    -1.504996    -1.615493      31.17
 O       4.438135     0.265330    -1.156721     178.99
 H       4.758871     0.850514    -0.277953      24.33
 C       3.797339    -1.346113     0.430347      99.81
 H       3.065592    -2.196174     0.571899      30.16
 O       5.119340    -1.957255     0.338828      74.49
 H       5.017568    -2.633049    -0.539157      25.09
 C       3.638348    -0.623461     1.867426     122.03
 O       4.327739     0.651938     1.798624     234.67
 H       3.896902     1.378899     2.429665      28.07
 H       4.166660    -1.252965     2.534318      31.19
 H       2.658868    -0.424242     2.071870      29.35
55
name = lig-Water-frame_677
 C      -2.021326     3.405680     3.167436      48.37
 H      -2.692429     4.111728     2.632738      22.70
 C      -1.389703     1.144041     3.217124      65.74
 H      -1.552833     0.024342     3.043662      26.59
 C      -0.242823     1.316853     3.906521      -3.74
 O       0.876172     0.470788     4.362365     134.02
 C       0.656054    -1.028443     4.319282     114.36
 H       1.706209    -1.312763     4.492335      26.27
 H       0.348913    -1.199772     3.157548      26.89
 H      -0.080102    -1.422543     5.088207      26.25
 C      -0.110984     2.707923     4.421035     -24.63
 O       1.352252     3.053006     4.910856      76.85
 H       1.159132     3.974896     5.172813      22.68
 C      -0.940299     3.763428     3.839250      66.86
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 H      -0.726500     4.746097     4.003655      30.76
 C      -2.371045     2.086939     2.818073      30.47
 C      -3.450425     1.691409     1.891031      85.29
 H      -4.252180     2.591622     1.789979      26.63
 O      -4.110772     0.472064     2.416779     250.45
 H      -5.051714     0.467608     2.321533      26.67
 C      -2.905896     1.576017     0.334183      92.07
 H      -2.372428     2.413211     0.051998      28.80
 C      -4.031400     1.594398    -0.799367      84.88
 O      -4.881185     0.399750    -0.801407     222.94
 H      -4.485559    -0.447132    -0.627137      28.95
 H      -3.396896     1.735121    -1.753868      27.27
 H      -4.734016     2.596598    -0.679194      26.00
 C       1.456833     1.000383    -0.528913      86.30
 H       2.215271     1.807023    -0.354177      30.59
 C       1.016962    -1.371835    -0.609735      58.81
 H       1.208427    -2.398423    -0.975880      25.87
 C      -0.258199    -1.130125    -0.228135      26.41
 O      -1.114267    -2.241591    -0.437356     229.77
 C      -1.297061    -2.603735    -1.755694      98.50
 H      -1.926048    -3.702963    -1.819338      24.82
 H      -1.968712    -1.885143    -2.627328      25.80
 H      -0.368738    -2.677774    -2.397725      27.92
 C      -0.814843     0.175398    -0.052200      -4.87
 O      -2.222452     0.296423     0.127729     144.21
 C       0.148410     1.288076    -0.195506      54.95
 H      -0.346427     2.268535     0.115703      26.06
 C       1.904431    -0.294100    -0.671960      17.71
 C       3.446369    -0.707782    -0.830549     101.49
 H       3.569503    -1.657842    -1.631265      26.25
 O       4.469876     0.279197    -1.184087     208.82
 H       4.723405     0.812038    -0.368519      28.64
 C       3.672656    -1.383157     0.417057      98.47
 H       3.113519    -2.370334     0.404520      27.65
 O       5.142092    -1.937225     0.297614      71.43
 H       5.104257    -2.613282    -0.469088      28.56
 C       3.655844    -0.591608     1.800521     111.07
 O       4.309943     0.662849     1.792598     278.08
 H       3.956420     1.236232     2.397976      33.37
 H       4.295697    -1.095005     2.630614      27.86
 H       2.537700    -0.234247     2.089374      27.29
55
name = lig-Water-frame_678
 C      -2.133177     3.433960     3.177583      46.46
 H      -2.714282     4.217626     2.662694      21.19
 C      -1.396304     0.985572     3.163657      54.67
 H      -1.748127     0.006028     3.017320      25.32
 C      -0.252886     1.370385     3.952505       1.76
 O       0.842216     0.444292     4.333461     161.10
 C       0.655106    -0.951082     4.348740     131.03
 H       1.651882    -1.436539     4.374518      26.22
 H       0.398858    -1.229818     3.314929      28.76
 H      -0.229620    -1.212570     4.958414      26.60
 C      -0.008113     2.706738     4.407951       8.17
 O       1.312546     3.046772     4.881711      60.18
 H       1.320368     4.069312     5.158975      22.58
 C      -0.890460     3.741910     3.868430      86.60
 H      -0.496998     4.818651     4.151380      28.71
 C      -2.324264     2.063332     2.900387       7.53
 C      -3.446923     1.706109     1.885284      88.87
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 H      -4.249908     2.387667     1.902305      29.60
 O      -4.120077     0.454385     2.409171     215.32
 H      -5.119304     0.658154     2.233058      24.79
 C      -2.965012     1.632164     0.307896      71.50
 H      -2.089191     2.390532     0.006795      26.63
 C      -4.028778     1.563192    -0.792409      99.89
 O      -4.897537     0.383794    -0.799192     198.81
 H      -4.346589    -0.427357    -0.765156      28.57
 H      -3.283067     1.711342    -1.674015      27.26
 H      -4.729506     2.434633    -0.758055      27.87
 C       1.493114     1.028089    -0.525321      62.53
 H       2.206258     1.966568    -0.797490      23.65
 C       1.055213    -1.408866    -0.620858      53.65
 H       1.430573    -2.513376    -0.774327      22.47
 C      -0.292060    -1.067445    -0.317090      30.10
 O      -1.125236    -2.201366    -0.396359     217.39
 C      -1.345217    -2.680004    -1.707483     125.88
 H      -1.587200    -3.626435    -1.861663      29.41
 H      -1.910863    -1.868391    -2.486942      27.19
 H      -0.365111    -2.745740    -2.385724      26.85
 C      -0.753557     0.113611    -0.009775       6.76
 O      -2.214883     0.292642     0.060174     114.53
 C       0.161509     1.308441    -0.182252      55.88
 H      -0.116518     2.327326     0.077829      26.44
 C       1.997031    -0.256708    -0.693025      20.51
 C       3.359273    -0.710711    -0.808224      95.56
 H       3.518636    -1.414592    -1.673315      26.03
 O       4.482208     0.296492    -1.220033     225.74
 H       4.641037     0.729397    -0.394785      32.12
 C       3.645250    -1.475718     0.479375      99.59
 H       3.027238    -2.334045     0.494421      28.84
 O       5.158528    -1.918842     0.271682     140.62
 H       5.173041    -2.596247    -0.359376      31.22
 C       3.649779    -0.560923     1.750010     127.67
 O       4.326594     0.696652     1.745711     269.07
 H       3.852864     1.307040     2.445841      26.93
 H       3.987776    -1.226162     2.535425      29.72
 H       2.628160    -0.540144     2.091303      29.87
55
name = lig-Water-frame_679
 C      -2.185774     3.449069     3.199679      77.68
 H      -2.748526     4.294079     2.836519      19.23
 C      -1.404371     0.884977     3.164008      25.81
 H      -1.813257    -0.141923     2.886518      21.84
 C      -0.224404     1.375547     4.022745       4.98
 O       0.800522     0.473542     4.305816     140.30
 C       0.639540    -0.890146     4.333415     120.71
 H       1.486615    -1.568988     4.622432      27.09
 H       0.276956    -1.390052     3.255158      26.31
 H      -0.278113    -1.161809     5.008992      26.92
 C       0.089014     2.733681     4.328091      18.47
 O       1.255072     3.040766     4.849980     195.58
 H       1.342943     3.872815     5.325615      27.98
 C      -0.823317     3.720610     3.937173      91.67
 H      -0.521859     4.711890     4.134355      22.28
 C      -2.290085     2.022215     2.927807     -18.77
 C      -3.441956     1.692954     1.878881      80.33
 H      -4.287224     2.509354     1.977596      26.43
 O      -4.130765     0.448341     2.383601     251.96
 H      -5.049231     0.809925     2.182437      25.85
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 C      -2.973103     1.646449     0.315798      78.80
 H      -2.266841     2.395017     0.173367      27.61
 C      -4.011609     1.532337    -0.775915      91.09
 O      -4.908908     0.371598    -0.803512     188.35
 H      -4.132705    -0.350122    -0.839967      27.02
 H      -3.449643     1.559214    -1.819580      26.78
 H      -4.768730     2.417373    -0.813585      26.18
 C       1.538441     1.101815    -0.537867      53.11
 H       2.084131     1.879778    -0.971357      23.91
 C       1.123257    -1.371311    -0.621483      48.70
 H       1.464863    -2.340748    -0.620376      24.45
 C      -0.278787    -1.133603    -0.436059       9.17
 O      -1.166398    -2.176599    -0.337712     212.76
 C      -1.341746    -2.724155    -1.742933      80.91
 H      -1.658508    -3.936746    -1.684200      22.88
 H      -2.134973    -1.876165    -2.098346      24.00
 H      -0.267669    -2.702209    -2.123621      25.57
 C      -0.747539     0.233421     0.023796      15.76
 O      -2.189448     0.279290     0.004285     124.85
 C       0.153505     1.273948    -0.151417      64.21
 H       0.012630     2.358392    -0.015330      23.63
 C       2.010702    -0.273230    -0.729516      19.15
 C       3.351712    -0.692784    -0.828641      86.44
 H       3.399977    -1.347182    -1.790252      25.15
 O       4.457172     0.299175    -1.245322     125.17
 H       4.647704     0.808140    -0.257087      24.08
 C       3.735304    -1.535612     0.529885      84.29
 H       2.902707    -2.346654     0.826684      25.79
 O       5.152569    -1.894169     0.276962      99.11
 H       5.171911    -2.815897    -0.398442      25.28
 C       3.624000    -0.593978     1.726568      94.50
 O       4.344328     0.735650     1.690856     242.19
 H       3.783751     1.397417     2.265264      26.10
 H       3.920536    -1.384242     2.520570      27.30
 H       2.480239    -0.607374     2.000054      26.17
55
name = lig-Water-frame_680
 C      -2.094463     3.405293     3.280303      73.42
 H      -2.850237     4.235415     3.051111      26.17
 C      -1.389701     0.899376     3.240971      44.91
 H      -1.561227    -0.099272     2.855327      21.72
 C      -0.234206     1.300638     4.034307      23.87
 O       0.799052     0.531626     4.291021     180.19
 C       0.557215    -0.908134     4.301025     126.77
 H       1.375053    -1.351361     4.882558      27.46
 H       0.275952    -1.386015     3.365686      27.44
 H      -0.197333    -1.131395     5.040664      28.25
 C       0.092487     2.747038     4.200432      33.44
 O       1.265502     3.025889     4.844462     183.54
 H       1.090540     3.826719     5.529717      30.47
 C      -0.848050     3.703572     3.966368      80.98
 H      -0.590344     4.798208     4.133729      16.75
 C      -2.300005     1.989987     2.880286       8.62
 C      -3.443103     1.671214     1.891830      92.91
 H      -4.038579     2.598744     1.923805      24.76
 O      -4.142670     0.469137     2.337573     268.72
 H      -5.104297     0.631928     2.244178      27.88
 C      -2.964769     1.590302     0.363856      71.12
 H      -2.402552     2.635557     0.226255      20.24
 C      -4.029654     1.528700    -0.788714      84.20
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 O      -4.884812     0.350466    -0.808216     258.93
 H      -4.291944    -0.374929    -0.779100      29.50
 H      -3.567860     1.506602    -1.839250      26.12
 H      -4.709547     2.501765    -0.801797      25.80
 C       1.547663     1.092496    -0.554470      50.19
 H       2.152477     2.061865    -1.064564      21.07
 C       1.128435    -1.291338    -0.614349      47.40
 H       1.558212    -2.428992    -0.579918      22.00
 C      -0.242041    -1.157728    -0.492553       6.86
 O      -1.213162    -2.175977    -0.289903     201.51
 C      -1.329895    -2.790419    -1.729486      81.32
 H      -1.848046    -3.625908    -1.576513      25.82
 H      -2.332424    -2.039582    -2.180898      22.33
 H      -0.304883    -2.667942    -2.165261      25.28
 C      -0.771276     0.305706    -0.008731      10.59
 O      -2.153659     0.291994    -0.024322     141.33
 C       0.192610     1.279545    -0.125143      58.69
 H      -0.176407     2.357274    -0.083872      20.69
 C       1.955342    -0.223931    -0.751494      38.59
 C       3.442963    -0.700962    -0.876683      89.42
 H       3.347238    -1.467947    -1.812398      24.40
 O       4.407783     0.302172    -1.222486     205.32
 H       4.627487     0.793439    -0.486763      29.86
 C       3.842034    -1.537817     0.524845     111.27
 H       3.225903    -2.294273     0.891292      28.69
 O       5.142176    -1.915181     0.292106     226.43
 H       5.094704    -2.686824    -0.221913      32.83
 C       3.594325    -0.660427     1.746254      88.10
 O       4.339453     0.746136     1.637918     260.12
 H       3.809059     1.426772     1.977811      30.48
 H       4.074918    -1.130408     2.621315      26.49
 H       2.515918    -0.329120     1.731301      24.87
55
name = lig-Water-frame_681
 C      -1.993715     3.299884     3.356022      47.43
 H      -2.784900     3.970876     3.262267      29.35
 C      -1.375874     0.985563     3.334251      59.50
 H      -1.326146    -0.027265     2.920811      22.77
 C      -0.277364     1.292444     3.983676      22.33
 O       0.833966     0.542081     4.289122     161.15
 C       0.482460    -0.932160     4.321788     105.88
 H       1.460270    -1.153847     4.867391      26.26
 H       0.335665    -1.414165     3.253442      24.55
 H      -0.433489    -1.054618     5.086556      25.86
 C       0.055350     2.696642     4.094973      16.91
 O       1.301547     3.025078     4.870135     148.57
 H       0.923516     3.753156     5.413743      29.94
 C      -0.916441     3.725490     3.960423      84.02
 H      -0.704747     4.790176     4.189568      18.83
 C      -2.298212     1.976368     2.834026      29.43
 C      -3.429594     1.641489     1.897295      96.75
 H      -4.012574     2.628729     1.821520      25.48
 O      -4.156001     0.494302     2.294668     258.62
 H      -5.180443     0.504267     2.243894      26.58
 C      -2.947786     1.533530     0.391493      96.00
 H      -2.544394     2.503824     0.193772      23.93
 C      -4.059012     1.533982    -0.792496      77.53
 O      -4.870771     0.334767    -0.808989     258.65
 H      -4.412633    -0.525672    -0.642565      27.88
 H      -3.396776     1.642731    -1.797188      25.12
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 H      -4.672897     2.462635    -0.715236      27.07
 C       1.537912     1.102644    -0.591282      55.40
 H       2.091229     1.887531    -0.782473      26.44
 C       1.084436    -1.291776    -0.603431      53.77
 H       1.521783    -2.177186    -0.674982      24.74
 C      -0.262643    -1.084906    -0.444853      16.85
 O      -1.232257    -2.185542    -0.290126     216.31
 C      -1.371886    -2.780965    -1.661101     101.81
 H      -1.976524    -3.824050    -1.509203      23.82
 H      -2.056432    -2.410618    -2.473071      25.69
 H      -0.442572    -2.835829    -2.454961      24.29
 C      -0.764143     0.253182    -0.117523      17.03
 O      -2.122305     0.347901    -0.019045     171.28
 C       0.216661     1.351587    -0.113953      63.89
 H      -0.282739     2.275187    -0.066515      18.40
 C       1.980349    -0.154716    -0.771027      37.29
 C       3.492833    -0.725432    -0.906837     103.39
 H       3.580651    -1.484559    -1.632130      27.21
 O       4.361826     0.296938    -1.218902     180.77
 H       4.581272     0.859988    -0.340462      23.71
 C       3.903330    -1.467955     0.485698      99.13
 H       3.360983    -2.543573     0.650410      24.77
 O       5.185338    -1.953326     0.329174     177.53
 H       5.096751    -2.779766    -0.246428      28.73
 C       3.612444    -0.641210     1.758954      99.06
 O       4.338046     0.721609     1.576873     233.69
 H       3.669617     1.543237     1.787384      25.82
 H       4.002837    -0.903063     2.764994      26.36
 H       2.586216    -0.301877     1.697412      26.55
55
name = lig-Water-frame_682
 C      -2.037679     3.173505     3.357658      74.61
 H      -2.903475     3.929234     3.325740      22.98
 C      -1.431221     1.022915     3.347228      59.76
 H      -1.379550    -0.035229     3.002442      22.88
 C      -0.217408     1.390775     3.949537      14.10
 O       0.846259     0.506717     4.283674     158.77
 C       0.434792    -0.927652     4.382644     126.67
 H       1.349289    -1.380920     4.715347      28.69
 H       0.466835    -1.373783     3.320598      26.54
 H      -0.465801    -1.050330     4.852742      29.01
 C       0.057066     2.674214     4.079844      33.31
 O       1.300405     3.011447     4.874360     165.59
 H       1.061157     3.895737     5.331934      25.41
 C      -0.887107     3.728514     3.974084      47.86
 H      -0.819964     4.751651     4.280777      15.79
 C      -2.255939     1.956881     2.839643      39.39
 C      -3.420013     1.632563     1.871302     102.98
 H      -4.136283     2.502982     1.759503      25.82
 O      -4.174554     0.489212     2.275637     274.67
 H      -5.119301     0.763961     2.086732      25.75
 C      -2.947076     1.484485     0.373845      97.46
 H      -2.345795     2.457241     0.133589      22.87
 C      -4.037087     1.510827    -0.765064      76.67
 O      -4.879293     0.327616    -0.824046     258.71
 H      -4.379663    -0.518013    -0.427807      25.17
 H      -3.375898     1.734577    -1.650716      26.19
 H      -4.840047     2.425092    -0.570441      24.28
 C       1.492493     1.148339    -0.606898      38.34
 H       2.364402     2.085030    -0.497767      23.85
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 C       1.049720    -1.250545    -0.608016      32.87
 H       1.500827    -2.357904    -0.826687      21.87
 C      -0.331691    -1.014548    -0.346378      25.19
 O      -1.226386    -2.182758    -0.344199     207.71
 C      -1.427096    -2.833475    -1.610487      99.18
 H      -1.680766    -3.829456    -1.442219      26.93
 H      -2.171125    -2.217395    -2.617649      22.70
 H      -0.540321    -3.070759    -2.212153      26.74
 C      -0.714639     0.224909    -0.239432      19.65
 O      -2.105522     0.409259     0.007889     208.04
 C       0.183535     1.374532    -0.132907      77.06
 H      -0.253862     2.454638     0.025878      20.61
 C       2.038223    -0.206386    -0.792921      22.90
 C       3.470971    -0.724927    -0.875268      84.87
 H       3.842994    -1.653833    -1.669597      24.06
 O       4.360474     0.328374    -1.220447     155.61
 H       4.405989     0.728206    -0.237454      25.74
 C       3.893735    -1.437050     0.455016     102.73
 H       3.272995    -2.241135     0.345917      29.36
 O       5.293001    -2.000930     0.370918     116.16
 H       5.214805    -2.874923    -0.333297      24.60
 C       3.669365    -0.549272     1.745328     115.84
 O       4.330648     0.706709     1.511794     258.01
 H       3.672717     1.405290     1.687427      30.04
 H       3.780296    -0.965028     2.814965      27.97
 H       2.458067    -0.502327     1.827049      27.04
55
name = lig-Water-frame_683
 C      -2.144424     3.198646     3.360913      58.79
 H      -2.948795     3.863744     3.225646      22.80
 C      -1.426307     0.957865     3.331907      50.77
 H      -1.669777    -0.052933     3.087251      23.27
 C      -0.133320     1.415108     3.907011       3.79
 O       0.832902     0.455870     4.283406     169.68
 C       0.447478    -0.901778     4.403567     116.77
 H       1.141890    -1.697795     4.884298      26.75
 H       0.358664    -1.327183     3.322836      26.72
 H      -0.686971    -1.148702     4.808964      25.67
 C       0.141958     2.786868     4.173635      28.57
 O       1.276449     3.000134     4.861189     173.55
 H       1.306449     3.958336     5.218366      25.65
 C      -0.868441     3.662702     3.959117      67.17
 H      -0.887635     4.726746     4.422387      23.35
 C      -2.270466     1.910657     2.826944      11.47
 C      -3.404741     1.627023     1.827656      95.58
 H      -4.139893     2.457240     1.812643      25.59
 O      -4.205679     0.473805     2.265897     282.62
 H      -5.073488     0.890753     2.037358      25.12
 C      -2.921324     1.506496     0.328042     107.25
 H      -2.271868     2.379385     0.179628      25.72
 C      -4.030550     1.493452    -0.686485      94.64
 O      -4.882544     0.312465    -0.843547     319.49
 H      -4.384793    -0.291650    -0.353485      30.79
 H      -3.512100     1.793076    -1.758465      24.89
 H      -4.740336     2.251670    -0.529312      26.43
 C       1.518363     1.210729    -0.587242      26.59
 H       2.163065     1.894808    -0.388189      26.85
 C       1.049416    -1.227726    -0.640032      50.63
 H       1.154679    -2.232341    -0.853517      24.92
 C      -0.347951    -1.075513    -0.291409      11.15
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 O      -1.215650    -2.153053    -0.396469     230.10
 C      -1.477046    -2.870937    -1.630370      95.09
 H      -1.846496    -3.883740    -1.295729      25.41
 H      -2.097607    -2.199421    -2.081957      26.68
 H      -0.314244    -3.138930    -1.898817      23.40
 C      -0.743280     0.346767    -0.298109      13.17
 O      -2.087734     0.418512     0.038108     203.97
 C       0.147767     1.382559    -0.195592      73.78
 H      -0.077324     2.338185     0.097476      25.34
 C       2.026055    -0.289056    -0.802196      17.04
 C       3.481445    -0.731701    -0.865059     105.32
 H       3.626760    -1.454330    -1.585043      28.87
 O       4.375566     0.380132    -1.205934     194.03
 H       4.467070     0.778879    -0.361768      29.54
 C       3.897789    -1.420747     0.443265      72.05
 H       2.959828    -2.187142     0.404368      26.12
 O       5.388487    -2.054681     0.401800     165.38
 H       5.400987    -2.691816    -0.196684      31.48
 C       3.677430    -0.500620     1.721094     128.36
 O       4.320456     0.705607     1.452183     270.12
 H       3.715668     1.410645     1.732509      30.54
 H       3.906856    -1.062219     2.625778      29.69
 H       2.634860    -0.475327     1.795185      29.79
55
name = lig-Water-frame_684
 C      -2.200166     3.270027     3.361057      35.14
 H      -3.023201     4.009761     3.094199      22.38
 C      -1.335887     0.880743     3.315351      36.89
 H      -1.799202    -0.156320     3.217591      23.92
 C      -0.100754     1.359844     3.847713       0.07
 O       0.831231     0.418858     4.305614     179.37
 C       0.414805    -0.940760     4.392066     130.38
 H       0.959064    -1.506952     5.105197      28.55
 H       0.222472    -1.302395     3.316427      27.58
 H      -0.509885    -0.991238     4.809923      30.85
 C       0.193577     2.847342     4.261927       6.96
 O       1.310685     3.016047     4.867076     182.04
 H       1.306960     3.927367     5.207997      26.09
 C      -0.945187     3.627737     3.936873      80.66
 H      -0.875750     4.538222     4.413957      29.58
 C      -2.328285     1.893477     2.815257     -25.69
 C      -3.384158     1.607137     1.795715      92.24
 H      -4.022030     2.578360     1.882509      25.55
 O      -4.234354     0.461480     2.248424     245.81
 H      -5.274309     0.693066     2.166144      24.23
 C      -2.876205     1.564617     0.302697     101.47
 H      -2.348131     2.550229     0.151702      26.00
 C      -4.040128     1.496717    -0.665301      91.31
 O      -4.869272     0.299870    -0.857730     261.99
 H      -4.437027    -0.386415    -0.267212      28.65
 H      -3.718498     1.722956    -1.688582      26.54
 H      -4.799847     2.483510    -0.383734      25.18
 C       1.541030     1.139698    -0.555031      33.21
 H       2.320080     2.118624    -0.319282      25.05
 C       0.987837    -1.248989    -0.672850      57.59
 H       1.149777    -2.396231    -0.899740      25.16
 C      -0.317331    -1.092401    -0.312631      11.05
 O      -1.217277    -2.107527    -0.390616     216.62
 C      -1.425817    -2.938184    -1.603252      85.96
 H      -2.257995    -3.692726    -1.290696      24.36
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 H      -2.321656    -2.071285    -2.244787      22.26
 H      -0.517453    -3.108148    -2.038816      28.00
 C      -0.826646     0.410299    -0.299857       4.55
 O      -2.082171     0.384653     0.071861     178.36
 C       0.178926     1.401819    -0.292296      65.94
 H      -0.082767     2.435317     0.198801      24.83
 C       1.980996    -0.260196    -0.786496      20.59
 C       3.520799    -0.694257    -0.855932      94.71
 H       3.388487    -1.454300    -1.880864      25.21
 O       4.388312     0.420603    -1.205778     122.29
 H       4.673612     1.036097    -0.316107      22.55
 C       3.892650    -1.446599     0.448614      82.50
 H       3.235744    -2.198600     0.751713      29.68
 O       5.432624    -2.066722     0.454101      63.77
 H       5.504783    -2.815575    -0.360026      23.03
 C       3.690830    -0.534368     1.661648     102.37
 O       4.318208     0.742974     1.405606     165.77
 H       3.832092     1.564734     1.919224      27.15
 H       4.314021    -1.080806     2.490634      28.08
 H       2.494014    -0.234139     1.749487      25.42
55
name = lig-Water-frame_685
 C      -2.233556     3.270830     3.311513      22.73
 H      -2.876141     4.124132     3.064164      19.63
 C      -1.283015     0.869862     3.268623      42.40
 H      -1.514374    -0.162801     3.325979      24.81
 C      -0.082508     1.304755     3.819228      13.95
 O       0.853358     0.406476     4.338389     169.01
 C       0.353617    -0.987231     4.368506      98.50
 H       1.118372    -1.334910     5.174013      24.92
 H       0.295906    -1.478955     3.371783      27.30
 H      -0.705487    -0.798288     4.963054      24.30
 C       0.086340     2.747629     4.235723     -16.67
 O       1.410550     3.066271     4.906487     149.40
 H       1.198689     3.980219     5.401802      22.16
 C      -1.012709     3.625830     3.955182      91.36
 H      -0.921630     4.710506     4.392735      29.93
 C      -2.336716     1.908052     2.859930      -7.71
 C      -3.398305     1.605602     1.794378     101.40
 H      -3.940544     2.521177     1.798022      27.44
 O      -4.261061     0.444339     2.222211     280.59
 H      -5.183006     0.632208     2.245254      29.52
 C      -2.855252     1.613946     0.304993      88.42
 H      -2.417515     2.638124     0.041458      25.74
 C      -4.100138     1.551761    -0.662139      89.94
 O      -4.840249     0.285432    -0.852598     229.15
 H      -4.637431    -0.534138    -0.232536      26.48
 H      -3.759170     1.779412    -1.841427      24.24
 H      -4.673218     2.344921    -0.338326      29.09
 C       1.593861     1.049162    -0.508633      64.10
 H       2.220213     1.838443    -0.482973      27.37
 C       0.950663    -1.328768    -0.720666      53.70
 H       1.422586    -2.288494    -0.876256      25.53
 C      -0.318868    -1.004440    -0.395055      17.84
 O      -1.237996    -2.082018    -0.352249     231.13
 C      -1.460603    -2.903414    -1.577299     116.57
 H      -2.056512    -3.726230    -1.454416      29.75
 H      -1.880349    -2.502309    -2.377541      29.92
 H      -0.627659    -3.312645    -2.445080      25.33
 C      -0.820454     0.363880    -0.280372       7.24
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 O      -2.119581     0.362173     0.116021     161.80
 C       0.191482     1.445572    -0.366578      59.75
 H      -0.074866     2.380290     0.020138      24.06
 C       1.954773    -0.174483    -0.744833      30.86
 C       3.515653    -0.657482    -0.891885     101.66
 H       3.559102    -1.184687    -1.702997      31.31
 O       4.411719     0.457223    -1.204426     194.31
 H       4.606233     0.897648    -0.411490      29.79
 C       3.929335    -1.480261     0.452315      81.37
 H       3.467047    -2.496098     0.854154      26.63
 O       5.432249    -2.064294     0.493655     102.15
 H       5.455317    -2.738545    -0.303920      26.06
 C       3.721864    -0.551889     1.606456     123.54
 O       4.326204     0.820764     1.377856     246.36
 H       3.995231     1.440067     1.980078      31.95
 H       4.301252    -0.939150     2.387820      31.31
 H       2.764212    -0.392570     1.853637      30.01
55
name = lig-Water-frame_686
 C      -2.214844     3.230338     3.253785      80.92
 H      -2.851447     4.070384     3.002020      25.47
 C      -1.280639     0.930552     3.205605      43.32
 H      -1.305056    -0.191710     3.164602      19.41
 C      -0.062365     1.292373     3.837325      21.04
 O       0.876342     0.403154     4.348799     170.83
 C       0.292262    -0.996274     4.420227     110.98
 H       1.108238    -1.416483     4.953417      27.69
 H       0.419882    -1.722715     3.495992      25.69
 H      -0.615632    -0.988905     4.849541      27.71
 C      -0.029093     2.611877     4.186171      13.72
 O       1.460509     3.131089     4.937440      15.48
 H       1.076419     3.849056     5.507610      32.24
 C      -1.035685     3.647210     4.016180      42.12
 H      -0.969306     4.669258     4.212524       2.61
 C      -2.312325     1.901950     2.909799      37.30
 C      -3.423883     1.613024     1.821719      87.10
 H      -4.168192     2.545895     1.732750      23.71
 O      -4.245349     0.421993     2.188313     272.73
 H      -5.224133     0.883742     2.186456      25.52
 C      -2.887498     1.618787     0.310269      84.57
 H      -2.304492     2.502332     0.046570      24.83
 C      -4.123199     1.571297    -0.700917      84.35
 O      -4.821164     0.272164    -0.843149     239.93
 H      -4.654577    -0.366878    -0.194937      30.53
 H      -3.804925     1.889253    -1.649331      27.68
 H      -4.971004     2.424351    -0.221650      24.81
 C       1.561708     1.053061    -0.463356      54.03
 H       2.464830     1.866777    -0.586226      23.10
 C       1.017821    -1.331307    -0.769519      38.42
 H       1.487297    -2.325369    -0.869735      22.75
 C      -0.356789    -0.941346    -0.517404      14.27
 O      -1.272227    -2.079674    -0.327720     189.75
 C      -1.443730    -2.881411    -1.600647      93.97
 H      -1.837914    -3.990414    -1.340735      24.58
 H      -1.959324    -2.269599    -2.687759      23.18
 H      -0.622371    -3.358922    -2.042832      26.77
 C      -0.741564     0.326643    -0.251053      20.09
 O      -2.160596     0.366190     0.154986     180.20
 C       0.170643     1.419092    -0.415825      57.10
 H      -0.083142     2.524281    -0.236926      21.51
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 C       1.972487    -0.254852    -0.715768      25.82
 C       3.476439    -0.601321    -0.895615      75.07
 H       3.785770    -1.341926    -1.933613      23.99
 O       4.431288     0.469612    -1.211849     139.60
 H       4.531742     0.908364    -0.224368      22.59
 C       3.999309    -1.531186     0.448776      90.56
 H       3.461702    -2.456782     0.510479      28.26
 O       5.404261    -2.036830     0.515449     188.59
 H       5.409379    -2.648819    -0.164988      31.98
 C       3.813248    -0.526396     1.572573      94.61
 O       4.342008     0.878775     1.344562     213.93
 H       3.948441     1.461175     2.097669      27.71
 H       4.284112    -0.922745     2.600278      27.59
 H       2.639874    -0.637781     2.041930      25.90
55
name = lig-Water-frame_687
 C      -2.132924     3.222292     3.245457      69.91
 H      -2.999995     3.880897     2.871960      28.31
 C      -1.279936     0.976918     3.152913      52.18
 H      -1.401672    -0.021407     2.689903      22.17
 C      -0.077590     1.279430     3.866442      22.80
 O       0.876538     0.382833     4.336078     152.68
 C       0.318420    -1.017650     4.462414     106.22
 H       1.049326    -1.639058     5.089333      26.73
 H       0.316064    -1.571073     3.544394      27.29
 H      -0.810020    -1.221142     4.926165      24.91
 C      -0.067319     2.606686     4.199581       6.61
 O       1.439029     3.162358     4.940407      32.73
 H       1.022795     3.892397     5.530519      29.24
 C      -1.052570     3.604673     4.039535      37.76
 H      -0.835035     4.716415     4.195163      11.37
 C      -2.308808     1.856557     2.896714      35.46
 C      -3.457377     1.645649     1.855009     105.69
 H      -4.173971     2.390243     1.900393      25.62
 O      -4.234827     0.423576     2.146429     327.96
 H      -5.093854     0.872297     2.139881      29.27
 C      -2.950091     1.579635     0.324324      79.57
 H      -2.142863     2.407057     0.153926      21.42
 C      -4.176995     1.585702    -0.674223      97.76
 O      -4.805306     0.280620    -0.850368     245.42
 H      -4.455992    -0.192819    -0.006864      26.96
 H      -3.793580     2.105181    -1.773101      24.18
 H      -4.929000     2.202737    -0.382704      27.19
 C       1.521148     1.115191    -0.450311      43.22
 H       2.374356     1.778545    -0.602182      24.52
 C       1.087550    -1.283264    -0.805753      55.54
 H       1.238274    -2.418869    -0.914698      22.51
 C      -0.355432    -1.002544    -0.641719      13.30
 O      -1.302595    -2.073660    -0.342054     208.29
 C      -1.429007    -2.883376    -1.659380     111.95
 H      -1.907939    -3.675813    -1.209053      28.15
 H      -1.975342    -2.272620    -2.207573      28.70
 H      -0.198288    -3.131485    -1.583962      21.07
 C      -0.731070     0.343896    -0.215785      13.28
 O      -2.162187     0.377304     0.177334     193.48
 C       0.171556     1.389355    -0.426124      55.61
 H      -0.131399     2.436528    -0.590334      21.75
 C       2.019689    -0.380570    -0.700125      26.40
 C       3.492914    -0.618490    -0.943566      95.39
 H       3.572451    -1.243153    -1.658429      30.65
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 O       4.439463     0.480377    -1.188150     131.47
 H       4.467487     1.002669    -0.282388      23.65
 C       4.074821    -1.525754     0.421004      89.36
 H       3.204553    -2.310757     0.288134      27.27
 O       5.368307    -1.985113     0.525031     132.48
 H       5.506529    -2.827836    -0.240415      23.02
 C       3.879994    -0.517510     1.641772     110.35
 O       4.343732     0.904258     1.326445     261.34
 H       3.832053     1.538737     2.002082      27.77
 H       4.360615    -0.839405     2.486024      31.82
 H       2.905179    -0.566531     1.798174      30.87
55
name = lig-Water-frame_688
 C      -2.098026     3.212417     3.244619      62.89
 H      -2.886078     3.799395     2.935239      29.18
 C      -1.270247     0.953438     3.085808      52.42
 H      -1.449506     0.150035     2.370340      22.22
 C      -0.132050     1.262872     3.896313       2.78
 O       0.852738     0.338215     4.322451     152.33
 C       0.353141    -1.068489     4.521316     107.08
 H       0.942034    -1.629469     5.238998      27.91
 H       0.190774    -1.313216     3.368127      24.54
 H      -0.618691    -1.093959     4.916725      29.20
 C       0.002036     2.686832     4.288610      10.92
 O       1.344720     3.160306     4.920333     138.37
 H       1.099531     4.031002     5.420706      28.85
 C      -1.042805     3.571814     4.029914      43.27
 H      -0.714055     4.575660     4.285936      11.55
 C      -2.319175     1.854377     2.840018      18.41
 C      -3.458266     1.644522     1.876562      95.19
 H      -4.194794     2.570454     2.131095      23.15
 O      -4.219188     0.427937     2.104002     294.84
 H      -5.223038     0.657683     2.184257      28.87
 C      -2.985594     1.559972     0.358124      88.47
 H      -2.387949     2.403266     0.235516      24.77
 C      -4.187718     1.606559    -0.684230      87.70
 O      -4.775682     0.285058    -0.846573     263.86
 H      -4.325818    -0.134856    -0.017622      26.58
 H      -3.899230     1.963203    -1.585460      29.01
 H      -5.159681     2.377484    -0.315754      24.19
 C       1.529471     1.074749    -0.480155      34.52
 H       2.243163     1.964138    -0.612469      23.95
 C       1.041926    -1.320332    -0.841371      50.66
 H       1.184577    -2.335940    -1.030671      23.93
 C      -0.350151    -1.046856    -0.687414      20.23
 O      -1.311437    -2.038160    -0.379106     217.53
 C      -1.334803    -2.895509    -1.605995     117.43
 H      -2.073255    -3.740103    -1.296762      24.95
 H      -2.083520    -2.119120    -2.351179      23.90
 H      -0.357043    -2.967177    -1.844200      28.03
 C      -0.791904     0.302562    -0.215091       8.65
 O      -2.132526     0.375826     0.187374     181.44
 C       0.175031     1.389762    -0.425684      44.20
 H      -0.228999     2.353121    -0.734034      20.78
 C       2.091646    -0.338435    -0.671855      10.26
 C       3.564935    -0.644029    -0.924701     100.70
 H       3.461077    -1.495842    -1.935733      23.18
 O       4.429602     0.489331    -1.174280     147.86
 H       4.443640     1.002505    -0.310044      26.38
 C       4.076465    -1.449586     0.384664     100.82
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 H       3.222917    -2.131524     0.449721      28.64
 O       5.362684    -1.975688     0.494435     238.83
 H       5.602831    -2.679525    -0.059323      29.81
 C       3.953086    -0.504954     1.674359      83.07
 O       4.332400     0.912797     1.328216     273.93
 H       3.813719     1.570595     1.744662      31.01
 H       4.637433    -0.868160     2.582388      27.02
 H       2.715741    -0.340797     1.715430      24.53
55
name = lig-Water-frame_689
 C      -2.119631     3.170460     3.241806      57.16
 H      -2.834287     4.107931     3.055043      21.91
 C      -1.265087     0.911666     3.014348      46.67
 H      -1.228393    -0.003977     2.337443      23.19
 C      -0.182114     1.272502     3.937987     -42.08
 O       0.820910     0.303284     4.321700     146.66
 C       0.372309    -1.083769     4.521045     108.23
 H       1.102854    -1.609723     5.183478      26.88
 H       0.276300    -1.473371     3.573879      26.95
 H      -0.713443    -0.877242     5.041689      25.45
 C       0.115489     2.714228     4.392668     -15.25
 O       1.206881     3.141083     4.885899      53.54
 H       1.086799     4.046381     5.276851      32.70
 C      -0.968532     3.564103     4.024831      49.60
 H      -0.866311     4.609261     4.335078      20.55
 C      -2.294998     1.894796     2.787360      36.35
 C      -3.484587     1.647074     1.886392     104.94
 H      -4.006280     2.507157     2.020025      27.79
 O      -4.210620     0.415735     2.075793     280.34
 H      -5.228740     0.536772     2.237138      28.76
 C      -3.017906     1.582953     0.398026      72.07
 H      -2.553995     2.663398     0.180133      22.87
 C      -4.233531     1.634903    -0.645111      82.61
 O      -4.734170     0.281585    -0.828965     245.62
 H      -4.407096    -0.318761    -0.208667      31.95
 H      -3.805691     1.935636    -1.831206      24.04
 H      -4.877963     2.312868    -0.293875      28.92
 C       1.589419     0.995217    -0.542483      50.90
 H       2.035094     2.067669    -0.601568      26.93
 C       0.987141    -1.344167    -0.867003      75.92
 H       1.418169    -2.397535    -1.202626      23.52
 C      -0.360154    -1.015244    -0.632463      23.56
 O      -1.300689    -2.011838    -0.435970     255.89
 C      -1.345731    -2.857142    -1.548361     141.45
 H      -1.717695    -3.908269    -1.608718      27.86
 H      -1.690876    -2.459014    -2.436797      30.26
 H      -0.344800    -3.163559    -2.373172      24.11
 C      -0.830777     0.250859    -0.268137      12.90
 O      -2.107793     0.364909     0.193597     162.47
 C       0.135466     1.348243    -0.417345      74.07
 H      -0.260854     2.411330    -0.650145      22.13
 C       2.092927    -0.230942    -0.657678      22.01
 C       3.641203    -0.707930    -0.911202     118.25
 H       3.681213    -1.222768    -1.715500      30.82
 O       4.414876     0.488509    -1.192039     154.57
 H       4.455824     0.914640    -0.153814      22.16
 C       4.041288    -1.337047     0.377379     110.80
 H       3.334087    -2.231421     0.718338      26.82
 O       5.387795    -1.968253     0.466306     199.04
 H       5.592543    -2.731403    -0.193396      26.33
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 C       3.970934    -0.454391     1.669375     117.38
 O       4.346978     0.908255     1.329234     277.83
 H       3.651827     1.663190     1.685245      26.38
 H       4.538576    -0.850761     2.426444      30.67
 H       3.027000    -0.391974     2.034471      29.17
55
name = lig-Water-frame_690
 C      -2.125809     3.196660     3.284157      50.70
 H      -2.704355     4.024840     3.154080      19.95
 C      -1.232803     0.900320     2.980676      34.94
 H      -1.051636    -0.085377     2.631506      23.36
 C      -0.201705     1.283092     3.971881     -13.21
 O       0.795203     0.299091     4.320576     131.52
 C       0.355598    -1.058775     4.535209     110.13
 H       1.247365    -1.511723     5.038853      26.09
 H       0.304124    -1.926753     3.655842      24.11
 H      -0.570332    -1.003859     5.115549      26.61
 C       0.050906     2.637042     4.390689       0.18
 O       1.165113     3.135550     4.895361     -33.45
 H       0.915881     4.082966     5.268366      28.13
 C      -0.892686     3.562715     4.013054      99.07
 H      -1.116764     4.635440     4.330817      25.26
 C      -2.257509     1.895280     2.728166      11.63
 C      -3.490822     1.623632     1.855950      90.43
 H      -4.202965     2.618518     1.827924      23.87
 O      -4.207979     0.380093     2.074235     304.65
 H      -5.083490     0.720808     2.219975      29.12
 C      -3.033300     1.667053     0.398668      74.95
 H      -2.546800     2.540804     0.178180      24.58
 C      -4.192314     1.596399    -0.640034      82.10
 O      -4.721376     0.276867    -0.827626     238.64
 H      -4.357777    -0.489467    -0.254209      27.40
 H      -3.885771     1.915622    -1.505487      30.74
 H      -4.984970     2.517033    -0.159886      25.30
 C       1.561883     1.035699    -0.603625      49.10
 H       2.184236     1.883902    -0.612793      29.87
 C       1.014092    -1.313197    -0.877626      68.28
 H       1.391498    -2.200139    -1.203937      25.18
 C      -0.337382    -1.002326    -0.545507      17.91
 O      -1.295558    -2.022047    -0.501025     234.14
 C      -1.304182    -2.888900    -1.613385     125.13
 H      -1.520577    -3.948584    -1.416086      27.07
 H      -1.841083    -2.375178    -2.668968      26.03
 H      -0.477420    -3.157168    -2.062805      29.69
 C      -0.825996     0.292615    -0.335118      24.33
 O      -2.119351     0.362747     0.201408     138.00
 C       0.098520     1.262032    -0.415115      72.94
 H      -0.142272     2.278033    -0.351737      25.98
 C       2.053720    -0.258728    -0.698950      -5.89
 C       3.654767    -0.687930    -0.865472      96.90
 H       3.902114    -1.433742    -1.928299      23.85
 O       4.413898     0.487314    -1.193180     154.57
 H       4.544220     0.846186    -0.319103      29.86
 C       4.018384    -1.302452     0.440033     102.58
 H       3.473330    -2.191830     0.742601      28.72
 O       5.432178    -1.957097     0.435301     101.12
 H       5.314937    -2.686050    -0.406248      24.09
 C       3.971696    -0.383527     1.630721     116.49
 O       4.368187     0.933795     1.337036     297.70
 H       3.699605     1.507981     1.724909      29.68
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 H       4.702846    -0.922986     2.415806      27.61
 H       2.967418    -0.517720     2.395684      24.99
55
name = lig-Water-frame_691
 C      -2.063587     3.204513     3.347027      57.46
 H      -2.925079     3.991943     3.099859      21.22
 C      -1.178305     0.946202     3.015581      43.29
 H      -1.150803    -0.197395     2.832980      22.73
 C      -0.208144     1.254309     3.965694      31.70
 O       0.769450     0.318259     4.306080     190.37
 C       0.371622    -1.078485     4.540728     119.11
 H       1.248609    -1.389505     5.109468      27.32
 H       0.196649    -1.771705     3.816811      29.14
 H      -0.575276    -1.243054     5.274407      26.26
 C      -0.093596     2.536747     4.331628      19.26
 O       1.199636     3.145044     4.951824      53.60
 H       0.821522     3.953587     5.353093      22.57
 C      -0.937619     3.576747     3.971164      58.67
 H      -0.903714     4.537299     4.405900      26.45
 C      -2.229422     1.875999     2.682381      -3.86
 C      -3.482959     1.630914     1.795278     105.09
 H      -4.227203     2.327616     1.868965      25.61
 O      -4.203129     0.351641     2.090175     275.77
 H      -5.153317     0.829472     2.203254      24.43
 C      -3.029808     1.705667     0.363506      76.19
 H      -2.270818     2.601112     0.162901      22.04
 C      -4.160469     1.560741    -0.567648      98.28
 O      -4.735214     0.258013    -0.839273     229.21
 H      -4.175540    -0.340998    -0.220011      27.32
 H      -3.807468     2.117184    -1.696678      24.44
 H      -4.911705     2.161898    -0.309709      28.63
 C       1.479708     1.091513    -0.655127      40.65
 H       2.465790     1.789656    -0.603697      25.57
 C       1.059288    -1.226417    -0.854874      70.30
 H       1.300815    -2.336734    -1.193158      24.13
 C      -0.293079    -1.040181    -0.487319      10.97
 O      -1.295691    -2.044442    -0.559954     196.35
 C      -1.285586    -2.942376    -1.752615     106.39
 H      -1.734011    -3.762940    -1.053720      24.77
 H      -2.042123    -2.518735    -2.308976      27.71
 H       0.053350    -3.022216    -1.863798      20.23
 C      -0.855594     0.322343    -0.365974      12.66
 O      -2.147977     0.381396     0.200772     140.32
 C       0.151707     1.244965    -0.425574      70.76
 H      -0.118036     2.299364     0.047050      22.98
 C       2.015701    -0.347584    -0.790806       4.29
 C       3.603310    -0.658430    -0.885438      97.93
 H       3.808846    -1.408910    -1.486587      30.14
 O       4.422417     0.475622    -1.204633      86.86
 H       4.748669     1.069213    -0.293567      20.21
 C       4.041011    -1.326537     0.523196      84.09
 H       3.282659    -2.199514     0.646552      27.79
 O       5.451485    -1.944592     0.379162     198.44
 H       5.282231    -2.475395    -0.284042      31.44
 C       3.974006    -0.361377     1.675704     131.21
 O       4.391746     0.970776     1.350756     296.60
 H       3.779124     1.632209     1.863989      26.33
 H       4.834775    -0.747174     2.163137      29.34
 H       3.125308    -0.453756     2.237896      28.09
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name = lig-Water-frame_692
 C      -2.101941     3.183017     3.313950      45.44
 H      -2.946171     3.772048     3.116510      23.88
 C      -1.187679     0.959866     3.048124      65.88
 H      -1.442839    -0.017747     2.792988      26.32
 C      -0.194705     1.187012     3.935645      40.81
 O       0.744743     0.329262     4.293554     198.46
 C       0.389695    -1.091906     4.603312     107.14
 H       1.294278    -1.428686     5.205173      26.80
 H       0.124018    -1.593581     3.522908      25.57
 H      -0.446482    -1.284966     5.343775      27.78
 C      -0.122742     2.544209     4.323770      14.33
 O       1.205405     3.113198     4.998889      71.18
 H       0.861162     3.947851     5.529129      21.23
 C      -0.995085     3.592456     3.962720      26.32
 H      -0.586808     4.523621     4.431809      14.13
 C      -2.191458     1.879058     2.692068      -6.90
 C      -3.431727     1.615970     1.764881     101.28
 H      -4.263112     2.422239     2.065238      23.42
 O      -4.206501     0.350373     2.109147     293.23
 H      -5.172465     0.511601     2.167276      28.73
 C      -2.954059     1.696847     0.321041     101.39
 H      -2.335366     2.520388     0.162716      28.03
 C      -4.124479     1.563525    -0.611457      99.62
 O      -4.731039     0.228768    -0.839297     265.27
 H      -4.156120    -0.257308    -0.307742      31.93
 H      -3.864712     1.953084    -1.445898      31.08
 H      -5.218358     2.127212    -0.253805      24.41
 C       1.517595     1.054887    -0.710332      44.42
 H       2.173771     1.801745    -0.580269      29.22
 C       1.038771    -1.268056    -0.831822      62.92
 H       1.235797    -2.284084    -0.995569      27.88
 C      -0.317934    -1.046308    -0.474775      20.09
 O      -1.281215    -2.047462    -0.598642     200.14
 C      -1.222573    -3.016123    -1.786493     110.08
 H      -1.739526    -3.762414    -1.291344      27.69
 H      -2.140401    -2.623760    -2.502239      25.48
 H      -0.289139    -3.041775    -2.082206      28.92
 C      -0.877961     0.265681    -0.359843      -5.88
 O      -2.173805     0.417257     0.185606     156.13
 C       0.187667     1.357115    -0.391716      50.81
 H      -0.073287     2.185533     0.135941      25.07
 C       2.042892    -0.289218    -0.897041      29.19
 C       3.515586    -0.607202    -0.836921      73.77
 H       3.724182    -1.651676    -1.605866      24.45
 O       4.445971     0.477447    -1.216040     133.25
 H       4.606667     0.914270    -0.445787      30.20
 C       4.055839    -1.367071     0.554160      81.44
 H       3.205111    -2.087249     0.602531      28.83
 O       5.433882    -1.900905     0.349276     117.90
 H       5.385332    -2.646794    -0.488813      22.15
 C       4.044644    -0.359988     1.723959     104.51
 O       4.403521     1.027889     1.363815     206.82
 H       3.994096     1.800360     1.949805      24.86
 H       4.993268    -0.659157     2.345174      27.75
 H       2.932325    -0.350325     2.275429      25.74
55
name = lig-Water-frame_693
 C      -2.205893     3.149071     3.219887      85.40
 H      -3.086748     3.866626     3.086222      26.23
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 C      -1.274683     0.925319     3.043002      61.95
 H      -1.628746    -0.072239     2.602643      24.07
 C      -0.177541     1.189104     3.916791      16.93
 O       0.754535     0.302133     4.314970     180.18
 C       0.420238    -1.102597     4.637668     117.58
 H       1.301283    -1.579082     5.006138      28.99
 H       0.249133    -1.428530     3.677124      29.15
 H      -0.496020    -1.137184     5.360522      27.14
 C      -0.044517     2.613987     4.356054      22.35
 O       1.163827     3.052346     5.035615     182.52
 H       1.010389     3.913887     5.499820      31.05
 C      -0.992934     3.579445     4.006269      94.77
 H      -0.707690     4.639429     4.182821      12.50
 C      -2.176988     1.904020     2.732976      30.84
 C      -3.403212     1.611525     1.808760     107.29
 H      -3.943390     2.489666     2.008021      26.99
 O      -4.178017     0.343589     2.120893     308.60
 H      -5.152760     0.476618     2.085108      30.58
 C      -2.892437     1.631229     0.303247      92.76
 H      -2.354259     2.650001     0.070015      25.12
 C      -4.188090     1.585396    -0.656560      86.74
 O      -4.709199     0.205111    -0.840500     199.09
 H      -4.132391    -0.509773    -0.350836      26.86
 H      -3.817100     2.007288    -1.845184      24.99
 H      -4.865407     2.158226    -0.234428      31.24
 C       1.565701     1.009572    -0.750480      39.36
 H       2.123486     2.066522    -0.579054      25.00
 C       1.001000    -1.332272    -0.799169      18.80
 H       1.334145    -2.431540    -0.844398      25.56
 C      -0.376662    -1.035351    -0.521701      26.52
 O      -1.268562    -2.066126    -0.630456     192.05
 C      -1.265213    -3.036216    -1.779702      87.39
 H      -1.535266    -4.217181    -1.591104      24.98
 H      -1.693475    -2.746350    -2.750042      26.41
 H      -0.149813    -3.249974    -2.574815      24.14
 C      -0.834923     0.268573    -0.318455       2.11
 O      -2.179382     0.440520     0.151573     174.02
 C       0.159610     1.396688    -0.349776      47.10
 H      -0.045043     2.465205     0.142045      21.39
 C       2.050370    -0.189830    -0.981604      27.50
 C       3.477122    -0.620446    -0.812431     103.65
 H       3.565144    -1.265535    -1.555500      31.36
 O       4.449420     0.452041    -1.246008      92.41
 H       4.476838     0.966198    -0.212765      19.24
 C       4.057100    -1.359233     0.529344      90.80
 H       3.301695    -2.178319     0.778526      28.83
 O       5.379762    -1.868258     0.314507     184.64
 H       5.579206    -2.596007    -0.379889      23.24
 C       4.134182    -0.350743     1.804491     117.97
 O       4.430892     1.075905     1.360490     216.13
 H       3.934071     1.721584     1.959948      25.57
 H       4.739914    -0.632933     2.648938      31.08
 H       3.139126    -0.303889     2.196980      29.21
55
name = lig-Water-frame_694
 C      -2.243807     3.202421     3.191809      54.91
 H      -3.050244     3.964171     3.008509      21.53
 C      -1.335066     0.847302     3.053798      55.13
 H      -1.473749    -0.103794     2.592714      23.29
 C      -0.191650     1.241570     3.895900      -7.04
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 O       0.804799     0.273662     4.364063     165.83
 C       0.443854    -1.085118     4.654471     100.78
 H       1.357563    -1.716873     4.912034      26.47
 H       0.144562    -1.683228     3.650646      25.89
 H      -0.529317    -1.023069     5.329657      25.48
 C       0.049774     2.670506     4.380757      14.41
 O       1.114635     2.975681     5.066197     142.53
 H       1.008314     3.968853     5.324471      37.90
 C      -1.025485     3.554212     4.016065      96.10
 H      -1.012062     4.652756     4.017334      17.76
 C      -2.246410     1.894335     2.741823      34.57
 C      -3.364381     1.597370     1.852332      90.59
 H      -3.999811     2.590568     1.843490      23.65
 O      -4.121481     0.343680     2.131984     270.04
 H      -5.085939     0.757906     1.975954      25.91
 C      -2.887417     1.590150     0.290668      93.84
 H      -2.395115     2.529588     0.044671      25.17
 C      -4.180908     1.574107    -0.753808      89.30
 O      -4.692203     0.194544    -0.843266     205.96
 H      -4.141036    -0.550749    -0.446819      27.03
 H      -4.013031     1.896916    -1.640284      30.36
 H      -4.865752     2.472531    -0.138860      25.83
 C       1.526816     1.123733    -0.736581      37.37
 H       2.258295     1.902332    -0.777389      24.46
 C       0.996359    -1.337796    -0.773743      30.05
 H       1.388379    -2.376596    -0.738047      24.52
 C      -0.374084    -1.049618    -0.623017       1.62
 O      -1.288958    -2.134544    -0.674983     194.70
 C      -1.233146    -3.087241    -1.836813     118.16
 H      -1.352517    -4.085649    -1.670429      28.38
 H      -1.727134    -2.622010    -2.783720      26.46
 H      -0.383100    -3.216251    -2.262205      30.34
 C      -0.779552     0.376017    -0.249510      16.49
 O      -2.142013     0.423949     0.095522     186.12
 C       0.134291     1.363787    -0.313503      65.23
 H      -0.000996     2.382820    -0.162641      25.11
 C       1.998644    -0.217380    -1.002186      -5.80
 C       3.484956    -0.616150    -0.810289      82.92
 H       3.615852    -1.414519    -1.812749      26.67
 O       4.435625     0.428072    -1.218419     104.75
 H       4.425678     1.019503    -0.445766      26.75
 C       4.040613    -1.324943     0.505786      91.16
 H       3.522396    -2.202925     0.999864      27.59
 O       5.343526    -1.835529     0.295123     228.21
 H       5.451207    -2.495225    -0.343973      28.12
 C       4.204395    -0.318961     1.839040      98.65
 O       4.483068     1.084261     1.356300     234.86
 H       3.711355     1.645087     1.843913      24.42
 H       4.676623    -0.679075     2.802474      28.39
 H       3.049513    -0.296853     2.239649      27.34
55
name = lig-Water-frame_695
 C      -2.182895     3.255230     3.227636      11.41
 H      -2.910419     3.998182     2.929149      20.14
 C      -1.333653     0.825913     3.112550      39.14
 H      -1.266289    -0.214136     2.695913      20.59
 C      -0.204344     1.276764     3.888440     -14.76
 O       0.861698     0.280868     4.403807     151.92
 C       0.441430    -1.091625     4.613163     121.14
 H       1.277296    -1.586981     5.075839      27.80
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 H      -0.014914    -1.727677     3.902538      27.23
 H      -0.388290    -1.125559     5.382941      27.51
 C       0.015631     2.652983     4.320610      16.71
 O       1.104119     2.936922     5.121861     156.23
 H       1.048911     3.941481     5.179569      35.02
 C      -1.090210     3.543712     3.982553      67.68
 H      -1.112441     4.674367     4.196465      21.65
 C      -2.336025     1.857966     2.752807       4.58
 C      -3.362666     1.597979     1.818602     113.64
 H      -4.168438     2.320763     1.744153      24.82
 O      -4.076593     0.376465     2.138449     292.48
 H      -4.932924     0.746465     2.041563      27.87
 C      -2.932899     1.566688     0.271285      89.71
 H      -2.287965     2.473986     0.065758      23.90
 C      -4.150898     1.550086    -0.732593      98.10
 O      -4.703358     0.202644    -0.858895     223.67
 H      -4.064973    -0.349795    -0.480557      30.91
 H      -3.985857     1.995571    -1.962468      23.42
 H      -4.844397     2.188359    -0.420949      29.09
 C       1.471097     1.189010    -0.723643      44.92
 H       2.341462     1.913988    -0.934907      24.10
 C       1.022825    -1.284227    -0.766751      59.34
 H       1.366110    -2.311306    -0.739502      24.89
 C      -0.350210    -1.054602    -0.721452     -15.50
 O      -1.320112    -2.207539    -0.719165     157.64
 C      -1.200701    -3.082050    -1.915518      64.59
 H      -1.612437    -4.122870    -1.461038      23.42
 H      -2.057761    -2.604956    -2.509254      23.14
 H       0.165968    -3.031092    -2.097636      19.99
 C      -0.771095     0.385928    -0.203813      17.56
 O      -2.078611     0.384593     0.028445     189.58
 C       0.187785     1.363183    -0.309491      65.05
 H      -0.197138     2.451426    -0.328352      23.17
 C       1.908799    -0.264904    -0.937048      22.11
 C       3.494233    -0.646091    -0.883831      91.81
 H       3.729477    -1.423591    -1.501031      31.23
 O       4.408855     0.406218    -1.188931      85.96
 H       4.473942     1.120457    -0.436128      24.06
 C       4.038279    -1.280260     0.545108      88.32
 H       3.411693    -2.092861     0.955627      29.24
 O       5.344191    -1.795616     0.285167     137.19
 H       5.151020    -2.558067    -0.543779      23.84
 C       4.186906    -0.272052     1.818764     115.77
 O       4.534159     1.065001     1.372655     271.86
 H       3.849682     1.693436     1.643383      29.20
 H       4.884004    -0.697936     2.596458      28.85
 H       3.150139    -0.265528     2.182621      27.68
55
name = lig-Water-frame_696
 C      -2.136806     3.208265     3.232172      46.52
 H      -2.815572     4.083562     2.831527      22.17
 C      -1.318800     0.868236     3.182149      39.10
 H      -1.237911    -0.187711     2.873451      21.48
 C      -0.187173     1.270864     3.909343       5.18
 O       0.887729     0.322616     4.410373     122.25
 C       0.417995    -1.095894     4.609912     104.18
 H       1.325053    -1.480721     5.185692      25.89
 H      -0.058896    -1.691471     3.741289      23.71
 H      -0.254706    -1.170098     5.619214      26.02
 C      -0.091188     2.591651     4.234995      12.75
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 O       1.092103     2.928454     5.160986     168.74
 H       1.154362     3.901065     5.266493      22.71
 C      -1.090664     3.585557     3.985153      17.04
 H      -0.961648     4.498511     4.503448      13.78
 C      -2.343949     1.842954     2.811026     -12.45
 C      -3.418379     1.578842     1.706766     109.89
 H      -4.245862     2.356484     1.801940      26.43
 O      -4.038592     0.395251     2.146015     273.13
 H      -5.069327     0.519290     2.209461      26.21
 C      -2.954145     1.561549     0.242128      90.79
 H      -2.264729     2.454227     0.109869      24.23
 C      -4.090629     1.520131    -0.764912     101.76
 O      -4.723739     0.219803    -0.878403     235.65
 H      -3.929155    -0.343571    -0.494284      27.43
 H      -3.768471     1.853223    -1.615380      30.18
 H      -5.150818     2.142375    -0.469365      23.64
 C       1.495380     1.137881    -0.735483      48.08
 H       2.146065     2.051902    -1.043772      24.79
 C       1.021554    -1.260185    -0.775999      59.64
 H       1.396569    -2.358250    -0.823656      23.33
 C      -0.378071    -1.031144    -0.758462      10.07
 O      -1.322979    -2.227105    -0.742907     196.11
 C      -1.145016    -3.073517    -1.946729     124.46
 H      -1.643972    -3.900195    -1.523380      26.13
 H      -1.974131    -2.762676    -2.609783      26.38
 H      -0.235062    -3.016696    -2.207506      31.00
 C      -0.743284     0.247918    -0.229858      14.87
 O      -2.062761     0.351575    -0.026825     186.08
 C       0.213644     1.452372    -0.315762      56.19
 H      -0.362353     2.370188    -0.322004      19.52
 C       1.895986    -0.219493    -0.832935      45.91
 C       3.470273    -0.656227    -0.886151      73.03
 H       3.785740    -1.661309    -1.580264      25.91
 O       4.378883     0.404813    -1.187075      58.05
 H       4.510461     0.971003    -0.208614      18.52
 C       4.033843    -1.215135     0.611805      94.26
 H       3.168524    -1.963708     0.772688      27.63
 O       5.345609    -1.786152     0.252399     208.24
 H       5.118627    -2.391907    -0.414853      31.41
 C       4.145938    -0.239668     1.740591     118.13
 O       4.603937     1.045170     1.384977     246.46
 H       3.967280     1.827681     1.675799      25.29
 H       5.043994    -0.634500     2.264866      27.32
 H       3.100520    -0.185967     2.307579      26.36
55
name = lig-Water-frame_697
 C      -2.156161     3.157137     3.185467      57.85
 H      -2.755109     3.904319     2.845048      29.11
 C      -1.317783     0.917610     3.240284      67.90
 H      -1.483125    -0.111756     2.959198      28.24
 C      -0.148347     1.207935     3.945847      25.59
 O       0.866517     0.377035     4.388711     130.94
 C       0.410148    -1.085979     4.674001     113.93
 H       1.372455    -1.540004     4.878282      29.02
 H       0.145346    -1.480728     3.680155      27.81
 H      -0.288979    -1.076034     5.484326      28.42
 C      -0.130436     2.592284     4.239748       1.96
 O       1.048483     2.916225     5.155850     111.68
 H       1.093623     3.917919     5.390100      21.17
 C      -1.015863     3.605431     4.024605      43.90
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 H      -0.844833     4.482503     4.769693       7.20
 C      -2.301503     1.843102     2.843173      10.66
 C      -3.484147     1.574566     1.642657      98.61
 H      -4.057776     2.532418     1.802596      27.62
 O      -4.031321     0.367627     2.154251     296.23
 H      -5.035279     0.369420     2.311242      29.00
 C      -2.928423     1.560432     0.229085     102.44
 H      -2.407550     2.489481     0.081046      28.15
 C      -4.100364     1.506790    -0.769835      94.86
 O      -4.710822     0.214753    -0.891530     198.60
 H      -4.099167    -0.554116    -0.679758      28.24
 H      -3.422750     1.872221    -1.842079      24.72
 H      -4.836736     2.163640    -0.528333      29.56
 C       1.524552     1.118479    -0.750489      49.12
 H       2.065267     1.987329    -1.040408      29.30
 C       0.990742    -1.283541    -0.801031      60.12
 H       1.385391    -2.222585    -0.931527      26.56
 C      -0.412265    -1.053911    -0.746499      25.35
 O      -1.293283    -2.183862    -0.759418     221.82
 C      -1.194009    -3.042638    -1.934992      96.63
 H      -1.442310    -4.164316    -1.636907      25.59
 H      -1.656616    -2.803467    -3.044457      25.43
 H       0.044923    -3.164865    -2.634404      23.24
 C      -0.690166     0.161015    -0.300841      15.16
 O      -2.110846     0.323598    -0.064542     157.45
 C       0.166391     1.453386    -0.331822      55.96
 H      -0.295926     2.450569    -0.259883      22.29
 C       1.986424    -0.175502    -0.739450      35.67
 C       3.446664    -0.668846    -0.833269     112.18
 H       3.464425    -1.425402    -1.575140      29.87
 O       4.346937     0.420200    -1.187509     106.84
 H       4.531971     0.745856    -0.237415      24.79
 C       3.977560    -1.174523     0.584903     113.08
 H       3.261032    -1.909771     0.831723      31.41
 O       5.333408    -1.770850     0.251370     176.25
 H       5.174600    -2.474600    -0.454532      28.15
 C       4.102769    -0.229797     1.682798     128.92
 O       4.676302     1.078132     1.374679     263.94
 H       4.068283     1.730111     1.805771      28.68
 H       5.013925    -0.668105     2.188643      28.95
 H       3.329998    -0.143305     2.520075      28.77
55
name = lig-Water-frame_698
 C      -2.135196     3.171994     3.183936      25.27
 H      -2.997986     3.918426     2.766234      26.27
 C      -1.324865     0.900415     3.281670      64.13
 H      -1.773764    -0.109588     3.001442      27.63
 C      -0.146837     1.175444     3.969401      24.64
 O       0.835700     0.408570     4.373410     164.06
 C       0.461701    -1.031436     4.696420     118.85
 H       1.379348    -1.644278     4.755823      28.36
 H       0.118021    -1.373120     3.713987      28.15
 H      -0.577579    -1.044484     5.413897      25.33
 C      -0.051458     2.615803     4.345600      -2.10
 O       0.990586     2.906189     5.127683     129.13
 H       0.870237     3.836405     5.412942      26.76
 C      -0.982976     3.591624     4.049514      52.12
 H      -0.998956     4.459090     4.607443      12.20
 C      -2.269374     1.855193     2.800856     -32.07
 C      -3.475629     1.580007     1.689179      92.95
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 H      -4.048090     2.516161     1.694384      27.37
 O      -4.044796     0.310042     2.156819     304.48
 H      -4.972007     0.505335     2.231516      28.81
 C      -2.898903     1.527587     0.222891     101.49
 H      -2.445664     2.603965     0.008042      26.10
 C      -4.030433     1.488436    -0.836790      97.17
 O      -4.705002     0.193522    -0.912406     206.47
 H      -4.212878    -0.591680    -0.816610      29.16
 H      -3.654126     1.677923    -1.722043      31.25
 H      -4.775770     2.460606    -0.567037      27.07
 C       1.495853     1.156046    -0.731757      31.21
 H       2.332415     2.038602    -0.993055      28.26
 C       0.997902    -1.261283    -0.826147      55.83
 H       1.419222    -2.347622    -1.082608      27.22
 C      -0.367523    -1.154231    -0.728937      25.46
 O      -1.265549    -2.134583    -0.801945     247.31
 C      -1.177121    -3.047356    -2.001148     132.31
 H      -1.195585    -4.118359    -1.796905      28.54
 H      -1.615588    -2.687271    -2.874739      30.34
 H      -0.304692    -3.147270    -2.304781      33.16
 C      -0.730347     0.258880    -0.353682      16.97
 O      -2.166857     0.300312    -0.091655     155.50
 C       0.119952     1.332434    -0.379984      75.40
 H      -0.112581     2.425001    -0.185840      26.57
 C       2.039039    -0.214187    -0.671242      12.52
 C       3.407198    -0.626959    -0.752851     126.47
 H       3.302570    -1.425384    -1.681182      26.81
 O       4.304951     0.428812    -1.199088      28.31
 H       4.786717     0.875038    -0.237252      22.34
 C       3.905506    -1.192837     0.468565     102.45
 H       3.378306    -2.082284     1.061760      29.15
 O       5.303039    -1.748740     0.270388     106.03
 H       5.258476    -2.627731    -0.431285      24.27
 C       4.135924    -0.214765     1.695325     115.30
 O       4.734937     1.129562     1.357501     247.36
 H       4.100253     1.745567     1.822657      29.17
 H       4.851155    -0.804208     2.286089      31.26
 H       3.344995    -0.151654     2.479215      30.29
55
name = lig-Water-frame_699
 C      -2.102757     3.241237     3.202572      70.62
 H      -2.845907     3.852205     2.927452      32.21
 C      -1.375389     0.830226     3.287754      42.34
 H      -1.689954    -0.153791     3.120528      26.42
 C      -0.212103     1.240334     3.974600      15.64
 O       0.843268     0.390714     4.391760     212.12
 C       0.479858    -0.957667     4.660829     129.79
 H       1.322867    -1.592359     5.042506      28.05
 H      -0.072395    -1.391880     3.756501      26.62
 H      -0.282514    -1.071064     5.319905      30.64
 C      -0.003480     2.590996     4.425344      24.15
 O       0.981080     2.917110     5.135908      65.61
 H       0.807576     3.847664     5.476106      28.06
 C      -1.023872     3.542808     4.028493      63.65
 H      -1.134397     4.652963     4.408138      21.12
 C      -2.252665     1.890693     2.721561     -45.58
 C      -3.376933     1.559420     1.787125      90.46
 H      -4.257392     2.327508     1.669314      22.93
 O      -4.069157     0.266588     2.147742     258.37
 H      -5.071368     0.642517     2.116926      20.87
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 C      -2.892500     1.502327     0.206950     106.78
 H      -2.323612     2.359247     0.031533      28.50
 C      -3.979366     1.470270    -0.861527      89.75
 O      -4.731906     0.190353    -0.940566     170.39
 H      -4.054357    -0.605610    -0.777417      24.44
 H      -3.627191     1.642373    -2.116519      24.00
 H      -4.658748     2.268607    -0.733682      28.25
 C       1.518376     1.146318    -0.689080      61.11
 H       2.175859     1.880405    -0.743631      29.80
 C       1.074938    -1.275914    -0.852392      77.89
 H       1.388287    -2.204520    -1.120781      27.71
 C      -0.282954    -1.151300    -0.685567      -1.54
 O      -1.271020    -2.126617    -0.864422     181.80
 C      -1.148761    -3.045279    -2.042196      71.08
 H      -1.433912    -4.109363    -1.746455      26.10
 H      -2.042492    -2.475064    -2.736447      22.78
 H       0.243416    -2.943012    -2.205301      21.51
 C      -0.863984     0.311233    -0.408316      14.31
 O      -2.188509     0.290573    -0.109864     199.06
 C       0.118873     1.249533    -0.445366      74.82
 H      -0.154095     2.216310    -0.152820      28.23
 C       1.949619    -0.206283    -0.634431      35.10
 C       3.375120    -0.587027    -0.758165     121.29
 H       3.463711    -1.349299    -1.539281      29.77
 O       4.284431     0.448163    -1.193383     125.99
 H       4.690388     0.911272    -0.512875      28.19
 C       3.894368    -1.272234     0.451519     104.55
 H       3.360332    -2.025144     0.902090      30.57
 O       5.269290    -1.742885     0.278092     249.35
 H       5.240932    -2.489554    -0.173381      33.96
 C       4.203453    -0.203368     1.717747      83.97
 O       4.775283     1.159354     1.354942     246.04
 H       4.110532     1.875994     1.697596      28.08
 H       4.842945    -0.879192     2.374365      27.13
 H       3.071325    -0.023021     2.141153      26.68
55
name = lig-Water-frame_700
 C      -2.064600     3.239023     3.198449      58.34
 H      -2.836317     4.148370     3.015989      26.58
 C      -1.445200     0.817710     3.264798      25.50
 H      -1.485064    -0.337058     3.170537      27.01
 C      -0.273385     1.294445     3.990863     -19.36
 O       0.857860     0.382156     4.416391     159.55
 C       0.476729    -0.923438     4.594361     122.97
 H       1.300494    -1.382042     5.149062      26.99
 H       0.046673    -1.489913     3.800900      28.10
 H      -0.234759    -0.999234     5.690483      22.96
 C      -0.102515     2.564600     4.407309      21.88
 O       1.049464     2.960202     5.206380      57.29
 H       0.973434     3.918305     5.549535      26.02
 C      -1.064650     3.528089     4.028047      61.72
 H      -0.957216     4.555930     4.229385      25.35
 C      -2.218078     1.911406     2.684250     -52.30
 C      -3.316685     1.507215     1.829380      96.56
 H      -4.115838     2.166661     1.858397      26.94
 O      -4.100040     0.254056     2.135977     246.82
 H      -5.045237     0.478808     2.078298      23.17
 C      -2.900698     1.473099     0.196847      91.82
 H      -2.042315     2.287600     0.054062      27.43
 C      -3.944475     1.432926    -0.950379     104.22
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 O      -4.743679     0.191397    -0.967836     222.58
 H      -4.077209    -0.451767    -0.639793      27.68
 H      -3.485996     1.609373    -1.816896      30.99
 H      -4.827878     2.248561    -0.796125      25.87
 C       1.507274     1.056408    -0.619276      75.93
 H       2.191141     2.102309    -0.424455      28.87
 C       1.114146    -1.301916    -0.858580      61.22
 H       1.603799    -2.325218    -1.153625      26.39
 C      -0.269971    -1.064282    -0.642304      -0.27
 O      -1.278243    -2.130371    -0.912532     190.69
 C      -1.082979    -2.999285    -2.070421     133.83
 H      -1.661972    -3.897882    -1.727316      27.17
 H      -1.836016    -2.685009    -2.651922      29.76
 H      -0.226838    -2.917363    -2.428977      31.74
 C      -0.934970     0.220887    -0.477446      17.41
 O      -2.198414     0.275154    -0.114241     201.79
 C       0.107911     1.255235    -0.501472      59.38
 H      -0.334759     2.269080    -0.173356      27.78
 C       1.877679    -0.169633    -0.645659      48.37
 C       3.371570    -0.554037    -0.785922      87.08
 H       3.565868    -1.397473    -1.632786      28.04
 O       4.259574     0.461584    -1.220929      14.86
 H       4.631460     1.127153    -0.267230      18.57
 C       3.963436    -1.294167     0.522478      88.73
 H       3.069018    -2.115339     0.750896      27.57
 O       5.243074    -1.733812     0.288040     176.31
 H       5.234189    -2.722668    -0.161813      25.73
 C       4.202692    -0.194749     1.707878     100.63
 O       4.804024     1.162638     1.359848     246.50
 H       4.134335     1.795249     1.623079      32.56
 H       4.838983    -0.638034     2.435145      29.16
 H       3.202659     0.071948     1.919120      30.48
55
name = lig-Water-frame_701
 C      -2.095302     3.222865     3.143257      55.82
 H      -2.642054     4.083520     2.945839      26.43
 C      -1.452744     0.851684     3.253335      86.55
 H      -1.463302    -0.174028     3.021949      28.11
 C      -0.306290     1.246924     4.014434     -21.20
 O       0.841457     0.431712     4.411328     140.06
 C       0.450132    -0.936076     4.644098     120.72
 H       1.469800    -1.337159     4.951464      27.80
 H       0.206860    -1.638499     3.737533      27.14
 H      -0.179619    -0.908075     5.415201      29.07
 C      -0.168227     2.616456     4.425457      -6.64
 O       1.099837     2.992631     5.259588     113.96
 H       1.075343     3.947029     5.481283      28.40
 C      -1.052594     3.546110     4.055901      41.65
 H      -0.705524     4.592029     4.288804      18.63
 C      -2.182642     1.871677     2.699602      -3.57
 C      -3.342209     1.432434     1.776080      81.16
 H      -4.017167     2.424347     2.003646      24.84
 O      -4.092495     0.237848     2.132642     247.01
 H      -5.095005     0.456231     2.085991      21.81
 C      -2.880902     1.471943     0.203287      99.57
 H      -2.262996     2.271988     0.075383      31.08
 C      -3.978875     1.425572    -0.977556      81.11
 O      -4.725549     0.198332    -0.998829     219.58
 H      -4.261570    -0.497898    -0.530352      28.01
 H      -3.143934     1.634956    -1.985137      25.52
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 H      -4.754677     2.231049    -0.902740      26.70
 C       1.425093     1.107136    -0.514222      52.48
 H       2.036153     1.823718    -0.273953      31.19
 C       1.079932    -1.334111    -0.846715      56.72
 H       1.613603    -2.222535    -1.065929      29.36
 C      -0.320907    -1.053587    -0.658221      34.17
 O      -1.262978    -2.110270    -0.926427     177.37
 C      -1.113014    -2.950589    -2.049253      94.51
 H      -1.425495    -3.962230    -1.741351      27.85
 H      -1.779140    -2.655344    -3.158970      24.13
 H       0.053921    -3.059958    -2.923130      23.71
 C      -0.853504     0.140345    -0.538836      21.95
 O      -2.223035     0.220606    -0.107398     161.80
 C       0.017260     1.297958    -0.527096      59.92
 H      -0.298562     2.291198    -0.382415      27.34
 C       1.953517    -0.243388    -0.703709     -11.98
 C       3.400470    -0.553794    -0.806833     102.85
 H       3.435325    -1.329516    -1.613048      26.21
 O       4.256272     0.517881    -1.217085     147.80
 H       4.385920     0.873674    -0.430198      30.78
 C       3.994163    -1.252123     0.599438     100.09
 H       3.255735    -1.926673     0.758600      30.44
 O       5.250514    -1.772280     0.285273     198.62
 H       5.255032    -2.774279    -0.089308      25.91
 C       4.175200    -0.194177     1.661991     103.81
 O       4.830124     1.145260     1.345257     258.35
 H       4.077027     1.737415     1.714171      30.45
 H       4.779653    -0.401938     2.621018      26.51
 H       3.057283     0.172440     2.110568      27.23
55
name = lig-Water-frame_702
 C      -2.094337     3.197838     3.103208      20.64
 H      -2.766397     4.027685     2.600328      24.94
 C      -1.367297     0.880571     3.270759      82.26
 H      -1.606260    -0.116316     2.757153      29.57
 C      -0.294321     1.204668     4.067285       4.37
 O       0.783959     0.501405     4.379861     177.92
 C       0.501637    -0.981668     4.677096      94.71
 H       1.451954    -1.405910     4.877674      28.15
 H       0.225644    -1.466205     3.785682      29.24
 H      -0.565195    -1.015430     5.439011      22.79
 C      -0.123856     2.639956     4.504781     -33.18
 O       1.096835     2.998142     5.267291     100.84
 H       1.058569     4.031888     5.362822      26.37
 C      -1.048076     3.612527     4.060821      45.51
 H      -0.733109     4.643533     4.353208      17.63
 C      -2.217283     1.828271     2.708127     -27.71
 C      -3.405652     1.427270     1.692143      96.03
 H      -3.927823     2.289437     1.772826      29.06
 O      -4.069966     0.220796     2.134067     242.30
 H      -5.063686     0.569854     2.141210      22.22
 C      -2.906862     1.445126     0.211778      89.33
 H      -2.389686     2.521309     0.052680      25.55
 C      -3.963013     1.438260    -0.997240     101.67
 O      -4.701399     0.207682    -1.045077     198.68
 H      -4.441924    -0.577419    -0.395144      26.39
 H      -3.380515     1.487356    -1.801459      30.62
 H      -4.684367     2.367537    -1.033160      26.72
 C       1.311932     1.103852    -0.421810      36.10
 H       2.155885     1.987491    -0.143030      22.06
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 C       1.029923    -1.319036    -0.819981      61.90
 H       1.401752    -2.376734    -1.027622      26.59
 C      -0.336084    -1.174292    -0.742581      38.28
 O      -1.244302    -2.093518    -0.931245     257.69
 C      -1.121791    -2.924857    -2.155052     130.16
 H      -1.082825    -4.011933    -1.828660      26.64
 H      -1.653077    -2.616820    -2.914096      30.77
 H      -0.273223    -3.033647    -2.476937      32.11
 C      -0.805146     0.188925    -0.548280      14.68
 O      -2.217017     0.145448    -0.104391     107.94
 C      -0.057368     1.327482    -0.536488      61.40
 H      -0.403030     2.400761    -0.565438      25.36
 C       2.006528    -0.288552    -0.757789       3.26
 C       3.444908    -0.578080    -0.807457      96.95
 H       3.468815    -1.418447    -1.617285      26.83
 O       4.249170     0.563400    -1.231723       6.30
 H       4.471004     1.077636    -0.142273      18.43
 C       4.023493    -1.162207     0.607181      88.83
 H       3.270044    -2.010103     1.083407      26.54
 O       5.295188    -1.837607     0.286959     242.03
 H       5.179364    -2.647958    -0.028843      32.77
 C       4.115562    -0.150938     1.695977     122.67
 O       4.825019     1.123432     1.312924     218.25
 H       4.219815     1.770782     1.820983      28.31
 H       4.596744    -0.510008     2.544952      29.37
 H       3.192153     0.023041     2.097506      31.73
55
name = lig-Water-frame_703
 C      -2.075163     3.197736     3.078256      26.78
 H      -2.733392     3.740384     2.392063      20.55
 C      -1.295990     0.864346     3.252870      19.81
 H      -1.495977    -0.076723     2.751772      29.73
 C      -0.273644     1.270267     4.141086      15.17
 O       0.753655     0.502598     4.369794     209.34
 C       0.511378    -0.993888     4.703231     101.48
 H       1.448420    -1.493028     5.153342      26.94
 H       0.123841    -1.320609     3.658269      27.59
 H      -0.230908    -1.185480     5.277774      30.93
 C      -0.069091     2.640818     4.580296      -1.91
 O       1.051030     3.001438     5.243156       2.84
 H       1.039667     3.985774     5.316726      31.55
 C      -1.047381     3.654557     4.037760      73.79
 H      -1.024774     4.712874     4.288341      24.83
 C      -2.288104     1.830366     2.713421     -87.49
 C      -3.404248     1.437965     1.621658      85.59
 H      -4.290274     2.324416     1.501978      24.65
 O      -4.063219     0.218646     2.134195     231.93
 H      -4.992802     0.486979     2.213434      23.63
 C      -2.958339     1.416775     0.182973     106.10
 H      -2.430989     2.307743     0.089313      26.72
 C      -3.951569     1.442160    -0.946730      88.02
 O      -4.704780     0.201531    -1.099348     191.64
 H      -4.491612    -0.345003    -0.328487      30.69
 H      -3.307807     1.418230    -2.102489      23.94
 H      -4.577616     2.412550    -1.100552      25.88
 C       1.319142     1.051708    -0.362373      56.94
 H       1.857303     1.944615    -0.247043      25.54
 C       1.034795    -1.338345    -0.815051      61.76
 H       1.166169    -2.427331    -0.982155      25.35
 C      -0.320257    -1.190490    -0.825138      11.24
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 O      -1.268297    -2.135783    -0.949671     201.71
 C      -1.119666    -2.944478    -2.198059      49.86
 H      -1.259656    -3.977766    -1.951040      25.35
 H      -2.092307    -2.440340    -2.962736      22.13
 H       0.308544    -2.732369    -2.338690      19.43
 C      -0.856842     0.203207    -0.525468       6.29
 O      -2.175243     0.099823    -0.106824      80.45
 C      -0.085324     1.375818    -0.531827      59.06
 H      -0.595089     2.348538    -0.625058      23.54
 C       1.938879    -0.240128    -0.761031      37.32
 C       3.497814    -0.608287    -0.791402      92.14
 H       3.752223    -1.478368    -1.522391      27.01
 O       4.250822     0.614428    -1.193261     108.79
 H       4.557466     1.063686    -0.537116      32.07
 C       4.033010    -1.133417     0.568085      94.57
 H       3.495390    -1.780256     1.164916      29.85
 O       5.350837    -1.868048     0.316098     132.76
 H       4.966749    -2.827805    -0.161930      25.99
 C       4.097360    -0.102414     1.743470      88.31
 O       4.790139     1.107444     1.289946     170.83
 H       4.437490     1.841571     1.790666      30.15
 H       4.647136    -0.788119     2.521715      25.56
 H       2.856897     0.070492     2.036716      26.89
55
name = lig-Water-frame_704
 C      -2.043128     3.177293     3.060454      37.42
 H      -2.648146     3.896548     2.471398      19.13
 C      -1.295429     0.888723     3.204296      -7.78
 H      -1.155932    -0.210012     2.937918      19.40
 C      -0.291389     1.376641     4.185405       5.18
 O       0.788035     0.433417     4.409645     187.46
 C       0.540684    -0.976272     4.659240      98.79
 H       1.364308    -1.375093     5.189178      26.48
 H       0.301052    -1.437014     3.729034      27.80
 H      -0.363986    -1.254833     5.596275      22.32
 C      -0.119005     2.682096     4.585275      26.24
 O       1.019584     3.011670     5.228804       0.96
 H       1.022345     4.017228     5.354747      32.75
 C      -1.050105     3.635438     3.992190      86.34
 H      -1.261427     4.744394     4.219807      17.94
 C      -2.314334     1.833263     2.727732      30.95
 C      -3.425614     1.477856     1.599252      98.09
 H      -4.206827     2.079421     1.500599      30.53
 O      -4.048085     0.218799     2.126606     229.81
 H      -5.114253     0.380880     2.248986      23.44
 C      -2.982261     1.345476     0.133782      93.06
 H      -2.202140     2.215444     0.041680      23.70
 C      -3.921709     1.428254    -0.984153     118.21
 O      -4.727746     0.203507    -1.141825     221.79
 H      -4.548393    -0.208861    -0.292554      31.59
 H      -3.379287     1.511509    -1.813505      30.31
 H      -4.569674     2.360163    -0.962296      28.09
 C       1.338117     1.000379    -0.370280      66.10
 H       1.956995     2.014520    -0.312277      23.48
 C       1.044934    -1.381084    -0.834933      46.76
 H       1.400754    -2.403358    -0.944843      25.24
 C      -0.335520    -1.078138    -0.864354       6.69
 O      -1.310531    -2.214203    -0.973061     204.95
 C      -1.076664    -2.921220    -2.242897     128.36
 H      -1.521605    -3.983076    -2.116071      25.48
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 H      -1.793242    -2.612964    -2.819165      30.43
 H      -0.274023    -2.658311    -2.582636      31.92
 C      -0.923281     0.165172    -0.506640      20.67
 O      -2.150030     0.089527    -0.103040     133.22
 C      -0.089047     1.357908    -0.513407      58.74
 H      -0.560047     2.328807    -0.509627      23.39
 C       1.864829    -0.185546    -0.720354      37.98
 C       3.528782    -0.596100    -0.749689      87.16
 H       3.826625    -1.344160    -1.476142      28.73
 O       4.242921     0.625084    -1.201670      31.17
 H       4.737354     1.210136    -0.328440      19.33
 C       4.074115    -1.105727     0.541221      85.06
 H       3.319559    -1.917865     1.032041      26.42
 O       5.376844    -1.900158     0.348080     196.97
 H       5.062000    -2.664997    -0.203243      29.20
 C       4.067344    -0.083780     1.762068     108.62
 O       4.754489     1.094817     1.288016     163.94
 H       4.489245     1.942384     1.835978      26.88
 H       4.614615    -0.639397     2.478663      27.06
 H       3.140345     0.172312     1.939275      32.59
55
name = lig-Water-frame_705
 C      -2.023572     3.165653     3.041654      53.97
 H      -2.537169     4.171217     2.787930      19.07
 C      -1.305233     0.945192     3.187242      21.37
 H      -0.986542    -0.107128     3.124233      19.06
 C      -0.323430     1.382740     4.164055     -16.88
 O       0.825657     0.390413     4.470482     128.77
 C       0.517667    -0.961632     4.668434     119.76
 H       1.548271    -1.288292     5.082149      25.21
 H       0.461687    -1.716381     3.766512      25.74
 H      -0.187351    -1.024691     5.301951      28.35
 C      -0.216067     2.758330     4.545604       3.66
 O       1.010612     3.047618     5.236147     127.11
 H       0.993027     4.060039     5.407332      22.39
 C      -1.084073     3.607919     3.937608      45.14
 H      -1.108812     4.605050     4.221099      25.00
 C      -2.297361     1.809122     2.703221      27.97
 C      -3.424909     1.461296     1.626642      80.62
 H      -4.296441     2.371921     1.655624      25.37
 O      -4.043373     0.210347     2.118230     267.40
 H      -4.975664     0.409235     2.099226      27.76
 C      -2.912906     1.282748     0.110786     104.24
 H      -2.199767     2.079526    -0.059339      29.02
 C      -3.936650     1.411029    -1.034482      90.22
 O      -4.753691     0.219462    -1.173633     144.77
 H      -4.716506    -0.339239    -0.268500      26.46
 H      -3.170511     1.667057    -2.065228      24.70
 H      -4.648207     2.313558    -0.677462      27.26
 C       1.318672     1.063610    -0.422246      50.53
 H       2.192618     1.806166    -0.351895      23.46
 C       1.030967    -1.366520    -0.867528      38.91
 H       1.707855    -2.286825    -0.974015      22.76
 C      -0.373627    -1.040196    -0.884686       0.71
 O      -1.323077    -2.266520    -0.988751     162.54
 C      -1.114219    -2.929484    -2.237677      95.86
 H      -1.324345    -3.990192    -2.223353      26.82
 H      -1.937388    -2.434307    -3.218527      24.54
 H      -0.047506    -2.683634    -3.203482      22.37
 C      -0.910250     0.164758    -0.508808      38.61
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 O      -2.205567     0.085670    -0.077673     188.98
 C      -0.067747     1.260028    -0.475881      72.06
 H      -0.320139     2.365765    -0.272235      24.66
 C       1.873123    -0.246214    -0.663301       5.50
 C       3.520564    -0.506824    -0.711193      76.88
 H       3.611873    -1.285170    -1.661768      26.09
 O       4.257956     0.643677    -1.206254     114.43
 H       4.502023     0.928721    -0.293221      23.40
 C       4.094222    -1.134429     0.580429     106.87
 H       3.313678    -1.844702     0.600387      27.81
 O       5.380459    -1.896676     0.389152     229.78
 H       5.242608    -2.631589    -0.253327      29.76
 C       4.091222    -0.103738     1.712819      99.34
 O       4.743328     1.117168     1.300533     201.73
 H       4.326745     1.803493     1.857924      28.80
 H       4.600092    -0.413130     2.686555      25.55
 H       2.897976     0.308451     2.074155      24.05
55
name = lig-Water-frame_706
 C      -2.058866     3.193566     3.012731      46.15
 H      -2.678865     4.007115     2.803688      24.34
 C      -1.273302     0.981449     3.228992      62.61
 H      -1.269799    -0.086419     2.932733      26.45
 C      -0.326670     1.342258     4.116822       2.53
 O       0.830985     0.433605     4.511002     142.04
 C       0.563837    -0.982207     4.661315      98.42
 H       1.509263    -1.298194     5.076991      26.81
 H       0.445471    -1.636503     3.789279      28.33
 H      -0.506085    -1.020923     5.410817      22.23
 C      -0.225471     2.751603     4.520504      -7.79
 O       0.978257     3.105401     5.242610      96.09
 H       0.984348     4.087946     5.408660      23.35
 C      -1.109855     3.610615     3.909870      76.13
 H      -0.863374     4.708933     4.221358      22.32
 C      -2.272389     1.810160     2.629977      -9.29
 C      -3.423078     1.448637     1.673432      93.88
 H      -3.929704     2.302601     1.756532      27.97
 O      -4.028188     0.203726     2.103053     250.88
 H      -5.082327     0.462138     1.964659      22.92
 C      -2.849362     1.266776     0.106789      96.09
 H      -2.212725     2.178640    -0.103789      28.22
 C      -3.941959     1.405336    -1.064265     110.88
 O      -4.783381     0.237545    -1.204616     243.57
 H      -4.774728    -0.395786    -0.506458      29.84
 H      -3.535308     1.694040    -1.964859      29.39
 H      -4.587117     2.230146    -0.741923      30.09
 C       1.349818     1.085067    -0.505907      38.14
 H       2.128679     1.841322    -0.378318      25.47
 C       1.027024    -1.304082    -0.899929      60.24
 H       1.495528    -2.220271    -1.124543      26.80
 C      -0.395826    -1.137746    -0.902601       7.33
 O      -1.288094    -2.281039    -1.013775     210.96
 C      -1.160750    -2.900824    -2.374866     126.89
 H      -1.094196    -4.028343    -2.207463      26.38
 H      -1.856572    -2.520784    -2.960733      30.35
 H      -0.295788    -2.881622    -2.800905      31.04
 C      -0.900272     0.155317    -0.512808      13.42
 O      -2.272441     0.059770    -0.047402     173.62
 C      -0.008328     1.225291    -0.405139      70.98
 H      -0.260565     2.171237    -0.086082      27.43
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 C       1.921144    -0.300410    -0.594153      -0.63
 C       3.469396    -0.425054    -0.745300      96.66
 H       3.408468    -1.142304    -1.499802      28.00
 O       4.265172     0.651150    -1.205283      91.08
 H       4.513521     1.130902    -0.156775      18.36
 C       4.101920    -1.189687     0.588642      92.94
 H       3.248137    -1.965267     0.642805      26.96
 O       5.368817    -1.860220     0.448570     179.90
 H       5.436527    -2.648986    -0.365466      24.29
 C       4.079491    -0.128912     1.707551     113.93
 O       4.739589     1.154997     1.312804     228.85
 H       4.094329     1.769995     1.811145      27.84
 H       4.501004    -0.323601     2.690740      28.08
 H       3.154460     0.000427     1.942928      32.54
55
name = lig-Water-frame_707
 C      -2.139179     3.214809     2.971701      26.00
 H      -3.058472     3.829325     2.521329      23.55
 C      -1.283604     0.943850     3.227223      55.56
 H      -1.603116    -0.003463     2.737115      30.07
 C      -0.244511     1.313065     4.113075      28.63
 O       0.800919     0.522560     4.529756     201.38
 C       0.566963    -0.985942     4.694779     105.78
 H       1.419376    -1.428200     5.278905      26.41
 H       0.334092    -1.388094     3.627385      28.25
 H      -0.223541    -1.221142     5.218811      30.42
 C      -0.161779     2.677218     4.499322       8.26
 O       0.918930     3.154308     5.237702      49.27
 H       0.926309     4.204157     5.352482      28.34
 C      -1.090388     3.660684     3.923313      62.02
 H      -0.895562     4.684183     4.033430      21.74
 C      -2.209243     1.860066     2.582942     -35.59
 C      -3.343763     1.408076     1.691531      67.34
 H      -4.058767     2.430307     1.724569      24.37
 O      -4.041572     0.213364     2.082159     231.29
 H      -5.002911     0.348313     1.975780      24.39
 C      -2.865615     1.328793     0.109501      82.78
 H      -2.184178     2.220192    -0.049128      25.73
 C      -3.969728     1.386362    -1.005133      84.11
 O      -4.821853     0.259479    -1.260573     221.63
 H      -4.627724    -0.464678    -0.616930      27.47
 H      -3.610939     1.696638    -2.240374      23.47
 H      -4.662458     2.390719    -0.837303      25.70
 C       1.441196     1.016538    -0.580886      44.76
 H       1.924794     2.139437    -0.399906      25.19
 C       1.010634    -1.265488    -0.934258      41.44
 H       1.193252    -2.354715    -1.321836      26.04
 C      -0.407112    -1.234523    -0.897120      19.22
 O      -1.224167    -2.274896    -1.054680     191.02
 C      -1.201762    -2.922777    -2.455905      64.85
 H      -1.264987    -3.990939    -2.168785      25.76
 H      -2.314742    -2.493212    -3.048006      22.34
 H       0.155028    -2.715508    -2.589178      21.86
 C      -0.912825     0.070500    -0.509502      -3.74
 O      -2.274419     0.013695    -0.031939     134.39
 C       0.037501     1.217554    -0.323503      43.76
 H      -0.455063     2.192065     0.092343      24.80
 C       1.962882    -0.235758    -0.544403      39.60
 C       3.417700    -0.399643    -0.764937      92.12
 H       3.489923    -1.303044    -1.617029      24.46
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 O       4.272349     0.674496    -1.168362     110.71
 H       4.521931     1.345516    -0.514326      23.87
 C       4.074525    -1.249070     0.554428      90.37
 H       3.385066    -1.984007     1.030004      28.00
 O       5.370071    -1.823429     0.495638     253.66
 H       5.402299    -2.413857    -0.160026      31.78
 C       4.108137    -0.180935     1.707739      77.83
 O       4.707986     1.195899     1.333402     207.92
 H       3.974783     1.865765     1.625356      27.55
 H       4.588707    -0.538885     2.616988      27.05
 H       2.794788    -0.128679     1.831201      25.61
55
name = lig-Water-frame_708
 C      -2.210227     3.250821     2.951252      57.60
 H      -2.978339     3.729380     2.493493      23.97
 C      -1.334565     0.897535     3.174790      64.70
 H      -1.524510    -0.124716     2.867933      28.25
 C      -0.177218     1.285458     4.099129      16.74
 O       0.780096     0.575741     4.571035     161.65
 C       0.587652    -0.955889     4.687855      86.39
 H       1.401145    -1.452692     5.248153      26.29
 H       0.449318    -1.150564     3.598990      27.79
 H      -0.456127    -1.332727     5.347674      24.30
 C      -0.119875     2.674230     4.446773      13.80
 O       0.864028     3.187768     5.232806     129.96
 H       0.824344     4.166945     5.299856      29.73
 C      -1.090769     3.657641     3.900876      60.38
 H      -0.974190     4.798860     3.982230      21.69
 C      -2.119642     1.907918     2.591956       0.84
 C      -3.289395     1.427674     1.657234      97.02
 H      -4.081283     2.055791     1.621033      27.43
 O      -4.032565     0.213436     2.070102     211.38
 H      -5.065260     0.423109     1.943414      21.49
 C      -2.927280     1.380870     0.126968      73.76
 H      -2.203024     2.154882    -0.040828      26.94
 C      -4.013216     1.431572    -0.992217     113.40
 O      -4.864979     0.271672    -1.299038     226.16
 H      -4.385816    -0.534410    -0.794715      25.28
 H      -3.509648     1.541409    -1.868085      28.62
 H      -4.635023     2.278737    -0.817802      29.15
 C       1.456803     1.057508    -0.591791      51.28
 H       1.933385     1.922046    -0.527320      29.68
 C       0.989916    -1.289090    -0.969240      45.29
 H       1.316864    -2.231544    -1.312304      28.13
 C      -0.374291    -1.225433    -0.861795      34.20
 O      -1.185174    -2.297735    -1.111295     232.40
 C      -1.210602    -2.924730    -2.485528     117.03
 H      -1.527416    -3.981381    -2.300890      27.21
 H      -1.971565    -2.626811    -3.050476      30.15
 H      -0.361078    -2.636326    -2.880591      30.22
 C      -0.910654    -0.002137    -0.471142      11.61
 O      -2.229550    -0.013988    -0.034581     112.34
 C       0.022108     1.156498    -0.259445      46.81
 H      -0.374849     2.066549     0.068728      27.90
 C       1.988132    -0.192181    -0.570337      20.87
 C       3.430983    -0.488668    -0.770964      92.21
 H       3.633632    -1.060231    -1.585853      28.28
 O       4.270362     0.691019    -1.174346      69.83
 H       4.462379     1.366055    -0.466288      24.66
 C       4.041634    -1.249262     0.554100      92.75
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 H       3.432725    -2.002423     1.127930      27.60
 O       5.381644    -1.770215     0.539387     186.58
 H       5.416038    -2.528943    -0.230236      24.66
 C       4.074080    -0.216164     1.688148      94.74
 O       4.644193     1.213347     1.362917     231.47
 H       3.980112     1.840216     1.643248      31.31
 H       4.683662    -0.761008     2.488347      26.23
 H       3.164655    -0.040457     1.899007      31.53
55
name = lig-Water-frame_709
 C      -2.171505     3.270794     2.991166      42.54
 H      -2.947409     4.026348     2.541980      20.55
 C      -1.316284     0.868286     3.155977      58.66
 H      -1.343993    -0.238982     3.073140      19.72
 C      -0.226694     1.307956     4.022053      24.85
 O       0.806186     0.556243     4.660982     188.68
 C       0.564834    -0.899200     4.682722     118.62
 H       1.506946    -1.298377     5.065839      26.95
 H       0.604541    -1.267835     3.624290      28.35
 H      -0.314957    -1.059358     5.143281      28.96
 C      -0.144730     2.745109     4.348199      12.29
 O       0.831501     3.187993     5.233681      91.15
 H       0.788194     4.231888     5.346471      24.94
 C      -1.129984     3.635519     3.828736      43.55
 H      -1.006896     4.673466     4.149023      26.41
 C      -2.097035     1.904958     2.591757      24.28
 C      -3.262201     1.439018     1.598828      90.90
 H      -4.200989     2.226482     1.645271      23.40
 O      -4.009386     0.202994     2.063774     200.00
 H      -4.943562     0.556076     1.903614      22.13
 C      -2.979419     1.362594     0.159041      67.91
 H      -2.203241     2.190163    -0.164983      22.19
 C      -4.047192     1.455440    -0.963081      68.52
 O      -4.889708     0.267315    -1.305158     217.15
 H      -4.377248    -0.482746    -1.079371      29.42
 H      -3.153163     1.642932    -1.928445      22.65
 H      -4.838909     2.402811    -0.750385      23.06
 C       1.372474     1.117202    -0.544396      28.64
 H       2.301752     2.016491    -0.646413      21.68
 C       1.046630    -1.302862    -0.977327      50.97
 H       1.665295    -2.217735    -1.267008      24.47
 C      -0.325678    -1.198011    -0.841647      25.89
 O      -1.172820    -2.344472    -1.173510     210.45
 C      -1.227193    -2.935031    -2.448128      97.34
 H      -1.506728    -4.043944    -2.484316      25.21
 H      -2.104101    -2.338142    -3.299589      22.49
 H      -0.411878    -2.705267    -3.556976      22.06
 C      -0.886857     0.006922    -0.384390      31.53
 O      -2.188306    -0.010820    -0.049148     143.38
 C      -0.003726     1.042738    -0.237732      70.31
 H      -0.323270     2.095942     0.043910      24.28
 C       1.968489    -0.231489    -0.679996     -11.89
 C       3.499547    -0.583601    -0.745253      76.05
 H       3.697422    -1.141967    -1.834291      22.53
 O       4.263843     0.698196    -1.202199      34.33
 H       4.335698     1.124399    -0.132589      19.21
 C       4.017926    -1.205214     0.572234     101.54
 H       3.294627    -2.045294     0.826987      25.62
 O       5.398634    -1.730487     0.544486     178.44
 H       5.508547    -2.585541    -0.102408      24.82
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 C       4.084003    -0.218102     1.666011      95.69
 O       4.579684     1.187381     1.389385     203.93
 H       3.859582     1.780874     1.946485      23.64
 H       4.703497    -0.684886     2.380598      26.25
 H       2.968617     0.116172     2.297525      23.47
55
name = lig-Water-frame_710
 C      -2.116713     3.256572     3.002528      51.28
 H      -2.720443     4.113734     2.777744      22.63
 C      -1.233769     0.863080     3.176766      37.67
 H      -1.370431    -0.207548     3.051384      20.54
 C      -0.273798     1.376564     3.960821      32.99
 O       0.813320     0.540366     4.738263     152.95
 C       0.589068    -0.814015     4.632865     107.87
 H       1.562281    -1.201531     5.147187      24.85
 H       0.604623    -1.464424     3.649067      26.30
 H      -0.488358    -1.024956     5.210416      24.65
 C      -0.185388     2.797206     4.241992      18.85
 O       0.800500     3.177307     5.225085     136.51
 H       0.864378     4.154177     5.435879      24.32
 C      -1.135379     3.644077     3.792788      47.50
 H      -1.084369     4.609885     4.301772      23.16
 C      -2.164135     1.860467     2.554815      31.44
 C      -3.302450     1.470588     1.595577     118.10
 H      -3.819816     2.370705     1.714371      26.88
 O      -3.966441     0.210233     2.053675     245.32
 H      -4.943380     0.415845     1.919480      25.12
 C      -2.972305     1.313276     0.150750      93.99
 H      -2.385955     2.117197    -0.135340      26.96
 C      -4.063183     1.467903    -0.973564     106.91
 O      -4.898666     0.287726    -1.295470     251.64
 H      -4.333480    -0.566415    -1.208399      28.58
 H      -3.472512     1.795475    -1.720614      30.30
 H      -4.702350     2.231514    -0.842419      28.51
 C       1.362604     1.098357    -0.493016      34.60
 H       1.930673     1.854564    -0.581350      22.05
 C       1.166173    -1.321111    -0.973011      54.60
 H       1.687377    -2.257666    -1.212375      23.42
 C      -0.285184    -1.223160    -0.859692      12.94
 O      -1.147501    -2.380237    -1.218313     236.27
 C      -1.267062    -2.902228    -2.561015     121.86
 H      -1.390752    -3.965523    -2.475648      26.08
 H      -2.098264    -2.353746    -2.916878      26.00
 H      -0.490066    -2.937364    -3.212286      28.48
 C      -0.856926    -0.007993    -0.298331      30.48
 O      -2.191438     0.019422    -0.062241     187.61
 C       0.005976     1.046585    -0.217806      49.66
 H      -0.475025     2.017873     0.015216      20.99
 C       1.932765    -0.248190    -0.815227      15.66
 C       3.564820    -0.631399    -0.808675     100.90
 H       3.617607    -1.364991    -1.493510      28.86
 O       4.247228     0.685969    -1.178798     103.42
 H       4.394654     0.996436    -0.306688      25.43
 C       4.001473    -1.181492     0.545891     105.54
 H       3.251021    -1.970888     0.588684      27.57
 O       5.416420    -1.705074     0.536585     214.02
 H       5.473193    -2.440159     0.023519      33.54
 C       4.034424    -0.164308     1.731412     117.19
 O       4.499085     1.146345     1.416961     278.56
 H       3.965703     1.672574     2.021276      26.33
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 H       4.845271    -0.550951     2.460467      25.34
 H       3.244134    -0.214928     2.296116      31.20
55
name = lig-Water-frame_711
 C      -2.103939     3.179428     2.947783      80.71
 H      -2.834152     4.018160     2.748579      22.01
 C      -1.211096     0.890666     3.152058      42.81
 H      -1.420062    -0.151775     2.928767      23.25
 C      -0.221891     1.448227     3.975573      -1.03
 O       0.779752     0.596250     4.757874     176.02
 C       0.605994    -0.796720     4.623190     129.00
 H       1.319785    -1.210685     5.299146      27.50
 H       0.533379    -1.257094     3.641676      29.81
 H      -0.239073    -1.178490     5.146586      28.87
 C      -0.151341     2.803121     4.206499      30.66
 O       0.764651     3.144228     5.198041     116.00
 H       0.839123     4.144925     5.390178      24.44
 C      -1.085699     3.712430     3.819800      68.77
 H      -1.253969     4.716406     4.343350      17.97
 C      -2.221593     1.809888     2.539968      22.13
 C      -3.338910     1.479581     1.634804     117.79
 H      -3.909684     2.525741     1.689989      22.71
 O      -3.929594     0.241348     2.046475     261.47
 H      -4.961482     0.192611     1.914125      27.27
 C      -2.944088     1.251781     0.111658      80.79
 H      -2.311807     2.248061    -0.096224      21.68
 C      -4.080825     1.414644    -0.963061      69.75
 O      -4.893362     0.309818    -1.280176     206.52
 H      -4.301091    -0.525012    -1.170887      28.09
 H      -3.547078     1.914150    -2.122850      22.69
 H      -4.879345     2.388766    -0.696009      23.64
 C       1.370106     0.961868    -0.458639      49.64
 H       1.829631     2.191754    -0.453949      20.52
 C       1.200402    -1.384277    -0.978277      58.64
 H       1.553727    -2.385867    -1.208335      23.68
 C      -0.250823    -1.283150    -0.892235       2.65
 O      -1.092245    -2.387674    -1.217993     196.06
 C      -1.313707    -2.880732    -2.670010      48.03
 H      -1.531778    -3.987278    -2.338711      22.29
 H      -2.446402    -2.319796    -2.834017      19.90
 H      -0.043907    -2.874727    -3.015322      19.96
 C      -0.817403    -0.093700    -0.256642      -3.79
 O      -2.229867     0.057811    -0.074535     182.38
 C       0.016801     1.135432    -0.185500      48.51
 H      -0.564283     2.007591     0.029813      19.47
 C       1.982923    -0.199006    -0.918797      36.55
 C       3.570338    -0.580449    -0.876402      88.38
 H       3.728030    -1.689239    -1.456108      25.25
 O       4.228950     0.630769    -1.181306      26.54
 H       4.631689     1.187030    -0.229775      16.67
 C       4.013174    -1.149338     0.515732      94.90
 H       3.285053    -2.025858     0.714740      27.52
 O       5.418694    -1.664145     0.535480      82.72
 H       5.400321    -2.584684    -0.158878      25.56
 C       4.043666    -0.177098     1.818995      96.87
 O       4.426156     1.108267     1.428449     196.25
 H       3.893744     1.870608     1.990097      20.88
 H       4.846226    -0.525980     2.409212      27.20
 H       2.919706    -0.421023     2.466963      24.54
55
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name = lig-Water-frame_712
 C      -2.092738     3.134635     2.900685      69.05
 H      -3.069658     3.624507     2.558315      22.96
 C      -1.238611     0.948153     3.095001      54.88
 H      -1.306279    -0.143524     2.891077      22.97
 C      -0.143498     1.427113     3.998723      22.16
 O       0.718596     0.701939     4.739466     156.64
 C       0.616645    -0.809230     4.643184      93.17
 H       1.382372    -1.333059     5.352976      25.59
 H       0.631342    -0.953890     3.456161      26.18
 H      -0.411452    -1.272489     5.137975      24.48
 C      -0.074500     2.831559     4.243845      29.81
 O       0.758156     3.120198     5.184916     115.50
 H       0.710085     4.125466     5.245381      25.94
 C      -1.091851     3.774337     3.813455      75.97
 H      -1.253510     4.728977     4.212777      16.21
 C      -2.206553     1.788194     2.575896      38.12
 C      -3.388018     1.487816     1.644052      98.59
 H      -4.211813     2.191012     1.562399      25.01
 O      -3.917335     0.256299     2.058928     290.14
 H      -4.848458     0.274497     1.829130      27.65
 C      -2.904154     1.277030     0.068841      91.10
 H      -2.300826     2.078457    -0.106875      26.91
 C      -4.096722     1.435813    -0.996196     124.92
 O      -4.885169     0.302994    -1.257400     291.48
 H      -4.355651    -0.424652    -1.040420      31.99
 H      -3.811153     1.679649    -1.874250      30.75
 H      -4.684022     2.096545    -0.553934      29.75
 C       1.395546     0.937441    -0.435430      42.65
 H       1.857809     1.788769    -0.334389      26.10
 C       1.164054    -1.430521    -1.002172      46.14
 H       1.528782    -2.493708    -1.273745      24.17
 C      -0.226820    -1.337951    -0.906697      14.17
 O      -1.035716    -2.383595    -1.191207     208.89
 C      -1.330336    -2.870154    -2.693611      95.25
 H      -1.671770    -3.833025    -2.515360      26.12
 H      -2.151103    -2.417957    -3.210370      27.19
 H      -0.484931    -2.655807    -3.150682      29.18
 C      -0.775669    -0.129644    -0.257869     -14.56
 O      -2.251745     0.052337    -0.098394     138.35
 C      -0.007416     1.122523    -0.155087      38.19
 H      -0.449898     2.194634     0.101119      20.65
 C       2.076320    -0.222191    -0.984399      40.13
 C       3.526848    -0.536368    -0.905438     121.12
 H       3.857823    -1.236505    -1.555640      32.04
 O       4.261511     0.599611    -1.203665     158.50
 H       4.497621     0.919110    -0.426199      31.41
 C       4.023756    -1.118830     0.540225      98.86
 H       3.464580    -1.957125     0.879063      30.62
 O       5.405876    -1.651550     0.501602     155.96
 H       5.417430    -2.356962    -0.118470      30.98
 C       4.012318    -0.268233     1.896884     107.42
 O       4.359910     1.114715     1.437548     241.99
 H       3.728548     1.786285     1.791252      28.38
 H       4.848291    -0.701080     2.537379      26.56
 H       3.097399    -0.236054     2.291670      30.81
55
name = lig-Water-frame_713
 C      -2.092164     3.158914     2.889114      57.17
 H      -2.999866     3.537213     2.519451      24.17
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 C      -1.207540     0.961475     3.077104      75.05
 H      -1.192113    -0.085033     2.898197      25.89
 C      -0.156869     1.408137     3.948497      14.45
 O       0.677512     0.761376     4.739694     145.94
 C       0.605137    -0.808784     4.661340     119.71
 H       1.463735    -1.201115     5.096490      29.32
 H       0.814652    -0.940609     3.661389      31.04
 H      -0.433973    -1.062052     4.846677      25.77
 C      -0.086746     2.852587     4.243839      12.68
 O       0.813496     3.148005     5.225273     181.29
 H       0.768994     4.129273     5.343635      29.75
 C      -1.134505     3.742129     3.744897      86.34
 H      -1.137352     4.877616     4.073798      19.31
 C      -2.183634     1.812998     2.599208      44.74
 C      -3.403487     1.455852     1.606808      83.73
 H      -4.360012     2.108530     1.593753      25.57
 O      -3.925531     0.236963     2.084390     252.31
 H      -4.903222     0.359687     1.790300      23.90
 C      -2.889652     1.330173     0.040744      66.98
 H      -2.099298     2.172101    -0.250136      25.08
 C      -4.088683     1.440334    -0.977322      72.32
 O      -4.896057     0.260968    -1.227922     156.13
 H      -4.370925    -0.576823    -0.829141      25.37
 H      -3.649810     1.853252    -2.176681      24.03
 H      -4.815203     2.263035    -0.301044      24.47
 C       1.410970     0.910451    -0.433231      -3.70
 H       2.311187     1.850094    -0.217747      24.83
 C       1.163443    -1.447430    -1.059496      56.41
 H       1.547701    -2.355058    -1.355732      26.31
 C      -0.214531    -1.333400    -0.886768      13.29
 O      -1.021832    -2.407422    -1.182643     209.07
 C      -1.355326    -2.836554    -2.647387      75.05
 H      -1.651346    -3.983574    -2.726937      24.00
 H      -1.982673    -2.196362    -3.556586      22.77
 H      -0.466302    -2.555673    -3.623162      23.36
 C      -0.782031    -0.084770    -0.294023       2.58
 O      -2.232740    -0.009150    -0.135563     123.40
 C      -0.003734     1.030848    -0.135733      68.07
 H      -0.201862     1.979102     0.148441      27.36
 C       2.057251    -0.314975    -0.984044      15.82
 C       3.492238    -0.503941    -0.880356      90.62
 H       3.855168    -1.134780    -1.871267      28.10
 O       4.327418     0.601202    -1.269085      54.08
 H       4.487417     1.001678    -0.140305      20.91
 C       4.033272    -1.112444     0.605505      92.41
 H       3.389338    -2.061860     0.857935      29.34
 O       5.398587    -1.621674     0.462990     120.16
 H       5.433786    -2.358020    -0.232004      27.34
 C       4.024791    -0.334152     1.891930      98.18
 O       4.323094     1.105352     1.435432     174.29
 H       3.545578     1.681834     1.857391      25.95
 H       4.661525    -0.775507     2.670473      28.70
 H       2.856893    -0.145967     2.392195      27.69
55
name = lig-Water-frame_714
 C      -2.115137     3.206711     2.889776      48.14
 H      -2.928779     4.019040     2.518069      23.19
 C      -1.140850     0.927103     3.081557      51.68
 H      -1.199710    -0.161142     2.822201      27.35
 C      -0.224763     1.477779     3.879475      14.84
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 O       0.672405     0.744672     4.761775     154.08
 C       0.593319    -0.730864     4.639539     103.88
 H       1.561694    -1.101359     5.251905      26.45
 H       0.955190    -1.144408     3.511785      28.79
 H      -0.477175    -1.053484     4.819896      26.68
 C      -0.161869     2.856300     4.218521       6.54
 O       0.884946     3.204775     5.275358      86.89
 H       0.896538     4.203337     5.556865      26.53
 C      -1.136582     3.702683     3.689082      54.70
 H      -1.033014     4.707532     3.829037      19.73
 C      -2.189153     1.849518     2.572177     -10.19
 C      -3.363342     1.418605     1.563492      86.45
 H      -4.054875     2.292820     1.716230      26.17
 O      -3.960769     0.194194     2.095629     242.90
 H      -4.982377     0.203639     1.988864      23.71
 C      -2.867979     1.371053     0.017209      68.75
 H      -2.185931     2.103382    -0.256303      28.52
 C      -4.080015     1.480962    -0.963664     115.80
 O      -4.893041     0.201409    -1.184118     190.00
 H      -4.497913    -0.565699    -0.713115      28.91
 H      -3.743225     1.911892    -1.754764      31.48
 H      -4.693482     2.183379    -0.652044      31.94
 C       1.476226     0.873353    -0.450765      90.93
 H       2.170506     1.553064    -0.190683      34.04
 C       1.178033    -1.435269    -1.133860      61.72
 H       1.626337    -2.442980    -1.547634      25.18
 C      -0.221139    -1.284056    -0.855979       4.56
 O      -1.047245    -2.454199    -1.209933     214.55
 C      -1.334949    -2.770916    -2.695119     109.12
 H      -1.499257    -3.784158    -2.722442      28.74
 H      -2.093176    -2.073871    -3.020571      28.47
 H      -0.459032    -2.820565    -3.229764      30.23
 C      -0.844951    -0.067877    -0.370135      21.99
 O      -2.192521    -0.071749    -0.176785     129.43
 C       0.103033     0.936402    -0.131734      52.76
 H      -0.253351     1.981518     0.377519      27.40
 C       1.942323    -0.362450    -0.904516      16.19
 C       3.526152    -0.515980    -0.885860      90.60
 H       3.570724    -1.298686    -1.599014      30.24
 O       4.405392     0.645395    -1.270104     109.12
 H       4.427245     1.187008    -0.520035      32.30
 C       4.017631    -1.187586     0.635462     100.96
 H       3.348089    -1.992506     0.682872      32.97
 O       5.404704    -1.585763     0.425607      66.86
 H       5.353390    -2.410050    -0.343533      25.66
 C       3.978670    -0.329065     1.868658     131.76
 O       4.303020     1.073467     1.438509     162.55
 H       3.708541     1.667847     2.016504      27.61
 H       4.575350    -0.710098     2.715156      31.75
 H       3.005033    -0.360898     2.281684      32.25
55
name = lig-Water-frame_715
 C      -2.190567     3.263642     2.859751      56.86
 H      -2.654370     4.108888     2.596748      22.08
 C      -1.159541     0.903906     3.029973      38.65
 H      -1.201099    -0.138858     2.787969      26.12
 C      -0.219974     1.538758     3.908048      16.23
 O       0.665016     0.712171     4.754617     181.83
 C       0.630259    -0.652455     4.580264     135.54
 H       1.146982    -0.971854     5.433953      28.35
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 H       0.830433    -1.090419     3.702468      33.93
 H      -0.327628    -1.198046     4.968290      28.89
 C      -0.193946     2.877000     4.248083      11.08
 O       0.926080     3.257659     5.290758      81.78
 H       0.803352     4.216698     5.520640      23.46
 C      -1.084437     3.691246     3.662184     103.67
 H      -0.963455     4.847361     3.722593      25.03
 C      -2.192331     1.848008     2.512334     -17.32
 C      -3.276017     1.401442     1.553475      91.05
 H      -3.838718     2.352685     1.642591      25.63
 O      -3.998777     0.152296     2.089164     204.99
 H      -4.985010     0.206600     2.092276      23.34
 C      -2.883374     1.337420     0.028695      61.93
 H      -2.126508     2.190724    -0.201574      24.57
 C      -4.073178     1.448818    -0.915681      74.15
 O      -4.879503     0.172654    -1.139764     142.75
 H      -4.478488    -0.545912    -0.628486      29.14
 H      -3.599116     1.943887    -2.089627      23.78
 H      -4.945038     2.366662    -0.710489      23.31
 C       1.484067     0.805162    -0.457834      71.15
 H       2.247914     1.719943    -0.073750      26.66
 C       1.135834    -1.459732    -1.212739      65.41
 H       1.515994    -2.327083    -1.613864      26.99
 C      -0.254006    -1.287589    -0.876726       6.77
 O      -1.076004    -2.486324    -1.231845     186.45
 C      -1.298217    -2.686241    -2.706605      80.77
 H      -1.717390    -3.810542    -2.606105      24.82
 H      -2.257892    -1.996270    -2.557798      21.00
 H      -0.083170    -2.812459    -3.005788      21.95
 C      -0.852979    -0.097532    -0.467515      13.02
 O      -2.178492    -0.091610    -0.214650     110.19
 C       0.192619     0.927870    -0.102281      54.95
 H      -0.234306     1.660679     0.412512      27.94
 C       1.942944    -0.361189    -0.810710      19.35
 C       3.545848    -0.535489    -0.849059      67.57
 H       3.680521    -1.558088    -1.469123      27.26
 O       4.451671     0.664303    -1.285445      37.54
 H       4.425034     1.428544    -0.561617      25.96
 C       4.010094    -1.248405     0.590883      87.24
 H       3.272333    -2.165482     0.636731      28.57
 O       5.409848    -1.579018     0.378417     166.67
 H       5.360764    -2.264775    -0.158689      35.26
 C       3.937003    -0.299148     1.826848     101.00
 O       4.292368     1.032585     1.458842     163.36
 H       3.922109     1.707882     2.099535      26.34
 H       4.672501    -0.598351     2.629130      27.83
 H       2.738096    -0.472954     2.250996      26.89
55
name = lig-Water-frame_716
 C      -2.190861     3.261592     2.853409      37.28
 H      -2.829813     4.179474     2.376039      18.49
 C      -1.209938     0.969529     2.980503      52.14
 H      -1.182183    -0.119878     2.784394      22.58
 C      -0.193774     1.496891     3.981177      16.10
 O       0.643967     0.738059     4.712159     199.00
 C       0.633447    -0.634092     4.593036     111.68
 H       1.130021    -1.022088     5.569548      24.43
 H       0.949556    -1.123590     3.485640      25.93
 H      -0.349304    -1.097744     4.886523      26.73
 C      -0.137174     2.899871     4.346256       3.81
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 O       0.917349     3.294842     5.258557      98.99
 H       0.695531     4.280543     5.399567      22.47
 C      -1.057382     3.760630     3.625388      70.86
 H      -0.934891     4.808393     3.760360      30.43
 C      -2.169022     1.837252     2.460663      18.74
 C      -3.212170     1.383975     1.558101      85.32
 H      -4.001980     2.239084     1.414239      25.74
 O      -4.009723     0.133254     2.064923     207.04
 H      -5.035768     0.438857     1.972251      21.12
 C      -2.886154     1.265023     0.064751      87.12
 H      -2.203943     2.096044    -0.106683      24.70
 C      -4.097299     1.434663    -0.947466     114.21
 O      -4.855657     0.180695    -1.093170     222.30
 H      -4.350104    -0.592282    -0.562610      23.99
 H      -3.713672     1.478484    -1.820364      30.15
 H      -4.722413     2.110785    -0.623572      30.29
 C       1.500699     0.836708    -0.398924      40.92
 H       2.139190     1.699521    -0.092510      27.15
 C       1.066672    -1.433739    -1.244706      57.57
 H       1.454424    -2.424042    -1.701873      25.13
 C      -0.296868    -1.377206    -0.969866      20.55
 O      -1.087277    -2.491428    -1.205801     245.93
 C      -1.262664    -2.650547    -2.631245     121.38
 H      -1.837773    -3.513699    -2.741029      28.14
 H      -1.985607    -1.915855    -3.016090      27.93
 H      -0.429244    -2.456221    -3.192477      29.36
 C      -0.770588    -0.108375    -0.540325      10.79
 O      -2.197973    -0.066399    -0.248293     122.14
 C       0.150107     0.898084    -0.089266      49.61
 H      -0.232306     1.812807     0.586788      22.82
 C       2.073531    -0.443061    -0.794308      15.23
 C       3.547906    -0.586246    -0.785068      76.40
 H       4.014364    -1.277377    -1.505947      26.67
 O       4.460513     0.643450    -1.301384       4.21
 H       4.330398     1.442407    -0.505012      25.03
 C       4.000023    -1.258151     0.517034      99.71
 H       3.489620    -2.154783     0.732083      28.73
 O       5.412008    -1.572489     0.354563      98.42
 H       5.488416    -2.555072    -0.221355      23.25
 C       3.871265    -0.304605     1.796853     107.41
 O       4.289220     1.011970     1.470923     157.37
 H       3.943007     1.696119     2.187480      26.11
 H       4.600873    -0.636400     2.498071      27.48
 H       2.852654    -0.368291     2.139596      28.98
55
name = lig-Water-frame_717
 C      -2.126753     3.261764     2.846427      31.17
 H      -2.914732     3.705068     2.355453      17.65
 C      -1.199102     1.058027     3.000696      61.04
 H      -1.213456    -0.012672     2.749840      21.14
 C      -0.231365     1.472957     4.021500      28.75
 O       0.650240     0.779858     4.675076     221.26
 C       0.625164    -0.707545     4.625855     102.26
 H       1.355256    -1.054826     5.312368      25.49
 H       1.075594    -0.944772     3.767761      32.21
 H      -0.531630    -0.879136     4.551670      24.25
 C      -0.092171     2.900566     4.403793      10.50
 O       0.872273     3.332515     5.200322      77.62
 H       0.820596     4.339199     5.411604      22.83
 C      -1.041948     3.810377     3.608595      72.08
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 H      -0.963652     4.916062     3.832672      32.85
 C      -2.142714     1.882540     2.443113      27.18
 C      -3.247282     1.349062     1.533848     103.78
 H      -4.046090     2.040969     1.449943      24.00
 O      -4.007244     0.156411     2.024188     276.49
 H      -4.913432     0.384976     1.869458      26.37
 C      -2.870401     1.168988     0.085042      96.64
 H      -2.202903     2.045856    -0.147210      22.53
 C      -4.088739     1.336875    -0.939121      61.29
 O      -4.842601     0.179098    -1.030993     244.83
 H      -4.358952    -0.561135    -0.686948      27.09
 H      -3.555654     1.399682    -2.148579      22.54
 H      -4.767697     2.316566    -0.478330      22.36
 C       1.525150     0.821086    -0.325698       4.79
 H       2.193154     1.774013    -0.030896      26.33
 C       1.079512    -1.420018    -1.255794      53.01
 H       1.380974    -2.376677    -1.661034      25.75
 C      -0.312295    -1.422684    -1.063149      22.61
 O      -1.099734    -2.488900    -1.174978     270.76
 C      -1.290674    -2.597683    -2.575881     115.60
 H      -1.808088    -3.549119    -2.967327      26.19
 H      -1.712135    -1.741769    -3.391227      23.16
 H      -0.468220    -2.317245    -3.475473      23.33
 C      -0.732085    -0.113270    -0.564256       6.87
 O      -2.201584    -0.023387    -0.285717     166.58
 C       0.062502     0.890875    -0.081306      55.32
 H      -0.157412     1.763659     0.433212      23.31
 C       2.132369    -0.488371    -0.825403       3.39
 C       3.594958    -0.639923    -0.772912      94.74
 H       4.049129    -1.149440    -1.680521      24.31
 O       4.421128     0.615025    -1.279722      90.19
 H       4.351130     1.154702    -0.627016      36.86
 C       4.030305    -1.218869     0.480430     101.70
 H       3.512009    -2.208441     0.787438      26.66
 O       5.426349    -1.600134     0.322391     133.13
 H       5.551174    -2.545270     0.012598      24.63
 C       3.843354    -0.343039     1.741119      97.12
 O       4.292948     1.031209     1.481074     136.20
 H       3.781075     1.534090     2.097501      30.52
 H       4.458560    -0.899346     2.571313      26.49
 H       2.670434    -0.272931     2.181334      25.43
55
name = lig-Water-frame_718
 C      -2.036956     3.240593     2.827262      68.66
 H      -3.030450     3.716584     2.412410      14.67
 C      -1.140234     1.104324     3.065811      59.29
 H      -1.203524     0.086480     2.727240      22.55
 C      -0.312532     1.541736     4.030961      41.45
 O       0.710971     0.773091     4.675178     214.06
 C       0.588628    -0.742280     4.636345      87.96
 H       1.361372    -1.156968     5.375763      23.78
 H       1.242477    -0.958495     3.584086      25.26
 H      -0.400719    -1.022333     4.505658      27.65
 C      -0.165150     2.912910     4.337104      17.02
 O       0.853759     3.374976     5.164722     -18.13
 H       0.897199     4.333766     5.399255      22.58
 C      -1.011134     3.823903     3.639817      62.18
 H      -1.065214     4.914487     3.868390      34.11
 C      -2.128963     1.945843     2.453550      18.55
 C      -3.312550     1.304594     1.517642      78.82
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 H      -4.099116     2.219230     1.587652      21.85
 O      -3.970145     0.179921     1.988731     247.40
 H      -5.046183     0.199253     1.832407      22.40
 C      -2.842106     1.122745     0.052723     104.47
 H      -2.237614     2.032468    -0.229411      22.63
 C      -4.027335     1.270904    -0.947952     118.74
 O      -4.873380     0.160778    -0.967327     283.78
 H      -4.339567    -0.716429    -0.810808      24.11
 H      -3.670568     1.633509    -1.789025      30.44
 H      -4.524502     2.111059    -0.776707      29.26
 C       1.527581     0.735504    -0.259957      21.69
 H       2.171271     1.684546     0.035130      26.73
 C       1.153390    -1.441177    -1.257379      51.92
 H       1.505687    -2.415980    -1.648068      23.86
 C      -0.259279    -1.327810    -1.090877       4.05
 O      -1.127972    -2.495327    -1.181710     216.10
 C      -1.334150    -2.538580    -2.687457     104.22
 H      -1.688469    -3.544668    -2.944424      26.35
 H      -1.896459    -1.665690    -2.877698      26.98
 H      -0.274188    -2.701051    -2.977709      25.40
 C      -0.803034    -0.141508    -0.553324      11.04
 O      -2.166623    -0.018862    -0.331428     198.86
 C       0.090185     0.891428    -0.110549      51.68
 H      -0.370794     1.854101     0.335331      20.21
 C       2.066756    -0.436027    -0.854349     -12.64
 C       3.660720    -0.672845    -0.870442     113.76
 H       3.781807    -1.469109    -1.749926      24.92
 O       4.356976     0.561935    -1.257715      -7.38
 H       4.405585     1.241041    -0.316258      24.26
 C       4.087412    -1.222624     0.500198     107.31
 H       3.416871    -2.054060     0.629930      29.42
 O       5.462550    -1.614551     0.318342     183.18
 H       5.434733    -2.633004    -0.018530      22.56
 C       3.823334    -0.397126     1.710484     108.12
 O       4.301239     1.047363     1.499298      97.60
 H       3.549025     1.589162     2.004126      25.67
 H       4.224759    -0.913438     2.524951      28.89
 H       2.747908    -0.254252     1.966198      27.68
55
name = lig-Water-frame_719
 C      -2.007602     3.279008     2.784563     118.09
 H      -2.741809     4.088103     2.673899      21.38
 C      -1.133959     1.107132     3.088505      50.44
 H      -1.057381     0.017551     2.799192      25.10
 C      -0.312812     1.601952     4.080790      32.33
 O       0.761777     0.746003     4.689591     138.17
 C       0.633317    -0.733914     4.576700     115.69
 H       0.968747    -1.173510     5.535180      27.60
 H       1.004505    -1.086552     3.722604      34.47
 H      -0.415201    -1.369713     4.649553      27.12
 C      -0.245972     2.986347     4.257059      17.91
 O       0.848720     3.388146     5.134251     242.12
 H       0.779255     4.422364     5.302125      23.93
 C      -1.020652     3.825973     3.671445      39.38
 H      -1.066346     4.850370     3.903660      16.11
 C      -2.111329     1.924055     2.473210      31.09
 C      -3.354586     1.345694     1.521088      91.32
 H      -3.934473     2.193060     1.500387      25.07
 O      -3.949937     0.165042     1.976593     283.68
 H      -4.914817     0.141816     1.845559      25.83
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 C      -2.833487     1.165954    -0.002836      86.72
 H      -2.238787     2.036320    -0.222779      25.01
 C      -3.942763     1.214952    -0.933923      81.05
 O      -4.923466     0.115949    -0.911161     193.14
 H      -4.432956    -0.801105    -1.001515      24.35
 H      -3.489634     1.667087    -2.070799      24.02
 H      -4.675229     2.215159    -0.704503      24.13
 C       1.478723     0.663084    -0.200132      68.28
 H       2.151812     1.488526     0.103180      26.07
 C       1.217759    -1.468714    -1.251838      37.24
 H       1.695679    -2.423192    -1.645764      25.63
 C      -0.201667    -1.244279    -1.074164      -1.50
 O      -1.142644    -2.478754    -1.206212     149.04
 C      -1.341313    -2.523673    -2.778002     101.16
 H      -1.907643    -3.494305    -2.913974      26.91
 H      -2.093484    -1.624056    -2.645170      22.15
 H      -0.270581    -2.792543    -2.724797      20.81
 C      -0.848874    -0.134389    -0.516130      23.04
 O      -2.126648    -0.073254    -0.380026     165.88
 C       0.147046     0.895142    -0.152292      57.19
 H      -0.438701     1.770654     0.155731      21.44
 C       2.014552    -0.378861    -0.881329      35.83
 C       3.647566    -0.688097    -0.989272      95.76
 H       3.722091    -1.589333    -1.623706      27.86
 O       4.296520     0.524650    -1.222652      48.58
 H       4.434815     0.895870    -0.308046      25.15
 C       4.131829    -1.246541     0.477838      99.21
 H       3.374052    -2.099660     0.541581      28.21
 O       5.506298    -1.640321     0.343128     170.93
 H       5.358433    -2.530013    -0.264577      23.09
 C       3.817845    -0.404577     1.675427     103.05
 O       4.298276     1.053748     1.536743     125.63
 H       3.586716     1.693822     1.813691      26.63
 H       4.232634    -0.832796     2.689536      27.41
 H       2.607986    -0.351624     1.734979      27.36
55
name = lig-Water-frame_720
 C      -2.010057     3.367793     2.757654      92.18
 H      -2.635339     4.262253     2.573670      26.37
 C      -1.149826     1.064342     3.098539      43.13
 H      -0.972529     0.041976     2.935996      24.24
 C      -0.251617     1.596438     4.125382      18.87
 O       0.772899     0.725606     4.697342     149.59
 C       0.625731    -0.739153     4.562144     115.39
 H       0.927861    -1.080872     5.566011      27.01
 H       1.107962    -1.327215     3.579608      27.77
 H      -0.332596    -1.112969     4.660815      30.48
 C      -0.185567     3.014156     4.289274       4.97
 O       0.827354     3.403025     5.090269     277.29
 H       0.752261     4.351132     5.270321      27.69
 C      -1.117454     3.867595     3.640453      50.65
 H      -1.000528     5.000172     3.948685      18.77
 C      -2.125536     1.880135     2.478913      43.29
 C      -3.299147     1.403361     1.521627      68.48
 H      -4.096541     2.333717     1.343525      22.80
 O      -3.923882     0.132874     1.986737     222.11
 H      -4.941351     0.233790     1.804173      23.82
 C      -2.819693     1.223330    -0.020603      74.88
 H      -2.104656     2.128667    -0.229205      23.11
 C      -3.934871     1.237384    -0.999649     105.84
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 O      -4.954001     0.078253    -0.876835     214.89
 H      -4.552385    -0.794597    -0.932905      26.80
 H      -3.578374     1.143857    -1.921142      29.95
 H      -4.552179     1.941497    -0.602593      28.77
 C       1.444663     0.650965    -0.155342      59.34
 H       2.282516     1.472531     0.286155      24.10
 C       1.230377    -1.471095    -1.241839      52.83
 H       1.677008    -2.316408    -1.654523      27.81
 C      -0.176010    -1.277351    -1.044566       2.64
 O      -1.129781    -2.428665    -1.221706     148.25
 C      -1.371105    -2.550202    -2.767877      98.53
 H      -2.174821    -3.312451    -2.970905      26.11
 H      -1.876512    -1.605742    -3.145715      26.51
 H      -0.347159    -2.502294    -3.338766      25.14
 C      -0.749438    -0.104063    -0.489043      22.13
 O      -2.140665    -0.132474    -0.410365     117.88
 C       0.099698     0.889604    -0.190728      62.00
 H      -0.195970     1.876711     0.161295      21.86
 C       2.050431    -0.412753    -0.925038      36.23
 C       3.539987    -0.685382    -1.012311      89.82
 H       3.906880    -1.591095    -1.772574      27.13
 O       4.268215     0.492121    -1.225273      12.84
 H       4.448847     0.793012    -0.170502      23.93
 C       4.135188    -1.280750     0.406271      87.57
 H       3.601428    -2.220778     0.639595      29.37
 O       5.536350    -1.664701     0.371061     119.79
 H       5.605620    -2.484150    -0.267089      24.05
 C       3.802306    -0.367432     1.678073     108.84
 O       4.299843     1.042605     1.560461     144.77
 H       3.627474     1.698145     1.829845      27.67
 H       4.174661    -0.658054     2.592014      30.25
 H       2.663022    -0.502875     1.529045      29.02
55
name = lig-Water-frame_721
55
name = lig-Water-frame_722
 C      -2.135660     3.384187     2.674963      56.82
 H      -2.790351     3.710855     1.995082      14.45
 C      -1.186111     1.052011     3.185862      55.68
 H      -1.351990     0.052185     2.888328      23.98
 C      -0.166652     1.520294     4.047429      21.38
 O       0.777339     0.737030     4.684424     185.50
 C       0.588792    -0.726574     4.606932     110.58
 H       1.166855    -1.160955     5.392580      26.96
 H       1.232830    -1.070170     3.612409      26.71
 H      -0.415233    -0.914771     4.478786      28.75
 C      -0.181594     2.951841     4.290571      -5.44
 O       0.902106     3.483846     5.091522     130.59
 H       0.882709     4.448606     5.385072      35.10
 C      -1.139155     3.909830     3.685682      72.89
 H      -1.052302     5.092837     3.758923      20.42
 C      -2.143235     1.968621     2.519638       1.29
 C      -3.131509     1.424950     1.473598      80.05
 H      -4.075065     2.211623     1.574511      23.56
 O      -3.868198     0.157230     1.996613     197.56
 H      -4.798483     0.176018     1.797006      26.37
 C      -2.762828     1.216718    -0.037840      70.86
 H      -2.016254     2.041912    -0.465756      20.97
 C      -4.060380     1.145529    -1.079396     105.00
 O      -4.978877     0.080453    -0.818494     275.14
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 H      -4.504397    -0.659127    -0.518454      27.04
 H      -3.634799     1.151494    -2.013241      27.81
 H      -4.480225     2.085656    -1.371488      26.37
 C       1.541677     0.650634    -0.225107      39.49
 H       2.135831     1.627009     0.378495      23.23
 C       1.144247    -1.506694    -1.278475      69.76
 H       1.394357    -2.332755    -1.816144      24.96
 C      -0.175998    -1.440790    -0.957211      33.19
 O      -1.067725    -2.318778    -1.393891     255.49
 C      -1.421641    -2.464672    -2.810288     100.69
 H      -2.208775    -3.338841    -2.740005      25.55
 H      -1.839198    -1.525790    -3.066570      26.45
 H      -0.656332    -3.059183    -3.519592      25.15
 C      -0.730415    -0.193782    -0.518528      -7.88
 O      -2.127015    -0.133696    -0.399861      99.54
 C       0.144347     1.018756    -0.142687      53.78
 H      -0.229695     1.906309     0.315085      20.42
 C       2.034608    -0.456755    -0.856204      53.22
 C       3.517417    -0.752188    -0.924701      92.69
 H       3.543862    -1.268422    -2.087220      25.65
 O       4.286796     0.499666    -1.243914      84.47
 H       4.370519     1.037687    -0.502610      33.49
 C       4.108946    -1.359333     0.372864      82.65
 H       3.543057    -2.289233     0.698135      29.08
 O       5.593402    -1.613774     0.427838     139.47
 H       5.506962    -2.512613     0.079888      29.37
 C       3.783495    -0.342989     1.592301     115.79
 O       4.295243     1.015277     1.557277     142.03
 H       3.780029     1.507802     2.176684      30.77
 H       4.123229    -0.928783     2.411097      30.77
 H       2.657706    -0.114775     1.907809      26.21
55
name = lig-Water-frame_723
 C      -2.142103     3.301058     2.699339      45.01
 H      -2.934368     3.912922     2.028533      19.30
 C      -1.247308     1.092663     3.202554      71.19
 H      -1.486072     0.040060     2.913049      21.75
 C      -0.173398     1.511058     3.972636      21.49
 O       0.791732     0.759251     4.687439     183.83
 C       0.618279    -0.685114     4.600198     112.22
 H       0.948811    -1.286446     5.531125      25.83
 H       0.926757    -0.908379     3.611810      28.07
 H      -0.463498    -1.271403     4.579371      25.85
 C      -0.242667     2.991673     4.250559     -25.86
 O       0.968214     3.500598     5.113346     180.31
 H       0.803687     4.477364     5.346847      23.70
 C      -1.132748     3.855959     3.672204      45.16
 H      -0.993457     4.872619     3.832893      23.24
 C      -2.090669     2.002868     2.561271      36.93
 C      -3.121470     1.380253     1.470020      85.70
 H      -3.762762     2.153814     1.413487      27.99
 O      -3.800045     0.199569     1.994344     209.41
 H      -4.853938     0.146675     1.785039      22.45
 C      -2.773409     1.174472    -0.108506      88.81
 H      -2.202082     1.925020    -0.491480      27.43
 C      -4.087953     1.114045    -1.098561      83.75
 O      -4.996570     0.126663    -0.791941     217.70
 H      -4.435235    -0.741036    -0.441557      20.42
 H      -3.368304     1.016532    -2.173281      23.13
 H      -4.613481     2.094096    -1.454208      23.69
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 C       1.537794     0.748562    -0.261323      54.47
 H       2.235686     1.339169     0.061582      29.70
 C       1.149175    -1.521216    -1.298209      62.87
 H       1.487624    -2.437730    -1.934262      22.82
 C      -0.202573    -1.408421    -0.924920      20.77
 O      -1.073391    -2.341449    -1.510031     239.72
 C      -1.459553    -2.458258    -2.842116     109.34
 H      -2.265911    -3.094814    -2.624309      27.15
 H      -2.047363    -1.340478    -3.007834      22.40
 H      -0.565886    -3.139935    -3.162327      23.10
 C      -0.757600    -0.156863    -0.490010       4.70
 O      -2.097290    -0.098712    -0.369117     159.71
 C       0.213472     0.957692    -0.124319      49.74
 H      -0.429086     1.773555     0.323267      21.73
 C       1.982777    -0.500452    -0.775098      25.19
 C       3.589224    -0.758134    -0.933372      99.60
 H       3.599905    -1.367583    -1.740358      30.88
 O       4.314436     0.495487    -1.280988     -10.73
 H       4.165557     1.318154    -0.428797      25.80
 C       4.073009    -1.336496     0.418581      92.02
 H       3.458913    -2.215994     0.584619      29.62
 O       5.575821    -1.580603     0.454488     114.53
 H       5.392350    -2.603342     0.068113      24.70
 C       3.757326    -0.374540     1.575566     108.24
 O       4.310434     1.002861     1.541667     116.92
 H       3.888560     1.500122     2.326905      27.09
 H       4.289612    -1.018391     2.398437      27.94
 H       2.714147    -0.202669     1.847272      27.40
55
name = lig-Water-frame_724
 C      -2.120264     3.322607     2.767178      45.47
 H      -2.764126     4.075663     2.474150      25.87
 C      -1.285025     1.087239     3.212985      74.01
 H      -1.426248     0.017935     3.081151      25.78
 C      -0.192703     1.563343     3.941010       1.93
 O       0.776761     0.783671     4.692471     168.17
 C       0.599155    -0.688482     4.595410     118.82
 H       1.081955    -1.114031     5.453818      28.31
 H       0.970903    -1.037074     3.526692      28.06
 H      -0.388399    -1.031038     4.718235      29.10
 C      -0.202688     3.006423     4.250491     -21.11
 O       0.982360     3.480140     5.099156     141.66
 H       0.830892     4.482099     5.381231      22.22
 C      -1.158393     3.789431     3.620567      56.98
 H      -1.011746     4.887522     3.922858      23.34
 C      -2.089484     1.930651     2.522313      30.15
 C      -3.115947     1.342306     1.460010      85.55
 H      -3.811225     2.340236     1.197743      26.09
 O      -3.741998     0.232534     1.995972     229.92
 H      -4.672448     0.265311     1.794729      25.57
 C      -2.823288     1.130428    -0.159345      89.39
 H      -2.231947     2.106905    -0.544748      26.39
 C      -4.017924     1.119921    -1.169585     102.15
 O      -5.019273     0.155851    -0.756714     168.65
 H      -4.622848    -0.733275    -0.659137      27.80
 H      -3.566945     0.663968    -1.942522      28.68
 H      -4.709801     1.994514    -1.091424      25.80
 C       1.540118     0.800328    -0.306249      29.85
 H       2.594615     1.479426    -0.118266      27.94
 C       1.160625    -1.516960    -1.280914      46.32
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 H       1.595314    -2.327384    -1.821272      25.68
 C      -0.249705    -1.352110    -0.972120      18.61
 O      -1.085378    -2.373625    -1.525924     235.80
 C      -1.530607    -2.435208    -2.847747     115.26
 H      -2.531147    -3.071345    -2.854017      26.05
 H      -1.728187    -1.570317    -3.478298      28.52
 H      -0.599099    -2.848909    -3.463733      26.13
 C      -0.703033    -0.102567    -0.442981      30.83
 O      -2.089265    -0.064991    -0.335569     142.37
 C       0.154559     0.855007    -0.103755      74.68
 H      -0.217428     1.776931     0.298714      28.30
 C       2.002855    -0.561860    -0.733850      -7.40
 C       3.610332    -0.702405    -0.921316      97.12
 H       3.941012    -1.741214    -1.641640      25.67
 O       4.338936     0.503576    -1.309134      95.10
 H       4.059275     1.062366    -0.673990      38.70
 C       4.045638    -1.247533     0.448481      89.45
 H       3.477308    -2.244680     0.554070      29.64
 O       5.498388    -1.598767     0.471859     109.32
 H       5.742402    -2.393950     0.019110      29.57
 C       3.768327    -0.418769     1.618184     110.63
 O       4.327853     0.980489     1.519928      93.52
 H       4.003106     1.492978     2.339078      25.19
 H       4.313637    -0.798303     2.468321      32.80
 H       2.532878    -0.534733     1.725435      28.60
55
name = lig-Water-frame_725
 C      -2.096330     3.333150     2.835109      33.79
 H      -2.834338     4.199532     2.605176      22.74
 C      -1.270510     1.035212     3.228961      41.56
 H      -1.303291    -0.045270     3.196230      26.38
 C      -0.194800     1.645575     3.979325      23.16
 O       0.735207     0.805831     4.678376     192.17
 C       0.588920    -0.675455     4.578006     109.83
 H       1.435200    -0.928090     5.329650      26.69
 H       1.049778    -1.222472     3.708492      29.63
 H      -0.568624    -0.752346     4.796676      25.72
 C      -0.082821     2.976224     4.269142      17.29
 O       0.946886     3.445889     5.055826     167.40
 H       0.931431     4.347499     5.407425      24.86
 C      -1.123511     3.787313     3.629968      51.92
 H      -1.246286     4.856601     3.895565      26.63
 C      -2.157870     1.873655     2.411551     -13.77
 C      -3.132622     1.400444     1.400657     106.16
 H      -3.843495     2.127576     1.336830      28.96
 O      -3.700888     0.244320     2.010563     211.11
 H      -4.679865     0.261888     1.791233      23.89
 C      -2.836399     1.154011    -0.173763     103.42
 H      -2.300682     2.002611    -0.422230      29.51
 C      -3.962378     1.097140    -1.165207      88.21
 O      -5.067348     0.169074    -0.720511     119.66
 H      -4.700842    -0.800203    -0.804592      25.94
 H      -3.684552     0.574577    -2.271940      24.80
 H      -4.463729     2.072510    -1.064398      27.52
 C       1.605912     0.752960    -0.364097      33.87
 H       2.074630     1.641957    -0.185756      33.92
 C       1.136338    -1.494005    -1.216899      53.27
 H       1.594391    -2.371804    -1.710959      27.24
 C      -0.257050    -1.315982    -1.092801      24.98
 O      -1.110449    -2.386137    -1.475229     208.17
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 C      -1.596794    -2.434206    -2.916154     107.33
 H      -2.406379    -3.031998    -3.140130      29.31
 H      -1.552654    -1.417885    -3.740258      25.82
 H      -0.810170    -2.814978    -3.795025      25.68
 C      -0.702239    -0.144046    -0.425571      20.24
 O      -2.082108    -0.048699    -0.312340     135.67
 C       0.149482     0.864920    -0.053841      57.88
 H      -0.083147     1.869193     0.304163      27.92
 C       2.084073    -0.539546    -0.741608      -4.46
 C       3.610961    -0.705660    -0.913601     125.22
 H       4.015414    -1.399119    -1.460988      30.56
 O       4.358234     0.481941    -1.365002      70.61
 H       4.049926     1.200384    -0.587927      29.73
 C       4.061682    -1.204362     0.447243     108.70
 H       3.531176    -2.107164     0.593140      33.31
 O       5.426953    -1.609738     0.503618     108.49
 H       5.779489    -2.289210    -0.185475      23.41
 C       3.768074    -0.432312     1.706553     134.13
 O       4.325448     0.946402     1.496140     108.04
 H       4.032607     1.478336     2.218818      28.08
 H       4.221884    -0.779524     2.682275      32.94
 H       2.728499    -0.564822     1.769408      32.10
55
name = lig-Water-frame_726
 C      -2.114429     3.281012     2.845322      39.01
 H      -2.910982     3.969714     2.492363      22.78
 C      -1.249743     1.029690     3.205588      35.49
 H      -1.185534    -0.092615     3.167983      23.51
 C      -0.204194     1.640568     4.033788      19.90
 O       0.702684     0.829498     4.641861     208.93
 C       0.596688    -0.629481     4.599019     119.73
 H       1.356219    -0.878084     5.289412      29.06
 H       0.884311    -1.204304     3.636879      29.04
 H      -0.430825    -0.896777     4.945799      28.23
 C      -0.012438     3.003073     4.253956      30.66
 O       0.930828     3.401079     5.021060     122.82
 H       0.869042     4.388851     5.393372      26.66
 C      -1.029891     3.816409     3.711047      54.04
 H      -1.283099     4.853706     3.940916      23.48
 C      -2.168283     1.882759     2.359391     -29.13
 C      -3.185026     1.452605     1.331591      87.94
 H      -4.133912     2.221414     1.474025      22.78
 O      -3.689205     0.233011     2.025121     174.88
 H      -4.708141     0.069360     1.814373      21.35
 C      -2.801717     1.182121    -0.150816      78.52
 H      -2.109948     2.101560    -0.452948      24.69
 C      -3.961243     1.032103    -1.160020     112.60
 O      -5.111932     0.182495    -0.688381     182.04
 H      -4.692659    -0.782832    -0.810804      23.63
 H      -3.745094     1.044727    -2.169827      28.07
 H      -4.174689     2.164860    -1.354947      26.68
 C       1.583311     0.679669    -0.395470      51.47
 H       1.878866     1.839334    -0.202489      26.05
 C       1.133010    -1.474776    -1.148511      42.94
 H       1.436470    -2.499688    -1.550230      24.79
 C      -0.233222    -1.301022    -1.215872      14.97
 O      -1.156494    -2.386703    -1.456605     132.46
 C      -1.592497    -2.391148    -3.059855      86.18
 H      -2.575709    -3.055601    -3.165190      25.31
 H      -1.693639    -1.323254    -3.177872      27.06
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 H      -0.911830    -3.121913    -3.633086      24.90
 C      -0.757708    -0.193862    -0.425608      -6.57
 O      -2.072319    -0.062496    -0.294194     106.50
 C       0.244080     0.908841    -0.024623      45.64
 H      -0.166899     1.892362     0.352041      24.13
 C       2.164052    -0.471434    -0.805418      59.29
 C       3.606615    -0.682211    -0.872332      86.20
 H       4.004271    -1.494786    -1.833863      24.65
 O       4.350894     0.473169    -1.407797      70.81
 H       4.391156     1.311524    -0.669345      24.52
 C       4.096918    -1.213589     0.476211     104.45
 H       3.369555    -2.133642     0.619583      29.50
 O       5.414403    -1.621585     0.537420     151.32
 H       5.379353    -2.156053    -0.334359      26.64
 C       3.804348    -0.409286     1.797586     111.54
 O       4.306241     0.902907     1.476385     120.79
 H       3.932688     1.603508     2.147545      25.30
 H       4.131928    -0.959619     2.744299      29.70
 H       2.550472    -0.276672     1.958912      27.86
55
name = lig-Water-frame_727
 C      -2.102776     3.200514     2.842793      58.30
 H      -2.892640     3.806675     2.379177      24.61
 C      -1.220570     1.069393     3.147782      61.58
 H      -1.190309     0.027894     2.997240      26.24
 C      -0.264218     1.568669     4.034585      15.34
 O       0.700552     0.837568     4.612275     180.46
 C       0.612674    -0.582583     4.630887     117.77
 H       1.322745    -0.995375     5.419454      26.91
 H       0.538731    -0.921937     3.528503      28.04
 H      -0.326901    -1.132324     5.087281      26.80
 C      -0.054779     3.037680     4.185492      15.19
 O       0.988516     3.395808     5.044622     179.27
 H       0.781682     4.305236     5.288494      30.90
 C      -1.011131     3.835332     3.752474      73.28
 H      -1.071677     4.946998     4.111708      20.33
 C      -2.106376     1.938524     2.391306       2.46
 C      -3.293344     1.484064     1.324623      86.15
 H      -4.040896     2.205821     1.310927      27.01
 O      -3.701955     0.205058     2.024273     230.93
 H      -4.584355    -0.028312     1.854462      27.23
 C      -2.746326     1.222035    -0.135393      82.78
 H      -2.100403     1.962114    -0.534516      26.82
 C      -3.990696     1.045688    -1.131358      96.81
 O      -5.120364     0.206849    -0.679423     244.40
 H      -4.734307    -0.668655    -0.635351      29.31
 H      -3.567937     0.955471    -2.282922      24.80
 H      -4.341297     2.062421    -1.274956      27.53
 C       1.527411     0.738261    -0.377953      49.66
 H       2.286710     1.549116    -0.341213      27.68
 C       1.192371    -1.481812    -1.110592      40.55
 H       1.388401    -2.481152    -1.357606      25.07
 C      -0.248408    -1.280948    -1.265928      -2.66
 O      -1.199544    -2.379324    -1.488128     141.40
 C      -1.603672    -2.395636    -3.123357      66.36
 H      -2.589926    -2.725619    -2.981044      26.08
 H      -1.828774    -1.170137    -3.011277      22.21
 H      -0.760439    -3.134272    -3.521893      22.18
 C      -0.737075    -0.171130    -0.437139       2.36
 O      -2.079876    -0.096616    -0.268498     141.35
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 C       0.254893     0.868070    -0.039772      67.49
 H      -0.113635     1.751333     0.379272      25.88
 C       2.160788    -0.451006    -0.908271      44.28
 C       3.657401    -0.674367    -0.882973     116.20
 H       3.667448    -1.355245    -1.597376      31.41
 O       4.354908     0.487760    -1.441486     152.50
 H       4.553676     1.080031    -0.844480      31.94
 C       4.054044    -1.253479     0.572291     108.09
 H       3.403219    -2.072840     0.610714      31.93
 O       5.434362    -1.649559     0.541376     177.93
 H       5.384889    -2.167099    -0.241741      31.45
 C       3.778006    -0.375509     1.854059     141.37
 O       4.294541     0.886755     1.486727     135.44
 H       3.814079     1.620844     1.951446      27.34
 H       4.223624    -0.979499     2.674120      31.19
 H       2.809177    -0.147535     2.046830      30.76
55
name = lig-Water-frame_728
 C      -2.062106     3.227900     2.865346      50.92
 H      -2.828027     3.925672     2.333589      23.71
 C      -1.189278     1.096633     3.066295      69.33
 H      -1.293477     0.012478     2.763815      23.37
 C      -0.324550     1.543984     3.994294      20.10
 O       0.717349     0.831628     4.616462     204.43
 C       0.594994    -0.571346     4.668293     117.82
 H       1.512683    -1.014660     5.150635      27.65
 H       0.532612    -0.834116     3.613532      29.52
 H      -0.322328    -1.005910     5.163029      27.52
 C      -0.091738     2.985579     4.157596      -2.33
 O       1.050122     3.398586     5.063612     135.17
 H       0.870904     4.361801     5.353075      29.41
 C      -1.096798     3.877830     3.732347      42.96
 H      -0.931827     4.839960     4.088994      16.02
 C      -2.059963     1.952628     2.425777      25.75
 C      -3.317234     1.459382     1.382781      61.53
 H      -4.139866     2.349634     1.178221      23.83
 O      -3.707819     0.193522     2.006088     222.13
 H      -4.730456    -0.043383     1.847648      24.41
 C      -2.748620     1.212621    -0.131255      79.41
 H      -2.059315     2.015435    -0.597348      24.22
 C      -4.000078     1.111447    -1.131449      78.20
 O      -5.102001     0.244062    -0.685043     190.66
 H      -4.702717    -0.722888    -0.390895      24.67
 H      -3.590914     0.524696    -1.914224      26.78
 H      -4.735787     2.022722    -1.050437      22.01
 C       1.585300     0.795410    -0.392222      41.48
 H       2.503329     1.440603    -0.294663      26.81
 C       1.230793    -1.500081    -1.124209      25.21
 H       1.598783    -2.606880    -1.252544      23.91
 C      -0.268330    -1.263175    -1.223864       0.02
 O      -1.215112    -2.351879    -1.548845     169.43
 C      -1.622470    -2.366023    -3.063172      84.39
 H      -2.679532    -2.729263    -3.002706      24.47
 H      -1.631302    -1.300231    -3.512110      26.13
 H      -0.693044    -2.824617    -3.636878      23.49
 C      -0.678053    -0.139704    -0.487122      21.60
 O      -2.089000    -0.122525    -0.228789     180.40
 C       0.166192     0.803922    -0.067397      59.46
 H      -0.099718     1.758640     0.515468      23.84
 C       2.075444    -0.430068    -0.979488      22.51
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 C       3.673974    -0.636928    -0.862342      70.83
 H       3.701136    -1.694114    -1.611386      26.21
 O       4.362771     0.474677    -1.494256      -3.03
 H       4.799238     1.081596    -0.554740      22.15
 C       3.980246    -1.269517     0.653360      84.73
 H       3.374669    -2.270761     0.697061      28.97
 O       5.461326    -1.680276     0.549271      82.92
 H       5.676271    -2.406185    -0.185961      24.16
 C       3.768582    -0.372569     1.859212     111.87
 O       4.308257     0.916124     1.507437     145.56
 H       3.689188     1.582108     1.832849      30.24
 H       4.452983    -0.793754     2.702716      28.74
 H       2.543569    -0.247090     2.220947      26.48
55
name = lig-Water-frame_729
 C      -2.052902     3.377761     2.869133      59.69
 H      -2.706849     4.042814     2.444665      24.80
 C      -1.180311     1.045651     2.953475      52.67
 H      -1.298295     0.028418     2.673306      24.27
 C      -0.288728     1.570687     3.978985      13.99
 O       0.726861     0.839438     4.639067     171.92
 C       0.582467    -0.587634     4.688038     111.81
 H       1.632796    -0.915037     4.868937      26.82
 H       0.582351    -1.105110     3.591747      26.92
 H      -0.381219    -0.792259     5.266272      25.52
 C      -0.118092     2.929502     4.197464       5.47
 O       1.070268     3.395423     5.045230     108.33
 H       1.004835     4.334173     5.458031      29.91
 C      -1.157943     3.862936     3.704654      55.63
 H      -1.016962     5.021622     3.947143      18.24
 C      -2.092131     1.952612     2.421527      18.22
 C      -3.260777     1.436966     1.453134      90.57
 H      -4.034359     2.161954     1.353893      27.11
 O      -3.735696     0.192751     1.975122     257.00
 H      -4.738377     0.136163     1.917482      26.72
 C      -2.794220     1.188620    -0.122760      78.82
 H      -2.134485     2.019315    -0.433652      25.68
 C      -4.025231     1.160366    -1.084355      91.66
 O      -5.086800     0.251178    -0.661437     246.92
 H      -4.676438    -0.561127    -0.412969      30.22
 H      -3.639013     0.487863    -1.944987      25.37
 H      -4.569750     2.052734    -1.262173      25.63
 C       1.630198     0.798226    -0.442166      38.66
 H       2.340670     1.663000     0.007208      25.77
 C       1.186447    -1.550721    -1.185614      56.03
 H       1.721318    -2.408680    -1.311760      27.17
 C      -0.229476    -1.311783    -1.156569      16.42
 O      -1.208425    -2.291461    -1.625075     221.32
 C      -1.618390    -2.313438    -2.971126     102.24
 H      -2.517018    -2.938039    -3.229548      25.40
 H      -1.543936    -1.225437    -3.813933      23.30
 H      -0.821438    -2.807302    -3.712765      24.94
 C      -0.714098    -0.146540    -0.561464      11.68
 O      -2.079846    -0.125993    -0.187776     163.62
 C       0.175342     0.848646    -0.072873      50.79
 H      -0.235936     1.574544     0.565405      24.19
 C       2.028198    -0.386185    -0.996235      12.26
 C       3.608142    -0.681763    -0.866048      85.64
 H       4.038214    -1.460981    -1.331110      32.63
 O       4.394401     0.460247    -1.486822     120.37
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 H       4.819077     0.820640    -0.727524      28.95
 C       3.933165    -1.307143     0.654127      77.30
 H       3.412966    -2.206021     0.817361      30.51
 O       5.487704    -1.707553     0.570667      93.20
 H       5.633673    -2.519324     0.020469      27.38
 C       3.759357    -0.382952     1.881809     124.21
 O       4.319153     0.968692     1.530189     168.86
 H       3.562276     1.643118     1.770972      28.95
 H       4.396883    -0.621498     2.696686      29.75
 H       2.826904    -0.488895     2.186701      32.07
55
name = lig-Water-frame_730
 C      -2.101261     3.461820     2.804320      35.66
 H      -2.871449     4.306269     2.405434      16.80
 C      -1.171629     1.020791     2.875759      25.00
 H      -1.183912    -0.078755     2.652440      22.90
 C      -0.203790     1.570844     3.954311      -9.90
 O       0.727203     0.851277     4.648566     139.54
 C       0.584928    -0.621535     4.653066     111.23
 H       1.611751    -0.914787     5.032665      26.40
 H       0.369052    -1.175737     3.763338      29.08
 H      -0.231186    -0.812175     5.465343      24.58
 C      -0.146797     2.961252     4.282812       7.49
 O       1.052822     3.376127     4.997662      93.22
 H       0.893444     4.235912     5.414443      32.22
 C      -1.103544     3.860876     3.739717      55.45
 H      -1.196820     4.872297     3.783147      19.26
 C      -2.162011     1.992108     2.408395      -5.29
 C      -3.157307     1.404491     1.502016      96.50
 H      -4.074555     2.193174     1.580286      24.62
 O      -3.769419     0.189458     1.955322     251.81
 H      -4.750243     0.253895     2.004557      26.91
 C      -2.853010     1.177546    -0.071650      75.58
 H      -2.178082     2.010092    -0.326593      24.63
 C      -4.030675     1.140823    -1.050116      99.35
 O      -5.097724     0.267598    -0.618355     262.31
 H      -4.563051    -0.614037    -0.489378      26.26
 H      -3.649830     0.992939    -2.108679      25.25
 H      -4.203562     2.226264    -1.552415      24.13
 C       1.577247     0.835351    -0.443624      42.04
 H       2.050363     1.624448     0.012185      27.01
 C       1.130818    -1.536455    -1.260528      57.42
 H       1.735853    -2.462586    -1.608067      25.06
 C      -0.193951    -1.410753    -1.125129      23.04
 O      -1.191640    -2.219172    -1.671225     276.93
 C      -1.566098    -2.244817    -2.985429     121.90
 H      -2.397098    -2.923015    -3.153071      26.66
 H      -1.777237    -1.334433    -3.460608      29.13
 H      -0.872214    -3.018311    -3.561413      26.00
 C      -0.769167    -0.130064    -0.602743      -9.14
 O      -2.065349    -0.115645    -0.158414     115.96
 C       0.239129     0.898036    -0.109203      34.90
 H      -0.302848     1.578667     0.608134      22.46
 C       2.055895    -0.403670    -0.992406      33.62
 C       3.513895    -0.732597    -0.854507      67.08
 H       4.242086    -1.548967    -1.464457      25.00
 O       4.417519     0.417309    -1.453191      38.32
 H       4.932654     0.873640    -0.656619      26.22
 C       3.959035    -1.309438     0.624070      67.48
 H       3.316263    -2.256348     0.841970      28.41
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 O       5.486805    -1.726996     0.604472      90.68
 H       5.390346    -2.567553     0.114158      29.76
 C       3.821138    -0.384977     1.869850      93.39
 O       4.289930     1.019883     1.558036     164.68
 H       3.622026     1.690274     1.751678      30.84
 H       4.422583    -0.745676     2.847448      25.50
 H       2.592213    -0.537998     2.250480      25.36
55
name = lig-Water-frame_731
 C      -2.161260     3.463391     2.729215      48.67
 H      -2.810806     4.164097     2.425556      21.49
 C      -1.135909     1.081081     2.882962      49.70
 H      -1.101893     0.016598     2.625822      21.69
 C      -0.160281     1.555512     3.884390       1.17
 O       0.728305     0.840892     4.636942     168.23
 C       0.610749    -0.642808     4.673368     107.10
 H       1.474111    -1.028838     5.159951      25.52
 H       0.039123    -1.166301     3.729906      24.36
 H      -0.043169    -0.955998     5.517677      25.71
 C      -0.162568     3.008406     4.355709       1.95
 O       1.006359     3.353735     4.942671      75.02
 H       0.755228     4.272001     5.381555      26.60
 C      -1.061143     3.848045     3.748435     111.35
 H      -1.098788     5.014961     3.932272      23.34
 C      -2.171394     2.045267     2.420642      20.99
 C      -3.158844     1.401001     1.497844     104.78
 H      -3.921945     2.177233     1.574836      25.46
 O      -3.782837     0.165329     1.960199     227.00
 H      -4.846241     0.294053     2.071041      22.27
 C      -2.878373     1.189174     0.005930      75.82
 H      -2.177842     2.025442    -0.384594      24.58
 C      -4.007159     1.160639    -1.062754      95.63
 O      -5.104431     0.289645    -0.585652     235.70
 H      -4.629092    -0.643959    -0.625358      25.42
 H      -3.567838     1.003196    -2.105155      27.15
 H      -4.220981     2.199518    -1.150972      28.38
 C       1.500292     0.832575    -0.440344      25.36
 H       2.250254     1.768714    -0.025798      24.48
 C       1.185334    -1.495780    -1.345127      53.64
 H       1.415994    -2.377586    -1.956295      25.32
 C      -0.252104    -1.426462    -1.118290      15.22
 O      -1.178462    -2.173822    -1.655396     226.12
 C      -1.508396    -2.262277    -3.042514      66.17
 H      -2.542203    -2.749118    -2.846577      22.69
 H      -1.956890    -0.907706    -3.408114      21.65
 H      -0.661974    -2.939382    -3.558910      23.78
 C      -0.736646    -0.103984    -0.596332       2.54
 O      -2.060263    -0.103828    -0.140901     105.33
 C       0.190655     0.897251    -0.171286      50.15
 H      -0.072115     1.758639     0.488071      24.29
 C       2.077483    -0.456146    -0.973921      28.81
 C       3.526925    -0.800048    -0.854912      88.63
 H       3.628935    -1.548562    -1.571695      29.94
 O       4.434535     0.362215    -1.393760     -32.97
 H       4.873441     1.012149    -0.539830      24.40
 C       4.018275    -1.285588     0.608487      93.66
 H       3.373569    -2.141186     0.750516      29.57
 O       5.443514    -1.750224     0.628800     129.88
 H       5.283593    -2.628291     0.054376      27.41
 C       3.850349    -0.382279     1.879279     115.59
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 O       4.249922     1.039294     1.585803     149.09
 H       3.568307     1.700696     1.897450      29.30
 H       4.367689    -0.839603     2.636780      28.18
 H       2.909535    -0.286225     2.097874      31.55
55
name = lig-Water-frame_732
 C      -2.133154     3.389539     2.735046      34.48
 H      -2.946884     4.159345     2.301485      23.76
 C      -1.081082     1.205862     2.949714      81.04
 H      -1.138139     0.203541     2.550313      25.08
 C      -0.168533     1.573921     3.820371      19.22
 O       0.735091     0.798604     4.612443     202.92
 C       0.595774    -0.663511     4.711697      97.93
 H       1.658814    -1.205262     4.893284      24.33
 H       0.188610    -1.008538     3.877317      31.45
 H      -0.131718    -0.943635     5.608529      24.08
 C      -0.194063     2.970691     4.333594      13.31
 O       0.959531     3.371113     4.926893     128.70
 H       0.937597     4.257553     5.347121      19.33
 C      -1.097276     3.886367     3.706529      90.75
 H      -0.844058     4.825072     4.133223      21.98
 C      -2.120071     2.070985     2.435146      29.87
 C      -3.235544     1.414255     1.475515      79.54
 H      -4.063941     2.281563     1.366065      25.53
 O      -3.786405     0.140673     1.992031     252.14
 H      -4.733865     0.142817     1.995116      26.49
 C      -2.831234     1.207554     0.037855      88.36
 H      -2.231980     1.991885    -0.341320      27.82
 C      -3.975607     1.195742    -1.033424      73.92
 O      -5.099389     0.313236    -0.587790     212.09
 H      -4.826244    -0.581002    -0.607834      28.87
 H      -3.541746     0.721921    -1.962111      26.02
 H      -4.589298     2.198850    -0.711840      24.63
 C       1.527391     0.783580    -0.447482      47.24
 H       2.187459     1.466131    -0.273928      29.04
 C       1.197418    -1.453861    -1.437432      62.55
 H       1.341075    -2.276746    -2.152709      24.71
 C      -0.258699    -1.299323    -1.116061      11.66
 O      -1.191897    -2.180357    -1.619170     246.97
 C      -1.511266    -2.231017    -3.086651     108.64
 H      -2.445150    -2.666330    -2.986864      26.75
 H      -1.623606    -1.367924    -3.333736      32.71
 H      -0.608555    -2.537206    -3.753614      26.11
 C      -0.698090    -0.116393    -0.550419      27.08
 O      -2.064283    -0.091206    -0.132173     105.53
 C       0.095173     0.919742    -0.226159      65.92
 H      -0.060290     1.872982     0.226262      26.47
 C       2.066779    -0.461884    -0.920220       8.14
 C       3.589034    -0.820254    -0.854679     102.06
 H       3.290546    -1.699276    -1.671348      24.65
 O       4.454169     0.307051    -1.318409     125.17
 H       4.535722     0.772262    -0.604093      37.05
 C       4.074824    -1.247632     0.588934     107.23
 H       3.396737    -2.141949     0.779687      28.76
 O       5.376089    -1.795413     0.626988     158.38
 H       5.488523    -2.511202     0.017711      30.09
 C       3.882525    -0.346003     1.828922      96.94
 O       4.224839     1.043668     1.609668     116.49
 H       3.534632     1.578707     2.183906      26.37
 H       4.531234    -0.942824     2.678414      25.53
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 H       2.659633    -0.152365     2.113222      23.69
55
name = lig-Water-frame_733
 C      -2.088173     3.393765     2.794918      20.86
 H      -2.824942     3.934459     2.304480      23.57
 C      -1.093906     1.285107     2.956269      65.29
 H      -1.135270     0.250841     2.528710      25.65
 C      -0.131305     1.626252     3.871368      40.86
 O       0.748939     0.755148     4.575909     185.87
 C       0.592340    -0.684685     4.777406     116.13
 H       1.539516    -1.066812     4.606285      28.27
 H       0.197228    -1.102286     3.651563      25.50
 H      -0.088348    -0.845027     5.558085      27.13
 C      -0.246152     2.922269     4.221402      40.28
 O       0.939989     3.397983     4.942436     160.63
 H       0.994474     4.323846     5.326649      13.26
 C      -1.136167     3.885362     3.669915      58.96
 H      -0.894231     4.900038     4.092214      21.46
 C      -2.086144     2.039950     2.416792       2.83
 C      -3.324654     1.449455     1.480210      73.61
 H      -4.144812     2.164926     1.261759      26.25
 O      -3.753784     0.136782     2.033809     213.61
 H      -4.824668    -0.039845     1.870252      21.92
 C      -2.755840     1.200072     0.019767      79.21
 H      -2.093654     2.155944    -0.250465      24.36
 C      -3.981922     1.210428    -0.919515      95.67
 O      -5.103786     0.342990    -0.605226     236.68
 H      -4.858255    -0.701656    -0.520858      23.86
 H      -3.618615     0.890056    -1.896152      27.65
 H      -4.608385     2.077387    -0.920617      27.44
 C       1.517559     0.680203    -0.462360      50.45
 H       2.375209     1.625086    -0.330477      26.34
 C       1.120495    -1.394241    -1.501662      70.86
 H       1.535070    -2.218915    -2.193436      23.71
 C      -0.189326    -1.180515    -1.178694      15.65
 O      -1.212230    -2.211481    -1.582018     180.09
 C      -1.484879    -2.217554    -3.077697      72.06
 H      -2.421677    -2.930064    -3.430217      23.20
 H      -1.517933    -0.793425    -3.594437      23.23
 H      -0.666232    -2.512722    -3.843499      24.57
 C      -0.744659    -0.122463    -0.462621      23.96
 O      -2.076848    -0.081006    -0.131007     150.53
 C       0.119182     0.987040    -0.279990      61.41
 H      -0.386445     2.027942    -0.035342      22.16
 C       2.060589    -0.461299    -0.863084      26.01
 C       3.608624    -0.824726    -0.876414     103.98
 H       3.823738    -1.679749    -1.477317      29.75
 O       4.471977     0.225987    -1.276678      65.30
 H       4.269922     0.856779    -0.285644      26.05
 C       4.064537    -1.255994     0.554174     107.66
 H       3.358386    -2.048430     0.893621      29.73
 O       5.354872    -1.838490     0.621150     134.35
 H       5.553694    -2.479193    -0.129122      26.23
 C       3.869169    -0.313639     1.789744     134.57
 O       4.214436     1.048981     1.633743     180.66
 H       3.720652     1.576269     2.274348      28.19
 H       4.419679    -0.688112     2.550360      32.37
 H       2.933369    -0.505980     2.073101      31.27
55
name = lig-Water-frame_734
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 C      -2.078430     3.409352     2.833225      52.29
 H      -2.847857     4.081863     2.320931      19.63
 C      -1.119501     1.238041     2.917744      40.59
 H      -1.041993     0.208079     2.670448      28.65
 C      -0.105020     1.615588     3.950939      24.61
 O       0.775578     0.744572     4.536052     131.23
 C       0.559710    -0.689511     4.719070     110.50
 H       1.703234    -1.056582     4.734576      27.13
 H       0.085084    -1.151580     3.981099      31.76
 H      -0.065329    -0.945371     5.746213      26.29
 C      -0.216559     2.982219     4.150061      34.95
 O       0.925153     3.414076     4.960666     371.82
 H       0.752818     4.379899     5.304851      23.14
 C      -1.139615     3.875876     3.669355      10.49
 H      -1.225494     4.976749     3.802191      17.99
 C      -2.123303     2.030920     2.381398      -6.56
 C      -3.334189     1.447115     1.503110      75.46
 H      -4.256587     2.154626     1.423931      25.05
 O      -3.728225     0.152423     2.073439     233.39
 H      -4.643243    -0.063425     1.845306      25.30
 C      -2.712128     1.223652     0.011682      92.54
 H      -2.119943     2.014250    -0.185245      26.78
 C      -3.994323     1.193218    -0.836450     102.42
 O      -5.121276     0.342313    -0.610176     312.94
 H      -4.713893    -0.540713    -0.527163      27.47
 H      -3.682781     1.241570    -1.975544      24.83
 H      -4.382367     2.326431    -1.154494      24.41
 C       1.518679     0.712595    -0.440516      57.70
 H       2.101421     1.463533    -0.293901      28.35
 C       1.108319    -1.328635    -1.538898      54.95
 H       1.512293    -2.123206    -2.037400      26.19
 C      -0.200291    -1.148977    -1.274359       8.43
 O      -1.224523    -2.231345    -1.585057     222.60
 C      -1.469139    -2.124501    -3.097252     124.09
 H      -2.126839    -2.790085    -3.524876      29.22
 H      -1.615529    -1.273770    -3.404690      32.89
 H      -0.515703    -2.660556    -3.607446      25.92
 C      -0.775796    -0.070197    -0.377102       8.31
 O      -2.098714    -0.075936    -0.133148     150.13
 C       0.159921     1.046814    -0.333679      57.14
 H      -0.308077     1.931319    -0.255945      22.36
 C       2.072390    -0.549047    -0.875662      34.13
 C       3.609205    -0.839977    -0.868729      90.65
 H       4.221027    -1.724323    -1.471492      25.29
 O       4.488384     0.193026    -1.206660     131.42
 H       4.362976     0.936790    -0.617060      30.99
 C       4.002768    -1.291916     0.547451      89.68
 H       3.281237    -2.060456     0.863269      29.28
 O       5.382428    -1.879214     0.606425      69.30
 H       5.382033    -2.491230    -0.235585      28.36
 C       3.867108    -0.310015     1.735427     107.33
 O       4.220590     1.058739     1.628617     182.06
 H       3.778990     1.789125     2.275425      22.76
 H       4.569129    -0.664484     2.679862      27.73
 H       2.746288    -0.703448     2.132988      26.35
55
name = lig-Water-frame_735
 C      -2.154154     3.387795     2.790307      47.91
 H      -2.784741     4.276217     2.503233      19.83
 C      -1.102629     1.135305     2.918207      36.46
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 H      -1.053222     0.016904     2.731848      24.56
 C      -0.185872     1.577906     3.941876     -19.26
 O       0.812707     0.755924     4.501085     156.30
 C       0.559004    -0.693996     4.699949     125.32
 H       1.466779    -1.089262     4.950292      29.62
 H      -0.221117    -1.321684     3.960884      25.13
 H       0.180174    -0.891320     5.637738      30.10
 C      -0.075362     3.067182     4.166126      11.15
 O       0.895532     3.442836     4.972395     163.01
 H       0.665639     4.276725     5.401675      25.74
 C      -1.141455     3.901701     3.670928      51.96
 H      -1.296618     4.952763     3.729355      19.54
 C      -2.191091     2.048869     2.370994      28.85
 C      -3.273731     1.427580     1.537445      96.19
 H      -4.178468     2.122133     1.671105      27.84
 O      -3.682076     0.179337     2.112478     217.93
 H      -4.670507    -0.008137     1.881125      24.83
 C      -2.779463     1.230362     0.048778      79.21
 H      -2.008998     2.094732    -0.319051      24.65
 C      -4.005707     1.258729    -0.877698     105.22
 O      -5.125581     0.349689    -0.605526     277.27
 H      -4.655153    -0.554609    -0.567362      26.20
 H      -3.670989     1.114259    -1.901584      29.10
 H      -4.138007     2.323773    -0.787112      29.55
 C       1.530563     0.744082    -0.421758      31.46
 H       2.266344     1.731568    -0.122550      24.28
 C       1.149014    -1.295489    -1.559449      50.54
 H       1.393745    -2.357586    -2.066180      24.26
 C      -0.340077    -1.137936    -1.306380       0.10
 O      -1.225619    -2.216174    -1.624307     196.08
 C      -1.382472    -2.134431    -3.073116      81.30
 H      -2.305848    -2.832576    -3.376468      24.40
 H      -1.890855    -0.773949    -3.474137      22.72
 H      -0.365972    -2.492690    -3.386305      25.54
 C      -0.727307    -0.039065    -0.388215      21.98
 O      -2.120868    -0.068393    -0.128744     133.97
 C       0.169001     1.033002    -0.376407      54.09
 H      -0.045883     2.233305    -0.291286      22.75
 C       2.088154    -0.593715    -0.917558      29.32
 C       3.622863    -0.893572    -0.832471     104.03
 H       3.921376    -1.638344    -1.571503      29.25
 O       4.525863     0.208533    -1.176864      89.42
 H       4.440600     1.097933    -0.692120      28.35
 C       3.951030    -1.337958     0.582293      82.05
 H       3.265210    -2.253470     0.754473      28.71
 O       5.402189    -1.912390     0.564778      84.43
 H       5.322283    -2.587549    -0.084706      31.26
 C       3.849669    -0.354706     1.766284     123.27
 O       4.232882     1.082654     1.590269     237.64
 H       3.689301     1.718070     2.119624      28.63
 H       4.489286    -0.768780     2.426390      31.17
 H       2.882547    -0.309560     2.105790      30.09
55
name = lig-Water-frame_736
 C      -2.216363     3.378363     2.759421      52.03
 H      -2.905819     4.159219     2.502034      21.48
 C      -1.105227     1.057975     2.944180      57.20
 H      -1.216775     0.038064     2.687109      26.56
 C      -0.285437     1.582408     3.877761      -7.10
 O       0.841733     0.764429     4.463021     101.67
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 C       0.532981    -0.702657     4.687517     112.74
 H       1.566971    -1.315341     4.798214      27.55
 H      -0.085510    -1.173599     4.013193      28.95
 H       0.047888    -0.650511     5.825645      26.54
 C      -0.014829     3.092172     4.155643      -4.85
 O       0.905674     3.477195     5.005525     120.78
 H       0.776788     4.336615     5.689891      22.37
 C      -1.132028     3.894730     3.652607      36.61
 H      -1.089754     5.025665     3.949763      19.99
 C      -2.199742     2.029727     2.411916      37.88
 C      -3.206086     1.415047     1.574982     100.46
 H      -4.062117     2.149934     1.623689      29.02
 O      -3.638964     0.191707     2.154104     202.59
 H      -4.665740     0.071913     1.992643      24.62
 C      -2.861683     1.238075     0.079274      95.83
 H      -2.248632     1.951027    -0.290844      30.22
 C      -3.996801     1.336025    -0.934809      76.10
 O      -5.115148     0.373700    -0.597684     201.77
 H      -4.729211    -0.617824    -0.578523      24.91
 H      -3.603673     0.907464    -1.938211      25.96
 H      -4.398322     2.426254    -0.530385      25.51
 C       1.600140     0.771200    -0.416020      36.44
 H       2.241652     1.510867    -0.111430      28.21
 C       1.106733    -1.359493    -1.588183      39.37
 H       1.272679    -2.274340    -1.995262      26.08
 C      -0.414453    -1.118917    -1.275729       2.93
 O      -1.227403    -2.165873    -1.662724     235.11
 C      -1.359222    -2.122069    -3.055529     122.89
 H      -2.153934    -2.779633    -3.167549      28.52
 H      -1.686989    -1.112221    -3.355389      27.99
 H      -0.255121    -2.130614    -3.585861      25.22
 C      -0.723073    -0.060947    -0.498832      30.86
 O      -2.120680    -0.050161    -0.113438     130.58
 C       0.203487     1.058898    -0.393257      59.70
 H       0.120717     2.037869    -0.167820      27.00
 C       2.118615    -0.517723    -0.935363       3.34
 C       3.611159    -0.902115    -0.791647      93.76
 H       3.614883    -1.722884    -1.692493      25.94
 O       4.575166     0.230093    -1.183311      -8.19
 H       4.317877     1.159916    -0.506884      26.89
 C       3.926358    -1.414541     0.612789      85.88
 H       3.348615    -2.279525     0.794201      31.62
 O       5.397407    -1.929777     0.525816      40.32
 H       5.375684    -2.854938     0.006872      24.27
 C       3.830923    -0.366704     1.789545      93.30
 O       4.263058     1.077210     1.514888     167.23
 H       3.590114     1.594764     2.081799      27.73
 H       4.572920    -0.966003     2.563312      26.40
 H       2.752992    -0.081720     2.214893      26.39
55
name = lig-Water-frame_737
 C      -2.205536     3.384276     2.784347      36.00
 H      -3.193997     3.895674     2.339805      20.83
 C      -1.188049     1.058500     2.950146      75.91
 H      -1.325960    -0.002373     2.637891      26.94
 C      -0.262859     1.616526     3.848457     -32.96
 O       0.847187     0.765839     4.408896      96.67
 C       0.539414    -0.676908     4.755909     129.05
 H       1.376106    -1.233787     4.518214      30.88
 H      -0.157307    -1.118655     3.836806      27.58
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 H      -0.016016    -0.617750     5.577253      32.40
 C      -0.100294     3.065043     4.099333     -10.79
 O       0.961431     3.504386     5.063135     170.70
 H       0.815027     4.333557     5.662674      19.56
 C      -1.100798     3.884219     3.630142      48.76
 H      -0.979339     4.809909     4.084658      22.76
 C      -2.129607     1.979670     2.492618      21.64
 C      -3.191916     1.415124     1.587439      89.11
 H      -4.036379     2.219785     1.428601      29.48
 O      -3.618582     0.185120     2.206040     194.93
 H      -4.531634     0.049228     2.042735      28.14
 C      -2.914170     1.217765     0.090542      90.11
 H      -2.213173     2.166217    -0.221188      26.52
 C      -4.013647     1.373097    -0.943066     105.73
 O      -5.107245     0.401194    -0.594034     254.63
 H      -4.745339    -0.459002    -0.564456      31.26
 H      -3.637941     1.244200    -1.917225      30.26
 H      -4.717781     2.215985    -0.920926      26.73
 C       1.643059     0.742419    -0.445139      48.37
 H       2.443955     1.561743    -0.050440      25.55
 C       1.025016    -1.377719    -1.545202      33.02
 H       1.326171    -2.419282    -2.044795      25.21
 C      -0.331408    -1.148052    -1.258733      24.57
 O      -1.233087    -2.107313    -1.666653     205.98
 C      -1.314110    -2.122624    -3.056393      97.62
 H      -2.037635    -3.005426    -3.367063      26.76
 H      -1.783847    -0.859104    -3.472300      24.62
 H      -0.437962    -2.134828    -3.759005      27.06
 C      -0.790710    -0.008247    -0.615452      14.11
 O      -2.102968    -0.027973    -0.096957     136.51
 C       0.279806     1.038860    -0.387717      46.82
 H      -0.112270     2.081307     0.112110      25.26
 C       2.097620    -0.419664    -0.961678      -1.36
 C       3.575959    -0.875803    -0.797069      91.70
 H       3.636530    -1.719011    -1.527896      28.77
 O       4.595169     0.249870    -1.178943     128.53
 H       4.362256     0.737687    -0.521248      35.55
 C       3.945129    -1.474381     0.617770      83.00
 H       3.254520    -2.374331     0.987607      29.84
 O       5.374299    -1.954657     0.491521      85.40
 H       5.415811    -2.869533     0.101501      25.96
 C       3.830082    -0.375253     1.828352     110.03
 O       4.294453     1.031060     1.428542     173.30
 H       3.747031     1.639021     2.070094      27.43
 H       4.351068    -0.715001     2.643464      32.00
 H       2.811834    -0.352491     2.220644      32.51
55
name = lig-Water-frame_738
 C      -2.164003     3.365406     2.828929      80.31
 H      -3.004815     3.725335     2.416934      29.21
 C      -1.248858     1.085114     2.986233      69.15
 H      -1.275063     0.046286     2.699131      30.81
 C      -0.150090     1.622092     3.840200      17.08
 O       0.833945     0.775532     4.349961     140.88
 C       0.507039    -0.612480     4.727927     121.23
 H       1.502086    -1.213483     4.571133      28.05
 H      -0.178801    -0.948066     3.964493      28.30
 H      -0.141486    -0.819783     5.782480      27.17
 C      -0.163566     2.989620     4.098870       6.61
 O       1.003607     3.466496     5.060683     164.01
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 H       0.649458     4.406115     5.511289      15.80
 C      -1.109377     3.883632     3.586602      58.20
 H      -1.091035     4.913032     4.140076      27.09
 C      -2.095789     1.971929     2.535926      16.43
 C      -3.224101     1.426741     1.580461      76.78
 H      -4.041993     2.169860     1.511575      30.65
 O      -3.610488     0.176198     2.263571     124.21
 H      -4.619979    -0.108537     1.973096      18.66
 C      -2.880052     1.256682     0.075621      98.21
 H      -2.299421     2.102573    -0.016728      29.91
 C      -4.085017     1.359853    -0.931615     100.66
 O      -5.110731     0.433498    -0.602726     231.88
 H      -4.603751    -0.538411    -0.548048      25.09
 H      -3.640834     1.545689    -2.033240      25.04
 H      -4.721699     2.349661    -1.196185      25.15
 C       1.671224     0.773668    -0.467905      57.09
 H       2.428678     1.476205    -0.035610      31.23
 C       1.035335    -1.371275    -1.460810      76.07
 H       1.356126    -2.247482    -1.947779      29.87
 C      -0.226154    -1.186739    -1.251754       2.56
 O      -1.241366    -2.069142    -1.667004     193.56
 C      -1.333776    -2.110559    -3.107898      90.02
 H      -1.827950    -2.984628    -3.538312      27.09
 H      -1.930897    -0.912815    -3.536802      25.12
 H      -0.310395    -2.293758    -3.752737      26.59
 C      -0.813664     0.118444    -0.704473     -17.10
 O      -2.081160     0.001543    -0.095266     142.50
 C       0.270906     1.021531    -0.345686      47.91
 H      -0.184475     1.755968     0.248723      30.16
 C       2.050801    -0.420338    -1.026592      23.71
 C       3.537763    -0.841558    -0.821464      78.16
 H       3.861565    -1.760767    -1.516648      29.55
 O       4.583210     0.216710    -1.189951       1.82
 H       4.510292     0.799327    -0.094493      20.78
 C       3.971975    -1.501886     0.637798      94.10
 H       3.312298    -2.225092     0.953187      33.95
 O       5.342686    -1.975509     0.474716     101.28
 H       5.356439    -2.832838    -0.017794      22.91
 C       3.845194    -0.389600     1.826500      99.61
 O       4.310025     0.960084     1.358959     104.46
 H       4.006233     1.672213     1.948077      27.76
 H       4.430467    -0.550628     2.874446      27.98
 H       2.706741    -0.529816     2.103005      31.54
55
name = lig-Water-frame_739
 C      -2.099451     3.313197     2.871235      52.32
 H      -2.989974     4.063591     2.465565      25.16
 C      -1.184170     1.097335     3.088024      55.57
 H      -1.216742     0.063159     2.767428      27.58
 C      -0.080584     1.581524     3.804520      29.19
 O       0.834874     0.785487     4.314100     228.00
 C       0.460388    -0.558352     4.699378     124.50
 H       1.396810    -1.042834     4.855061      28.41
 H      -0.292213    -1.005016     3.945544      26.63
 H       0.170102    -0.769555     5.643889      29.80
 C      -0.131958     2.936412     4.169529      -6.86
 O       0.993281     3.396315     4.998691     169.84
 H       0.721201     4.216230     5.438961      22.59
 C      -1.126289     3.912629     3.582345      59.53
 H      -1.285329     4.884158     3.929609      31.79
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 C      -2.163464     2.004126     2.499809      14.39
 C      -3.261415     1.421973     1.595972      73.37
 H      -4.197249     2.142295     1.767420      26.89
 O      -3.640779     0.165802     2.303223     198.09
 H      -4.473133    -0.171373     1.971270      23.66
 C      -2.848011     1.313473     0.070951      81.06
 H      -2.133198     2.247306    -0.098894      25.39
 C      -4.149248     1.390912    -0.959200      99.36
 O      -5.109650     0.428079    -0.621358     278.79
 H      -4.696397    -0.423114    -0.601759      29.81
 H      -3.706653     1.229306    -1.921213      29.25
 H      -4.425317     2.476868    -0.878204      27.74
 C       1.645639     0.821093    -0.494036      51.15
 H       2.386126     1.508073    -0.018406      29.78
 C       1.160609    -1.368712    -1.382664      60.67
 H       1.470642    -2.319189    -1.914144      26.32
 C      -0.279469    -1.143769    -1.229399      -5.82
 O      -1.244259    -2.054217    -1.689864     185.22
 C      -1.335299    -2.092628    -3.181883      96.58
 H      -1.947759    -2.995796    -3.458993      26.58
 H      -2.014003    -1.275925    -3.596098      27.32
 H      -0.263171    -2.165522    -3.496989      27.34
 C      -0.741772     0.178617    -0.778490       6.52
 O      -2.057907     0.053218    -0.115305     116.90
 C       0.203099     0.997068    -0.286726      40.60
 H      -0.078155     1.841236     0.467131      25.52
 C       2.051195    -0.454048    -1.078455      25.87
 C       3.535521    -0.832280    -0.863848      80.71
 H       3.956748    -1.663142    -1.518592      27.83
 O       4.532581     0.191921    -1.141823     110.15
 H       4.836177     0.627924    -0.458504      34.98
 C       4.007536    -1.448747     0.653266      87.00
 H       3.226557    -2.344046     0.879223      28.69
 O       5.313962    -1.998153     0.473477     114.22
 H       5.289301    -2.759228    -0.257806      21.50
 C       3.871065    -0.425611     1.829873     114.09
 O       4.320178     0.876056     1.293075     178.25
 H       4.075862     1.677841     1.903853      26.50
 H       4.426840    -0.557387     2.725222      28.70
 H       2.752090    -0.379449     1.878228      30.78
55
name = lig-Water-frame_740
 C      -2.121167     3.323727     2.854976      47.19
 H      -2.688893     4.108100     2.619864      26.67
 C      -1.141201     1.124036     3.134457      52.74
 H      -1.185814     0.058435     2.842047      27.16
 C      -0.084844     1.579837     3.765434      26.92
 O       0.879490     0.771161     4.308266     223.36
 C       0.438581    -0.521820     4.663263     108.06
 H       1.416801    -1.069850     4.789628      26.37
 H      -0.215622    -1.237528     3.976743      25.48
 H       0.073980    -0.407150     5.848200      24.12
 C      -0.074087     2.972089     4.241696      -4.54
 O       0.964238     3.299972     4.912242      98.43
 H       0.807791     4.191610     5.490546      21.16
 C      -1.069592     3.881235     3.647313      49.39
 H      -1.304078     4.983434     3.872295      29.22
 C      -2.210502     1.972468     2.471516       5.83
 C      -3.314819     1.419701     1.649091      88.29
 H      -4.175197     2.036790     1.749914      27.82
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 O      -3.664298     0.157906     2.322460     206.19
 H      -4.540687    -0.176012     1.963730      21.49
 C      -2.827602     1.382000     0.063360      81.34
 H      -2.191896     2.185665    -0.272013      27.13
 C      -4.117814     1.430844    -0.953705      78.80
 O      -5.144143     0.428528    -0.634736     206.21
 H      -4.702351    -0.505107    -0.671642      26.56
 H      -3.788311     0.917560    -1.953549      24.48
 H      -4.431216     2.479871    -0.608502      26.23
 C       1.563616     0.834798    -0.532139      40.11
 H       2.343063     1.596770     0.001443      27.31
 C       1.187281    -1.431334    -1.351284      34.25
 H       1.535958    -2.439125    -1.755778      23.89
 C      -0.333426    -1.076468    -1.247175       3.81
 O      -1.246112    -2.039642    -1.718623     152.37
 C      -1.333122    -2.136779    -3.211435      39.62
 H      -1.945161    -3.079865    -3.274433      22.93
 H      -2.192201    -1.027042    -3.810958      22.50
 H      -0.150096    -1.911707    -3.493099      23.99
 C      -0.706693     0.134504    -0.805821      22.68
 O      -2.034556     0.128843    -0.156783     106.57
 C       0.214503     1.042174    -0.203167      45.43
 H       0.083435     1.899973     0.503185      24.46
 C       2.140268    -0.395721    -1.059026       2.13
 C       3.580720    -0.829168    -0.863428     100.19
 H       3.801209    -1.712086    -1.641822      26.60
 O       4.479762     0.168707    -1.154134      80.69
 H       5.044530     0.626209    -0.315591      23.12
 C       3.985704    -1.413693     0.641435     115.59
 H       3.372662    -2.204422     0.785991      30.90
 O       5.303153    -2.012331     0.470293     160.14
 H       5.265754    -2.654011    -0.218800      28.80
 C       3.886429    -0.443011     1.773281     115.02
 O       4.341553     0.816545     1.241274     206.82
 H       3.994670     1.453016     1.887431      28.65
 H       4.442510    -0.813598     2.764913      25.81
 H       2.783174    -0.236006     1.949126      27.86
55
name = lig-Water-frame_741
 C      -2.117740     3.338561     2.843482      35.62
 H      -2.868004     4.220222     2.465810      24.49
 C      -1.205110     1.131375     3.067722      48.69
 H      -1.165139     0.075647     2.924918      31.29
 C      -0.082748     1.652235     3.785600      11.22
 O       0.938845     0.759734     4.284543     201.21
 C       0.455349    -0.532176     4.716701     115.03
 H       1.344039    -1.178268     4.683273      28.28
 H      -0.144576    -1.157291     4.027846      29.47
 H      -0.128253    -0.217255     5.493510      29.27
 C      -0.101738     3.003568     4.208850      22.54
 O       1.002460     3.251042     4.897866     187.41
 H       0.887590     4.114469     5.356102      21.53
 C      -1.009798     3.813951     3.734546      53.16
 H      -0.993650     4.863698     4.004778      30.08
 C      -2.195250     1.947193     2.510078     -16.81
 C      -3.342560     1.400333     1.689371      59.80
 H      -4.306183     2.141641     1.573512      23.54
 O      -3.685647     0.148507     2.315137     181.84
 H      -4.698183    -0.109944     2.058236      17.01
 C      -2.837934     1.400663     0.038776      74.02
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 H      -2.238847     2.333817    -0.278978      25.84
 C      -4.030231     1.416717    -0.911076      97.57
 O      -5.195363     0.429917    -0.631547     221.92
 H      -4.710458    -0.506032    -0.660331      25.29
 H      -3.818448     1.323987    -1.969219      27.32
 H      -4.700816     2.374367    -0.815347      25.28
 C       1.533286     0.849080    -0.544828      68.68
 H       2.177997     1.550030    -0.157242      31.05
 C       1.148817    -1.450309    -1.329654      28.13
 H       1.449666    -2.452953    -1.567856      25.35
 C      -0.284288    -1.093269    -1.332292       7.92
 O      -1.253885    -2.013176    -1.749349     249.52
 C      -1.353325    -2.113452    -3.212476     111.47
 H      -1.738198    -3.127049    -3.376666      26.80
 H      -1.798865    -1.444426    -3.602532      33.59
 H      -0.391159    -1.972390    -3.733794      29.22
 C      -0.737586     0.133622    -0.718724       5.55
 O      -2.022941     0.204101    -0.213743     146.49
 C       0.269413     1.088908    -0.160901      47.53
 H      -0.018068     1.931892     0.453984      26.68
 C       2.171869    -0.351518    -1.006879      -9.70
 C       3.631894    -0.853954    -0.829130     121.17
 H       3.513026    -1.682323    -1.581276      26.28
 O       4.480878     0.194089    -1.212052     100.70
 H       4.849074     0.380650    -0.210308      25.34
 C       3.943564    -1.410780     0.562437     113.42
 H       3.200278    -2.318322     0.836971      28.16
 O       5.313515    -1.987552     0.484219     132.46
 H       5.244070    -2.814501    -0.146457      24.64
 C       3.890060    -0.458874     1.714858     123.17
 O       4.380575     0.786988     1.225267     231.06
 H       3.951930     1.419363     1.834509      28.55
 H       4.358740    -0.997188     2.557918      28.62
 H       2.849789    -0.283704     2.199936      28.37
55
name = lig-Water-frame_742
 C      -2.087916     3.384137     2.855855      71.49
 H      -2.860857     3.883032     2.379998      27.43
 C      -1.228585     1.128560     3.004730      40.94
 H      -1.235900     0.029947     2.868608      24.34
 C      -0.114507     1.658367     3.803123      14.21
 O       0.986344     0.778289     4.226661     185.69
 C       0.486019    -0.553612     4.755921      78.00
 H       1.323064    -1.233047     4.993096      27.63
 H      -0.230326    -0.922497     3.830583      25.13
 H      -0.374222    -0.369157     5.583247      24.54
 C      -0.081678     2.934651     4.152891      31.81
 O       1.090501     3.249440     4.932118      93.61
 H       0.979602     4.177311     5.298108      28.72
 C      -1.070604     3.809379     3.754429      68.70
 H      -0.733573     4.799153     4.166935      20.33
 C      -2.194552     1.985179     2.564909       9.97
 C      -3.361888     1.401481     1.681278      80.58
 H      -4.139458     2.058927     1.599296      31.63
 O      -3.727483     0.140437     2.286377     216.47
 H      -4.655428    -0.038815     2.232879      22.76
 C      -2.849807     1.405098     0.025720      75.18
 H      -2.367600     2.418463    -0.022234      27.73
 C      -4.022841     1.400610    -0.878119     104.87
 O      -5.212468     0.428297    -0.627715     236.47
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 H      -4.855983    -0.435151    -0.542472      29.46
 H      -3.681000     1.687135    -1.987997      25.70
 H      -4.657268     2.297799    -0.963496      26.75
 C       1.599972     0.854303    -0.539277      52.00
 H       2.382024     1.812749    -0.275967      27.07
 C       1.111330    -1.377867    -1.302657      55.05
 H       1.353533    -2.529743    -1.462106      26.13
 C      -0.204558    -1.111114    -1.404583       3.54
 O      -1.255164    -1.982616    -1.783823     202.56
 C      -1.324161    -2.152875    -3.167006      79.83
 H      -1.630550    -3.222569    -3.590187      23.95
 H      -2.227052    -1.053897    -3.734976      22.76
 H      -0.377912    -2.183845    -3.955264      24.56
 C      -0.729442     0.169829    -0.572839       2.60
 O      -2.039115     0.257298    -0.278561     160.32
 C       0.240284     1.081801    -0.174906      60.03
 H      -0.187682     2.054261     0.358720      26.84
 C       2.092364    -0.386292    -0.946968      42.18
 C       3.596170    -0.869548    -0.826474     110.39
 H       3.638865    -1.761785    -1.552581      28.80
 O       4.515973     0.220320    -1.275347     135.85
 H       4.775897     0.557330    -0.404742      28.60
 C       3.880404    -1.473917     0.478883     115.17
 H       3.192618    -2.191235     0.759134      32.13
 O       5.322480    -1.956700     0.491943     136.49
 H       5.314599    -2.922423     0.157169      26.30
 C       3.862970    -0.495223     1.676364     107.99
 O       4.432160     0.781398     1.251094     243.36
 H       3.996814     1.623156     1.684590      29.35
 H       4.568299    -0.971705     2.469349      27.14
 H       2.903507    -0.405514     2.148693      31.26
55
name = lig-Water-frame_743
 C      -2.060027     3.402216     2.879016      59.68
 H      -2.924757     3.973983     2.351731      21.33
 C      -1.186482     1.113493     2.988647      50.98
 H      -1.364216     0.094531     2.668473      26.38
 C      -0.150319     1.519545     3.785838      20.01
 O       1.002785     0.795848     4.171825     211.84
 C       0.462802    -0.545243     4.760822     108.81
 H       1.257717    -1.127931     5.307903      27.86
 H       0.028744    -0.934269     3.925531      30.10
 H      -0.183456    -0.582282     5.589589      28.80
 C       0.010622     2.886193     4.151016     -16.66
 O       1.157153     3.270203     4.958853      90.23
 H       1.015573     4.261487     5.294385      26.10
 C      -1.141174     3.858344     3.756057      60.70
 H      -0.854592     4.856326     4.144344      21.67
 C      -2.222380     2.034770     2.591087      37.04
 C      -3.326171     1.397702     1.651669      75.86
 H      -4.282757     2.193833     1.717981      27.36
 O      -3.752304     0.139465     2.250837     183.83
 H      -4.834245    -0.026482     2.299241      21.03
 C      -2.879191     1.410008     0.087448      80.55
 H      -2.375936     2.386636     0.083245      29.49
 C      -4.089645     1.403567    -0.902484      88.33
 O      -5.194339     0.450636    -0.638515     228.56
 H      -4.860924    -0.548068    -0.361070      24.28
 H      -3.535275     1.419413    -1.854763      27.85
 H      -4.567650     2.512664    -0.677778      26.02
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 C       1.702507     0.906156    -0.502521      61.85
 H       2.345026     1.625415    -0.456175      31.75
 C       1.104883    -1.347118    -1.285637      65.95
 H       1.369865    -2.294534    -1.486119      29.74
 C      -0.224666    -1.038667    -1.390243     -12.32
 O      -1.228974    -1.958367    -1.815600     231.62
 C      -1.346145    -2.160830    -3.236666     128.46
 H      -1.812480    -3.097015    -3.393565      28.69
 H      -2.017776    -1.552024    -3.496293      31.52
 H      -0.344415    -2.078015    -3.654755      28.72
 C      -0.678027     0.149373    -0.481131       0.21
 O      -2.076476     0.285040    -0.346357     146.07
 C       0.204762     1.098004    -0.205638      66.55
 H      -0.085877     1.988838     0.162903      30.39
 C       2.017384    -0.438278    -0.879849      51.95
 C       3.511609    -0.862173    -0.906897      81.11
 H       3.950963    -1.669881    -1.609503      27.58
 O       4.542375     0.216318    -1.338614      44.00
 H       4.743685     1.041498    -0.567255      23.17
 C       3.870400    -1.508508     0.453831      88.09
 H       3.084654    -2.393969     0.637721      30.08
 O       5.314096    -1.942687     0.494571     123.03
 H       5.409906    -2.872898     0.270230      28.28
 C       3.859643    -0.536134     1.658512      90.82
 O       4.484860     0.799841     1.289005     257.50
 H       4.023515     1.573289     1.593108      32.77
 H       4.719301    -0.791909     2.336292      26.94
 H       2.739502    -0.447687     2.075461      28.21
55
name = lig-Water-frame_744
 C      -2.112748     3.411590     2.868643      40.54
 H      -2.761956     4.266084     2.566863      20.66
 C      -1.193785     1.099558     2.959639      54.16
 H      -1.358943     0.120363     2.504072      26.64
 C      -0.115926     1.423085     3.785995      15.72
 O       0.984922     0.764072     4.143932     212.36
 C       0.483647    -0.520674     4.775310      96.72
 H       1.373841    -0.939770     5.219682      28.83
 H       0.265068    -1.413969     3.860072      25.05
 H      -0.309488    -0.368229     5.623102      26.16
 C       0.049590     2.901382     4.164571     -15.53
 O       1.184392     3.299631     4.961794     137.15
 H       0.965569     4.151095     5.305210      33.53
 C      -1.078990     3.877693     3.801994      44.54
 H      -1.218875     4.971836     4.007118      17.81
 C      -2.223019     2.031153     2.592137      52.85
 C      -3.318324     1.433565     1.643430     102.64
 H      -4.096864     2.056261     1.702260      32.14
 O      -3.780165     0.138216     2.215973     248.75
 H      -4.723357     0.022973     2.157930      27.30
 C      -2.929093     1.404057     0.183949      76.12
 H      -2.286133     2.349775    -0.058186      27.68
 C      -4.156630     1.440209    -0.882740      91.94
 O      -5.162167     0.467937    -0.654006     273.92
 H      -4.695223    -0.300467    -0.316881      28.97
 H      -3.660155     1.050437    -1.887769      25.61
 H      -4.510705     2.397622    -0.617777      28.17
 C       1.691542     0.897309    -0.457965      41.34
 H       2.611945     1.786796    -0.513547      28.27
 C       1.067707    -1.350485    -1.285711      46.38
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 H       1.537031    -2.378246    -1.743181      25.19
 C      -0.325829    -0.938186    -1.302042      10.41
 O      -1.189348    -1.925538    -1.811655     152.26
 C      -1.337586    -2.208931    -3.287792      79.64
 H      -1.920925    -3.233116    -3.138290      23.57
 H      -2.369458    -1.293318    -3.748379      23.42
 H      -0.186788    -1.932630    -3.540949      23.51
 C      -0.683291     0.067762    -0.475303      14.00
 O      -2.105454     0.286783    -0.410027      90.58
 C       0.300243     1.145440    -0.243413      33.96
 H      -0.053178     2.253236     0.129237      26.19
 C       2.035847    -0.418512    -0.815909      39.10
 C       3.485963    -0.839590    -0.994083      75.42
 H       3.795936    -1.501550    -1.785382      28.81
 O       4.545201     0.229461    -1.390881      76.09
 H       4.506815     0.892328    -0.792088      35.81
 C       3.882840    -1.523395     0.458461      95.27
 H       3.294581    -2.409204     0.495423      33.39
 O       5.293707    -1.932610     0.487707      72.88
 H       5.441969    -2.907768     0.087577      23.20
 C       3.857867    -0.540388     1.646723     115.65
 O       4.529473     0.822804     1.313783     232.32
 H       3.871561     1.467563     1.730056      31.78
 H       4.555413    -0.898905     2.421218      31.14
 H       2.916184    -0.423994     2.024513      31.70
55
name = lig-Water-frame_745
 C      -2.136516     3.425652     2.908032      28.03
 H      -2.746602     4.300705     2.676086      20.08
 C      -1.218955     1.086358     2.929742      46.57
 H      -1.216400     0.073044     2.487016      26.60
 C      -0.079055     1.489832     3.777335      -1.04
 O       0.958389     0.668972     4.134060     194.14
 C       0.541069    -0.539893     4.774593     123.63
 H       1.535660    -0.784915     5.230490      28.63
 H       0.353099    -1.260585     4.184805      31.76
 H      -0.335975    -0.130831     5.272220      28.58
 C       0.019482     2.943156     4.178970       3.92
 O       1.178614     3.313836     4.939925      99.29
 H       0.854048     4.206351     5.443384      29.54
 C      -0.978511     3.839898     3.822197      63.33
 H      -1.318293     4.875623     4.014105      15.82
 C      -2.214344     2.014907     2.564741      35.51
 C      -3.299383     1.448216     1.676085      81.14
 H      -4.271434     2.249358     1.634254      24.85
 O      -3.776326     0.145884     2.177461     209.95
 H      -4.803673     0.017083     1.987070      22.89
 C      -2.947572     1.403858     0.196729      85.39
 H      -2.397093     2.239569    -0.089053      29.29
 C      -4.160222     1.445341    -0.834767      88.06
 O      -5.153218     0.483077    -0.650189     253.75
 H      -4.579673    -0.280842    -0.343529      26.51
 H      -3.860945     1.180387    -1.863793      26.43
 H      -4.693444     2.588623    -0.933372      25.04
 C       1.674277     0.907464    -0.416684      76.39
 H       2.340861     1.605832    -0.379445      33.08
 C       1.047211    -1.340149    -1.291615      38.58
 H       1.332639    -2.121872    -1.872475      27.30
 C      -0.364645    -0.957718    -1.240117      12.70
 O      -1.182158    -1.888829    -1.791973     207.73
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 C      -1.363784    -2.195734    -3.279497     112.91
 H      -1.620322    -3.208047    -3.254147      29.12
 H      -2.030908    -1.489787    -3.860868      28.53
 H      -0.434440    -2.119202    -3.838117      29.63
 C      -0.737013     0.109804    -0.463917       6.92
 O      -2.126843     0.267556    -0.454143      92.13
 C       0.393742     1.209679    -0.264868      52.47
 H       0.054058     2.104524    -0.007915      29.93
 C       2.077698    -0.400505    -0.807525      25.42
 C       3.526828    -0.805178    -1.035576      96.70
 H       3.315312    -1.523215    -2.011686      27.48
 O       4.507176     0.223893    -1.447208      41.41
 H       4.347911     0.904063    -0.607747      29.86
 C       3.936256    -1.498694     0.421912      94.87
 H       3.290759    -2.438993     0.569331      31.45
 O       5.290436    -1.943410     0.460958     141.88
 H       5.350131    -2.710062    -0.096391      27.33
 C       3.896847    -0.521514     1.629435     114.47
 O       4.540094     0.835727     1.342503     161.20
 H       3.854892     1.373477     1.895512      29.96
 H       4.248455    -1.148747     2.582377      31.04
 H       2.780339    -0.256630     2.064089      29.68
55
name = lig-Water-frame_746
 C      -2.081487     3.397289     3.001475      44.00
 H      -2.951310     4.121062     2.665053      25.83
 C      -1.182641     1.095870     2.940942      20.48
 H      -1.112434     0.073661     2.602528      28.32
 C      -0.083488     1.621236     3.731546       0.73
 O       0.944389     0.602441     4.093211     162.38
 C       0.624725    -0.524452     4.807017     109.11
 H       1.383399    -0.810026     5.568817      27.22
 H       0.191786    -1.460773     3.975995      24.95
 H      -0.342324    -0.288341     5.320370      28.27
 C       0.006783     2.939953     4.201725      23.39
 O       1.139958     3.345722     4.921556     147.19
 H       0.897326     4.103464     5.494372      26.08
 C      -0.973587     3.793259     3.772561      56.47
 H      -0.901372     4.786710     4.284493      26.33
 C      -2.208683     2.029016     2.531633     -38.28
 C      -3.341973     1.473785     1.701731      87.70
 H      -4.060577     2.153025     1.657238      31.17
 O      -3.766366     0.163848     2.139904     204.01
 H      -4.754697    -0.025961     1.932205      22.35
 C      -2.955852     1.402817     0.122801      78.97
 H      -2.369796     2.439283    -0.057561      27.61
 C      -4.162684     1.503885    -0.810036     100.01
 O      -5.168815     0.475722    -0.613056     220.87
 H      -4.719109    -0.492035    -0.479339      23.91
 H      -3.676551     1.507943    -1.929567      26.07
 H      -4.651519     2.369656    -1.030994      27.71
 C       1.690414     0.866923    -0.387860      44.72
 H       2.457211     1.847202    -0.133625      28.59
 C       1.045281    -1.244017    -1.273907      61.00
 H       1.188733    -2.149149    -2.040731      26.58
 C      -0.303002    -1.034345    -1.196267      -2.30
 O      -1.227217    -1.871674    -1.796368     195.75
 C      -1.335989    -2.175484    -3.212361     107.35
 H      -1.529745    -3.312803    -3.399059      26.18
 H      -2.112884    -1.455697    -4.026074      25.62
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 H      -0.476903    -2.353480    -4.082857      26.40
 C      -0.767792     0.250038    -0.458367     -12.28
 O      -2.157093     0.252465    -0.466350      99.56
 C       0.338647     1.211866    -0.276396      56.46
 H       0.046172     2.343718     0.000989      27.49
 C       2.081688    -0.402417    -0.851256      53.11
 C       3.545091    -0.812528    -1.068473     129.29
 H       3.333341    -1.475552    -1.799216      32.34
 O       4.431862     0.229840    -1.469074      53.02
 H       4.511153     0.779439    -0.548924      29.33
 C       3.984665    -1.454875     0.355936     103.69
 H       3.210980    -2.190667     0.709843      32.62
 O       5.312810    -1.947337     0.419294     153.86
 H       5.350645    -2.699789    -0.238535      24.17
 C       3.880372    -0.495415     1.638782     136.13
 O       4.525100     0.824046     1.391832     146.45
 H       4.086625     1.480456     1.922364      31.75
 H       4.175653    -1.034581     2.486515      34.32
 H       2.919084    -0.233334     1.766709      32.21
55
name = lig-Water-frame_747
 C      -2.061953     3.338486     3.063553      62.69
 H      -2.883263     3.879293     2.813104      29.28
 C      -1.123604     1.163854     2.967533      43.80
 H      -1.095558     0.076129     2.744958      25.85
 C      -0.080921     1.653204     3.685643      27.33
 O       0.951506     0.615884     4.020676     172.90
 C       0.616870    -0.562804     4.837400     128.27
 H       1.230875    -0.896383     5.697368      27.82
 H       0.451269    -1.190770     4.155169      32.34
 H      -0.274763    -0.594313     5.535930      28.48
 C       0.027144     2.897997     4.213071      13.45
 O       1.101043     3.374146     4.913736     140.44
 H       0.874135     4.169382     5.499492      24.70
 C      -0.999768     3.808352     3.744637      67.59
 H      -0.602808     4.656576     4.291641      20.39
 C      -2.165641     2.027524     2.530665       4.17
 C      -3.359060     1.467125     1.673494      67.51
 H      -4.285203     2.331633     1.736172      26.33
 O      -3.750979     0.181950     2.116444     235.33
 H      -4.671893    -0.007187     1.971845      26.50
 C      -2.945110     1.459273     0.040154      94.20
 H      -2.406088     2.310413    -0.043415      30.31
 C      -4.143038     1.519317    -0.847504      82.28
 O      -5.185880     0.450235    -0.575621     250.06
 H      -4.858809    -0.409575    -0.629554      29.46
 H      -3.544999     1.605153    -1.744768      27.83
 H      -4.869135     2.603292    -0.726883      24.54
 C       1.729986     0.860038    -0.359912      49.73
 H       2.340208     1.585115     0.041136      33.05
 C       1.056611    -1.199200    -1.309144      72.37
 H       1.286533    -2.056179    -1.901802      29.70
 C      -0.259198    -1.023240    -1.116155      -3.24
 O      -1.287946    -1.865291    -1.815701     159.27
 C      -1.289680    -2.200940    -3.213740     112.33
 H      -1.803961    -3.144938    -3.196910      28.13
 H      -2.207367    -1.467059    -3.701103      25.35
 H      -0.309519    -2.169402    -3.668695      28.31
 C      -0.751764     0.330369    -0.519007       4.05
 O      -2.188278     0.268179    -0.444899     139.35
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 C       0.190952     1.231827    -0.264726      70.66
 H       0.133177     2.246933     0.004898      28.45
 C       2.085152    -0.365689    -0.899696      52.73
 C       3.525727    -0.831464    -1.035239     110.27
 H       3.745912    -1.802969    -1.865426      27.09
 O       4.365425     0.244950    -1.462487      52.32
 H       4.657771     0.698480    -0.685007      31.98
 C       4.007546    -1.373174     0.324108     100.29
 H       3.212301    -2.095208     0.622195      32.62
 O       5.349383    -1.946477     0.357766     138.39
 H       5.472610    -2.841783    -0.196151      19.98
 C       3.848961    -0.445780     1.590178     113.86
 O       4.527874     0.805634     1.439203     127.38
 H       4.210736     1.608374     1.972963      28.44
 H       4.336231    -0.914506     2.603956      29.12
 H       2.650089    -0.268142     1.550350      29.84
55
name = lig-Water-frame_748
 C      -2.096313     3.276384     3.074390      31.00
 H      -3.039683     4.042585     2.940289      26.98
 C      -1.103361     1.213632     2.954511      63.06
 H      -1.143138     0.153462     2.817009      28.60
 C      -0.005210     1.574970     3.693369      43.72
 O       0.965190     0.667849     3.963594     148.86
 C       0.572189    -0.585386     4.911194      75.26
 H       1.524683    -0.824084     5.521454      25.89
 H       0.672460    -1.522675     3.998995      23.60
 H      -0.359744    -0.555979     5.466716      26.90
 C       0.023095     2.897807     4.185877       2.18
 O       1.085602     3.396276     4.929685     103.31
 H       0.749121     4.294756     5.381388      25.59
 C      -0.946070     3.815801     3.791191      55.11
 H      -0.869619     4.956018     4.007673      19.43
 C      -2.118469     1.990793     2.545901       6.91
 C      -3.369829     1.501460     1.613333      81.12
 H      -4.138826     2.104328     1.759811      29.77
 O      -3.721863     0.195812     2.109670     209.91
 H      -4.787419     0.000642     1.987956      22.25
 C      -2.947285     1.505904     0.028103      88.02
 H      -2.224901     2.459405    -0.187725      26.33
 C      -4.181346     1.560592    -0.867655      88.55
 O      -5.198675     0.459170    -0.556003     174.96
 H      -4.704028    -0.488873    -0.725479      24.50
 H      -3.746611     1.494191    -1.993116      26.90
 H      -4.654516     2.341386    -0.485685      30.39
 C       1.659539     0.858994    -0.337467      39.78
 H       2.469951     1.564316     0.229264      31.42
 C       1.073063    -1.210129    -1.373277      51.50
 H       1.493785    -2.157868    -1.842469      26.93
 C      -0.303084    -0.957997    -1.067924       8.52
 O      -1.326338    -1.839112    -1.772881     147.49
 C      -1.270026    -2.221094    -3.213137      98.22
 H      -1.926928    -3.145483    -3.096316      25.36
 H      -2.064085    -1.375739    -3.429925      24.37
 H      -0.142210    -1.933702    -3.303462      24.76
 C      -0.783146     0.289376    -0.624158      14.69
 O      -2.198140     0.309881    -0.405070     130.89
 C       0.162023     1.265865    -0.240232      69.90
 H      -0.020351     2.313771     0.132955      26.96
 C       2.102554    -0.309644    -0.944506      29.28
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 C       3.528523    -0.880634    -1.004570     122.12
 H       3.849648    -1.611694    -1.559050      33.80
 O       4.312946     0.264247    -1.465942     -32.99
 H       4.858651     0.767105    -0.600015      25.57
 C       4.020457    -1.311533     0.342852     104.97
 H       3.332591    -2.237467     0.454236      30.38
 O       5.390523    -1.937980     0.287966     136.24
 H       5.424273    -2.853284    -0.015506      24.72
 C       3.792626    -0.394749     1.543887     142.38
 O       4.558610     0.816073     1.464832     171.18
 H       4.062615     1.483155     2.070892      28.51
 H       4.128937    -0.825685     2.387483      35.10
 H       2.775630    -0.360171     1.665628      31.64
55
name = lig-Water-frame_749
 C      -2.144405     3.297548     3.083568      29.45
 H      -2.877174     3.960965     2.994579      25.91
 C      -1.068581     1.173554     2.927630      39.64
 H      -1.203703     0.094180     2.683213      30.86
 C       0.057980     1.523139     3.725518      24.11
 O       1.001462     0.685182     3.952457     155.61
 C       0.590196    -0.630066     4.909260      85.22
 H       1.528109    -0.574073     5.356856      27.76
 H       0.647128    -1.383232     4.272083      29.16
 H      -0.437711    -0.368925     5.283472      27.70
 C       0.043756     2.932311     4.152887      -9.15
 O       1.083712     3.418506     4.960828      62.32
 H       0.786405     4.254054     5.294824      30.18
 C      -0.952204     3.827597     3.819587      60.67
 H      -1.179620     4.852099     3.736609      18.46
 C      -2.153555     1.988808     2.534798      -3.07
 C      -3.299727     1.509399     1.561754      70.36
 H      -4.284674     2.263818     1.746900      23.64
 O      -3.711931     0.199275     2.106649     225.63
 H      -4.628387     0.020717     1.985539      26.11
 C      -2.917927     1.561932     0.030214     101.24
 H      -2.388722     2.375607    -0.263134      28.83
 C      -4.209771     1.545568    -0.892088      81.58
 O      -5.186491     0.470460    -0.557287     228.53
 H      -4.617563    -0.340883    -0.581988      27.44
 H      -4.337296     1.516174    -1.988133      26.27
 H      -4.743918     2.610049    -0.390328      26.00
 C       1.539165     0.914834    -0.299729      43.09
 H       2.362850     1.473978     0.209007      30.73
 C       1.083224    -1.219215    -1.426209      29.79
 H       1.458011    -2.257376    -1.736368      27.52
 C      -0.356356    -0.953034    -1.137752      22.39
 O      -1.350435    -1.802375    -1.645340     169.41
 C      -1.249687    -2.191176    -3.130581      83.00
 H      -1.580846    -3.240773    -3.347988      27.20
 H      -1.941363    -1.203084    -3.762640      24.42
 H      -0.266976    -2.091441    -3.511373      29.05
 C      -0.840775     0.260841    -0.690130       7.82
 O      -2.190035     0.350742    -0.363580     136.11
 C       0.227809     1.281488    -0.220174      50.28
 H      -0.271410     2.183013     0.275096      25.85
 C       2.075461    -0.306510    -0.993313      17.62
 C       3.542119    -0.830922    -0.944100      98.39
 H       3.733905    -1.833205    -1.769965      26.54
 O       4.308216     0.304125    -1.458197      53.66
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 H       4.702656     0.689425    -0.723626      33.66
 C       4.023181    -1.334137     0.382479     108.47
 H       3.467815    -2.230982     0.535691      32.35
 O       5.424903    -1.891285     0.237642      93.54
 H       5.236430    -2.905424    -0.009486      22.96
 C       3.767390    -0.373335     1.498813     119.84
 O       4.580433     0.855461     1.486534     196.64
 H       4.001158     1.361940     2.051170      31.93
 H       4.010280    -1.080703     2.509223      28.85
 H       2.612178    -0.190627     1.774093      28.67
55
name = lig-Water-frame_750
 C      -2.132313     3.309659     3.096540      38.49
 H      -3.050350     4.087492     2.873243      23.38
 C      -1.041915     1.090989     2.894791      25.60
 H      -1.115991     0.087479     2.484737      30.24
 C       0.016823     1.566847     3.723552     -20.22
 O       1.084910     0.642512     3.981514     139.69
 C       0.626727    -0.591822     4.866973      88.35
 H       1.442214    -0.471133     5.742205      26.21
 H       0.526917    -1.555184     4.116214      25.87
 H      -0.326728    -0.282543     5.262019      30.99
 C       0.098074     2.969656     4.137990       1.99
 O       1.099140     3.412674     4.977929     -24.45
 H       0.863126     4.380526     5.464225      26.95
 C      -1.062336     3.792408     3.784890      69.40
 H      -1.065242     4.974831     3.860102      20.92
 C      -2.200271     2.016266     2.524413     -10.54
 C      -3.252883     1.535188     1.557650      90.32
 H      -3.985940     2.222710     1.569540      30.01
 O      -3.684868     0.207299     2.098867     194.84
 H      -4.679794     0.015611     1.891571      23.89
 C      -2.914384     1.574866    -0.002931      81.43
 H      -2.379605     2.602391    -0.300500      25.73
 C      -4.302802     1.572963    -0.854269     104.81
 O      -5.163187     0.488461    -0.551470     258.45
 H      -4.659493    -0.346583    -0.399993      26.78
 H      -4.409397     1.719222    -2.006531      26.28
 H      -4.739452     2.449797    -0.706886      30.50
 C       1.490749     0.939375    -0.292705      16.11
 H       2.219408     1.643319     0.190540      28.73
 C       1.062458    -1.216926    -1.444569      48.59
 H       1.255199    -2.216586    -1.724376      27.58
 C      -0.370840    -0.966008    -1.279484       1.70
 O      -1.376679    -1.806182    -1.541265     219.42
 C      -1.256698    -2.104207    -3.041992     116.37
 H      -1.373000    -3.137665    -3.413445      28.01
 H      -1.556277    -1.630672    -3.917715      29.08
 H      -0.223297    -2.241854    -3.653772      26.43
 C      -0.837028     0.300629    -0.696005       0.53
 O      -2.172979     0.375656    -0.328312     140.82
 C       0.191583     1.247499    -0.210937      62.37
 H      -0.179545     2.022172     0.357553      29.05
 C       1.992610    -0.323323    -1.008687      13.82
 C       3.531520    -0.778890    -0.958332     116.05
 H       3.436604    -1.470587    -1.627082      30.36
 O       4.324691     0.330777    -1.455022      39.40
 H       4.656293     0.830133    -0.587659      30.96
 C       4.026702    -1.378335     0.401109      98.95
 H       3.354049    -2.289496     0.803097      30.28
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 O       5.428588    -1.838656     0.213105     117.10
 H       5.330061    -2.716572    -0.216552      25.18
 C       3.756122    -0.399329     1.551979     124.55
 O       4.584951     0.876890     1.502644     185.94
 H       4.037465     1.592411     2.112257      27.31
 H       3.950933    -0.931843     2.362364      34.24
 H       2.777187     0.015630     1.543702      31.11
55
name = lig-Water-frame_751
 C      -2.181997     3.320911     3.057080      48.60
 H      -2.937214     3.944954     2.770020      28.91
 C      -1.068535     1.074751     2.852195      31.83
 H      -0.905950     0.088706     2.378001      28.84
 C      -0.025265     1.610652     3.702643     -36.08
 O       1.158501     0.594169     4.029316      86.61
 C       0.691907    -0.498192     4.819762     135.86
 H       1.089942    -0.779099     5.762001      30.88
 H       0.527298    -1.433001     4.184200      28.33
 H      -0.311534    -0.306327     5.274255      30.30
 C       0.098353     3.000394     4.122493       6.90
 O       1.123282     3.412290     4.989546     151.31
 H       0.893481     4.161461     5.545442      24.59
 C      -1.110154     3.790367     3.774195      77.56
 H      -0.855283     4.720062     4.173876      19.18
 C      -2.163588     2.001864     2.538798      18.21
 C      -3.207452     1.546923     1.557184      69.60
 H      -4.108003     2.413769     1.547693      26.76
 O      -3.661899     0.225670     2.081673     180.55
 H      -4.654274     0.058493     1.805581      24.94
 C      -2.928201     1.595043    -0.058125      88.85
 H      -2.404341     2.499233    -0.213382      29.63
 C      -4.366891     1.595029    -0.839794      81.57
 O      -5.163658     0.501623    -0.534379     233.25
 H      -4.653183    -0.419494    -0.277552      23.42
 H      -3.895409     1.721983    -1.889996      26.95
 H      -5.055453     2.661404    -0.623928      25.21
 C       1.526889     0.904794    -0.331568     -53.56
 H       2.115692     1.864516     0.091766      29.14
 C       0.972154    -1.217218    -1.448587      45.89
 H       1.214293    -2.313293    -1.876650      25.48
 C      -0.358197    -0.874235    -1.371350      -3.73
 O      -1.405727    -1.855097    -1.524290     186.97
 C      -1.203190    -2.099827    -2.999536      81.35
 H      -1.635194    -3.187704    -3.050998      24.95
 H      -1.801644    -1.406267    -3.922483      23.94
 H      -0.138429    -2.097499    -3.076136      26.09
 C      -0.783170     0.328404    -0.690745      20.95
 O      -2.151994     0.387906    -0.309468     169.66
 C       0.070789     1.186276    -0.210984      43.22
 H      -0.053621     2.121636     0.526939      28.69
 C       1.932588    -0.282375    -0.950660     -20.64
 C       3.455128    -0.696429    -0.965713     102.01
 H       3.410763    -1.539039    -1.945184      23.99
 O       4.367492     0.350041    -1.429048      52.67
 H       4.474354     1.013354    -0.547314      26.97
 C       4.005245    -1.410004     0.408046     100.84
 H       3.388481    -2.180624     0.743550      33.02
 O       5.405576    -1.787587     0.208302      92.76
 H       5.526563    -2.566947    -0.467597      21.30
 C       3.786494    -0.383242     1.593831     111.83
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 O       4.581549     0.892958     1.519884     182.27
 H       4.230422     1.589459     2.063468      29.44
 H       3.984154    -0.855738     2.745899      28.06
 H       2.724763    -0.037207     1.354041      30.68
55
name = lig-Water-frame_752
 C      -2.214657     3.306191     2.999709      57.89
 H      -3.091396     4.009457     2.644479      24.19
 C      -1.078942     1.123085     2.833842      59.57
 H      -0.819511     0.169576     2.379522      30.21
 C      -0.017827     1.617220     3.677767     -45.21
 O       1.206009     0.597665     4.072756      42.77
 C       0.690144    -0.422889     4.805639     135.50
 H       1.229464    -1.026475     5.681185      28.46
 H       0.600641    -1.399310     4.131509      27.88
 H      -0.367532    -0.285690     5.075448      29.16
 C       0.039029     2.982570     4.104339      12.30
 O       1.146635     3.381495     4.970221     148.36
 H       0.790174     4.183588     5.636520      15.57
 C      -1.059284     3.788418     3.807721      91.73
 H      -1.001454     4.779254     4.460435      19.43
 C      -2.090459     1.954466     2.538192      24.29
 C      -3.220632     1.585100     1.542682      82.07
 H      -3.998826     2.226612     1.733926      29.24
 O      -3.646792     0.258202     2.052977     235.95
 H      -4.524650     0.105510     1.823949      29.62
 C      -2.967691     1.597838    -0.042143      82.62
 H      -2.320714     2.526432    -0.284915      26.46
 C      -4.354457     1.663873    -0.830272     101.38
 O      -5.190135     0.489424    -0.510600     243.19
 H      -4.582602    -0.232716    -0.449250      30.00
 H      -3.787932     1.561698    -1.801474      27.83
 H      -4.957411     2.364710    -0.538450      29.05
 C       1.499458     0.915684    -0.375555      79.10
 H       2.160905     1.654748    -0.107836      36.22
 C       0.902010    -1.219683    -1.447681      39.40
 H       1.257778    -2.053796    -1.862352      25.75
 C      -0.397866    -0.776555    -1.388544      17.08
 O      -1.406263    -1.873977    -1.551161     204.43
 C      -1.203578    -2.155558    -2.986905     102.45
 H      -1.772230    -3.031759    -2.927606      27.69
 H      -1.815500    -1.336148    -3.213164      27.08
 H      -0.126455    -2.026049    -2.878770      26.09
 C      -0.819398     0.316899    -0.696964      27.16
 O      -2.138000     0.385824    -0.318204     174.83
 C       0.091523     1.201200    -0.164131      64.87
 H      -0.177716     1.994937     0.396848      32.04
 C       1.924594    -0.250363    -0.885146     -37.06
 C       3.359809    -0.667390    -1.014982     101.33
 H       3.608988    -1.284648    -1.721077      27.95
 O       4.400207     0.380256    -1.375548     115.26
 H       4.386279     0.954688    -0.707856      41.25
 C       3.998335    -1.374682     0.394744      77.63
 H       3.305920    -2.368927     0.571441      30.20
 O       5.373374    -1.751410     0.213595      92.34
 H       5.496585    -2.380897    -0.594470      19.82
 C       3.830341    -0.345189     1.656054     125.63
 O       4.600021     0.878035     1.505105     191.10
 H       4.131382     1.567100     2.218692      24.56
 H       3.857884    -0.647834     2.596161      35.31
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 H       2.717275    -0.306565     1.507161      34.28
55
name = lig-Water-frame_753
 C      -2.170994     3.302208     2.974951      43.68
 H      -3.043062     3.921400     2.692997      22.44
 C      -0.989412     1.156354     2.858005      58.15
 H      -0.958785     0.170650     2.385379      31.70
 C       0.038976     1.593126     3.652523       9.70
 O       1.228332     0.691368     4.088305      89.31
 C       0.634603    -0.477710     4.816755     111.97
 H       1.456608    -0.687004     5.474231      28.54
 H       0.658731    -1.271475     3.963730      27.57
 H      -0.399315    -0.227098     5.035066      27.51
 C       0.011424     2.925602     4.122642       2.09
 O       1.133915     3.345951     4.936827      47.77
 H       0.868154     4.130759     5.428545      30.52
 C      -1.053994     3.813411     3.848506      50.01
 H      -1.332289     4.689066     4.319203      13.60
 C      -2.090129     1.975777     2.481910       1.86
 C      -3.225135     1.582081     1.543294      71.97
 H      -4.137040     2.332557     1.867306      22.93
 O      -3.621260     0.293438     2.023581     185.73
 H      -4.637085     0.063920     1.789882      22.09
 C      -2.984921     1.619146     0.036091      87.06
 H      -2.384782     2.449850    -0.388675      25.49
 C      -4.261134     1.651784    -0.813033      83.01
 O      -5.218856     0.493503    -0.493512     165.63
 H      -4.525495    -0.335571    -0.678049      22.98
 H      -4.205436     1.553158    -2.015128      24.88
 H      -4.950918     2.659323    -0.507123      23.66
 C       1.426487     0.979392    -0.394818      69.82
 H       2.472017     1.612279    -0.150529      33.56
 C       0.909568    -1.129742    -1.402094      36.75
 H       1.343556    -2.121039    -1.949102      24.69
 C      -0.484888    -0.791206    -1.367039      25.66
 O      -1.371589    -1.848899    -1.542835     226.39
 C      -1.244098    -2.207075    -2.920906      95.10
 H      -1.826251    -3.219117    -3.315459      25.12
 H      -1.789508    -1.200544    -3.278140      25.02
 H      -0.184541    -2.299846    -3.530014      25.97
 C      -0.893265     0.355743    -0.670733      24.15
 O      -2.168739     0.376668    -0.340710     157.47
 C       0.173129     1.225944    -0.135050      65.50
 H      -0.357904     2.147627     0.391172      27.12
 C       1.900184    -0.303729    -0.893366      15.40
 C       3.338760    -0.627613    -0.999506      89.21
 H       3.670560    -1.485442    -1.856713      25.52
 O       4.408630     0.402130    -1.340714      -4.58
 H       4.371352     1.171579    -0.493567      29.78
 C       3.968325    -1.326650     0.385244      90.32
 H       3.438273    -2.191753     0.458811      33.85
 O       5.343356    -1.717415     0.214355     121.84
 H       5.307652    -2.300377    -0.514620      27.71
 C       3.844352    -0.336392     1.646996     125.05
 O       4.609535     0.865556     1.493044     163.66
 H       4.112639     1.452767     2.101937      28.41
 H       3.984246    -0.834947     2.806037      30.01
 H       2.718798    -0.208803     1.743592      32.50
55
name = lig-Water-frame_754
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 C      -2.060818     3.295742     2.987097      44.26
 H      -2.950032     3.930479     2.792295      26.69
 C      -0.913929     1.155292     2.849726      10.29
 H      -1.074030     0.132814     2.482103      30.21
 C       0.150933     1.560545     3.645311      39.33
 O       1.197078     0.834364     4.085477     166.08
 C       0.609216    -0.540788     4.774088      75.14
 H       1.435136    -0.465997     5.539965      23.12
 H       0.578611    -1.306326     3.984161      25.74
 H      -0.372829    -0.288343     5.298707      25.93
 C       0.017547     2.902359     4.178821     -19.46
 O       1.105033     3.290048     4.882855     -47.85
 H       0.926012     4.221219     5.337912      29.27
 C      -1.116669     3.790266     3.844836      43.14
 H      -1.416715     4.839512     4.267899      16.64
 C      -2.088344     2.045767     2.421591     -15.43
 C      -3.260851     1.587102     1.586340      93.38
 H      -3.998547     2.353191     1.679471      28.66
 O      -3.617592     0.304143     2.000286     217.07
 H      -4.532328     0.038348     1.722794      24.65
 C      -2.976881     1.627512     0.071194      91.51
 H      -2.410972     2.504155    -0.285681      26.92
 C      -4.247102     1.629056    -0.804558     114.96
 O      -5.213659     0.509760    -0.486772     272.38
 H      -4.844693    -0.372137    -0.650516      28.31
 H      -4.337863     1.730621    -1.884243      28.00
 H      -4.572903     2.570163    -0.650602      29.49
 C       1.501673     1.023423    -0.407784      57.43
 H       2.183701     1.659960    -0.103351      34.51
 C       0.928690    -1.077276    -1.387844      53.83
 H       1.109441    -1.967663    -1.842425      26.89
 C      -0.518992    -0.829994    -1.297957      19.55
 O      -1.324972    -1.843688    -1.526159     249.44
 C      -1.332240    -2.243722    -2.958239     135.65
 H      -1.781733    -3.055418    -3.291993      30.04
 H      -1.584284    -1.544512    -3.771622      29.45
 H      -0.508875    -2.509050    -3.654602      29.43
 C      -0.900590     0.400715    -0.633792      20.11
 O      -2.257088     0.382073    -0.350412     179.20
 C       0.122777     1.283037    -0.113643      58.70
 H      -0.163214     2.262381     0.292441      28.99
 C       1.862320    -0.303478    -0.924219      27.85
 C       3.423451    -0.635212    -0.970993     122.46
 H       3.362721    -1.357718    -1.679949      30.84
 O       4.384039     0.451126    -1.298192      91.46
 H       4.444003     1.028358    -0.520164      33.06
 C       3.931555    -1.227678     0.380220      87.45
 H       3.273770    -2.249417     0.592418      30.91
 O       5.318518    -1.676693     0.216569      83.74
 H       5.251233    -2.471867    -0.491583      22.86
 C       3.825352    -0.393903     1.655394     132.73
 O       4.622803     0.839619     1.471152     125.67
 H       4.146463     1.672267     2.012175      24.45
 H       4.303360    -0.964929     2.365835      36.33
 H       2.837339     0.097444     1.920564      27.40
55
name = lig-Water-frame_755
 C      -2.004525     3.306182     2.978186      55.01
 H      -2.899771     4.050359     2.867334      24.60
 C      -0.918870     1.153949     2.793004      17.21
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 H      -1.002487     0.077984     2.606752      27.05
 C       0.185943     1.602945     3.622789      25.21
 O       1.163282     0.921095     4.097380     144.84
 C       0.625402    -0.529659     4.749757      66.45
 H       1.300321    -0.749638     5.585246      24.79
 H       0.483833    -1.512473     4.023161      23.49
 H      -0.241643    -0.404931     5.342530      26.52
 C      -0.013862     2.911421     4.201475     -12.21
 O       1.098179     3.259811     4.855983      98.06
 H       0.967380     4.148188     5.338038      22.73
 C      -1.125635     3.755787     3.879245      65.94
 H      -1.105015     4.752356     4.220069      27.87
 C      -2.004496     2.060655     2.400279       9.32
 C      -3.267644     1.606367     1.606812      62.77
 H      -4.126460     2.479525     1.646476      26.22
 O      -3.626816     0.288839     2.003173     218.83
 H      -4.453190     0.034957     1.604946      26.61
 C      -2.959333     1.600247     0.038276      91.04
 H      -2.373390     2.599695    -0.056195      25.77
 C      -4.262069     1.577982    -0.786966      89.19
 O      -5.226400     0.568852    -0.475148     247.41
 H      -4.776575    -0.372322    -0.550375      24.87
 H      -3.967981     1.771477    -1.977206      24.92
 H      -4.716955     2.706435    -0.468679      25.04
 C       1.533521     1.021861    -0.409905      42.34
 H       2.172322     1.986446     0.062553      29.57
 C       0.848526    -1.082978    -1.408215      66.21
 H       1.046278    -2.152076    -1.859660      23.28
 C      -0.445523    -0.797441    -1.183212      16.51
 O      -1.317275    -1.877780    -1.557165     212.77
 C      -1.411724    -2.267641    -3.071951      61.87
 H      -2.253692    -3.256892    -2.886014      22.92
 H      -1.713567    -1.549107    -3.891344      26.70
 H      -0.259973    -2.722747    -3.178635      23.27
 C      -0.899204     0.405460    -0.591377      10.85
 O      -2.334354     0.412486    -0.352647     187.15
 C       0.074244     1.338885    -0.139075      75.86
 H      -0.034118     2.378490     0.269416      29.92
 C       1.926579    -0.170934    -0.914432      23.35
 C       3.480988    -0.618471    -0.913271     122.48
 H       3.417028    -1.450739    -1.798638      30.20
 O       4.343511     0.487222    -1.284458      57.11
 H       4.489250     0.955794    -0.354027      31.13
 C       3.856672    -1.186464     0.371013     105.69
 H       3.256103    -1.941290     0.668918      36.22
 O       5.293230    -1.650208     0.212277      92.39
 H       5.360185    -2.500840    -0.276236      24.19
 C       3.818656    -0.404497     1.645434     126.24
 O       4.653333     0.830762     1.446113      99.53
 H       4.238052     1.633037     1.835367      29.19
 H       4.555700    -1.134434     2.253420      31.32
 H       2.885080    -0.070139     2.032246      27.13
55
name = lig-Water-frame_756
 C      -2.030128     3.351465     2.947015      37.72
 H      -2.808815     4.001351     2.759140      24.04
 C      -0.931639     1.160843     2.743017      62.03
 H      -0.900004     0.082466     2.591962      28.46
 C       0.064490     1.707040     3.557430      24.22
 O       1.171016     0.896492     4.145062      98.46
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 C       0.667164    -0.514301     4.737481      96.50
 H       1.406388    -1.010704     5.438661      27.30
 H       0.521185    -1.279087     4.059827      28.96
 H      -0.378000    -0.307303     5.194683      26.99
 C      -0.049973     2.908871     4.175703      18.34
 O       1.126312     3.263612     4.871647     109.01
 H       0.946747     4.024408     5.456589      26.05
 C      -1.046164     3.729039     3.953838      65.51
 H      -0.855516     4.792465     4.280225      24.87
 C      -1.923631     2.019611     2.393459      11.38
 C      -3.248284     1.638853     1.590733      64.17
 H      -4.070375     2.303988     1.817777      28.24
 O      -3.638523     0.272909     2.036397     186.78
 H      -4.483612     0.002682     1.441662      22.90
 C      -2.971391     1.596965     0.027774     115.88
 H      -2.397425     2.468764    -0.112808      29.64
 C      -4.273739     1.629432    -0.780991     108.09
 O      -5.236983     0.617475    -0.468108     244.59
 H      -4.611977    -0.188836    -0.441423      26.69
 H      -3.820926     1.568196    -1.762311      28.90
 H      -4.917113     2.354915    -0.447866      25.89
 C       1.490835     1.097538    -0.357932      47.77
 H       2.150009     1.804413    -0.036246      32.10
 C       0.862702    -1.089800    -1.414536      88.25
 H       1.126565    -2.079171    -1.763082      25.67
 C      -0.408032    -0.789511    -1.096489      14.38
 O      -1.342218    -1.886444    -1.603294     220.11
 C      -1.459978    -2.358527    -3.129887      91.05
 H      -2.212404    -2.879784    -2.873553      29.61
 H      -1.824072    -1.457190    -3.695686      28.50
 H      -0.539905    -2.766423    -3.000578      28.73
 C      -0.926540     0.420719    -0.520031      18.73
 O      -2.334927     0.437997    -0.368729     212.52
 C       0.077877     1.370423    -0.208858      54.81
 H      -0.123507     2.429554     0.280004      27.28
 C       2.007675    -0.083804    -0.927512      22.76
 C       3.449618    -0.581217    -0.936535     116.01
 H       3.781755    -1.311414    -1.648952      32.43
 O       4.305460     0.528079    -1.273453      72.30
 H       4.634300     0.843857    -0.268283      30.77
 C       3.818538    -1.189910     0.371858      85.83
 H       3.022566    -2.091247     0.640462      31.69
 O       5.268484    -1.628146     0.226564     110.48
 H       5.354097    -2.494280    -0.204343      25.62
 C       3.883655    -0.377790     1.639789     145.53
 O       4.701043     0.816085     1.405713     133.68
 H       4.150436     1.586035     1.880181      25.90
 H       4.413672    -0.996942     2.341694      36.73
 H       2.822150    -0.445395     2.170168      29.80
55
name = lig-Water-frame_757
 C      -2.011859     3.372906     2.954494      12.68
 H      -2.915887     4.060872     2.496262      22.45
 C      -0.912971     1.144700     2.715186      66.77
 H      -0.858897     0.107793     2.383036      26.68
 C      -0.026092     1.706386     3.520842      17.63
 O       1.163658     0.828094     4.188750     120.55
 C       0.694622    -0.458578     4.731518     104.63
 H       1.525103    -0.942039     5.292158      27.34
 H       0.517623    -1.091399     3.642051      25.78
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 H      -0.264257    -0.246676     5.091208      28.84
 C       0.020599     2.903876     4.177969       9.39
 O       1.158337     3.275864     4.902019      36.53
 H       0.856246     3.968114     5.692757      23.59
 C      -1.038907     3.783163     3.973364      55.03
 H      -0.870156     4.800568     4.361143      24.54
 C      -1.959236     2.033567     2.376137       8.59
 C      -3.181501     1.610465     1.576265      66.37
 H      -4.052874     2.341543     1.932323      24.64
 O      -3.652401     0.270547     2.070585     188.30
 H      -4.399191    -0.012872     1.545999      26.16
 C      -3.022099     1.635012     0.070981      99.35
 H      -2.359875     2.509005    -0.416758      25.53
 C      -4.288067     1.707213    -0.758023      83.88
 O      -5.224655     0.624696    -0.458956     224.76
 H      -4.778356    -0.260401    -0.434863      27.32
 H      -3.939162     1.418538    -1.922306      24.68
 H      -4.996632     2.658613    -0.647641      23.74
 C       1.435650     1.147334    -0.325724      49.17
 H       2.305031     1.916365    -0.006583      27.52
 C       1.002699    -1.028063    -1.365775      57.20
 H       1.272439    -2.036610    -1.768021      25.94
 C      -0.448488    -0.840138    -1.078961      -2.47
 O      -1.380512    -1.849341    -1.615643     168.31
 C      -1.498867    -2.359893    -3.101543      60.18
 H      -2.558216    -3.044292    -3.071234      23.14
 H      -1.633950    -1.469056    -3.680539      27.35
 H      -0.428935    -3.125812    -3.459945      23.34
 C      -0.935402     0.421790    -0.457215      21.02
 O      -2.280914     0.444810    -0.396251     171.69
 C       0.077259     1.412581    -0.268537      61.87
 H      -0.267334     2.283355     0.162826      27.08
 C       1.987194    -0.075997    -0.974211      29.40
 C       3.401654    -0.508778    -0.980391     105.01
 H       3.789360    -1.339257    -1.703708      29.10
 O       4.299169     0.588044    -1.248223     102.86
 H       4.671860     0.867482    -0.493142      34.71
 C       3.801846    -1.258556     0.401789      94.39
 H       3.183442    -2.057873     0.434457      33.63
 O       5.238482    -1.614894     0.251657     123.20
 H       5.248514    -2.522534    -0.313489      24.68
 C       3.932485    -0.373552     1.651928     148.98
 O       4.725292     0.818051     1.380086     154.69
 H       4.207749     1.534243     1.914521      26.53
 H       4.467821    -0.951816     2.543379      32.41
 H       2.972791    -0.305838     2.053914      30.78
55
name = lig-Water-frame_758
 C      -1.992423     3.383806     2.965858      61.23
 H      -2.677483     3.976351     2.568483      26.37
 C      -0.939169     1.124378     2.661234      32.20
 H      -0.855268     0.156284     2.160644      26.63
 C       0.028388     1.609597     3.582175     -12.48
 O       1.142589     0.791045     4.207129     170.42
 C       0.714240    -0.410243     4.620052     123.92
 H       1.508003    -0.798688     5.268384      27.51
 H       0.545517    -0.959708     3.810494      29.65
 H      -0.254065    -0.374880     5.327693      27.28
 C       0.102863     2.944237     4.193760     -13.68
 O       1.180179     3.290436     4.958630      98.22
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 H       0.914670     3.921875     5.630790      26.23
 C      -1.063075     3.851316     3.933179      57.50
 H      -1.105290     4.843299     4.390974      27.20
 C      -2.025170     2.086726     2.377076      30.23
 C      -3.148019     1.569750     1.589596      94.25
 H      -3.894939     2.387601     1.778520      27.71
 O      -3.638271     0.285914     2.112622     176.95
 H      -4.462341    -0.010726     1.665177      24.32
 C      -3.037359     1.711121     0.069140      90.67
 H      -2.535585     2.502271    -0.326643      28.60
 C      -4.334959     1.748220    -0.774712     105.16
 O      -5.223110     0.626734    -0.434047     257.02
 H      -4.897677    -0.344698    -0.594474      23.63
 H      -4.147256     1.651876    -1.806296      28.96
 H      -4.631742     2.787350    -0.957643      27.77
 C       1.452105     1.167938    -0.335058      55.67
 H       2.121775     1.994360    -0.018001      27.86
 C       1.079019    -0.976559    -1.296150      56.58
 H       1.443175    -1.912805    -1.846769      26.29
 C      -0.455421    -0.899227    -1.119253       1.99
 O      -1.419874    -1.802953    -1.617597     184.40
 C      -1.511992    -2.368469    -3.030377     112.79
 H      -2.383967    -2.883722    -3.362271      27.84
 H      -1.333821    -1.530052    -3.795546      27.53
 H      -0.846069    -3.027021    -3.664816      27.16
 C      -0.885570     0.349012    -0.460776      13.03
 O      -2.246704     0.456397    -0.416975     124.09
 C       0.053517     1.436332    -0.302642      41.60
 H      -0.453382     2.485133     0.131910      24.46
 C       1.899943    -0.046713    -0.995224      61.25
 C       3.397740    -0.444044    -0.993611      92.88
 H       3.366997    -1.253231    -1.803957      29.21
 O       4.298468     0.652385    -1.266774      22.31
 H       4.792339     1.032205    -0.294070      20.81
 C       3.850004    -1.283825     0.412608      90.11
 H       3.179171    -2.303447     0.436806      26.71
 O       5.207343    -1.642079     0.258870     200.62
 H       5.227363    -2.339058    -0.370883      29.99
 C       3.969911    -0.405136     1.683609     116.72
 O       4.737437     0.829621     1.366068     155.07
 H       4.352228     1.586902     1.876706      28.55
 H       4.517812    -0.887841     2.512072      31.04
 H       2.935712     0.199231     1.940854      26.84
55
name = lig-Water-frame_759
 C      -1.967060     3.371338     2.982483      50.80
 H      -2.798953     4.228893     2.663056      22.90
 C      -0.971483     1.159135     2.635123      12.75
 H      -0.915896     0.221008     2.076166      28.38
 C       0.134991     1.525513     3.686772     -30.98
 O       1.118678     0.840722     4.180353     191.58
 C       0.695508    -0.425063     4.572682     123.18
 H       1.548332    -0.816254     5.229232      27.24
 H       0.439645    -1.367929     3.749939      25.15
 H      -0.011968    -0.508718     5.341313      29.63
 C       0.103967     2.992313     4.174209     -24.19
 O       1.210206     3.280377     5.010406     127.76
 H       0.977826     4.189970     5.656483      15.32
 C      -1.026856     3.868945     3.876374      57.16
 H      -1.367916     4.853162     4.354863      21.84
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 C      -2.009336     2.096273     2.414238      57.80
 C      -3.175476     1.564411     1.586855      85.76
 H      -4.017790     2.432611     1.690228      27.42
 O      -3.604536     0.312149     2.156975     166.48
 H      -4.596610     0.082456     1.808033      21.38
 C      -3.031337     1.732071     0.025984      64.81
 H      -2.467463     2.819329    -0.090782      23.81
 C      -4.350884     1.732217    -0.799872      89.88
 O      -5.250562     0.646702    -0.400360     247.22
 H      -4.755417    -0.106767    -0.800426      27.52
 H      -4.038769     1.715281    -2.016661      25.32
 H      -4.710703     2.816136    -0.783978      26.83
 C       1.434513     1.205681    -0.373456      53.74
 H       2.080902     2.065687    -0.060829      26.19
 C       0.978449    -1.043661    -1.282673      60.15
 H       1.512124    -1.775780    -1.830577      26.93
 C      -0.386387    -0.925300    -1.177132      21.69
 O      -1.454674    -1.779912    -1.626685     194.11
 C      -1.481704    -2.292081    -2.990597      96.17
 H      -2.602343    -2.628869    -3.082944      24.61
 H      -1.247455    -1.490812    -3.678259      27.98
 H      -0.790716    -3.293482    -3.407468      24.41
 C      -0.822534     0.261821    -0.528156       1.93
 O      -2.241271     0.477663    -0.435054      79.03
 C       0.016924     1.448216    -0.298962      49.00
 H      -0.305450     2.333817    -0.057440      27.28
 C       1.906535     0.080065    -0.933203      36.42
 C       3.378340    -0.388864    -0.971553      92.83
 H       3.300009    -1.070177    -1.869596      28.35
 O       4.319494     0.720248    -1.284831     146.21
 H       4.506356     0.909934    -0.390547      27.60
 C       3.885911    -1.289995     0.395981     100.02
 H       3.278043    -2.099315     0.619905      30.50
 O       5.205257    -1.685507     0.255132     211.80
 H       5.289538    -2.351027    -0.527300      26.31
 C       3.940679    -0.376174     1.703835     111.52
 O       4.780292     0.841789     1.339377     156.40
 H       4.357070     1.646700     1.910212      27.99
 H       4.465656    -0.941740     2.537053      30.95
 H       3.073305     0.113097     1.899134      28.94
55
name = lig-Water-frame_760
 C      -1.993200     3.401102     2.979298      56.69
 H      -2.764458     4.041505     2.887260      23.97
 C      -0.925260     1.220490     2.692377      48.68
 H      -1.012031     0.259759     2.171786      32.37
 C       0.101150     1.595712     3.708650     -38.13
 O       1.133255     0.870834     4.147017     130.38
 C       0.711741    -0.568534     4.563032     112.31
 H       1.625019    -0.918632     4.987165      30.01
 H       0.463054    -1.203537     3.867805      32.22
 H      -0.156034    -0.404197     5.333736      28.82
 C       0.088216     2.991859     4.152591      -7.07
 O       1.228347     3.282228     5.054536     213.29
 H       1.021176     4.072648     5.573167      19.96
 C      -0.958148     3.855643     3.828052      64.48
 H      -1.230325     4.747983     4.294275      24.00
 C      -1.973777     2.076351     2.443669      24.06
 C      -3.245189     1.622151     1.573194      84.32
 H      -4.126903     2.273877     1.756291      28.11
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 O      -3.587817     0.339503     2.195609     197.34
 H      -4.472739     0.158499     1.998074      27.45
 C      -2.983053     1.732265    -0.009146      88.71
 H      -2.518336     2.625100     0.030330      29.37
 C      -4.325157     1.736874    -0.857918      95.63
 O      -5.261429     0.688358    -0.386710     241.19
 H      -4.752278    -0.063799    -0.786376      28.23
 H      -4.046866     1.611919    -1.825004      30.77
 H      -5.026481     2.525989    -0.371997      24.78
 C       1.375933     1.306483    -0.405766      60.89
 H       2.163864     2.162068    -0.133465      27.82
 C       0.926499    -1.089526    -1.290370      48.76
 H       1.508967    -1.919470    -1.865337      25.08
 C      -0.363270    -0.941771    -1.230540      26.16
 O      -1.452392    -1.761765    -1.620303     231.93
 C      -1.468996    -2.233226    -2.963167      88.88
 H      -2.584798    -2.220016    -2.775296      22.08
 H      -1.219773    -1.364777    -3.628040      27.22
 H      -0.764883    -3.297839    -2.885276      23.01
 C      -0.807704     0.285648    -0.603028      16.45
 O      -2.233676     0.492666    -0.464207     117.43
 C       0.005825     1.359429    -0.304326      61.39
 H      -0.395293     2.527093    -0.089790      25.88
 C       1.929091     0.115388    -0.858276     -11.68
 C       3.347231    -0.340727    -0.944626      82.04
 H       3.575294    -0.974850    -1.916160      26.84
 O       4.324614     0.759730    -1.309987      99.17
 H       4.491915     1.076594    -0.258309      25.46
 C       3.906660    -1.222678     0.381144      91.59
 H       3.098412    -2.065486     0.713776      28.76
 O       5.242598    -1.744118     0.231953     194.68
 H       5.271154    -2.417829    -0.555459      24.79
 C       3.936435    -0.327900     1.670421     101.73
 O       4.825873     0.858701     1.326668     164.06
 H       4.373175     1.502800     1.856189      32.45
 H       4.307802    -0.980869     2.570252      30.91
 H       2.771754    -0.118061     2.041537      29.74
55
name = lig-Water-frame_761
 C      -2.001152     3.401824     2.983542      43.53
 H      -3.040997     4.011064     2.949165      21.51
 C      -0.848981     1.267617     2.790163      66.72
 H      -0.932852     0.238239     2.457258      31.62
 C      -0.000590     1.734544     3.667153      13.19
 O       1.165101     0.841329     4.120555      31.28
 C       0.739595    -0.663614     4.599841      89.18
 H       1.760315    -1.112136     4.904886      27.43
 H       0.320907    -1.185585     3.505192      28.36
 H      -0.108101    -0.388475     5.190019      29.87
 C       0.117533     2.962330     4.168322      24.98
 O       1.231169     3.244679     5.036319       4.13
 H       0.886541     4.101541     5.733156      17.23
 C      -0.904161     3.832565     3.777333      50.77
 H      -0.838843     4.864080     4.344787      22.11
 C      -1.991322     2.100560     2.444857     -53.02
 C      -3.281583     1.670700     1.582177      68.77
 H      -4.208557     2.348166     1.841983      25.29
 O      -3.569424     0.365775     2.231720     150.81
 H      -4.556322     0.061987     2.030698      23.73
 C      -2.955235     1.669379    -0.009562      81.35
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 H      -2.298142     2.692420    -0.191061      24.22
 C      -4.315471     1.756716    -0.812364      89.17
 O      -5.238376     0.709906    -0.401039     205.28
 H      -5.006231    -0.295092    -0.509500      26.37
 H      -4.158647     1.649352    -2.078660      24.80
 H      -4.936238     2.519269    -0.474522      25.99
 C       1.381906     1.386304    -0.445611      75.10
 H       1.980038     2.195095    -0.231870      31.89
 C       1.040238    -1.091064    -1.309232      49.86
 H       1.321840    -2.001437    -1.733862      25.41
 C      -0.444772    -0.917833    -1.245417      12.70
 O      -1.407708    -1.717918    -1.562262     248.81
 C      -1.481051    -2.167437    -2.923156      99.83
 H      -2.558696    -2.321122    -3.191505      26.83
 H      -1.053154    -1.512285    -3.687612      28.72
 H      -0.987714    -3.178045    -2.672128      24.65
 C      -0.861894     0.363909    -0.674898      24.48
 O      -2.223098     0.501003    -0.502078     183.59
 C      -0.019803     1.343304    -0.302500      75.84
 H      -0.518374     2.176299    -0.100300      30.22
 C       1.899513     0.048376    -0.810664       4.27
 C       3.381573    -0.304929    -0.938159     100.92
 H       3.594232    -0.988214    -1.729909      28.49
 O       4.314557     0.790169    -1.293948     120.39
 H       4.646013     1.394059    -0.515879      27.88
 C       3.898729    -1.144710     0.379879      95.12
 H       3.143221    -1.872703     0.502956      30.79
 O       5.277196    -1.798300     0.197604     189.02
 H       5.156737    -2.505310    -0.447600      29.44
 C       3.915929    -0.298369     1.615298     126.82
 O       4.843958     0.859378     1.337661     145.82
 H       4.376729     1.628255     1.912513      27.79
 H       4.332522    -0.872218     2.456980      33.04
 H       2.936659    -0.196780     1.924172      31.93
55
name = lig-Water-frame_762
 C      -2.021915     3.412123     3.001023      60.75
 H      -2.956943     3.940647     2.937051      28.02
 C      -0.899731     1.287904     2.815212      46.15
 H      -0.722340     0.193009     2.735383      29.83
 C       0.041629     1.753530     3.673349       1.43
 O       1.172469     0.793593     4.094921      43.75
 C       0.772993    -0.703508     4.538317     116.65
 H       1.584952    -1.229958     4.942375      29.65
 H       0.385482    -1.063801     3.708892      30.07
 H      -0.048385    -0.626508     5.330914      28.24
 C       0.162692     3.001785     4.215558      32.93
 O       1.203672     3.221315     5.008904      -1.15
 H       0.904915     3.932246     5.650391      24.00
 C      -0.858318     3.862928     3.764367      59.69
 H      -0.623882     4.808494     4.119856      24.08
 C      -2.028755     2.142791     2.432708     -29.13
 C      -3.262340     1.689702     1.619960      72.66
 H      -4.073716     2.500276     1.763143      27.55
 O      -3.575440     0.386435     2.259735     165.33
 H      -4.458166    -0.033580     1.943294      24.71
 C      -2.931891     1.639712    -0.009537     101.59
 H      -2.389056     2.407597    -0.406865      28.16
 C      -4.291549     1.731075    -0.790053     103.50
 O      -5.228338     0.707474    -0.410719     285.08
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 H      -4.981163    -0.218694    -0.314341      28.05
 H      -4.255185     1.846334    -1.777268      30.46
 H      -4.675170     2.882557    -0.728021      26.11
 C       1.385708     1.342918    -0.500560      54.57
 H       1.939755     2.438026    -0.266752      28.99
 C       1.094719    -1.026788    -1.300185      57.61
 H       1.378476    -2.122494    -1.577145      23.74
 C      -0.425233    -0.795874    -1.211815      20.42
 O      -1.403480    -1.691162    -1.502015     256.58
 C      -1.521673    -2.128611    -2.894704      89.62
 H      -2.361210    -2.458481    -3.583919      25.94
 H      -0.770704    -1.686143    -3.620150      28.72
 H      -1.025202    -3.364217    -2.956272      24.52
 C      -0.931104     0.394767    -0.752193      30.79
 O      -2.247040     0.500486    -0.534784     199.03
 C      -0.011764     1.385263    -0.305780      43.98
 H      -0.694382     2.320462     0.091117      26.58
 C       1.868221    -0.029615    -0.805532      15.00
 C       3.466528    -0.263297    -0.896666     104.98
 H       3.492375    -1.154536    -1.734926      27.20
 O       4.301561     0.831254    -1.295784     176.34
 H       4.582174     1.389672    -0.667131      32.39
 C       3.917703    -1.069801     0.336524      91.25
 H       3.120353    -1.930841     0.358102      28.29
 O       5.283733    -1.821539     0.169784     100.33
 H       5.029068    -2.675524    -0.422197      26.71
 C       3.945072    -0.283232     1.553327     112.92
 O       4.828640     0.876840     1.377296     158.98
 H       4.481943     1.617351     1.906241      30.82
 H       4.534868    -0.851885     2.413416      29.83
 H       2.832523     0.134382     1.816134      28.84
55
name = lig-Water-frame_763
 C      -1.999709     3.435536     3.036396      54.03
 H      -2.887192     4.150795     2.884084      30.39
 C      -0.998080     1.288585     2.819272      24.85
 H      -0.823950     0.239527     2.670251      32.37
 C       0.164526     1.661021     3.706780     -25.94
 O       1.157203     0.736120     4.080328     115.23
 C       0.779277    -0.657710     4.489982     107.56
 H       1.679381    -1.272473     4.928032      26.96
 H       0.309110    -1.312881     3.523258      26.65
 H       0.128056    -0.869486     5.389995      26.91
 C       0.155255     3.035874     4.207722      22.85
 O       1.204211     3.212398     4.999371     110.74
 H       1.034060     4.075660     5.686501      16.46
 C      -0.827443     3.907779     3.763550      75.65
 H      -0.718052     5.066266     3.904563      22.81
 C      -2.046747     2.158778     2.433582       0.16
 C      -3.190465     1.687319     1.643181      80.48
 H      -3.981303     2.513481     1.670224      29.33
 O      -3.593983     0.407158     2.274131     164.09
 H      -4.347601     0.043888     1.855512      27.84
 C      -2.953840     1.611379    -0.019092      86.22
 H      -2.379078     2.586845    -0.435093      27.83
 C      -4.258310     1.725124    -0.744861     100.46
 O      -5.246884     0.727941    -0.405864     214.14
 H      -4.624621    -0.086948    -0.393389      27.09
 H      -4.054667     1.764584    -2.023625      25.79
 H      -4.491189     2.697824    -0.564363      29.95
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 C       1.357827     1.275367    -0.535430      68.04
 H       1.924950     2.059553    -0.375075      36.76
 C       1.023420    -0.986803    -1.277221      64.69
 H       1.497027    -1.922096    -1.391182      26.67
 C      -0.328383    -0.688936    -1.198192      18.50
 O      -1.431627    -1.701486    -1.471268     184.40
 C      -1.475103    -2.183808    -2.912690     100.52
 H      -2.475399    -2.098192    -3.398497      28.25
 H      -0.584267    -1.657796    -3.324321      29.05
 H      -1.196155    -3.161458    -3.154385      29.42
 C      -0.942762     0.460098    -0.783983      28.61
 O      -2.312218     0.467992    -0.559310     148.50
 C      -0.029103     1.478202    -0.323754      50.11
 H      -0.298372     2.377381     0.221927      32.51
 C       1.927228    -0.019022    -0.819699      -4.80
 C       3.525805    -0.265887    -0.882766     123.90
 H       3.572404    -0.893518    -1.684755      32.40
 O       4.279834     0.860732    -1.341416      78.44
 H       4.484790     1.422870    -0.359409      26.95
 C       3.956793    -1.056747     0.257748     111.29
 H       3.214858    -1.864342     0.401476      30.75
 O       5.259369    -1.823463     0.142673     163.96
 H       5.101330    -2.561123    -0.451956      30.06
 C       3.982362    -0.249450     1.556293     131.90
 O       4.829264     0.913301     1.404805     122.28
 H       4.416507     1.553911     2.030322      30.11
 H       4.359690    -0.856298     2.314088      34.43
 H       3.062356     0.256018     1.722920      31.77
55
name = lig-Water-frame_764
 C      -1.958680     3.484442     3.068478      43.32
 H      -2.624235     4.371875     2.750198      28.25
 C      -1.008754     1.275122     2.873239      27.70
 H      -1.237356     0.267691     2.328102      31.77
 C       0.185977     1.567333     3.697092      22.13
 O       1.133562     0.670942     4.080831     173.71
 C       0.787058    -0.655920     4.426738     132.87
 H       1.792537    -0.966032     4.578137      29.66
 H       0.423320    -1.312711     3.711941      30.59
 H       0.117294    -0.709144     5.283655      29.55
 C       0.138062     2.984869     4.148353       3.99
 O       1.246335     3.253911     5.032959     151.67
 H       1.070828     4.050457     5.540892      24.86
 C      -0.836461     3.980483     3.752558      61.11
 H      -0.891969     5.033381     3.825280      22.03
 C      -2.022273     2.177948     2.480368      -7.11
 C      -3.124935     1.664532     1.620761      81.34
 H      -4.023783     2.437112     1.647176      26.80
 O      -3.605934     0.440740     2.279111     123.72
 H      -4.467012     0.120196     1.717633      21.83
 C      -2.956989     1.618119    -0.022961      96.97
 H      -2.468511     2.548921    -0.128417      29.86
 C      -4.223618     1.733599    -0.766021      98.89
 O      -5.239090     0.745227    -0.396904     196.63
 H      -4.639859    -0.043648    -0.635701      28.07
 H      -3.922707     1.556634    -1.693064      30.38
 H      -4.727480     2.719006    -0.279298      24.97
 C       1.325335     1.178212    -0.554252      50.68
 H       2.249462     2.008657    -0.331556      31.20
 C       0.978477    -0.954364    -1.226568      63.27
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 H       1.402045    -1.973674    -1.408293      27.51
 C      -0.322980    -0.678993    -1.225318       5.51
 O      -1.430937    -1.723252    -1.452959     166.93
 C      -1.410384    -2.193034    -2.926117      71.60
 H      -2.398612    -1.539062    -3.060939      23.15
 H      -0.660543    -1.514542    -3.324252      28.32
 H      -1.227988    -3.484685    -3.053255      22.62
 C      -0.928391     0.585359    -0.754272       7.81
 O      -2.362676     0.416292    -0.581532     128.53
 C      -0.035493     1.559761    -0.364386      74.24
 H      -0.076396     2.539182     0.240470      30.33
 C       2.002837     0.050695    -0.852867      13.20
 C       3.516813    -0.266344    -0.942934      91.59
 H       3.718537    -0.882907    -2.000840      26.31
 O       4.270495     0.918397    -1.346745     131.42
 H       4.370385     1.279254    -0.480657      34.07
 C       4.028322    -1.084642     0.239802     110.82
 H       3.178010    -1.825688     0.473767      29.33
 O       5.233645    -1.787129     0.120142     181.03
 H       5.166480    -2.520083    -0.650233      23.99
 C       4.029795    -0.220627     1.542212     111.82
 O       4.858798     0.973264     1.426733     143.18
 H       4.365042     1.514524     2.188550      27.19
 H       4.132807    -1.004461     2.501668      28.54
 H       2.924674     0.115490     1.762185      30.54
55
name = lig-Water-frame_765
 C      -1.923451     3.554447     3.046517      56.63
 H      -2.519031     4.335211     2.622048      25.95
 C      -0.993323     1.220116     2.910829      55.03
 H      -1.334203     0.456389     2.301318      26.96
 C       0.092309     1.530146     3.653605      37.33
 O       1.111755     0.650293     4.068614     162.30
 C       0.821863    -0.678313     4.388129      99.12
 H       1.929506    -0.945632     4.486995      26.01
 H       0.311027    -1.358764     3.490138      26.44
 H       0.089334    -0.518413     5.284547      25.15
 C       0.166994     2.912667     4.106761     -17.06
 O       1.287579     3.286215     5.035927      65.39
 H       0.924050     4.219353     5.573673      19.33
 C      -0.838814     3.988046     3.745516      59.45
 H      -0.784922     5.084956     4.029837      20.41
 C      -1.965410     2.222138     2.567617     -14.49
 C      -3.109412     1.640013     1.580860      90.68
 H      -3.952318     2.382702     1.697204      27.61
 O      -3.625962     0.472334     2.256876     186.49
 H      -4.455442     0.192386     1.838711      24.51
 C      -2.951829     1.613420     0.045169     102.10
 H      -2.298685     2.579527    -0.087992      26.76
 C      -4.246251     1.790186    -0.726137      88.98
 O      -5.198457     0.736682    -0.400752     153.79
 H      -5.084838    -0.204867    -0.710319      27.68
 H      -3.900333     1.603633    -1.927495      25.47
 H      -4.862996     2.634635    -0.529593      27.35
 C       1.392739     1.198730    -0.533534      52.44
 H       2.004594     1.920705    -0.262938      28.27
 C       1.028929    -0.958822    -1.171893      57.29
 H       1.094132    -2.021235    -1.531541      23.96
 C      -0.443231    -0.689323    -1.237540     -14.31
 O      -1.368061    -1.735227    -1.431221     215.05
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 C      -1.363172    -2.159553    -2.902315     106.03
 H      -2.193928    -1.571685    -3.161724      26.73
 H      -0.617692    -1.645236    -3.605268      26.95
 H      -1.522613    -3.195283    -2.881564      26.76
 C      -0.936885     0.639320    -0.724468       4.01
 O      -2.357919     0.400610    -0.595378     136.23
 C      -0.009567     1.635439    -0.405014      62.77
 H      -0.130820     2.693668     0.106458      24.83
 C       2.010710     0.044578    -0.928338      57.67
 C       3.491421    -0.279554    -1.099009      89.90
 H       3.625910    -0.893221    -1.878595      30.56
 O       4.265995     0.974513    -1.339810      70.75
 H       4.451906     1.476623    -0.438658      25.48
 C       4.061044    -1.108748     0.271715     102.37
 H       3.161883    -1.775222     0.488766      28.31
 O       5.242202    -1.751672     0.075794     213.47
 H       5.146621    -2.438685    -0.660531      26.15
 C       4.036808    -0.233397     1.541654     110.16
 O       4.879682     1.025772     1.470601     232.88
 H       4.531584     1.618261     2.138730      29.35
 H       4.231521    -0.776839     2.383206      31.10
 H       2.943363    -0.099991     1.646667      30.71
55
name = lig-Water-frame_766
 C      -1.900297     3.608302     2.975708      47.02
 H      -2.726420     4.314672     2.437401      22.09
 C      -1.048676     1.194624     2.897286      61.76
 H      -1.081057     0.123951     2.413786      23.34
 C       0.038140     1.531831     3.660398      13.79
 O       1.092258     0.697757     4.025167     190.36
 C       0.850118    -0.728749     4.347891     111.84
 H       1.733323    -1.288810     4.658452      27.91
 H       0.302846    -1.141712     3.527217      29.25
 H       0.265016    -0.777538     5.217432      27.84
 C       0.207040     2.900075     4.101663     -10.70
 O       1.287170     3.323542     5.008201     196.72
 H       0.965150     3.971938     5.577507      25.71
 C      -0.767653     3.941863     3.779350      85.59
 H      -0.497384     4.888174     4.301620      17.30
 C      -1.927170     2.239621     2.626196      16.53
 C      -3.116491     1.649818     1.591180      83.02
 H      -3.890199     2.553519     1.730713      27.65
 O      -3.635344     0.490008     2.233390     198.99
 H      -4.528869     0.176487     1.929534      22.06
 C      -2.934656     1.631380     0.112655     107.21
 H      -2.243954     2.385869    -0.261448      27.74
 C      -4.265995     1.797846    -0.746551     105.70
 O      -5.177352     0.714213    -0.397306     174.53
 H      -5.254221    -0.216838    -0.786960      24.71
 H      -4.104159     1.938282    -1.723050      30.84
 H      -4.858699     2.745248    -0.752748      28.24
 C       1.443251     1.297868    -0.497418      28.28
 H       2.084628     2.267524    -0.091465      20.79
 C       0.990619    -0.995866    -1.160745      43.68
 H       1.136431    -1.973230    -1.560318      23.56
 C      -0.491783    -0.658590    -1.193600      13.29
 O      -1.269184    -1.741059    -1.426882     204.51
 C      -1.339848    -2.060402    -2.869674      98.32
 H      -2.351935    -1.724545    -3.531449      24.36
 H      -0.452472    -2.060535    -3.552853      26.44
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 H      -1.704427    -3.300737    -2.862411      23.57
 C      -0.961296     0.578457    -0.726663      12.06
 O      -2.322637     0.449042    -0.582200     158.94
 C       0.050971     1.674157    -0.448208      48.13
 H      -0.277597     2.648540    -0.114496      23.50
 C       1.968575    -0.019677    -1.023134      22.24
 C       3.478530    -0.250498    -1.173206      70.08
 H       3.606062    -1.103214    -2.070899      25.63
 O       4.261902     1.014759    -1.343070      40.10
 H       4.503680     1.531441    -0.389538      19.81
 C       4.026684    -1.087597     0.288881      71.73
 H       3.244415    -1.882219     0.471068      26.03
 O       5.297002    -1.724368     0.017463     165.41
 H       5.083003    -2.526444    -0.564889      27.86
 C       4.034807    -0.230576     1.517630      86.36
 O       4.892646     1.047405     1.497634     220.54
 H       4.547037     1.749752     2.177604      26.16
 H       4.619688    -0.730391     2.493999      23.54
 H       2.944647     0.033965     1.597289      26.62
55
name = lig-Water-frame_767
 C      -1.864261     3.638775     2.897831      54.98
 H      -2.627570     4.201279     2.568255      21.27
 C      -1.095929     1.156826     2.875431      57.35
 H      -0.927327     0.147585     2.700708      20.14
 C       0.047631     1.555596     3.715051      -2.77
 O       1.094159     0.742010     3.987826     164.74
 C       0.861435    -0.760136     4.319743      85.28
 H       1.698618    -1.460648     4.583945      25.28
 H       0.278659    -1.208896     3.423452      25.08
 H       0.198221    -1.038779     5.284980      24.06
 C       0.226895     2.928995     4.121654      24.19
 O       1.278990     3.317197     4.943073     147.95
 H       0.925235     3.979112     5.779612      24.19
 C      -0.674574     3.867648     3.821958      64.85
 H      -0.414994     4.763629     4.327544      23.62
 C      -1.965462     2.213110     2.589615      38.89
 C      -3.135362     1.730914     1.668739      92.59
 H      -3.852565     2.589439     1.693528      29.21
 O      -3.639391     0.491487     2.216560     150.10
 H      -4.626131     0.182601     1.928524      19.69
 C      -2.929949     1.660106     0.089873     104.33
 H      -2.309621     2.508762    -0.262881      26.76
 C      -4.284351     1.783508    -0.751834      87.98
 O      -5.191521     0.699552    -0.388824     169.57
 H      -4.872010    -0.052152    -0.947695      27.76
 H      -4.020244     1.951585    -1.976538      26.68
 H      -4.812925     2.803599    -0.447269      27.60
 C       1.477823     1.424103    -0.474276      33.13
 H       2.176250     2.152584    -0.183120      21.65
 C       0.890687    -1.009017    -1.191292      39.96
 H       1.364973    -2.004285    -1.537559      22.19
 C      -0.406242    -0.632457    -1.121387      37.57
 O      -1.199596    -1.757550    -1.458267     233.93
 C      -1.379800    -2.041220    -2.867804     119.63
 H      -2.048558    -1.654861    -3.570219      28.38
 H      -0.329027    -2.308774    -3.182613      25.87
 H      -1.674022    -3.074970    -2.779162      27.30
 C      -0.941590     0.511274    -0.733908      25.05
 O      -2.299689     0.526258    -0.540904     184.68
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 C       0.106908     1.625038    -0.496015      44.18
 H      -0.456513     2.704166    -0.311077      21.21
 C       1.910390    -0.014936    -1.076217      -0.99
 C       3.471701    -0.242736    -1.179156      81.36
 H       3.717263    -0.814491    -1.968332      28.87
 O       4.253699     1.033321    -1.355895     166.76
 H       4.399160     1.246445    -0.476248      27.62
 C       3.991226    -1.053112     0.244622      64.51
 H       3.358122    -2.001853     0.446693      24.30
 O       5.357963    -1.694270    -0.046911     117.10
 H       5.092307    -2.660080    -0.394255      25.51
 C       4.067241    -0.197559     1.539722     105.73
 O       4.899711     1.058039     1.494569     273.75
 H       4.371101     1.611667     2.161528      27.06
 H       4.496752    -0.746762     2.239733      27.61
 H       3.041357     0.228361     1.845026      23.92
55
name = lig-Water-frame_768
 C      -1.742607     3.573810     2.879300      64.22
 H      -2.643025     4.432748     2.745795      24.83
 C      -1.050533     1.177673     2.934745      44.29
 H      -1.166284     0.045648     2.694963      25.57
 C       0.037486     1.585701     3.745708      14.08
 O       1.126730     0.730207     3.982212     150.40
 C       0.826604    -0.800247     4.301117     101.16
 H       1.885201    -1.185491     4.258911      27.38
 H       0.375354    -1.311083     3.373412      28.42
 H       0.178406    -0.879085     5.079969      28.42
 C       0.248500     2.906298     4.155284      25.75
 O       1.289591     3.307352     4.912975     154.55
 H       1.000666     3.912311     5.596466      34.73
 C      -0.684204     3.844031     3.797676      75.74
 H      -0.543239     4.928327     4.181922      21.14
 C      -2.040373     2.184042     2.492575      26.50
 C      -3.164627     1.821318     1.726768      80.32
 H      -4.060995     2.622060     1.716453      25.82
 O      -3.655619     0.487306     2.208624     140.81
 H      -4.501291     0.290342     1.873691      25.46
 C      -2.935726     1.722517     0.020022      87.18
 H      -2.510397     2.792900    -0.093973      26.48
 C      -4.283662     1.808887    -0.743102     107.73
 O      -5.193664     0.686607    -0.415856     195.48
 H      -4.594300     0.046315    -0.850817      29.43
 H      -4.054104     1.697102    -1.711908      30.70
 H      -4.706574     2.575864    -0.193788      29.17
 C       1.494155     1.437685    -0.520912      33.01
 H       2.360008     2.189990    -0.302891      21.85
 C       0.945448    -0.981161    -1.247229      46.94
 H       1.250426    -1.952517    -1.451823      25.41
 C      -0.349433    -0.713793    -1.084621      27.63
 O      -1.186560    -1.762334    -1.475628     238.20
 C      -1.354371    -2.087007    -2.849777      73.83
 H      -1.884393    -1.161246    -3.591207      24.46
 H      -0.321552    -2.211617    -3.147599      26.84
 H      -1.882309    -3.236786    -2.720805      22.69
 C      -0.865923     0.545425    -0.707999      22.98
 O      -2.277929     0.593413    -0.492248     182.38
 C       0.077975     1.575513    -0.533613      57.49
 H      -0.277548     2.494717    -0.407443      27.45
 C       1.864178     0.076112    -1.060818       5.00
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 C       3.446773    -0.230493    -1.117264      79.90
 H       3.844334    -0.810202    -2.116557      26.47
 O       4.227346     1.024029    -1.376401      75.26
 H       4.460918     1.173423    -0.272321      24.66
 C       3.983979    -1.019056     0.156619      71.64
 H       3.349950    -1.847896     0.386753      29.15
 O       5.397410    -1.658530    -0.099704      96.34
 H       5.250823    -2.536846    -0.411803      28.93
 C       4.087795    -0.132752     1.542542      98.12
 O       4.890553     1.052611     1.478206     230.46
 H       4.360632     1.632856     2.064997      27.38
 H       4.429674    -1.077010     2.350009      25.69
 H       3.155082     0.123940     2.018131      27.04
55
name = lig-Water-frame_769
 C      -1.674421     3.490097     2.878110      50.44
 H      -2.241890     4.290971     2.851172      27.67
 C      -1.032786     1.220816     2.990442      47.02
 H      -1.398145     0.288929     2.676802      32.18
 C       0.050461     1.570417     3.753501      25.74
 O       1.151804     0.681069     3.994090     125.16
 C       0.831628    -0.796277     4.216448     107.96
 H       1.895428    -0.940145     4.253368      28.95
 H       0.379524    -1.312888     3.342729      29.60
 H       0.120431    -0.756662     5.191708      27.25
 C       0.235782     2.882312     4.179270      13.63
 O       1.348063     3.285375     4.909828      28.18
 H       1.012165     4.077737     5.512770      32.79
 C      -0.734529     3.875791     3.738608      59.36
 H      -0.711740     4.886447     3.937112      22.02
 C      -2.010807     2.187696     2.455356      -6.06
 C      -3.268529     1.859935     1.696688      77.61
 H      -4.079596     2.557512     1.880453      27.39
 O      -3.655279     0.503083     2.207909     109.60
 H      -4.592586     0.300704     1.727017      19.61
 C      -2.958222     1.830925    -0.003792     100.77
 H      -2.540825     2.794592    -0.134889      28.86
 C      -4.273143     1.816469    -0.666152      86.10
 O      -5.165936     0.675780    -0.466784     132.90
 H      -4.708260    -0.252093    -0.588246      24.97
 H      -4.136586     1.771819    -1.879996      26.14
 H      -4.888741     2.795200    -0.183087      24.92
 C       1.497897     1.356336    -0.624594      72.98
 H       2.218707     2.224990    -0.511175      27.89
 C       1.087513    -0.916204    -1.296566      70.80
 H       1.248826    -2.045979    -1.486699      24.79
 C      -0.369146    -0.809360    -1.079225       9.03
 O      -1.221787    -1.764681    -1.445245     241.64
 C      -1.314189    -2.138271    -2.856350     104.98
 H      -1.546082    -1.211300    -3.141049      31.60
 H      -0.361825    -2.215060    -3.466923      28.69
 H      -2.132721    -2.877929    -2.996106      27.24
 C      -0.796473     0.567954    -0.673107      27.09
 O      -2.227596     0.653998    -0.451750     164.89
 C       0.060585     1.555558    -0.550780      58.52
 H      -0.272989     2.740488    -0.312695      24.50
 C       1.900855     0.191514    -0.998554      48.95
 C       3.430952    -0.224188    -1.096041     105.25
 H       3.532473    -0.857981    -1.921711      32.53
 O       4.200238     1.004023    -1.339060     154.20
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 H       4.614331     1.411285    -0.613614      29.64
 C       4.013922    -0.961851     0.081182      79.77
 H       3.176632    -1.780387     0.349770      29.50
 O       5.408610    -1.587597    -0.135202      95.72
 H       5.301848    -2.507395    -0.696002      23.57
 C       4.110696    -0.158390     1.549319     119.49
 O       4.874562     1.037472     1.461425     207.10
 H       4.500230     1.878916     1.961192      25.49
 H       4.475701    -0.857811     2.146880      33.93
 H       3.022398    -0.028563     1.997380      29.47
55
name = lig-Water-frame_770
 C      -1.683472     3.423026     2.853228      52.72
 H      -2.392883     4.389877     2.528079      25.25
 C      -1.099715     1.271367     2.991092      54.56
 H      -1.337999     0.201143     2.723145      35.76
 C       0.111938     1.526154     3.763308      -8.97
 O       1.147017     0.638518     4.001702     187.42
 C       0.847056    -0.728973     4.150267     130.39
 H       1.847488    -1.208712     4.510751      27.65
 H       0.297225    -1.300881     3.263694      27.83
 H       0.361303    -0.907010     5.048170      29.98
 C       0.200818     2.911817     4.191769      -7.85
 O       1.411986     3.268511     4.936114     103.79
 H       1.139605     4.226441     5.327815      25.04
 C      -0.695388     3.866366     3.716723      42.10
 H      -0.705987     5.000895     3.889986      22.98
 C      -1.921088     2.192120     2.469168      45.62
 C      -3.330208     1.840208     1.628182      70.50
 H      -4.129923     2.645688     2.080920      26.82
 O      -3.671657     0.538601     2.183531     120.51
 H      -4.532826     0.179520     1.822791      21.55
 C      -2.980989     1.918494     0.046453      83.16
 H      -2.344172     2.849122    -0.337768      26.66
 C      -4.304523     1.837057    -0.651528     122.51
 O      -5.132840     0.651249    -0.509665     218.79
 H      -4.906617    -0.257727    -0.408936      24.64
 H      -4.240445     2.160732    -1.637294      30.78
 H      -4.887667     2.612435    -0.484493      30.83
 C       1.430122     1.380372    -0.720567      63.80
 H       2.044898     2.233831    -0.644758      31.46
 C       1.120136    -0.882462    -1.318761      79.55
 H       1.592042    -1.836585    -1.587898      26.78
 C      -0.315102    -0.822304    -1.087294      21.11
 O      -1.277057    -1.808403    -1.381424     237.22
 C      -1.257270    -2.136052    -2.882429      77.52
 H      -1.610452    -0.986121    -3.229613      26.80
 H      -0.447669    -2.555118    -3.507604      28.55
 H      -2.279488    -2.725900    -3.204466      26.63
 C      -0.809638     0.504303    -0.647558       8.18
 O      -2.169290     0.713368    -0.413707     145.92
 C       0.104709     1.648649    -0.537414      60.06
 H      -0.255721     2.510636    -0.271401      30.38
 C       2.040382     0.150628    -0.959886      49.31
 C       3.423322    -0.163291    -1.065563     110.83
 H       3.321702    -0.962406    -1.987680      28.90
 O       4.182483     0.991550    -1.339750     173.94
 H       4.692942     1.482101    -0.663486      27.14
 C       4.038113    -0.927800     0.088141     110.71
 H       3.358843    -1.691577     0.249152      31.98
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 O       5.380015    -1.520018    -0.180147     104.43
 H       5.260123    -2.184891    -0.877799      29.31
 C       4.083195    -0.198053     1.500839     124.85
 O       4.870372     1.041192     1.443551     162.25
 H       4.503056     1.816863     1.891512      29.60
 H       4.859821    -0.897091     2.255242      28.18
 H       3.086472    -0.054614     1.754773      28.69
55
name = lig-Water-frame_771
 C      -1.748466     3.524174     2.822312      62.00
 H      -2.385424     4.031821     2.189931      26.18
 C      -1.102606     1.210468     3.006498      69.21
 H      -1.131755     0.145554     2.821661      33.30
 C       0.124034     1.526785     3.755285       2.13
 O       1.141107     0.626146     4.004542     184.53
 C       0.889368    -0.719487     4.110646     144.90
 H       1.649647    -1.410785     4.379905      30.13
 H       0.406773    -1.134604     3.276293      31.36
 H       0.199806    -1.024238     5.072369      27.18
 C       0.231548     2.913515     4.210201      19.07
 O       1.448535     3.272783     4.958876     161.88
 H       1.356260     4.116635     5.271326      31.00
 C      -0.642348     3.868424     3.700807      59.69
 H      -0.495737     4.892634     3.979842      26.34
 C      -1.923667     2.163203     2.443834     -36.66
 C      -3.297950     1.837889     1.611403      87.68
 H      -3.980836     2.580254     1.864927      30.72
 O      -3.690378     0.571883     2.147275     146.42
 H      -4.594951     0.162279     1.900337      19.86
 C      -2.978204     1.979589     0.112883      82.65
 H      -2.451415     2.773905    -0.234404      29.58
 C      -4.331443     1.841077    -0.688828      91.87
 O      -5.128046     0.649562    -0.551176     194.27
 H      -4.640844    -0.239685    -0.449701      24.92
 H      -4.123001     2.248128    -1.816588      26.96
 H      -5.184895     2.712333    -0.274588      23.97
 C       1.408859     1.463050    -0.796250      30.86
 H       2.123508     2.440920    -0.721006      29.98
 C       1.121731    -0.873624    -1.310862      65.30
 H       1.744253    -1.692322    -1.715863      27.43
 C      -0.253364    -0.771515    -1.090670      28.16
 O      -1.308479    -1.876366    -1.333828     190.14
 C      -1.268563    -2.063443    -2.923279      96.29
 H      -1.349030    -1.216805    -3.541717      30.83
 H      -0.460250    -2.808571    -3.169844      28.63
 H      -2.264359    -2.619110    -3.142856      28.90
 C      -0.815081     0.472601    -0.620711      16.90
 O      -2.139698     0.748278    -0.373576     133.12
 C       0.101380     1.650977    -0.529948      50.01
 H      -0.357855     2.735999    -0.151743      28.84
 C       2.063137     0.074909    -0.936689      27.96
 C       3.476448    -0.119173    -1.056020     123.93
 H       3.572839    -0.755134    -1.902723      34.42
 O       4.185964     1.009271    -1.395807     112.76
 H       4.660200     1.272250    -0.415927      27.59
 C       4.075364    -0.912699     0.144514     101.19
 H       3.426973    -1.942406     0.255060      30.65
 O       5.332670    -1.434504    -0.230155      78.48
 H       5.209530    -2.057964    -0.988110      26.38
 C       4.123921    -0.255782     1.440852     141.09
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 O       4.873212     1.052421     1.412784     134.32
 H       4.293092     1.670703     1.955533      30.13
 H       4.630425    -0.773627     2.108633      38.63
 H       2.996813    -0.033473     1.756726      31.07
55
name = lig-Water-frame_772
 C      -1.776628     3.598375     2.792431      35.16
 H      -2.407161     4.249784     2.047561      22.26
 C      -1.029823     1.106458     3.042210      48.17
 H      -1.120843     0.051468     2.797576      30.07
 C       0.086032     1.564811     3.739726      23.75
 O       1.160681     0.653611     4.017391     165.49
 C       0.869493    -0.786486     4.130123     114.59
 H       1.884440    -1.385812     4.122134      28.00
 H       0.414226    -1.041638     3.005129      29.01
 H       0.044997    -0.897008     4.767670      29.65
 C       0.310240     2.877773     4.219161      20.36
 O       1.462336     3.257753     4.962185      85.43
 H       1.407610     4.250888     5.420548      23.83
 C      -0.624395     3.883951     3.663266      41.94
 H      -0.294291     4.873148     4.055625      24.64
 C      -1.977965     2.152417     2.433398     -58.87
 C      -3.174217     1.835902     1.632743      76.59
 H      -4.037652     2.751263     1.655340      26.34
 O      -3.712965     0.586770     2.111614     126.39
 H      -4.729467     0.389146     1.813032      18.48
 C      -2.990396     1.951594     0.147815      74.26
 H      -2.504167     3.060099    -0.035973      26.62
 C      -4.380036     1.905994    -0.741677     106.71
 O      -5.113630     0.644059    -0.601447     222.05
 H      -4.323815     0.026827    -0.724633      28.19
 H      -4.066617     1.958372    -1.740572      29.93
 H      -4.932358     2.477388    -0.184667      30.10
 C       1.492115     1.529789    -0.844042      50.95
 H       2.080046     2.333320    -0.812380      34.16
 C       1.144340    -0.900352    -1.285863      62.74
 H       1.494017    -1.847538    -1.855079      25.48
 C      -0.282278    -0.727490    -1.081546       3.47
 O      -1.293604    -1.902748    -1.333382     172.54
 C      -1.291482    -2.039643    -2.920367      82.26
 H      -0.960681    -1.157650    -3.751343      27.00
 H      -0.514724    -2.815106    -2.807103      25.84
 H      -2.319142    -2.632116    -3.057836      26.68
 C      -0.782881     0.522437    -0.589149      25.42
 O      -2.151876     0.749033    -0.332993     161.53
 C       0.034708     1.625894    -0.514527      55.47
 H      -0.254563     2.588788    -0.260753      30.43
 C       1.955044     0.133518    -0.921434      17.13
 C       3.544875    -0.124491    -1.056862      94.33
 H       3.891447    -0.827173    -1.999970      31.22
 O       4.234263     1.067768    -1.422440     166.87
 H       4.508848     1.253562    -0.602547      35.08
 C       4.070721    -0.969382     0.155836     120.64
 H       3.481146    -1.771146     0.338490      35.85
 O       5.320653    -1.347167    -0.287764      63.27
 H       5.192891    -2.118415    -0.993996      22.24
 C       4.133451    -0.252308     1.407138     145.55
 O       4.861219     1.068845     1.379803      91.03
 H       4.188298     1.566774     1.982512      29.31
 H       4.551400    -1.051295     2.344509      30.66
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 H       3.195304    -0.085297     1.778401      31.31
55
name = lig-Water-frame_773
 C      -1.757342     3.593344     2.754135      45.76
 H      -2.180039     4.591053     2.436465      21.77
 C      -1.012040     1.079914     3.033374      42.29
 H      -1.194034     0.017362     2.727439      30.38
 C       0.094785     1.556218     3.750450      16.31
 O       1.187850     0.691406     4.044320     146.50
 C       0.840110    -0.840706     4.054300     111.24
 H       1.837928    -1.133348     4.153005      30.48
 H       0.547022    -1.080080     3.109172      33.99
 H      -0.065746    -1.002792     4.779197      27.84
 C       0.336469     2.891962     4.182213      12.34
 O       1.466615     3.250104     4.963651      73.18
 H       1.167278     4.057462     5.475038      27.78
 C      -0.599291     3.886448     3.632783      63.93
 H      -0.306240     4.935679     3.938261      19.66
 C      -1.965310     2.170230     2.507355     -38.65
 C      -3.111994     1.850670     1.647087      97.93
 H      -3.792283     2.635039     1.770824      29.87
 O      -3.749761     0.603458     2.080444     177.86
 H      -4.591321     0.525476     1.671692      23.69
 C      -2.973264     1.907538     0.122308     104.15
 H      -2.628548     2.861152     0.094771      31.21
 C      -4.369038     1.921135    -0.751650      82.76
 O      -5.062402     0.642928    -0.666562     231.39
 H      -4.369050     0.056863    -0.986558      29.42
 H      -4.083748     2.018887    -1.876203      27.85
 H      -5.012918     2.875559    -0.165723      25.51
 C       1.498819     1.513570    -0.844443      81.90
 H       2.273793     2.468258    -0.868725      30.63
 C       1.077118    -0.954873    -1.253972      72.95
 H       1.248592    -1.876037    -1.672259      26.09
 C      -0.348342    -0.731111    -1.065769      -1.23
 O      -1.245107    -1.845530    -1.358189     242.06
 C      -1.293506    -2.058042    -2.878226      97.35
 H      -0.770190    -1.319522    -3.406415      31.69
 H      -0.566218    -2.863835    -2.926806      27.26
 H      -2.373103    -2.470508    -3.177624      26.01
 C      -0.792677     0.586795    -0.561330      24.61
 O      -2.189475     0.730038    -0.299667     198.06
 C       0.084102     1.616935    -0.529544      65.78
 H      -0.374368     2.670094    -0.301036      27.89
 C       1.926854     0.256824    -0.957912      15.76
 C       3.541047    -0.163491    -1.107672      88.40
 H       3.779228    -0.845210    -1.897797      32.20
 O       4.291650     1.128167    -1.436614      35.44
 H       4.623902     1.689165    -0.545270      25.16
 C       4.046441    -0.987179     0.110620      98.21
 H       3.232414    -1.877765     0.400104      31.88
 O       5.362709    -1.305217    -0.361552     105.01
 H       5.296767    -2.135242    -0.807051      26.52
 C       4.175620    -0.250160     1.470712     136.19
 O       4.824115     1.067516     1.359263      92.27
 H       4.367770     1.684269     1.919848      30.38
 H       4.487697    -0.922823     2.136119      36.13
 H       3.052966    -0.028545     1.814413      31.25
55
name = lig-Water-frame_774
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 C      -1.650176     3.563981     2.781556      74.72
 H      -2.172036     4.512214     2.678121      23.50
 C      -1.048576     1.152211     2.994904      70.41
 H      -1.224845     0.156522     2.708367      26.96
 C       0.150283     1.505580     3.774292     -11.53
 O       1.190908     0.705602     4.076600     132.30
 C       0.810060    -0.818367     3.984426      97.52
 H       1.817824    -1.184128     4.455714      27.82
 H       0.572900    -1.278649     2.852117      27.15
 H       0.182441    -1.231889     4.815175      27.06
 C       0.302130     2.938391     4.101212      12.67
 O       1.441484     3.243069     4.963178     201.04
 H       1.025996     3.904702     5.561951      28.72
 C      -0.555415     3.873392     3.611102      73.16
 H      -0.454537     4.924454     3.720407      21.45
 C      -1.896053     2.190732     2.605683      33.86
 C      -3.114217     1.832153     1.649909      77.69
 H      -3.815650     2.772999     2.067003      25.40
 O      -3.757763     0.630341     2.069638     156.97
 H      -4.646698     0.429591     1.445712      20.38
 C      -2.960029     1.841832     0.084889      99.01
 H      -2.382672     2.895893    -0.170891      25.82
 C      -4.321602     1.946572    -0.728496     114.50
 O      -5.005441     0.662785    -0.737545     250.33
 H      -4.562024    -0.137661    -1.179156      26.45
 H      -4.155148     2.358523    -1.731834      29.19
 H      -4.904631     2.723994    -0.586754      31.31
 C       1.473467     1.538430    -0.812180      85.81
 H       2.135767     2.278131    -0.860431      31.46
 C       0.942850    -0.918557    -1.183569      61.00
 H       1.334024    -2.039928    -1.446452      25.69
 C      -0.396840    -0.745458    -1.040383      17.30
 O      -1.199368    -1.744847    -1.391891     252.98
 C      -1.263663    -2.123498    -2.790668      86.79
 H      -0.751296    -1.107463    -3.294716      26.46
 H      -0.732446    -3.058989    -3.235072      26.17
 H      -2.364629    -2.231176    -3.278636      24.87
 C      -0.853176     0.604222    -0.555584       9.39
 O      -2.221204     0.699486    -0.283380     184.27
 C       0.164626     1.686061    -0.547430      66.27
 H      -0.415799     2.631862    -0.366740      24.50
 C       1.990041     0.238587    -1.062719       4.25
 C       3.464649    -0.128847    -1.132699      78.40
 H       3.543856    -0.846430    -2.096237      26.18
 O       4.353532     1.164896    -1.434015      66.69
 H       4.526131     1.872556    -0.696751      27.31
 C       4.000410    -0.961891     0.077795      93.08
 H       3.435504    -1.791121     0.187993      32.21
 O       5.417860    -1.302110    -0.427441      54.65
 H       5.467556    -2.309127    -0.714384      24.79
 C       4.142839    -0.211467     1.505484     114.79
 O       4.800542     1.058826     1.342331     116.47
 H       4.486114     1.791675     1.963461      28.89
 H       4.809668    -0.963989     2.321448      27.14
 H       3.151913    -0.028110     1.771285      30.53
55
name = lig-Water-frame_775
 C      -1.529830     3.528676     2.847431      68.09
 H      -2.504870     4.181251     2.596672      22.69
 C      -1.024034     1.246725     2.997583      66.54
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 H      -1.295539     0.195048     2.665913      25.87
 C       0.157247     1.511084     3.765738      -0.37
 O       1.170783     0.661519     4.108678     182.62
 C       0.854243    -0.797574     3.934497     130.22
 H       1.652996    -1.304423     4.391772      31.22
 H       0.695325    -1.167828     3.034987      32.76
 H       0.117011    -1.183110     4.710582      28.41
 C       0.311648     2.912863     4.042372      16.12
 O       1.384552     3.243845     4.951449     160.37
 H       1.031749     3.879100     5.794440      25.98
 C      -0.511037     3.892803     3.581028      66.40
 H      -0.417483     5.036224     3.693601      20.22
 C      -1.872349     2.202775     2.627628      46.13
 C      -3.155469     1.867439     1.691296      88.19
 H      -3.784604     2.641352     1.913715      29.43
 O      -3.762278     0.645984     2.056869     255.63
 H      -4.500010     0.309593     1.571956      26.62
 C      -2.928873     1.867738     0.065363      99.85
 H      -2.299345     2.532484    -0.389217      28.25
 C      -4.219116     1.929724    -0.742452      94.20
 O      -4.971402     0.691535    -0.809571     206.86
 H      -4.645776    -0.117738    -1.278820      28.66
 H      -3.930215     2.391482    -1.759309      27.86
 H      -5.165406     2.724793    -0.397981      24.99
 C       1.488727     1.509901    -0.792595       0.37
 H       2.202088     2.482498    -0.808982      22.72
 C       0.932558    -0.851877    -1.113185      58.25
 H       1.312503    -1.772059    -1.188931      29.19
 C      -0.435686    -0.675488    -0.992700      24.74
 O      -1.211444    -1.694289    -1.414299     241.31
 C      -1.211391    -2.153861    -2.766094     112.91
 H      -0.874437    -1.273304    -3.308972      28.12
 H      -0.902828    -3.079908    -3.143056      28.01
 H      -2.296234    -1.832880    -3.096314      24.96
 C      -0.879055     0.608353    -0.577617      14.58
 O      -2.239253     0.644681    -0.287942     189.93
 C       0.102709     1.736639    -0.548463      59.94
 H      -0.227372     2.762866    -0.383925      25.18
 C       1.984887     0.155291    -1.159581      14.76
 C       3.395278    -0.053532    -1.160341      81.62
 H       3.498893    -0.575058    -2.131931      27.64
 O       4.391027     1.166061    -1.447936     125.84
 H       4.316654     1.694485    -0.700952      29.27
 C       4.028630    -0.886876     0.039201      78.32
 H       3.506994    -1.993483     0.033854      26.78
 O       5.451117    -1.323587    -0.478645      34.05
 H       5.482754    -2.320683    -0.645324      27.87
 C       4.125609    -0.205121     1.516339     111.46
 O       4.795411     1.068168     1.324332     147.43
 H       4.443369     1.650935     2.092805      27.68
 H       4.772976    -0.684904     2.129313      31.70
 H       3.058211    -0.075535     1.978903      28.61
55
name = lig-Water-frame_776
 C      -1.571860     3.502658     2.857616      51.16
 H      -2.365934     4.017250     2.516133      23.38
 C      -0.953557     1.242843     3.017210      62.64
 H      -1.242193     0.277703     2.725968      30.90
 C       0.136126     1.559312     3.729384      36.67
 O       1.142812     0.585747     4.138417     140.39
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 C       0.909262    -0.770984     3.966992     124.95
 H       1.831822    -1.410927     4.241775      27.84
 H       0.729437    -1.041261     2.731381      29.12
 H      -0.186716    -0.907631     4.371857      27.65
 C       0.384880     2.863633     4.048808       9.84
 O       1.323084     3.252039     4.958198      94.09
 H       1.079056     3.797112     5.624735      37.34
 C      -0.431094     3.979570     3.570986       0.31
 H      -0.182553     4.936487     3.867222      16.81
 C      -1.910695     2.214438     2.574924       1.45
 C      -3.162900     1.920038     1.713815      75.57
 H      -4.044837     2.820052     1.708342      25.34
 O      -3.736467     0.644240     2.073061     214.23
 H      -4.612457     0.325942     1.600631      23.41
 C      -2.884342     1.888747     0.084899      81.25
 H      -2.162990     2.689987    -0.402835      25.85
 C      -4.168840     1.939402    -0.783059     108.41
 O      -4.961654     0.717071    -0.881778     203.78
 H      -4.417058     0.048962    -1.320723      31.58
 H      -3.749497     2.187401    -1.771154      28.62
 H      -4.783111     2.397357    -0.146094      28.93
 C       1.503381     1.468695    -0.799221      -1.77
 H       2.065814     2.367148    -0.722609      25.92
 C       1.002742    -0.771912    -1.054276      59.28
 H       1.309474    -1.938965    -1.106392      26.34
 C      -0.428764    -0.574574    -0.962053      13.77
 O      -1.262229    -1.686497    -1.389064     162.72
 C      -1.204514    -2.100143    -2.779199      88.60
 H      -0.540815    -1.398705    -3.564385      26.06
 H      -0.902404    -3.258210    -2.837492      25.56
 H      -2.339605    -1.911434    -2.990367      25.15
 C      -0.897524     0.652473    -0.601896      25.21
 O      -2.257150     0.572188    -0.300327     171.17
 C       0.009533     1.742268    -0.549014      43.24
 H      -0.028495     2.901746    -0.317453      25.84
 C       1.875688     0.175462    -1.180025      61.24
 C       3.426049     0.011223    -1.204699      74.28
 H       3.721829    -0.568398    -2.173134      30.38
 O       4.385686     1.138101    -1.462463      88.01
 H       4.121280     1.593541    -0.462266      23.57
 C       4.084673    -0.860268    -0.013632      98.82
 H       3.579081    -1.749467     0.048199      30.18
 O       5.459409    -1.332049    -0.502250      55.94
 H       5.310825    -2.285320    -0.709108      28.38
 C       4.086925    -0.191983     1.451714     116.50
 O       4.780002     1.101382     1.324010     128.90
 H       4.432650     1.552181     2.082234      29.17
 H       4.841635    -0.905590     2.191053      28.00
 H       3.201114    -0.180953     2.098995      29.00
55
name = lig-Water-frame_777
 C      -1.642165     3.538080     2.861807      43.41
 H      -2.295806     4.496199     2.393394      21.85
 C      -0.963189     1.202651     2.985336      72.31
 H      -1.076495     0.096880     2.793544      32.34
 C       0.178309     1.550518     3.710197      28.82
 O       1.124978     0.562498     4.176360     142.31
 C       0.905960    -0.772980     3.921179     163.30
 H       1.754731    -1.337584     4.259885      30.88
 H       0.891295    -0.825420     2.922800      32.93
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 H      -0.114940    -0.990820     4.197388      30.25
 C       0.420228     2.924417     4.065176      26.00
 O       1.320683     3.232297     4.977054     115.14
 H       0.894002     4.030084     5.631098      20.83
 C      -0.359721     3.973617     3.556006      46.89
 H       0.006880     4.981673     4.019089      22.77
 C      -1.933526     2.188554     2.521037       8.55
 C      -3.186390     1.982920     1.678078      85.21
 H      -3.868640     2.708004     1.755929      31.48
 O      -3.706403     0.636240     2.098394     161.02
 H      -4.676985     0.569999     1.719708      23.00
 C      -2.817081     1.877548     0.102441      85.59
 H      -2.285691     2.812268    -0.026840      28.73
 C      -4.104580     1.919086    -0.806471      89.16
 O      -4.946316     0.730369    -0.959008     208.56
 H      -4.190167     0.142005    -1.292690      30.35
 H      -3.857420     2.257690    -1.843561      27.88
 H      -4.715478     2.730726    -0.067145      25.09
 C       1.383817     1.468226    -0.806090      61.35
 H       2.137831     2.307022    -0.689574      27.54
 C       0.989721    -0.828768    -1.013698      62.12
 H       1.251244    -1.826995    -1.150230      30.03
 C      -0.356117    -0.551390    -0.979517      -8.78
 O      -1.297353    -1.653005    -1.324090     159.80
 C      -1.203388    -2.035231    -2.813841     111.91
 H      -0.321729    -1.878512    -3.430332      29.24
 H      -0.977579    -3.014385    -2.531089      28.58
 H      -2.296825    -2.236013    -3.264293      26.96
 C      -0.943542     0.723808    -0.612939      15.23
 O      -2.274793     0.534979    -0.305926     159.62
 C       0.016128     1.755652    -0.551847      88.57
 H      -0.199986     2.693711    -0.225885      32.92
 C       1.890856     0.301168    -1.153017      47.52
 C       3.514133     0.011349    -1.284297      93.03
 H       3.794188    -0.753627    -2.094838      32.18
 O       4.323221     1.126624    -1.424039     152.78
 H       4.410922     1.633255    -0.623369      28.30
 C       4.134548    -0.822888    -0.066177      91.02
 H       3.388809    -1.765739     0.127585      30.42
 O       5.440609    -1.324099    -0.500445     117.97
 H       5.191897    -2.290422    -0.890834      23.55
 C       4.133035    -0.221248     1.375198     136.22
 O       4.746232     1.131499     1.334193     109.36
 H       4.440303     1.737913     2.127368      24.52
 H       4.624458    -0.985525     1.880818      34.20
 H       3.161370    -0.171308     1.943033      30.91
55
name = lig-Water-frame_778
 C      -1.667735     3.648518     2.858698      56.88
 H      -2.041975     4.498152     2.530312      23.08
 C      -1.000049     1.154144     2.932430      63.62
 H      -1.018402     0.088402     2.785356      31.08
 C       0.231699     1.523035     3.695674      -3.58
 O       1.114295     0.616117     4.236708     103.78
 C       0.878616    -0.782856     3.849216     114.06
 H       1.647104    -1.336806     4.467448      27.38
 H       1.082160    -0.864616     2.622569      29.18
 H      -0.062827    -1.428531     4.287824      24.99
 C       0.404861     2.970772     4.044099      22.94
 O       1.363312     3.232534     5.058110     137.07
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 H       0.963170     4.042267     5.490038      25.21
 C      -0.356492     3.921024     3.525735      59.09
 H      -0.150394     4.913055     3.845088      28.40
 C      -1.923644     2.199344     2.495450      -8.15
 C      -3.159148     1.943565     1.618918      83.59
 H      -3.925342     2.900981     1.948404      25.85
 O      -3.697392     0.659810     2.118366     163.99
 H      -4.587439     0.567159     1.876019      25.38
 C      -2.825950     1.836123     0.128305     109.52
 H      -2.219496     2.799604     0.071061      26.92
 C      -4.075173     1.965699    -0.783143     116.80
 O      -4.899085     0.748114    -1.030173     237.50
 H      -4.267289     0.011072    -1.210199      30.88
 H      -3.973196     2.458975    -1.790466      27.33
 H      -4.642134     2.826261    -0.638472      29.07
 C       1.275097     1.565397    -0.810500      64.57
 H       2.110246     2.317620    -0.677807      29.06
 C       0.988698    -0.871126    -1.011303      50.57
 H       1.330048    -1.959252    -1.265214      27.70
 C      -0.337566    -0.567308    -1.012579       8.45
 O      -1.311592    -1.573951    -1.264886     167.06
 C      -1.213190    -2.055436    -2.800460      85.43
 H      -0.193556    -1.834056    -3.330888      28.18
 H      -1.022239    -3.154328    -2.446200      25.88
 H      -2.112307    -2.130806    -3.510312      26.82
 C      -0.937797     0.722659    -0.640721      18.78
 O      -2.272475     0.565066    -0.296007     171.58
 C      -0.002289     1.766905    -0.542052      81.73
 H      -0.487918     2.736775    -0.050275      27.62
 C       1.981122     0.319962    -1.109684      -5.04
 C       3.566070    -0.034861    -1.310602     115.92
 H       3.667407    -0.753505    -2.205070      30.87
 O       4.274252     1.155448    -1.413826     153.50
 H       4.605250     1.619519    -0.594725      27.08
 C       4.114161    -0.813191    -0.108531     115.06
 H       3.434501    -1.599581     0.081326      33.18
 O       5.403481    -1.327657    -0.497024     137.27
 H       5.336272    -2.198483    -0.898444      27.06
 C       4.179238    -0.224388     1.275973     130.91
 O       4.715546     1.159396     1.355250     111.76
 H       4.406384     1.762417     2.073500      26.68
 H       4.801269    -1.115841     1.898456      29.12
 H       3.064070    -0.119822     1.491333      29.12
55
name = lig-Water-frame_779
 C      -1.602243     3.665263     2.858799      49.37
 H      -2.226618     4.659405     2.471371      20.62
 C      -0.985841     1.163545     2.907314      53.88
 H      -1.223583     0.115896     2.621301      30.30
 C       0.214271     1.543084     3.663689       7.98
 O       1.088932     0.664581     4.296122     122.73
 C       0.879592    -0.830987     3.777563     118.40
 H       1.615110    -1.249199     4.471072      28.05
 H       1.124654    -1.005245     2.830402      33.35
 H       0.056331    -1.352266     4.124559      29.41
 C       0.426116     2.896031     4.039385      10.35
 O       1.410037     3.236484     5.121369      82.94
 H       1.147432     4.061188     5.658184      24.73
 C      -0.449264     3.900393     3.471692      52.79
 H      -0.315669     4.990814     3.650137      28.18
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 C      -1.885428     2.266788     2.491204     -28.00
 C      -3.141522     1.888379     1.621852     105.87
 H      -3.731584     2.655947     1.780206      32.62
 O      -3.692104     0.699647     2.142177     188.47
 H      -4.692184     0.376695     1.863339      19.91
 C      -2.899523     1.829181     0.137914     110.16
 H      -2.122931     2.575225    -0.170052      27.94
 C      -4.069289     2.037758    -0.815500      96.81
 O      -4.847450     0.780189    -1.083036     251.21
 H      -4.379859    -0.054301    -1.113525      30.93
 H      -3.598963     2.346108    -1.815605      28.14
 H      -4.928685     2.857322    -0.657497      25.95
 C       1.336993     1.640304    -0.835476      19.61
 H       1.886432     2.561716    -0.684563      30.94
 C       1.073160    -0.862463    -1.052438      53.62
 H       1.363960    -1.911232    -1.327560      27.81
 C      -0.385155    -0.582417    -1.037584      17.18
 O      -1.328073    -1.494087    -1.250557     169.74
 C      -1.190387    -2.160738    -2.734672      65.07
 H      -0.293318    -1.503942    -3.039526      27.43
 H      -1.166357    -3.224195    -2.686763      26.91
 H      -1.920673    -1.610166    -3.554935      25.12
 C      -0.879171     0.648973    -0.678736      23.64
 O      -2.244749     0.631661    -0.276880     189.92
 C      -0.137611     1.807057    -0.493576      58.93
 H      -0.406185     2.711226    -0.082346      29.04
 C       1.995093     0.258596    -1.042355      -7.16
 C       3.541882    -0.059940    -1.281803     119.68
 H       3.511740    -0.493403    -2.358936      29.52
 O       4.250054     1.224219    -1.446730      78.33
 H       4.663116     1.318580    -0.407057      29.76
 C       4.095347    -0.828182    -0.164373     123.20
 H       3.381819    -1.766453     0.005176      29.08
 O       5.392288    -1.324758    -0.495247     123.75
 H       5.369979    -2.345531    -0.810460      23.47
 C       4.202296    -0.204847     1.193522     145.41
 O       4.705577     1.176130     1.358540     162.57
 H       4.249737     1.612236     2.111462      29.09
 H       4.743103    -0.768055     1.917075      33.81
 H       3.145367    -0.166977     1.337291      32.19
55
name = lig-Water-frame_780
 C      -1.600811     3.628363     2.781741      30.06
 H      -2.328364     4.303530     2.521967      24.19
 C      -0.966134     1.248134     2.884033      57.17
 H      -1.368380     0.306997     2.488648      25.89
 C       0.169768     1.563064     3.648969       7.72
 O       1.041865     0.663187     4.318916     136.41
 C       0.934423    -0.846142     3.792800      77.25
 H       1.745074    -1.289877     4.373078      25.51
 H       1.228244    -1.052156     2.608619      26.48
 H      -0.282353    -1.129151     3.958584      23.75
 C       0.439833     2.859840     4.056803      -9.30
 O       1.443895     3.222260     5.132624     -67.02
 H       1.154598     4.001241     5.850759      30.40
 C      -0.471815     3.915593     3.488506      65.39
 H      -0.250859     5.008943     3.614949      20.35
 C      -1.835932     2.303364     2.488986      -2.76
 C      -3.098092     1.845825     1.651187      70.31
 H      -3.950326     2.823403     1.655038      25.84
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 O      -3.715989     0.708578     2.181961     215.13
 H      -4.495022     0.345998     1.724709      24.63
 C      -2.939115     1.852227     0.113822      99.57
 H      -2.285476     2.631315    -0.232661      26.90
 C      -4.090868     2.090257    -0.910440     102.56
 O      -4.821741     0.832332    -1.128139     255.80
 H      -4.253925     0.012446    -0.968058      28.59
 H      -3.315888     2.146509    -1.689770      27.97
 H      -4.886161     2.627964    -0.462438      27.32
 C       1.394706     1.660637    -0.837960      19.17
 H       1.793560     2.750152    -0.766203      26.64
 C       1.114576    -0.810246    -1.116317      65.29
 H       1.456111    -1.820308    -1.342875      26.17
 C      -0.352895    -0.609658    -1.058099      11.88
 O      -1.377364    -1.483657    -1.281329     199.47
 C      -1.158702    -2.165358    -2.657995      85.50
 H      -0.230080    -1.664611    -2.881625      27.45
 H      -1.260092    -3.318277    -2.860427      25.23
 H      -1.871840    -1.504369    -3.201298      26.05
 C      -0.869561     0.630979    -0.669175      17.47
 O      -2.216622     0.665477    -0.265864     202.71
 C      -0.147045     1.805045    -0.484167      59.64
 H      -0.407041     2.862178    -0.101012      25.70
 C       1.950050     0.241820    -0.962496      34.87
 C       3.443595     0.001357    -1.292333     107.07
 H       3.517018    -0.428331    -2.280327      29.61
 O       4.242296     1.275170    -1.448539     166.32
 H       4.549537     1.359041    -0.637229      34.64
 C       4.098061    -0.909658    -0.216757     120.84
 H       3.468464    -1.792653    -0.063075      28.47
 O       5.423274    -1.345765    -0.513113     173.43
 H       5.275875    -2.306557    -0.640308      28.82
 C       4.174586    -0.144561     1.139870     121.62
 O       4.707064     1.189914     1.338578     166.71
 H       4.105250     1.499227     2.112615      28.17
 H       4.729263    -0.758750     1.991975      29.29
 H       3.076775    -0.181540     1.611958      28.21
55
name = lig-Water-frame_781
 C      -1.615203     3.575252     2.697210      66.02
 H      -2.512147     4.293199     2.447666      21.45
 C      -0.962383     1.349865     2.845421     102.90
 H      -1.212203     0.356487     2.510726      28.33
 C       0.158708     1.545446     3.683175     -31.03
 O       0.986096     0.614875     4.297824     121.49
 C       0.964833    -0.819220     3.800065     106.01
 H       1.685038    -1.460097     4.380791      26.98
 H       1.185589    -0.796119     2.797094      33.33
 H       0.017650    -0.996737     3.858481      29.99
 C       0.413695     2.938928     4.088379     -10.93
 O       1.458624     3.192694     5.107650     150.35
 H       0.974567     3.814648     5.666308      27.81
 C      -0.409587     3.936577     3.562654      68.94
 H      -0.114994     4.924843     3.771016      20.50
 C      -1.829223     2.269876     2.454510      59.64
 C      -3.106246     1.906172     1.662056      85.69
 H      -3.765903     2.622933     1.764288      31.69
 O      -3.730701     0.698611     2.230242     202.33
 H      -4.415772     0.396033     1.595914      27.03
 C      -2.926165     1.888970     0.092085      83.84
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 H      -2.456455     2.978933     0.001090      26.29
 C      -4.079843     2.045646    -0.974157     101.96
 O      -4.817021     0.871808    -1.175764     263.48
 H      -4.100706     0.269686    -0.871099      29.77
 H      -3.526061     2.383460    -1.925061      27.56
 H      -4.760002     2.877316    -0.524251      27.38
 C       1.365570     1.650962    -0.799619      56.36
 H       2.002237     2.486473    -0.888200      29.35
 C       1.051885    -0.779424    -1.180819      89.15
 H       1.637939    -1.799766    -1.380780      25.10
 C      -0.286086    -0.625364    -1.060706      13.82
 O      -1.420120    -1.535404    -1.320132     225.25
 C      -1.124724    -2.120556    -2.579675     101.98
 H       0.021960    -2.188035    -3.001006      25.75
 H      -1.380458    -3.181950    -2.734990      29.56
 H      -2.057389    -1.552270    -3.136649      24.39
 C      -0.887816     0.683068    -0.615467      17.35
 O      -2.205926     0.656855    -0.269169     184.47
 C       0.000874     1.785244    -0.513611      65.38
 H      -0.505185     2.745062    -0.270238      27.04
 C       1.921917     0.354932    -0.903525      45.31
 C       3.352365     0.098899    -1.310105      85.64
 H       3.533767    -0.548876    -2.313174      27.26
 O       4.213298     1.296658    -1.462738      95.00
 H       4.591347     1.693684    -0.501935      25.66
 C       4.107842    -0.940576    -0.243688      92.36
 H       3.443972    -1.866922    -0.053054      29.23
 O       5.470895    -1.366194    -0.539626     158.84
 H       5.404472    -2.388862    -0.700698      24.93
 C       4.101241    -0.132810     1.171198     116.35
 O       4.700290     1.204589     1.301613     158.91
 H       4.210541     1.659511     2.000244      31.43
 H       4.711948    -0.892408     1.741988      30.07
 H       3.205931    -0.098410     1.668277      31.44
55
name = lig-Water-frame_782
 C      -1.588810     3.603994     2.676968      75.67
 H      -2.338329     4.394990     2.413452      26.00
 C      -0.896169     1.339642     2.832329      68.50
 H      -0.954566     0.252178     2.599214      27.74
 C       0.159063     1.556057     3.742928      -4.64
 O       0.942072     0.560538     4.268649     156.15
 C       1.003867    -0.744537     3.815574      92.69
 H       1.517388    -1.452973     4.444315      27.39
 H       1.317762    -0.609465     2.663835      30.85
 H      -0.187107    -1.311463     3.896781      25.11
 C       0.391811     2.978305     4.121486      14.96
 O       1.446616     3.157874     5.044639     226.71
 H       0.896295     3.873777     5.689825      19.52
 C      -0.388776     3.951012     3.603715      73.01
 H      -0.082312     5.023048     3.967982      19.63
 C      -1.889231     2.254094     2.373331      33.94
 C      -3.124722     1.936920     1.651191      63.98
 H      -3.907453     2.889900     2.024921      23.80
 O      -3.725344     0.697050     2.259122     158.40
 H      -4.531117     0.412590     1.595325      24.04
 C      -2.899498     1.963176     0.080158      94.61
 H      -2.439834     2.892859     0.098008      29.38
 C      -4.051219     2.053316    -1.009337     120.36
 O      -4.816530     0.890654    -1.217175     272.86
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 H      -4.162741     0.233230    -0.948501      31.99
 H      -3.932281     2.567554    -2.009516      26.70
 H      -4.528854     3.023924    -0.822207      28.17
 C       1.367424     1.629467    -0.746703      97.52
 H       2.259211     2.317743    -0.945933      32.93
 C       1.033492    -0.757887    -1.222675      88.41
 H       1.495645    -1.612085    -1.468660      28.72
 C      -0.337380    -0.594159    -1.022905       6.98
 O      -1.394027    -1.587341    -1.327727     236.92
 C      -1.127386    -2.107565    -2.574368     127.47
 H      -0.231955    -2.307219    -2.946723      32.00
 H      -1.571087    -3.214220    -2.377422      27.29
 H      -1.783497    -1.674881    -3.428383      28.48
 C      -0.834643     0.708448    -0.570233      24.09
 O      -2.202271     0.659922    -0.276849     155.41
 C       0.085209     1.764994    -0.548483      77.30
 H      -0.407324     2.697662    -0.451038      29.05
 C       1.889400     0.449888    -0.904297      22.85
 C       3.342260     0.158275    -1.318009      95.82
 H       3.337822    -0.320562    -2.237435      28.52
 O       4.182893     1.310210    -1.472422     112.56
 H       4.338435     1.858078    -0.588499      27.92
 C       4.086270    -0.893636    -0.239757      88.09
 H       3.455177    -1.826351    -0.057971      28.98
 O       5.511492    -1.374757    -0.566578     118.97
 H       5.572170    -2.349210    -0.904242      23.36
 C       4.065186    -0.179752     1.203326      86.01
 O       4.697650     1.217281     1.244509     103.65
 H       4.376944     1.829633     1.942058      30.45
 H       4.769252    -0.922088     1.723776      29.07
 H       2.965103    -0.047574     1.684659      28.53
55
name = lig-Water-frame_783
 C      -1.514998     3.655765     2.716337      48.85
 H      -2.094961     4.553083     2.399045      23.87
 C      -0.823493     1.260851     2.827494      23.65
 H      -0.878097     0.212821     2.610609      30.71
 C       0.138251     1.601835     3.780303      24.59
 O       0.913516     0.552332     4.279396     226.12
 C       0.952825    -0.716062     3.775664     116.29
 H       1.619686    -1.242627     4.524215      27.50
 H       1.454462    -0.800816     2.819486      35.44
 H       0.177364    -1.304775     3.765844      33.91
 C       0.390759     2.915661     4.147647      24.93
 O       1.404729     3.160160     5.003607     216.74
 H       1.320504     3.848531     5.652220      26.03
 C      -0.434643     3.990478     3.598626      30.56
 H      -0.292619     4.950530     3.936227      21.98
 C      -1.880429     2.283340     2.329016     -54.29
 C      -3.219945     1.972319     1.647935      93.81
 H      -3.768584     2.734485     1.900772      32.07
 O      -3.719779     0.712007     2.238674     186.53
 H      -4.574911     0.462404     1.943228      26.58
 C      -2.902341     2.011456     0.052427      81.93
 H      -2.056420     2.865828    -0.118832      25.73
 C      -4.014423     2.142421    -1.043014      97.85
 O      -4.827402     0.897127    -1.242042     208.14
 H      -4.343787     0.021441    -1.144185      30.92
 H      -3.736902     2.378461    -2.104819      27.67
 H      -4.755392     2.965543    -0.661548      27.63
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 C       1.480270     1.669591    -0.703471      54.68
 H       2.118911     2.524474    -0.813547      33.22
 C       1.020388    -0.674887    -1.217116      59.88
 H       1.400705    -1.748592    -1.718882      26.80
 C      -0.428656    -0.551426    -0.976055      22.88
 O      -1.316490    -1.583576    -1.294979     215.16
 C      -1.222132    -2.193511    -2.617672     115.01
 H       0.028550    -2.352131    -2.828732      25.33
 H      -1.690115    -3.095874    -2.277791      29.34
 H      -1.355039    -1.705022    -3.695073      27.57
 C      -0.774422     0.675458    -0.540405      34.15
 O      -2.187375     0.703124    -0.278415     163.39
 C       0.020649     1.791074    -0.559233      62.77
 H      -0.276542     2.945006    -0.580398      25.47
 C       1.886797     0.359093    -0.971580      37.31
 C       3.377085     0.187187    -1.276900      95.71
 H       3.158454    -0.159848    -2.443749      25.29
 O       4.150098     1.339804    -1.494733     168.30
 H       4.121563     1.733158    -0.653911      32.94
 C       4.060542    -0.810814    -0.226829      95.30
 H       3.452127    -1.727066    -0.125232      29.76
 O       5.536687    -1.340891    -0.592204      79.96
 H       5.413474    -2.290082    -0.912216      26.37
 C       4.043988    -0.226602     1.228535     103.57
 O       4.695921     1.217699     1.166548      25.56
 H       4.451327     1.729523     2.051056      25.48
 H       4.729493    -0.781796     1.996429      30.70
 H       3.083681    -0.174058     1.513194      32.89
55
name = lig-Water-frame_784
 C      -1.458620     3.680627     2.758577      59.86
 H      -1.947915     4.652390     2.302470      22.53
 C      -0.839774     1.234328     2.796712      21.90
 H      -0.982481     0.166467     2.525908      30.61
 C       0.110308     1.594653     3.774662      28.72
 O       0.889983     0.606098     4.324990     183.00
 C       0.965335    -0.737607     3.748281      92.44
 H       1.721012    -1.030131     4.461019      26.95
 H       1.593753    -0.937294     2.767465      31.11
 H      -0.103656    -1.463023     3.607976      26.58
 C       0.347568     2.908445     4.158111      28.10
 O       1.405311     3.154338     4.987595     118.65
 H       1.429742     4.027887     5.558945      27.35
 C      -0.474681     3.962338     3.593757      44.31
 H      -0.437683     5.086203     3.909136      23.07
 C      -1.775435     2.311325     2.352002     -61.65
 C      -3.259949     1.978763     1.613710      66.43
 H      -4.079413     2.955478     1.812663      26.25
 O      -3.711307     0.738263     2.202780     141.51
 H      -4.762620     0.536655     2.113564      23.16
 C      -2.869541     2.036524     0.002514     100.72
 H      -2.135811     2.669295    -0.229376      30.86
 C      -4.000219     2.220991    -1.065325      90.33
 O      -4.855952     0.906399    -1.254793     197.44
 H      -4.360017     0.054149    -1.331860      31.99
 H      -3.341031     2.282968    -1.960693      28.05
 H      -4.874963     2.657645    -0.616187      26.21
 C       1.508282     1.709228    -0.661595      -0.89
 H       1.963591     2.744286    -0.606255      25.68
 C       0.953895    -0.660530    -1.219179      86.33
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 H       1.237211    -1.462310    -1.704161      32.94
 C      -0.409014    -0.557384    -0.972946      39.96
 O      -1.252277    -1.548221    -1.254882     206.04
 C      -1.211480    -2.296082    -2.674482     109.23
 H      -0.280176    -2.572683    -2.567753      30.48
 H      -1.849087    -3.273308    -2.595758      28.43
 H      -1.422911    -1.636193    -3.524551      29.84
 C      -0.826944     0.688589    -0.496892      18.46
 O      -2.176734     0.767235    -0.273539     179.07
 C       0.033805     1.884956    -0.570735      45.11
 H      -0.313999     2.829037    -0.555029      25.99
 C       1.937235     0.287870    -1.035016      -4.15
 C       3.406912     0.152099    -1.290911     104.80
 H       3.401197    -0.265806    -2.220699      30.32
 O       4.118514     1.383689    -1.519858      67.51
 H       4.087114     1.798768    -0.454061      21.38
 C       4.077494    -0.742860    -0.214101      99.16
 H       3.394843    -1.712441    -0.274114      30.57
 O       5.523534    -1.271705    -0.613823      92.81
 H       5.273299    -2.259712    -0.726264      27.22
 C       4.089692    -0.233143     1.226658     105.84
 O       4.674294     1.201987     1.107400      31.75
 H       4.471197     1.430270     2.002822      28.23
 H       4.552665    -0.733116     2.058818      33.85
 H       2.902064    -0.204651     1.535510      29.88
55
name = lig-Water-frame_785
 C      -1.479434     3.668803     2.723931      50.43
 H      -1.982614     4.443253     2.279987      20.03
 C      -0.925623     1.267661     2.758441      66.50
 H      -1.151821     0.255324     2.447156      27.04
 C       0.076928     1.549684     3.731291       1.23
 O       0.873234     0.655792     4.367478     164.68
 C       0.985148    -0.794035     3.724856      93.01
 H       1.670741    -1.247165     4.487852      26.54
 H       1.483401    -0.717977     2.733027      29.49
 H       0.105002    -1.171912     3.700618      31.32
 C       0.285340     2.955119     4.163087      -1.80
 O       1.441327     3.148856     4.993459     102.17
 H       1.105075     4.054466     5.311512      26.96
 C      -0.449200     3.948907     3.655142      39.22
 H      -0.335248     4.965811     3.900017      21.98
 C      -1.691060     2.327954     2.386659      23.55
 C      -3.243135     2.045460     1.572237      76.88
 H      -3.968109     2.697292     1.694348      30.77
 O      -3.725315     0.761255     2.158966     176.40
 H      -4.724874     0.693931     1.970351      25.13
 C      -2.867632     2.008913    -0.009746      86.64
 H      -2.162239     2.999247    -0.170509      23.59
 C      -3.985289     2.187607    -1.062444      92.63
 O      -4.882104     0.925948    -1.267311     235.33
 H      -4.211139     0.258664    -1.464356      31.65
 H      -3.333552     2.532741    -1.928785      28.41
 H      -4.833605     2.906060    -0.839443      26.77
 C       1.444266     1.704975    -0.641578      43.05
 H       2.047963     2.616543    -0.439621      26.42
 C       0.926108    -0.661066    -1.230867      47.87
 H       1.276777    -1.663809    -1.838208      25.50
 C      -0.357079    -0.536502    -0.979095      25.92
 O      -1.251097    -1.554835    -1.233268     179.08
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 C      -1.190946    -2.395865    -2.674848      70.30
 H      -0.121400    -3.014123    -2.598996      23.98
 H      -2.011113    -3.140818    -2.958499      26.11
 H      -1.574813    -1.433073    -3.281073      24.17
 C      -0.888588     0.779431    -0.474268      17.81
 O      -2.193022     0.817633    -0.269032     207.45
 C       0.103591     1.904568    -0.569579      54.88
 H      -0.482517     2.945384    -0.406104      19.65
 C       1.973080     0.361188    -1.053648      24.68
 C       3.451898     0.102723    -1.314903      90.56
 H       3.845269    -0.704933    -2.215813      27.60
 O       4.080684     1.438629    -1.504538      84.45
 H       4.240655     1.851719    -0.712908      30.14
 C       4.123230    -0.743176    -0.209066     111.21
 H       3.497914    -1.589333    -0.272960      33.22
 O       5.468829    -1.190630    -0.626200     103.60
 H       5.484966    -2.180038    -0.562247      26.46
 C       4.093777    -0.190780     1.186113     138.85
 O       4.637922     1.152780     1.077762      80.10
 H       4.470287     1.505217     2.030926      23.93
 H       4.557200    -0.917301     2.055950      30.86
 H       3.118219    -0.066879     1.485387      30.52
55
name = lig-Water-frame_786
 C      -1.491531     3.639427     2.696307      92.67
 H      -2.295880     4.426118     2.207541      26.88
 C      -0.985795     1.281124     2.763727      66.66
 H      -1.317844     0.315739     2.392244      24.54
 C       0.038436     1.538165     3.684470      -1.36
 O       0.872008     0.662042     4.394652      98.02
 C       1.047100    -0.778551     3.740642      87.09
 H       1.516540    -1.539626     4.397541      25.80
 H       1.361927    -0.522314     2.707820      26.92
 H      -0.186824    -1.166707     3.785715      22.03
 C       0.283537     2.900987     4.171254     -17.14
 O       1.442621     3.159794     4.987465      13.46
 H       1.132016     3.974659     5.456119      27.11
 C      -0.454151     3.979727     3.690493      91.06
 H      -0.105027     5.019825     3.997937      13.85
 C      -1.741088     2.372427     2.361909      50.42
 C      -3.128395     2.064767     1.530215      63.68
 H      -4.030773     2.938881     1.753184      25.92
 O      -3.742544     0.797012     2.102693     197.32
 H      -4.610836     0.683699     1.731709      26.85
 C      -2.892909     2.036890     0.028352     121.76
 H      -2.474152     2.970812     0.003396      28.18
 C      -4.010113     2.139101    -1.058654     110.47
 O      -4.874414     0.970853    -1.281681     272.04
 H      -4.128572     0.353992    -1.579796      29.59
 H      -3.648317     2.567869    -2.038311      27.49
 H      -4.461157     3.173523    -1.030519      27.70
 C       1.433511     1.655831    -0.647512      67.71
 H       2.201295     2.362561    -0.406784      28.84
 C       1.046034    -0.671101    -1.283550      67.08
 H       1.262891    -1.613561    -1.697348      24.10
 C      -0.389861    -0.469308    -0.971011      13.88
 O      -1.290021    -1.606095    -1.220787     158.39
 C      -1.155449    -2.442915    -2.647238      95.90
 H      -0.347941    -3.014013    -2.919541      30.02
 H      -2.102237    -3.004152    -2.827635      26.50
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 H      -1.209604    -1.583457    -3.214896      29.60
 C      -0.846194     0.855579    -0.515997      45.78
 O      -2.223779     0.848267    -0.271590     226.94
 C       0.050579     1.898460    -0.529320      29.67
 H      -0.211576     2.859945    -0.244754      21.59
 C       1.947924     0.452495    -1.066203      23.79
 C       3.523933     0.063256    -1.342620      99.43
 H       3.832763    -0.532802    -2.074380      33.81
 O       4.049997     1.468717    -1.526800      35.00
 H       4.376137     1.882408    -0.648091      25.86
 C       4.167159    -0.773335    -0.205688     114.66
 H       3.458885    -1.766307    -0.118140      30.55
 O       5.426300    -1.109229    -0.629835     118.16
 H       5.672814    -2.060488    -0.513760      22.56
 C       4.102995    -0.154948     1.151848     139.66
 O       4.617262     1.109555     1.095657     125.88
 H       4.479383     1.769545     1.847491      22.94
 H       4.621169    -0.860023     1.767418      34.24
 H       2.975351     0.025241     1.493551      27.90
55
name = lig-Water-frame_787
 C      -1.509660     3.707450     2.703266      57.63
 H      -2.211823     4.348587     2.425285      30.60
 C      -1.030907     1.271567     2.790790      49.61
 H      -1.353140     0.277905     2.424123      23.05
 C       0.027050     1.539681     3.679260      17.15
 O       0.885991     0.623627     4.407179     125.57
 C       1.002250    -0.725326     3.781724     126.62
 H       1.566702    -1.526784     4.253780      27.83
 H       1.336090    -0.549575     2.676179      28.70
 H       0.103565    -1.104263     3.680262      29.10
 C       0.310081     2.834435     4.164874     -15.34
 O       1.415482     3.164579     4.971004      33.88
 H       1.342182     3.849492     5.795701      25.52
 C      -0.488137     4.005509     3.681943      47.45
 H      -0.036347     4.968916     3.992795      14.00
 C      -1.873865     2.376313     2.290680      21.07
 C      -3.068546     2.087782     1.539216     113.18
 H      -3.564202     2.938253     1.765334      29.19
 O      -3.735163     0.853309     2.049547     160.71
 H      -4.577848     0.530992     1.435933      23.30
 C      -2.963182     2.075591     0.058470      98.36
 H      -2.362969     3.123506    -0.111864      25.90
 C      -4.047580     2.154182    -1.072556     104.02
 O      -4.847588     1.029093    -1.291805     256.72
 H      -4.278500     0.301255    -1.622378      30.47
 H      -3.614905     2.153536    -2.136873      26.90
 H      -4.509680     3.126161    -0.796397      28.87
 C       1.451589     1.617045    -0.660082      59.06
 H       2.275111     2.380043    -0.396866      27.30
 C       1.100846    -0.630666    -1.308519     128.49
 H       1.445168    -1.697907    -1.641757      23.04
 C      -0.380359    -0.438783    -0.999549      22.51
 O      -1.317383    -1.660308    -1.213707     148.10
 C      -1.141958    -2.419192    -2.598832      67.74
 H      -0.257750    -3.162518    -2.960207      25.40
 H      -2.193487    -2.925756    -2.500767      23.89
 H      -0.772951    -1.631917    -3.497022      26.95
 C      -0.828186     0.844589    -0.599124      45.63
 O      -2.219368     0.866413    -0.286158     221.21
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 C       0.016203     1.906671    -0.459192      69.55
 H      -0.103245     2.970437    -0.044283      22.10
 C       1.938743     0.420322    -1.114403      29.63
 C       3.536430     0.114065    -1.311943      92.87
 H       3.603364    -0.371061    -2.507276      29.52
 O       4.042612     1.483374    -1.561735       4.45
 H       4.497681     1.667932    -0.564502      24.91
 C       4.116842    -0.822624    -0.203234     118.93
 H       3.608533    -1.695358    -0.048952      31.91
 O       5.453488    -1.038212    -0.635706     116.28
 H       5.623997    -2.037446    -0.542525      25.28
 C       4.051298    -0.133762     1.145369     133.37
 O       4.647599     1.132093     1.115118     127.33
 H       4.325859     1.749804     1.771319      26.13
 H       4.792154    -0.854303     1.788706      29.74
 H       3.021435    -0.214452     1.474693      28.00
55
name = lig-Water-frame_788
 C      -1.528170     3.759225     2.743445      37.45
 H      -2.252303     4.743477     2.540176      21.46
 C      -1.097355     1.283840     2.805064      61.98
 H      -1.245126     0.245037     2.560704      25.63
 C       0.045641     1.528932     3.720816     -23.13
 O       0.898918     0.563782     4.405354     148.71
 C       0.958756    -0.649137     3.784583     136.05
 H       1.781619    -1.238484     4.305437      27.72
 H       1.388782    -0.638235     2.781731      30.24
 H      -0.155150    -1.264584     3.588641      22.45
 C       0.302764     2.872245     4.139388     -15.37
 O       1.406578     3.141325     4.963658     105.62
 H       1.160910     3.705803     5.725127      30.09
 C      -0.498509     3.950151     3.652236      45.78
 H      -0.211772     4.956418     3.916710      22.01
 C      -1.890853     2.349772     2.293452       0.16
 C      -3.092807     2.087748     1.542774      74.52
 H      -3.677875     3.210541     1.832492      22.59
 O      -3.723349     0.914293     1.997858     217.77
 H      -4.352280     0.537893     1.400688      27.35
 C      -2.969089     2.134805     0.021758      86.19
 H      -2.301101     2.865077    -0.312507      30.31
 C      -4.050519     2.197482    -1.092789     101.50
 O      -4.866470     1.059198    -1.283271     244.91
 H      -4.383938     0.271934    -1.555844      31.30
 H      -3.312310     2.165078    -1.912429      29.39
 H      -4.883771     2.894577    -0.733082      26.03
 C       1.449344     1.637798    -0.656234      38.95
 H       2.072087     2.442766    -0.456007      29.62
 C       1.031812    -0.634033    -1.325282      54.94
 H       1.593578    -1.600314    -1.525028      23.68
 C      -0.313737    -0.484781    -1.076100      20.94
 O      -1.295603    -1.681968    -1.225032     211.12
 C      -1.085154    -2.361282    -2.567666     117.95
 H      -0.423149    -3.208000    -2.320105      27.59
 H      -1.907353    -2.952960    -2.694624      29.54
 H      -0.918549    -1.811639    -3.380931      31.09
 C      -0.886063     0.795173    -0.676669      24.34
 O      -2.193654     0.873964    -0.312807     179.41
 C       0.097019     1.932932    -0.386872      84.94
 H      -0.264097     2.899049     0.104373      23.51
 C       1.987986     0.349555    -1.161083      43.93
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 C       3.450110     0.183201    -1.362192     122.42
 H       3.378308    -0.155175    -2.264273      32.85
 O       4.077338     1.475119    -1.551648     160.54
 H       4.472085     1.636587    -0.791018      34.27
 C       4.056685    -0.801129    -0.233333      91.25
 H       3.538748    -1.926595    -0.145377      27.45
 O       5.522837    -0.997110    -0.630413     147.02
 H       5.532030    -1.966758    -0.694369      30.18
 C       4.036563    -0.174039     1.167351     148.20
 O       4.686844     1.186729     1.129663     146.45
 H       4.124450     1.677911     1.850881      26.47
 H       4.625814    -0.713644     1.846284      36.27
 H       2.969322    -0.307792     1.599183      28.74
55
name = lig-Water-frame_789
 C      -1.595891     3.771457     2.774681      43.34
 H      -2.004457     4.675213     2.575561      19.83
 C      -1.110859     1.301883     2.854952      63.75
 H      -1.256544     0.231569     2.604154      30.63
 C       0.047626     1.542447     3.770739     -48.16
 O       0.880960     0.555316     4.393948     128.67
 C       0.912895    -0.661378     3.751647     135.21
 H       1.663756    -1.037140     4.431043      29.13
 H       1.431451    -0.589531     2.696980      30.89
 H       0.079691    -1.237827     3.808215      27.09
 C       0.292855     2.908099     4.104579      21.04
 O       1.403037     3.097319     4.956957     169.27
 H       0.972548     3.823135     5.580675      21.80
 C      -0.491910     3.888689     3.614344      50.67
 H      -0.412961     4.995787     3.926824      23.04
 C      -1.823660     2.376431     2.368644      -8.30
 C      -3.197464     2.163397     1.517710      92.52
 H      -3.871843     2.880375     1.688973      29.33
 O      -3.701635     0.964937     1.969072     255.91
 H      -4.343160     0.586010     1.346035      28.60
 C      -2.916588     2.157464    -0.034199      76.99
 H      -2.172910     2.962600    -0.355737      27.07
 C      -4.049673     2.226471    -1.083103     111.10
 O      -4.917653     1.053127    -1.270520     209.33
 H      -4.322225     0.241296    -1.412700      30.14
 H      -3.311664     2.665578    -1.870349      27.82
 H      -4.888585     2.902664    -1.024207      27.69
 C       1.451324     1.654392    -0.659185      44.04
 H       2.105476     2.608349    -0.513219      28.85
 C       1.007728    -0.676770    -1.343534      52.85
 H       1.403453    -1.660459    -1.541637      26.23
 C      -0.337955    -0.546747    -1.153125      25.13
 O      -1.241808    -1.653001    -1.254275     239.03
 C      -1.022334    -2.359803    -2.464696      84.86
 H      -0.332943    -3.084093    -1.929885      24.03
 H      -1.932302    -3.028439    -3.022799      25.64
 H      -0.910599    -1.635825    -3.489464      24.99
 C      -0.886077     0.780616    -0.725482      16.31
 O      -2.188955     0.858357    -0.348440     172.50
 C       0.142977     1.874530    -0.340747      62.99
 H      -0.287913     2.733434     0.110810      28.05
 C       1.961530     0.381483    -1.148183      47.64
 C       3.347285     0.242468    -1.394202      95.19
 H       3.480031    -0.438068    -2.523228      26.02
 O       4.118811     1.453296    -1.545640      82.62
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 H       4.596095     1.815331    -0.609822      23.55
 C       4.026842    -0.770436    -0.287671      89.39
 H       3.582788    -1.655413    -0.387990      32.18
 O       5.574639    -0.974091    -0.611015     132.99
 H       5.594548    -1.955446    -0.886613      27.67
 C       4.027774    -0.215529     1.175506     117.23
 O       4.680417     1.219874     1.159275      92.20
 H       4.212647     1.757458     1.875220      27.48
 H       4.630310    -0.843989     2.028031      31.41
 H       2.997044    -0.035798     1.637427      29.34
55
name = lig-Water-frame_790
 C      -1.626290     3.700568     2.809409      44.07
 H      -2.141362     4.678792     2.365486      19.62
 C      -1.052913     1.303662     2.950588      54.60
 H      -1.413257     0.355626     2.570825      31.43
 C       0.009152     1.564580     3.795070      35.17
 O       0.826614     0.621267     4.375023     159.05
 C       0.945995    -0.707664     3.714896     123.21
 H       1.576051    -1.311248     4.450948      28.26
 H       1.242598    -0.589731     2.717573      32.17
 H      -0.103715    -1.394326     3.932469      26.15
 C       0.321938     2.867034     4.080410      27.14
 O       1.381336     3.073203     4.966993     114.29
 H       1.238936     3.993405     5.438012      24.37
 C      -0.504713     3.920922     3.587069      57.21
 H      -0.349295     4.852714     4.008152      28.08
 C      -1.838596     2.458668     2.419640     -37.93
 C      -3.230627     2.236984     1.467025      61.07
 H      -4.233641     3.026814     1.635185      25.47
 O      -3.687098     0.974172     1.955858     187.34
 H      -4.533874     0.626291     1.369377      23.90
 C      -2.834018     2.161789    -0.077438      94.60
 H      -2.206301     3.099190    -0.168175      25.53
 C      -4.047395     2.275825    -1.093931     101.98
 O      -4.945411     1.029235    -1.263560     218.17
 H      -4.299334     0.292810    -1.228782      31.52
 H      -3.780227     2.747668    -2.091783      26.15
 H      -4.689775     3.234738    -1.028049      26.99
 C       1.488016     1.682787    -0.666646      88.45
 H       2.179576     2.452995    -0.594533      32.83
 C       1.040396    -0.708858    -1.355509      56.35
 H       1.214432    -1.846925    -1.698386      23.14
 C      -0.430508    -0.544512    -1.196957      14.69
 O      -1.218864    -1.579578    -1.274736     250.83
 C      -0.971531    -2.407423    -2.423221     127.15
 H      -0.031507    -3.045045    -2.298342      26.78
 H      -1.804340    -2.831653    -2.743743      30.12
 H      -0.559828    -1.750026    -3.060710      31.32
 C      -0.810193     0.777566    -0.740188      33.78
 O      -2.209125     0.838312    -0.388808     193.93
 C       0.097481     1.729395    -0.336594      65.95
 H      -0.246336     2.790090     0.149929      26.41
 C       1.838743     0.459434    -1.115005      40.80
 C       3.351769     0.231782    -1.459502     100.59
 H       3.612846    -0.315420    -2.195990      30.63
 O       4.168332     1.440753    -1.536206     155.58
 H       4.378076     1.703472    -0.568284      28.32
 C       4.064697    -0.688298    -0.340917      80.25
 H       3.456870    -1.748222    -0.560796      28.19
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 O       5.586547    -0.962646    -0.591282     137.45
 H       5.706397    -1.893850    -0.915611      26.08
 C       4.035834    -0.212500     1.195843     121.59
 O       4.648688     1.213619     1.190039      94.59
 H       4.401500     1.839340     1.935232      24.72
 H       4.517929    -0.885878     1.787449      34.81
 H       3.039865     0.114243     1.512736      29.32
55
name = lig-Water-frame_791
 C      -1.634177     3.719340     2.836025      35.71
 H      -2.315479     4.363243     2.279464      15.09
 C      -1.064892     1.340602     2.991411      57.77
 H      -1.459630     0.392226     2.632532      31.34
 C      -0.028523     1.547184     3.800446      42.24
 O       0.786997     0.664604     4.356451     170.85
 C       0.937075    -0.778679     3.750359     110.47
 H       1.640714    -1.455753     4.198559      29.52
 H       1.080964    -0.682439     2.574092      30.60
 H      -0.055732    -1.143477     3.751972      30.17
 C       0.338142     2.883687     4.068425      19.85
 O       1.374840     3.069024     4.981492     167.07
 H       1.446610     3.915649     5.364931      30.67
 C      -0.479000     3.959434     3.609605      42.64
 H      -0.162552     4.966361     4.106442      23.94
 C      -1.936261     2.446058     2.428354     -62.85
 C      -3.237889     2.287552     1.433374      79.66
 H      -3.890611     3.048777     1.511419      30.26
 O      -3.695667     0.962044     1.937256     182.13
 H      -4.547188     0.735002     1.646598      25.52
 C      -2.791040     2.165673    -0.117036     102.66
 H      -2.173200     3.049276    -0.192016      26.53
 C      -4.066196     2.361583    -1.140528      80.20
 O      -4.949375     1.033844    -1.242011     223.51
 H      -4.300858     0.333648    -1.072796      31.02
 H      -4.000577     2.315040    -2.273225      24.47
 H      -4.525821     3.206620    -0.558786      26.98
 C       1.459886     1.698853    -0.660138      75.11
 H       2.300963     2.464650    -0.579267      30.93
 C       0.988519    -0.720224    -1.362882      63.67
 H       1.393170    -1.579717    -1.718203      27.47
 C      -0.398492    -0.470391    -1.211772      24.71
 O      -1.256037    -1.531231    -1.283923     173.73
 C      -0.853492    -2.455751    -2.392337      86.10
 H      -0.059443    -3.242002    -2.531476      26.14
 H      -1.984787    -2.925095    -2.564627      24.71
 H      -0.257313    -1.673771    -3.142617      24.95
 C      -0.798166     0.735179    -0.726067      32.11
 O      -2.218554     0.841298    -0.430564     210.24
 C       0.071549     1.673049    -0.331845      78.65
 H      -0.242059     2.505610     0.061025      31.22
 C       1.805691     0.443908    -1.141810      -0.46
 C       3.410055     0.236543    -1.439883      79.05
 H       3.669258    -0.410810    -2.567820      25.39
 O       4.199793     1.434156    -1.531239     170.81
 H       4.245189     1.599887    -0.564913      31.68
 C       4.110175    -0.648471    -0.376712     100.82
 H       3.624196    -1.525922    -0.373377      33.18
 O       5.569980    -0.942502    -0.579016     148.55
 H       5.652991    -1.897947    -0.768270      28.12
 C       4.031086    -0.137853     1.156433     120.99
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 O       4.622409     1.182971     1.208612      84.55
 H       4.454357     1.709163     2.116532      22.42
 H       4.563352    -1.071405     1.736413      30.47
 H       2.853599    -0.041838     1.418935      28.11
55
name = lig-Water-frame_792
 C      -1.638883     3.754360     2.841200      41.96
 H      -2.357461     4.511298     2.424122      17.26
 C      -1.201672     1.380671     2.940206      62.75
 H      -1.361345     0.291251     2.779603      25.59
 C      -0.042537     1.558917     3.798841      -5.81
 O       0.802088     0.628493     4.353896     118.28
 C       0.892311    -0.790443     3.742050      91.00
 H       1.779144    -1.386526     4.125977      27.19
 H       1.076523    -0.721900     2.728611      34.79
 H      -0.254779    -1.178299     3.751168      24.38
 C       0.323943     2.954522     4.073492      19.90
 O       1.394765     3.043412     4.983519     176.90
 H       1.397203     4.024798     5.434090      26.58
 C      -0.427694     4.009835     3.670632      32.72
 H      -0.153234     4.984235     3.937041      22.31
 C      -2.027957     2.390451     2.437820      14.82
 C      -3.155962     2.237639     1.413970      66.19
 H      -3.812500     3.344252     1.521895      25.00
 O      -3.710395     0.965596     1.926000     147.06
 H      -4.731163     0.755541     1.782397      22.11
 C      -2.796412     2.154648    -0.173023      83.30
 H      -1.967798     2.951998    -0.451867      24.12
 C      -4.082586     2.395083    -1.163976      87.62
 O      -4.949848     1.064859    -1.193069     229.05
 H      -4.312654     0.338358    -0.896684      29.86
 H      -3.837626     2.362019    -2.198527      27.83
 H      -4.620811     3.030444    -0.464884      27.02
 C       1.412319     1.667988    -0.658617      49.38
 H       2.094720     2.493172    -0.451578      29.71
 C       0.948414    -0.652457    -1.365135      70.42
 H       1.662527    -1.520624    -1.767259      24.79
 C      -0.328189    -0.457027    -1.213222      39.90
 O      -1.294928    -1.513041    -1.301834     186.94
 C      -0.756787    -2.476155    -2.415968     122.38
 H      -0.238701    -3.491089    -2.121460      27.18
 H      -1.641425    -2.909997    -2.682983      29.78
 H      -0.580224    -1.940852    -3.266493      30.08
 C      -0.883023     0.700457    -0.680752      27.12
 O      -2.208410     0.858534    -0.471961     200.43
 C       0.101467     1.706016    -0.329632      67.05
 H      -0.495557     2.654333     0.227514      21.63
 C       1.888145     0.381039    -1.206754      -4.53
 C       3.482703     0.198394    -1.466315     109.71
 H       3.438172    -0.132471    -2.369076      32.30
 O       4.214343     1.433906    -1.528688     114.78
 H       4.295924     1.784169    -0.452752      25.79
 C       4.169207    -0.612773    -0.361478     108.42
 H       3.602470    -1.689261    -0.157286      29.27
 O       5.546708    -0.920645    -0.582486     143.60
 H       5.510433    -1.944424    -0.517301      26.33
 C       3.999385    -0.092625     1.079358     140.54
 O       4.603008     1.146473     1.240423     188.98
 H       4.335129     1.516108     2.076717      27.37
 H       4.474809    -0.789246     1.659466      35.09
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 H       2.973602    -0.236840     1.367042      31.44
55
name = lig-Water-frame_793
 C      -1.634197     3.758720     2.839288      97.33
 H      -2.150676     4.801630     2.769765      33.42
 C      -1.297346     1.356748     2.916404      46.38
 H      -1.413717     0.304459     2.777377      20.40
 C      -0.081602     1.622996     3.763130     -14.10
 O       0.833367     0.558137     4.345907     101.68
 C       0.808794    -0.762921     3.726939      96.14
 H       1.621869    -1.192633     4.294045      26.15
 H       1.128828    -0.627420     2.597292      28.56
 H      -0.083271    -1.423304     3.993603      25.08
 C       0.320009     2.958036     4.113811      19.71
 O       1.430911     3.043022     4.983252     128.91
 H       1.194585     3.825862     5.514313      33.15
 C      -0.453278     4.062451     3.679192     107.93
 H      -0.166879     5.143932     3.822626      11.90
 C      -2.065915     2.420895     2.454346      49.84
 C      -3.086660     2.194720     1.402069     111.79
 H      -3.641928     3.020401     1.509837      29.25
 O      -3.749020     0.976943     1.913906     192.71
 H      -4.761800     0.816079     1.727702      23.55
 C      -2.797596     2.149693    -0.238139      88.41
 H      -2.098232     2.807822    -0.577984      29.96
 C      -4.083647     2.333360    -1.123254      86.71
 O      -4.939726     1.113733    -1.130486     261.50
 H      -4.405500     0.381587    -0.770742      30.07
 H      -3.635035     2.871418    -2.103152      26.17
 H      -4.894314     3.127809    -0.831935      26.07
 C       1.407185     1.585529    -0.672960      29.78
 H       1.917009     2.506474    -0.344634      28.37
 C       1.078801    -0.595311    -1.405802      60.54
 H       1.338249    -1.564642    -1.731844      23.48
 C      -0.391386    -0.493380    -1.182926      26.61
 O      -1.293583    -1.520212    -1.359614     200.07
 C      -0.724145    -2.525217    -2.403712      96.39
 H      -0.226664    -3.203898    -1.709391      23.99
 H      -1.743718    -3.080372    -2.892971      24.23
 H      -0.530860    -2.067873    -3.514929      25.39
 C      -0.905694     0.728055    -0.618662      39.27
 O      -2.224299     0.862016    -0.514032     212.77
 C       0.033561     1.781684    -0.308971      50.53
 H      -0.246291     2.585317     0.207999      21.61
 C       2.001405     0.395297    -1.233146      20.31
 C       3.508434     0.186041    -1.446722      94.84
 H       3.458287    -0.241522    -2.676787      24.53
 O       4.226165     1.455910    -1.508566     185.09
 H       4.342880     1.854222    -0.740883      33.36
 C       4.174183    -0.647024    -0.317884     125.84
 H       3.667401    -1.534073    -0.231341      31.32
 O       5.541499    -0.923912    -0.598062     155.71
 H       5.590083    -1.869798    -0.342848      28.96
 C       3.968448    -0.082198     0.984978     118.57
 O       4.591982     1.132206     1.264580     169.41
 H       4.158537     1.653362     2.102371      21.88
 H       4.596919    -0.778157     1.786004      27.51
 H       2.817264    -0.214514     1.369195      26.43
55
name = lig-Water-frame_794
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 C      -1.603423     3.794730     2.874233     -12.49
 H      -2.099718     4.699190     2.770671      28.51
 C      -1.290257     1.325065     2.960238      44.00
 H      -1.654964     0.309779     2.606394      21.30
 C      -0.132395     1.655926     3.720346       1.19
 O       0.822218     0.532127     4.317366     133.45
 C       0.760176    -0.722855     3.716654     119.13
 H       1.543813    -1.197368     4.369466      25.36
 H       0.964082    -0.716213     2.680325      30.09
 H      -0.084552    -1.434089     4.018540      26.31
 C       0.308109     2.928657     4.156956      11.05
 O       1.456947     3.056014     4.979293      44.96
 H       1.162056     3.709123     5.703135      28.18
 C      -0.512121     4.071643     3.652430      63.79
 H      -0.214406     5.115086     3.861244      18.98
 C      -2.038123     2.500798     2.465903      17.42
 C      -3.057524     2.141764     1.377554     100.31
 H      -3.939790     3.071754     1.463471      23.85
 O      -3.791073     0.987020     1.896813     223.19
 H      -4.652997     0.898012     1.568238      28.18
 C      -2.819687     2.130646    -0.244813      82.65
 H      -2.118202     3.042134    -0.615079      24.29
 C      -4.098234     2.294530    -1.080741     116.76
 O      -4.922707     1.169991    -1.078989     287.88
 H      -4.452917     0.406028    -0.727928      30.59
 H      -3.706807     2.817166    -1.904977      28.22
 H      -4.785371     3.121915    -1.022923      27.38
 C       1.404079     1.535897    -0.664708      58.99
 H       2.016900     2.430730    -0.346061      28.20
 C       1.137391    -0.594644    -1.456333      70.26
 H       1.205009    -1.672697    -1.778541      20.98
 C      -0.416252    -0.494834    -1.130951       6.89
 O      -1.278189    -1.538623    -1.460322     197.65
 C      -0.793055    -2.577378    -2.411304     103.83
 H       0.016901    -2.947735    -1.678705      25.91
 H      -1.568230    -3.219401    -2.648316      27.99
 H      -0.073997    -2.225392    -3.147874      29.25
 C      -0.867275     0.761015    -0.576051      32.23
 O      -2.282485     0.844889    -0.560469     207.54
 C      -0.009610     1.788058    -0.323881      49.77
 H      -0.090981     2.847884     0.298344      20.59
 C       2.086513     0.467309    -1.218368      45.07
 C       3.516614     0.195354    -1.467552     108.84
 H       3.801899    -0.294354    -2.279279      28.63
 O       4.237704     1.472182    -1.539596      81.50
 H       4.349594     1.940487    -0.571862      27.54
 C       4.149589    -0.694251    -0.339881      96.07
 H       3.532141    -1.732771    -0.390176      27.72
 O       5.563094    -0.940218    -0.616155     125.73
 H       5.801131    -1.861644    -0.328190      24.61
 C       3.938466    -0.114688     1.027434     138.34
 O       4.581467     1.163119     1.282254     199.76
 H       4.148985     1.763686     1.911535      25.66
 H       4.380083    -0.822776     1.607773      32.82
 H       2.930716    -0.022520     1.200851      29.61
55
name = lig-Water-frame_795
 C      -1.606827     3.831882     2.892161      16.05
 H      -2.370288     4.646523     2.410207      13.87
 C      -1.276485     1.350288     2.994919      59.56
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 H      -1.701403     0.466435     2.589968      23.26
 C      -0.137463     1.605799     3.721639      20.94
 O       0.766038     0.583708     4.274511     181.33
 C       0.737396    -0.728495     3.746514     109.99
 H       1.566092    -1.359697     4.142765      26.35
 H       0.836289    -0.860730     2.590092      26.87
 H      -0.395462    -1.179997     3.880107      24.47
 C       0.259096     2.932761     4.171307       6.52
 O       1.460376     3.077151     4.970228     153.23
 H       1.284683     3.644044     5.853231      22.89
 C      -0.495213     4.020615     3.676354      26.38
 H      -0.281626     5.008959     4.014313      34.94
 C      -1.963644     2.531250     2.466507       7.88
 C      -3.126938     2.173479     1.369466     100.09
 H      -3.844086     2.881896     1.352577      26.99
 O      -3.796638     0.992404     1.880730     215.94
 H      -4.736871     0.920158     1.349664      22.95
 C      -2.835833     2.140432    -0.191117     111.74
 H      -2.260179     2.950247    -0.384196      29.42
 C      -4.101224     2.302576    -1.039979      81.30
 O      -4.932072     1.197580    -1.038443     241.35
 H      -4.410880     0.371535    -0.776399      26.16
 H      -3.699561     2.264062    -2.254119      23.41
 H      -4.673658     3.244584    -0.628931      25.76
 C       1.411541     1.571753    -0.619080      53.88
 H       2.146312     2.316926    -0.418185      28.02
 C       1.074179    -0.619460    -1.484654      85.53
 H       1.541383    -1.597780    -1.900068      25.06
 C      -0.322391    -0.482353    -1.104971       6.97
 O      -1.278796    -1.527385    -1.571549     194.62
 C      -0.780720    -2.609789    -2.344654     113.13
 H       0.017236    -3.201413    -1.855191      28.01
 H      -1.611241    -3.479325    -2.500902      24.62
 H       0.033761    -2.204812    -3.045507      26.26
 C      -0.887463     0.747524    -0.568805      21.40
 O      -2.326143     0.824343    -0.611474     170.66
 C       0.047283     1.797585    -0.334770      56.66
 H      -0.161616     2.773686     0.106633      23.01
 C       2.066427     0.469866    -1.216460       7.91
 C       3.569687     0.243669    -1.442256      84.95
 H       4.017665    -0.468748    -2.383833      26.79
 O       4.261794     1.502307    -1.576358      87.79
 H       4.267997     1.751927    -0.535749      28.71
 C       4.103553    -0.756535    -0.386933      90.63
 H       3.583808    -1.679098    -0.484939      30.84
 O       5.593751    -0.956420    -0.637379     113.36
 H       5.821845    -1.932466    -0.409364      22.51
 C       3.919660    -0.144962     1.102143      98.46
 O       4.595875     1.186052     1.258683     125.01
 H       4.083041     1.780974     1.975214      23.10
 H       4.196995    -1.086152     1.836979      27.15
 H       2.715208     0.154512     1.119379      25.71
55
name = lig-Water-frame_797
 C      -1.672897     3.820569     2.811153      75.23
 H      -2.143485     4.832870     2.317404      15.53
 C      -1.243192     1.446006     2.992360      70.46
 H      -1.470670     0.412639     2.776521      28.86
 C      -0.119532     1.589181     3.802993      32.17
 O       0.730551     0.646119     4.211050     177.95
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 C       0.579576    -0.763802     3.688206     104.94
 H       1.350654    -1.347424     4.293232      26.51
 H       0.701445    -0.621936     2.589407      28.36
 H      -0.510069    -1.227857     4.129421      24.06
 C       0.227517     2.865019     4.208607      10.58
 O       1.416202     3.095227     4.931329     131.46
 H       1.197775     3.927373     5.585617      23.29
 C      -0.514634     4.023006     3.770726      39.01
 H      -0.229715     4.890502     4.266197      29.89
 C      -1.932544     2.527857     2.375365      23.42
 C      -3.242103     2.269272     1.450454     107.14
 H      -3.730934     3.125545     1.624579      30.82
 O      -3.774793     1.006063     1.838462     260.36
 H      -4.697803     0.760905     1.608545      25.77
 C      -2.862949     2.115348    -0.055333     102.35
 H      -2.128059     2.812740    -0.290730      28.27
 C      -4.024835     2.330213    -1.013316      71.99
 O      -5.060251     1.156553    -0.891887     158.94
 H      -4.472183     0.399346    -1.093311      28.93
 H      -3.676962     2.510933    -2.245735      25.85
 H      -4.609888     3.374412    -0.820788      26.15
 C       1.554775     1.653474    -0.573569      56.75
 H       2.095828     2.519190    -0.384792      28.24
 C       1.092985    -0.617624    -1.500876      69.12
 H       1.438664    -1.573751    -2.203327      23.37
 C      -0.304082    -0.534812    -1.173923      22.69
 O      -1.244212    -1.427430    -1.691436     179.89
 C      -0.655908    -2.723845    -2.237910     118.50
 H      -0.126819    -3.367574    -1.557447      28.81
 H      -1.763824    -3.188608    -2.600362      25.34
 H      -0.549917    -2.592595    -3.316119      26.66
 C      -0.853985     0.668745    -0.655620      15.72
 O      -2.272641     0.818976    -0.665682     142.23
 C       0.100370     1.736527    -0.364447      50.69
 H      -0.407703     2.774373    -0.137475      23.29
 C       1.886651     0.414579    -1.201759      12.21
 C       3.610144     0.257315    -1.473163      83.78
 H       3.423195    -0.065217    -2.627977      27.24
 O       4.307701     1.521589    -1.587255      63.40
 H       4.582379     2.037554    -0.612471      23.15
 C       4.152533    -0.737326    -0.331800      96.64
 H       3.583084    -1.681943    -0.497570      28.52
 O       5.598940    -1.010323    -0.666022     178.77
 H       5.637910    -2.027873    -0.541589      26.34
 C       3.836879    -0.204013     1.147797      92.13
 O       4.620461     1.111585     1.188186      85.46
 H       4.335399     1.629643     1.984130      25.96
 H       4.114190    -0.723063     2.210203      28.02
 H       2.602616     0.039041     1.254484      27.60
55
name = lig-Water-frame_798
 C      -1.598992     3.840134     2.807430      19.19
 H      -2.000221     4.755750     2.547499      31.11
 C      -1.212044     1.433581     2.969191      50.23
 H      -1.499664     0.414341     2.729893      24.37
 C      -0.174194     1.674555     3.808258      23.61
 O       0.782771     0.571368     4.216712     153.96
 C       0.474140    -0.737953     3.689331     120.21
 H       1.221184    -1.216675     4.252243      27.14
 H       0.606722    -0.758861     2.555096      29.02
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 H      -0.429078    -1.249473     4.036583      27.56
 C       0.233992     2.892768     4.228117      22.26
 O       1.384070     3.106077     4.932145     149.63
 H       1.210349     4.006369     5.324591      29.37
 C      -0.617342     4.004861     3.771453      35.12
 H      -0.250358     5.048015     4.162034      13.02
 C      -1.999865     2.523694     2.318561      32.22
 C      -3.219666     2.267274     1.503290      87.95
 H      -3.932811     3.304711     1.753608      22.44
 O      -3.754627     1.003264     1.858200     185.48
 H      -4.837309     0.864973     1.771874      21.93
 C      -2.854099     2.113350    -0.057981      87.55
 H      -2.086955     2.928195    -0.347384      24.32
 C      -4.033929     2.340128    -1.017672     100.39
 O      -5.103999     1.161358    -0.819383     160.18
 H      -4.636039     0.339797    -1.192473      27.34
 H      -3.627959     2.645650    -1.853654      31.08
 H      -4.650250     3.153695    -1.006259      28.69
 C       1.519881     1.640767    -0.579382      59.70
 H       2.191797     2.558853    -0.381120      25.83
 C       1.092514    -0.664229    -1.529869      81.21
 H       1.273913    -1.422771    -2.121380      22.41
 C      -0.379608    -0.554218    -1.248692      17.64
 O      -1.197132    -1.408852    -1.724855     201.78
 C      -0.732747    -2.759728    -2.255703     105.89
 H      -0.035072    -3.140723    -1.458293      26.99
 H      -1.717462    -3.230450    -2.147969      26.78
 H      -0.006627    -2.877831    -3.257111      25.19
 C      -0.765646     0.666172    -0.706165      26.16
 O      -2.211124     0.827605    -0.645589     152.16
 C       0.091501     1.700533    -0.386237      61.64
 H      -0.306281     2.678430    -0.146830      24.01
 C       1.977035     0.490261    -1.144723      17.22
 C       3.500217     0.276047    -1.476502      84.36
 H       3.672197    -0.115910    -2.470257      27.84
 O       4.331180     1.523040    -1.582778     182.32
 H       4.496551     1.885605    -0.733455      33.53
 C       4.193860    -0.708506    -0.308124     108.85
 H       3.601252    -1.647918    -0.423586      28.40
 O       5.566998    -1.043073    -0.659886     166.06
 H       5.772401    -1.989540    -0.394817      26.59
 C       3.812556    -0.172409     1.142497     120.09
 O       4.625451     1.031632     1.161976     140.23
 H       4.318809     1.720668     1.872534      25.34
 H       4.267966    -0.781759     1.861762      30.89
 H       2.841572    -0.039476     1.165072      31.14
55
name = lig-Water-frame_799
 C      -1.540558     3.830125     2.795443      91.73
 H      -2.142999     4.803515     2.548017      30.72
 C      -1.254103     1.443135     2.886397      43.38
 H      -1.532272     0.390475     2.643633      20.64
 C      -0.158519     1.666273     3.828750      -1.60
 O       0.793561     0.534279     4.214856     149.09
 C       0.413007    -0.707233     3.697373     102.21
 H       1.276930    -1.422470     4.064987      25.29
 H       0.488128    -0.940984     2.635083      28.75
 H      -0.733503    -1.222452     3.946099      23.21
 C       0.192321     2.999934     4.220172      20.19
 O       1.363451     3.130181     4.948877     193.94
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 H       1.365105     4.029222     5.300503      30.02
 C      -0.648062     3.977366     3.802546      72.36
 H      -0.466957     5.003035     3.899582      18.84
 C      -2.001188     2.519417     2.350598      37.25
 C      -3.196505     2.271081     1.520547      94.51
 H      -3.965361     2.937349     1.546325      25.55
 O      -3.762884     0.986138     1.912346     232.35
 H      -4.665916     1.012093     1.828883      27.18
 C      -2.831068     2.146236    -0.091902      81.21
 H      -2.228410     3.047098    -0.305329      24.51
 C      -4.086254     2.305423    -0.982685      66.04
 O      -5.105121     1.194149    -0.781333     178.41
 H      -4.828206     0.324249    -1.102504      28.71
 H      -3.471921     2.350237    -2.131028      23.95
 H      -4.851824     3.206303    -0.701185      23.78
 C       1.447839     1.642986    -0.580910      48.61
 H       2.145334     2.397931    -0.389415      28.58
 C       1.043592    -0.628780    -1.507062     102.11
 H       1.496979    -1.559544    -2.242879      23.40
 C      -0.288559    -0.527882    -1.334500      24.29
 O      -1.207567    -1.451746    -1.795600     238.54
 C      -0.772464    -2.784792    -2.233415     121.94
 H      -0.071127    -2.994392    -1.409457      27.72
 H      -1.688494    -3.517212    -1.996747      24.95
 H      -0.028971    -2.880929    -2.945908      27.90
 C      -0.752096     0.699240    -0.737460      33.94
 O      -2.153581     0.847511    -0.597359     145.01
 C       0.120626     1.682403    -0.414185      38.16
 H      -0.296066     2.765538     0.052000      20.94
 C       2.092280     0.486364    -1.133373      23.65
 C       3.443051     0.302576    -1.431845      83.40
 H       3.804654    -0.326430    -2.368963      25.87
 O       4.331256     1.506905    -1.595130     160.33
 H       4.379965     1.736383    -0.584278      33.09
 C       4.171060    -0.695836    -0.322278     100.28
 H       3.565814    -1.690325    -0.332999      27.91
 O       5.544100    -1.053151    -0.642520     131.06
 H       5.715985    -1.935767    -0.176132      26.02
 C       3.883656    -0.153479     1.080444     109.29
 O       4.636049     0.997416     1.158483     160.63
 H       4.190167     1.644392     1.717994      28.54
 H       4.297067    -1.079654     1.730614      27.54
 H       2.638629    -0.024650     1.190847      24.84
55
name = lig-Water-frame_800
 C      -1.576992     3.799397     2.745506     101.95
 H      -2.257312     4.620251     2.438459      29.92
 C      -1.269241     1.441288     2.836305      49.11
 H      -1.536454     0.467685     2.544125      22.73
 C      -0.127794     1.615085     3.819598      -8.65
 O       0.760744     0.555790     4.200728     152.59
 C       0.367911    -0.758996     3.706621     111.89
 H       1.013991    -1.527811     3.970856      28.42
 H       0.348060    -0.803198     2.539035      28.80
 H      -0.664578    -0.965327     4.017453      26.94
 C       0.171374     3.016575     4.220888      11.05
 O       1.351343     3.164356     4.972531     173.40
 H       1.533472     4.092930     5.489613      25.26
 C      -0.651476     4.017770     3.817324      74.72
 H      -0.485116     5.120888     3.954510      21.20
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 C      -1.960691     2.548918     2.428545      47.02
 C      -3.162164     2.208967     1.468397      76.86
 H      -4.106401     3.014534     1.416606      23.66
 O      -3.754709     0.967581     1.986922     193.22
 H      -4.766253     1.002333     1.767547      24.01
 C      -2.815655     2.182772    -0.111394      60.97
 H      -2.253884     3.114027    -0.322716      24.81
 C      -4.142405     2.247113    -0.972287     112.29
 O      -5.095807     1.243159    -0.757410     276.68
 H      -4.793723     0.312021    -0.888222      28.56
 H      -3.961844     2.038940    -1.913779      30.78
 H      -4.546122     3.108896    -0.589137      29.97
 C       1.481529     1.602046    -0.612343      35.48
 H       2.074300     2.519587    -0.287918      27.48
 C       1.132477    -0.584483    -1.515145      64.97
 H       1.561924    -1.318672    -1.970098      27.59
 C      -0.218077    -0.481785    -1.416301      30.65
 O      -1.253330    -1.493592    -1.881426     212.05
 C      -0.791715    -2.803360    -2.107698     113.67
 H      -0.132806    -3.115371    -1.265018      26.53
 H      -1.487794    -3.745146    -2.226887      24.15
 H      -0.200318    -2.815429    -3.221069      23.88
 C      -0.803317     0.724412    -0.770027      38.38
 O      -2.112985     0.882022    -0.533661     161.43
 C       0.103741     1.744381    -0.400232      49.92
 H      -0.241393     2.518678     0.086128      23.76
 C       2.043127     0.442650    -1.143378      34.20
 C       3.536359     0.275508    -1.410121     118.67
 H       3.554849    -0.426229    -2.301816      28.24
 O       4.306482     1.482920    -1.587272      93.10
 H       4.383725     1.696537    -0.489352      28.30
 C       4.084455    -0.704611    -0.355025     116.04
 H       3.526021    -1.622445    -0.384227      29.42
 O       5.526807    -1.038709    -0.615859     152.08
 H       5.554947    -1.937377    -0.115089      26.19
 C       3.943657    -0.218614     1.011023     142.12
 O       4.660902     1.016802     1.178582     137.93
 H       4.083283     1.633690     1.736978      26.83
 H       4.140842    -0.994608     1.708949      31.88
 H       2.985121    -0.023796     1.268978      31.04
55
name = lig-Water-frame_801
 C      -1.636723     3.820538     2.739317      62.79
 H      -2.290832     4.569192     2.315168      34.75
 C      -1.194592     1.416851     2.874031      52.75
 H      -1.562261     0.448563     2.409498      21.39
 C      -0.123637     1.578200     3.764239       6.13
 O       0.720437     0.597111     4.182108     152.39
 C       0.315241    -0.803159     3.664879      94.80
 H       0.939718    -1.659449     4.143523      24.75
 H       0.224382    -0.593672     2.641804      28.84
 H      -0.796436    -0.771079     4.284795      23.11
 C       0.181862     2.953585     4.240034     -23.22
 O       1.360223     3.202956     5.009133     185.19
 H       1.285288     3.980911     5.554232      26.11
 C      -0.666046     4.115697     3.770981      68.02
 H      -0.361302     5.078824     4.238920      14.32
 C      -1.971821     2.534807     2.442497      44.23
 C      -3.153589     2.162030     1.400056      98.07
 H      -3.761085     3.022130     1.516930      26.06
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 O      -3.750581     0.961308     2.056622     182.95
 H      -4.712293     0.739625     1.644055      22.78
 C      -2.808489     2.177045    -0.118350      66.08
 H      -2.181432     3.098418    -0.408884      22.14
 C      -4.148501     2.172368    -0.937355      83.59
 O      -5.124638     1.257541    -0.705077     264.51
 H      -4.618367     0.374663    -0.592015      26.95
 H      -4.152759     2.160548    -2.238632      23.93
 H      -4.449639     3.331408    -0.718848      25.36
 C       1.540241     1.598567    -0.628681      65.76
 H       2.037527     2.470890    -0.257435      29.17
 C       1.242325    -0.546857    -1.535245     104.99
 H       1.753617    -1.607038    -1.979869      24.86
 C      -0.262529    -0.435621    -1.482834      16.16
 O      -1.296352    -1.493899    -1.942478     172.84
 C      -0.743253    -2.845766    -2.034020     116.29
 H      -0.106522    -3.272954    -1.232550      27.39
 H      -1.605021    -3.643153    -2.299171      25.00
 H      -0.432201    -2.827362    -2.997789      26.44
 C      -0.813406     0.750017    -0.814262      36.91
 O      -2.115998     0.914929    -0.467436     202.30
 C       0.091218     1.763494    -0.407747      71.76
 H      -0.347497     2.718527     0.363921      19.11
 C       1.981017     0.435481    -1.152729      50.66
 C       3.614787     0.207571    -1.418985     118.95
 H       3.504468    -0.317711    -2.465152      27.72
 O       4.275789     1.452143    -1.545491     128.36
 H       4.505720     1.745794    -0.724705      29.62
 C       4.026398    -0.722104    -0.405547     117.09
 H       3.366426    -1.698071    -0.577138      24.97
 O       5.497425    -1.018701    -0.582006     168.06
 H       5.613095    -1.974229    -0.308434      24.86
 C       3.995588    -0.277957     0.992396     116.22
 O       4.692451     1.062162     1.209979     143.08
 H       4.132025     1.627546     1.834548      26.98
 H       4.320383    -0.994139     1.858966      28.61
 H       2.843244     0.028938     1.292268      27.26
55
name = lig-Water-frame_802
 C      -1.690386     3.887891     2.785092      23.10
 H      -2.289863     4.734021     2.199647      18.64
 C      -1.145822     1.393616     2.903459      68.93
 H      -1.415711     0.482447     2.463545      25.91
 C      -0.104446     1.600140     3.721300      38.18
 O       0.707857     0.606472     4.168337     177.90
 C       0.224357    -0.794288     3.696111     114.43
 H       0.900586    -1.487221     4.116901      28.08
 H       0.113883    -0.702278     2.524727      26.36
 H      -0.693870    -0.937820     4.138614      29.15
 C       0.154731     2.926736     4.229703     -37.46
 O       1.360483     3.219219     5.043321      69.33
 H       0.975585     4.009904     5.649073      23.90
 C      -0.631577     4.135615     3.726385      12.25
 H      -0.379445     5.021262     4.292374      16.61
 C      -1.987538     2.453949     2.400494     -40.12
 C      -3.113520     2.140726     1.397046      90.11
 H      -3.757838     3.137403     1.610200      25.65
 O      -3.753594     0.956702     2.087465     187.37
 H      -4.483965     0.583439     1.685245      28.01
 C      -2.809504     2.124899    -0.141524     103.55
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 H      -2.219280     2.952862    -0.415878      27.64
 C      -4.119238     2.207541    -0.990001     115.26
 O      -5.166502     1.226248    -0.613731     298.98
 H      -4.686062     0.429253    -0.401916      30.61
 H      -3.882743     2.399324    -1.931424      31.24
 H      -4.567853     3.133863    -0.890784      29.07
 C       1.502471     1.664867    -0.603181      51.50
 H       2.284859     2.398880    -0.273960      29.35
 C       1.201025    -0.635750    -1.611686      69.14
 H       1.651135    -1.534290    -1.874403      26.44
 C      -0.322928    -0.416578    -1.543418       4.44
 O      -1.301994    -1.453297    -1.956834     152.72
 C      -0.725672    -2.907035    -1.993961      83.39
 H      -0.065842    -3.276825    -1.219109      28.65
 H      -1.837595    -3.254505    -2.021632      23.66
 H      -0.067015    -2.978682    -3.094426      23.78
 C      -0.784789     0.787614    -0.861321      34.91
 O      -2.144625     0.915106    -0.411098     222.04
 C       0.118527     1.788566    -0.397565      41.00
 H      -0.172213     2.487738     0.152406      27.88
 C       2.062309     0.476857    -1.164419      11.58
 C       3.586118     0.175352    -1.468770     102.42
 H       3.740142    -0.060510    -2.606877      26.62
 O       4.251648     1.419723    -1.529358     102.64
 H       4.727043     1.827986    -0.600132      23.98
 C       4.035099    -0.804070    -0.436597     120.52
 H       3.434409    -1.627257    -0.613244      31.69
 O       5.472188    -1.006235    -0.567627     158.29
 H       5.702248    -1.990288    -0.511261      22.70
 C       3.978282    -0.274193     1.068939     104.19
 O       4.719642     1.095641     1.236762     159.25
 H       4.252749     1.598520     1.921564      30.45
 H       4.596673    -0.952575     1.678130      29.92
 H       2.945681    -0.133951     1.231640      28.84
55
name = lig-Water-frame_803
 C      -1.734071     3.902864     2.823056      37.29
 H      -2.150784     4.716981     2.408637      23.31
 C      -1.179938     1.406336     2.870882      53.39
 H      -1.270128     0.333755     2.560813      24.26
 C      -0.042925     1.672662     3.731082      38.74
 O       0.707017     0.567189     4.154161     137.55
 C       0.162812    -0.723903     3.714386     116.37
 H       1.019034    -1.399212     4.034288      26.58
 H       0.151948    -1.009782     2.695932      28.93
 H      -0.974037    -1.265373     4.094294      24.08
 C       0.122329     2.963927     4.194266      31.62
 O       1.317971     3.228881     5.075347     141.08
 H       1.006670     4.000917     5.707551      24.91
 C      -0.581484     4.061527     3.692860      45.55
 H      -0.464963     5.124532     4.118999      22.64
 C      -1.953335     2.429440     2.363094     -11.53
 C      -3.096349     2.163773     1.457555      88.91
 H      -3.876075     2.942163     1.501714      27.52
 O      -3.729647     0.959814     2.096975     123.31
 H      -4.565170     0.502113     1.577633      21.07
 C      -2.842259     2.063884    -0.143052      98.50
 H      -2.165574     3.010642    -0.391060      25.54
 C      -4.099637     2.259217    -1.009513      65.03
 O      -5.181945     1.205261    -0.532948     186.95
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 H      -4.825123     0.271295    -0.387698      25.38
 H      -3.499426     2.213362    -2.159486      23.90
 H      -4.809038     3.185292    -0.741862      24.85
 C       1.507841     1.714364    -0.587677      48.32
 H       2.330692     2.359135    -0.294216      29.04
 C       1.070394    -0.644734    -1.656677      44.51
 H       1.544496    -1.721212    -1.986539      25.10
 C      -0.346438    -0.429182    -1.594619       7.30
 O      -1.251873    -1.390961    -1.937596     169.69
 C      -0.731152    -2.918849    -2.017549      94.93
 H      -0.132355    -3.135472    -1.063250      28.43
 H      -1.752028    -3.323191    -1.836631      25.66
 H      -0.085854    -3.170089    -2.735167      28.72
 C      -0.766594     0.826033    -0.899125      32.74
 O      -2.151102     0.858943    -0.384242     199.96
 C       0.170403     1.763574    -0.423138      47.82
 H      -0.260506     2.786706     0.261706      24.02
 C       2.107915     0.466315    -1.216227      -4.89
 C       3.515206     0.209150    -1.520067      94.62
 H       3.784941    -0.173357    -2.595188      27.36
 O       4.265489     1.427992    -1.510755     179.63
 H       4.652129     1.519081    -0.609644      30.40
 C       4.099489    -0.855499    -0.421028      84.57
 H       3.478046    -1.899631    -0.488504      28.31
 O       5.473919    -1.006323    -0.589260     158.24
 H       5.666106    -1.980698    -0.559900      24.61
 C       3.980402    -0.238938     1.117440      92.51
 O       4.727387     1.099088     1.255933     138.43
 H       4.302035     1.628478     2.031537      28.09
 H       4.657994    -0.994727     1.596347      29.48
 H       2.830522    -0.237317     1.490072      27.47
55
name = lig-Water-frame_804
 C      -1.708224     3.801388     2.862707      54.18
 H      -2.240684     4.849186     2.526193      25.14
 C      -1.180362     1.428130     2.843684      37.29
 H      -1.302593     0.373867     2.617720      23.99
 C      -0.029438     1.711742     3.723348      15.34
 O       0.689767     0.527326     4.134549     157.16
 C       0.123078    -0.723643     3.755503     130.65
 H       0.949234    -1.361057     4.124983      27.56
 H       0.204406    -1.015915     2.615232      27.93
 H      -0.724167    -1.050189     4.138539      30.75
 C       0.166332     3.023910     4.194139      37.83
 O       1.243597     3.231786     5.101325     177.22
 H       1.182663     4.030644     5.676742      25.66
 C      -0.594817     4.016040     3.647056      62.88
 H      -0.400605     5.013798     3.858329      23.20
 C      -1.917450     2.509723     2.343145      -1.48
 C      -3.135794     2.162154     1.497567      84.13
 H      -3.994300     2.955154     1.500541      27.04
 O      -3.703808     0.944381     2.083054     131.76
 H      -4.542276     0.810988     1.558044      21.77
 C      -2.857030     2.057949    -0.094448     102.05
 H      -2.245278     2.856826    -0.302628      29.55
 C      -4.087285     2.263350    -1.022047      92.16
 O      -5.168246     1.200094    -0.475102     207.35
 H      -4.895882     0.223814    -0.665026      24.55
 H      -3.837163     1.917942    -1.902018      30.64
 H      -4.633453     3.141533    -0.781752      28.61
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 C       1.616738     1.664492    -0.629471      35.04
 H       2.194824     2.535865    -0.241769      27.07
 C       0.996718    -0.590272    -1.676526      72.22
 H       1.242699    -1.575047    -2.138769      26.35
 C      -0.328060    -0.409742    -1.604810      23.00
 O      -1.196763    -1.362422    -1.922980     189.73
 C      -0.764703    -2.859422    -1.964364      74.92
 H      -0.320576    -2.882546    -0.994254      27.73
 H      -1.651326    -3.738445    -1.869539      24.19
 H      -0.051549    -3.385802    -2.872560      23.43
 C      -0.775331     0.835169    -0.926132      39.21
 O      -2.129659     0.771712    -0.391175     180.65
 C       0.158709     1.791754    -0.417897      51.73
 H      -0.204952     2.589465     0.008178      28.20
 C       2.001053     0.430508    -1.288477      16.63
 C       3.479252     0.231844    -1.550321      93.83
 H       3.585348    -0.505155    -2.465063      28.39
 O       4.290160     1.435031    -1.494968     198.49
 H       4.577777     1.382404    -0.549198      29.18
 C       4.109558    -0.856483    -0.373258      95.23
 H       3.711813    -1.784465    -0.309145      31.76
 O       5.512624    -1.019530    -0.638613     172.11
 H       5.675327    -1.978607    -0.489518      27.10
 C       3.987961    -0.214667     1.134309     115.22
 O       4.705997     1.079101     1.280013     142.21
 H       4.292695     1.622651     1.988413      29.36
 H       4.566614    -1.002720     1.730927      30.02
 H       3.082561    -0.247244     1.768112      30.25
55
name = lig-Water-frame_805
 C      -1.684977     3.734770     2.860061      85.45
 H      -2.298763     4.492724     2.626784      32.18
 C      -1.120742     1.483182     2.843970      41.43
 H      -1.489266     0.513445     2.531015      23.68
 C      -0.070464     1.682881     3.689828      15.80
 O       0.667670     0.538343     4.119408     198.07
 C       0.172977    -0.770754     3.759753     102.97
 H       0.787758    -1.497834     4.320542      25.86
 H       0.104364    -0.754882     2.707350      28.50
 H      -0.976103    -0.790754     4.468045      23.50
 C       0.255476     3.044470     4.211817      24.42
 O       1.175842     3.221773     5.128571      53.57
 H       1.242985     4.230353     5.567951      23.41
 C      -0.611184     4.018453     3.622701      65.35
 H      -0.225236     5.102436     3.756828      19.78
 C      -1.929876     2.572537     2.322869      -1.08
 C      -3.201795     2.156883     1.507800      90.30
 H      -3.916245     3.047125     1.644280      27.47
 O      -3.683007     0.936040     2.050891     144.66
 H      -4.553218     0.937866     1.580612      22.02
 C      -2.857736     2.044689    -0.025318      84.07
 H      -2.094283     2.916627    -0.284548      25.38
 C      -4.097871     2.168892    -0.949093      79.84
 O      -5.141993     1.207661    -0.437081     210.79
 H      -4.849235     0.395042    -0.862421      26.49
 H      -4.137607     1.761932    -2.165829      24.77
 H      -4.459673     3.305356    -0.976974      27.25
 C       1.656438     1.581261    -0.687177      66.09
 H       2.144356     2.488380    -0.338568      26.94
 C       1.010337    -0.506779    -1.707389      79.67
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 H       1.259456    -1.435483    -2.294526      26.30
 C      -0.330778    -0.332617    -1.562854      17.04
 O      -1.194199    -1.389546    -1.937981     204.76
 C      -0.787577    -2.816312    -1.900721     106.79
 H      -0.258296    -2.849668    -0.900125      27.76
 H      -1.592242    -3.540506    -1.975947      26.95
 H      -0.258618    -3.056190    -2.696378      28.40
 C      -0.797546     0.825968    -0.920101      40.85
 O      -2.107449     0.697863    -0.417648     142.49
 C       0.174380     1.771153    -0.462636      88.92
 H      -0.302924     2.832620     0.069606      22.93
 C       1.886993     0.422988    -1.351695      48.14
 C       3.455378     0.173986    -1.533047      85.52
 H       3.522453    -0.470983    -2.447512      29.18
 O       4.302561     1.412767    -1.494568     104.94
 H       4.548605     1.496608    -0.386712      23.39
 C       4.094203    -0.761084    -0.303806      84.35
 H       3.593912    -1.860063    -0.230852      27.93
 O       5.562912    -1.036987    -0.691840     126.64
 H       5.762074    -1.985272    -0.380616      26.20
 C       4.039082    -0.227274     1.163207     121.18
 O       4.676180     1.052011     1.300145     145.52
 H       4.146447     1.608205     1.923256      28.68
 H       4.584371    -0.931777     1.820566      29.97
 H       3.034660    -0.124361     1.748936      28.80
55
name = lig-Water-frame_806
 C      -1.688781     3.757691     2.832322      32.80
 H      -2.551306     4.556373     2.550786      22.16
 C      -1.101158     1.546932     2.798305      76.10
 H      -1.551980     0.576372     2.464822      23.08
 C      -0.077122     1.638674     3.693183       0.13
 O       0.670631     0.583779     4.119949     202.27
 C       0.165854    -0.787110     3.829271     113.26
 H       0.688615    -1.655605     4.339513      25.53
 H      -0.065867    -0.805979     2.707993      26.77
 H      -0.720821    -0.745623     4.194745      31.27
 C       0.259616     3.014128     4.151435       1.12
 O       1.162152     3.229219     5.188934     109.02
 H       1.043704     4.109933     5.414831      31.42
 C      -0.528723     4.059727     3.667352      70.22
 H      -0.274726     5.071988     3.774566      22.79
 C      -1.968131     2.499804     2.301234       5.50
 C      -3.210153     2.176738     1.516926      87.11
 H      -3.918199     3.069618     1.689126      25.71
 O      -3.683924     0.934494     2.011179     145.90
 H      -4.699895     0.681036     1.648050      18.98
 C      -2.826030     2.031158    -0.005676      90.09
 H      -2.175365     2.789087    -0.241658      28.14
 C      -4.136098     2.053366    -0.907781     115.88
 O      -5.120855     1.248024    -0.401881     346.46
 H      -4.825763     0.332016    -0.798850      24.10
 H      -3.999092     1.972573    -1.903584      30.20
 H      -4.289526     3.112298    -1.087122      28.53
 C       1.536462     1.561714    -0.715337      50.52
 H       2.393936     2.253783    -0.521101      25.78
 C       1.010724    -0.480422    -1.782012     113.46
 H       1.519261    -1.325357    -2.492107      24.71
 C      -0.364856    -0.307177    -1.525704      17.52
 O      -1.231927    -1.401775    -1.955558     222.39
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 C      -0.785686    -2.734729    -1.793094      82.29
 H      -0.164571    -3.116925    -0.961124      27.13
 H      -1.929140    -3.230862    -1.998298      22.23
 H      -0.037832    -2.783313    -2.816445      21.96
 C      -0.819967     0.823072    -0.868305      48.54
 O      -2.109993     0.665024    -0.435975     138.54
 C       0.194668     1.775177    -0.513931      68.86
 H      -0.070365     2.656725    -0.002633      23.23
 C       1.945216     0.446452    -1.396139      37.44
 C       3.440171     0.091062    -1.450790      85.08
 H       3.731592    -0.273285    -2.579068      26.83
 O       4.295973     1.365335    -1.484577     153.73
 H       4.431714     1.630130    -0.670232      35.29
 C       4.067480    -0.695046    -0.256129      87.00
 H       3.493990    -1.545727    -0.280908      31.09
 O       5.586149    -1.052917    -0.720817      74.60
 H       5.760435    -1.935344    -0.325299      27.52
 C       4.081495    -0.252615     1.210146     118.67
 O       4.656392     1.053656     1.321318     160.42
 H       3.980170     1.613570     1.854781      27.93
 H       4.683105    -0.983103     1.881935      27.42
 H       2.943909    -0.094414     1.318815      26.88
55
name = lig-Water-frame_807
 C      -1.711696     3.838929     2.791634      20.64
 H      -2.387537     4.629072     2.566336      16.75
 C      -1.119900     1.520063     2.716891      70.45
 H      -1.324572     0.507388     2.490090      28.59
 C      -0.058989     1.644678     3.710557     -12.96
 O       0.706361     0.609361     4.139751     109.88
 C       0.156275    -0.770884     3.867639     100.98
 H       0.790035    -1.518544     4.241754      28.74
 H       0.050539    -1.096125     2.820635      29.87
 H      -1.142550    -0.852529     4.223876      24.23
 C       0.232290     2.947743     4.084393       5.68
 O       1.166250     3.212439     5.232176     184.23
 H       0.874613     4.185225     5.587891      18.44
 C      -0.485410     4.086895     3.676231      55.23
 H      -0.300912     5.168847     3.982985      20.16
 C      -1.994106     2.471251     2.325770      17.41
 C      -3.185813     2.181542     1.504271      89.04
 H      -3.992362     3.021850     1.564469      25.45
 O      -3.726279     0.910978     1.983131     209.94
 H      -4.509213     0.568503     1.724453      29.76
 C      -2.827604     1.987017    -0.028076      88.00
 H      -2.126113     2.866030    -0.353394      25.53
 C      -4.098460     2.005035    -0.864880      80.75
 O      -5.135974     1.267222    -0.373426     336.50
 H      -4.998777     0.273359    -0.367362      27.46
 H      -3.602510     1.792816    -2.031502      25.17
 H      -4.504838     3.108751    -0.817727      25.98
 C       1.457893     1.579012    -0.748746      53.94
 H       2.350966     2.129484    -0.555818      32.59
 C       1.019929    -0.486790    -1.898332      55.30
 H       1.428227    -1.233954    -2.494290      25.88
 C      -0.371803    -0.363265    -1.535363      15.02
 O      -1.281607    -1.344285    -1.931852     230.34
 C      -0.779297    -2.674515    -1.780402     133.98
 H      -0.269623    -3.186795    -0.909783      29.59
 H      -1.688962    -3.138228    -1.884065      28.55
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 H      -0.144457    -2.895201    -2.513504      30.66
 C      -0.822894     0.803440    -0.801573      41.87
 O      -2.141169     0.684538    -0.426132     129.07
 C       0.164528     1.786381    -0.552107      69.04
 H      -0.022790     2.788812     0.092920      23.98
 C       2.051080     0.440299    -1.422875      -6.63
 C       3.481037     0.082147    -1.381361     102.53
 H       3.808752    -0.335049    -2.291877      32.83
 O       4.273246     1.310355    -1.515102      40.84
 H       4.343221     1.819367    -0.526408      33.10
 C       4.085105    -0.681143    -0.251904      77.28
 H       3.392950    -1.662975    -0.279318      30.05
 O       5.560593    -1.061454    -0.717116      35.54
 H       5.676837    -1.966773    -0.316585      27.31
 C       4.096591    -0.263917     1.213367     134.59
 O       4.638984     1.086006     1.353811     152.98
 H       4.004651     1.627242     1.858338      30.05
 H       4.528689    -1.003438     1.843410      32.02
 H       2.961696    -0.259678     1.268451      30.87
55
name = lig-Water-frame_808
 C      -1.671899     3.894659     2.782460      56.27
 H      -2.268007     4.836740     2.504502      23.88
 C      -1.094589     1.423559     2.685522      43.08
 H      -1.148276     0.335767     2.365632      26.43
 C      -0.073559     1.666124     3.668031     -28.02
 O       0.742266     0.592193     4.161746      99.12
 C       0.084834    -0.747838     3.900910     118.03
 H       0.953387    -1.326368     4.449635      26.90
 H       0.268201    -1.120384     2.843789      30.16
 H      -0.755082    -0.928497     4.278980      32.13
 C       0.234142     2.947437     4.100765      -5.78
 O       1.154623     3.189211     5.236994     118.01
 H       0.904845     3.938783     5.886025      22.44
 C      -0.535701     4.096467     3.615704      36.76
 H      -0.284045     4.987071     4.217520      14.43
 C      -2.007862     2.548513     2.384497      -6.00
 C      -3.183124     2.144529     1.451362      97.72
 H      -3.949522     2.942244     1.435533      29.18
 O      -3.741073     0.883707     1.991209     171.05
 H      -4.703350     0.619020     1.560433      21.93
 C      -2.819503     1.963443    -0.054883     105.16
 H      -2.247106     2.783370    -0.445641      29.56
 C      -4.011282     2.026934    -0.880988      95.64
 O      -5.198834     1.259257    -0.338915     313.54
 H      -5.019304     0.325357    -0.092976      28.23
 H      -3.687013     1.618162    -1.730736      31.43
 H      -4.615542     2.901400    -0.674896      26.56
 C       1.518330     1.556325    -0.823044      32.98
 H       2.079565     2.473154    -0.330259      29.69
 C       1.047752    -0.461680    -1.985915      54.49
 H       1.237593    -1.521408    -2.664582      25.52
 C      -0.329726    -0.398399    -1.561128      24.76
 O      -1.325049    -1.262239    -1.878314     185.19
 C      -0.783650    -2.650495    -1.773467      91.05
 H      -0.483577    -2.767221    -0.673048      28.29
 H      -1.714765    -3.556323    -1.885703      25.61
 H      -0.035954    -3.131438    -2.639805      25.42
 C      -0.807025     0.737630    -0.761023      16.98
 O      -2.177144     0.735799    -0.392796     157.96
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 C       0.058572     1.836044    -0.543963      53.53
 H      -0.129382     2.789140     0.083631      26.36
 C       2.036796     0.402626    -1.430474      26.98
 C       3.555882     0.142703    -1.337032     114.91
 H       3.797843    -0.785616    -2.180920      31.56
 O       4.269417     1.295323    -1.538301      81.84
 H       4.189036     1.777523    -0.621063      31.00
 C       4.125676    -0.761215    -0.250076      96.76
 H       3.639035    -1.689251    -0.202131      35.37
 O       5.497407    -1.073631    -0.683760      61.08
 H       5.577239    -2.029742    -0.372404      27.26
 C       4.069306    -0.241188     1.168959     129.61
 O       4.625485     1.115921     1.387970     124.59
 H       4.031159     1.665692     2.026568      26.32
 H       4.485352    -1.080585     1.918669      29.55
 H       2.971240    -0.363941     1.608317      30.56
55
name = lig-Water-frame_809
 C      -1.628959     3.929569     2.777930      74.60
 H      -2.150297     4.859995     2.379253      24.72
 C      -1.069252     1.373668     2.694318      39.67
 H      -1.217046     0.460198     2.177459      26.46
 C      -0.070060     1.651878     3.606938     -33.69
 O       0.739874     0.578864     4.168825     140.58
 C       0.155640    -0.736976     3.936806     112.59
 H       0.752221    -1.240791     4.634332      27.24
 H       0.317519    -0.984050     2.866663      28.70
 H      -0.979537    -1.015269     4.591410      24.31
 C       0.217272     3.026420     4.160858       7.05
 O       1.138735     3.137396     5.219016     146.36
 H       0.896354     3.804818     5.891848      27.64
 C      -0.567187     4.058798     3.593038      62.13
 H      -0.360451     4.935378     4.186936      18.14
 C      -1.995952     2.591898     2.418566     -34.31
 C      -3.172468     2.097746     1.413827      87.38
 H      -3.994902     2.972580     1.384148      26.71
 O      -3.758915     0.855568     2.001673     166.93
 H      -4.682503     0.973983     1.561566      21.62
 C      -2.789929     1.964272    -0.050823     103.16
 H      -2.195393     2.853078    -0.444465      26.43
 C      -4.024456     2.030321    -0.867622      74.24
 O      -5.274348     1.257438    -0.298960     261.88
 H      -4.888446     0.305674    -0.199464      24.51
 H      -3.886156     1.545878    -2.018467      25.62
 H      -4.422599     3.095402    -0.975347      26.66
 C       1.536819     1.593386    -0.859873      40.31
 H       1.861706     2.411623    -0.331013      30.21
 C       1.045315    -0.494729    -2.062576      66.47
 H       1.210000    -1.279862    -2.579714      28.75
 C      -0.266165    -0.362683    -1.571522      16.52
 O      -1.359786    -1.229681    -1.843007     164.27
 C      -0.833205    -2.696181    -1.760162     117.12
 H      -0.528615    -2.441743    -0.754439      28.46
 H      -1.543682    -3.376377    -1.869071      31.31
 H      -0.076108    -2.928193    -2.426551      30.31
 C      -0.791180     0.693920    -0.737219      12.14
 O      -2.181484     0.756579    -0.360513     150.72
 C       0.016510     1.832651    -0.547717      38.84
 H      -0.321156     2.751104     0.023684      25.85
 C       1.999255     0.374737    -1.419999      11.38
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 C       3.585870     0.109233    -1.361875     113.95
 H       3.700071    -0.577601    -2.134430      33.92
 O       4.292645     1.316097    -1.563701     127.52
 H       4.170311     1.761217    -0.730402      31.97
 C       4.161392    -0.822594    -0.217408     104.16
 H       3.633781    -1.845200    -0.175767      31.39
 O       5.443939    -1.101707    -0.637083     114.91
 H       5.604239    -2.040171    -0.428339      26.25
 C       4.025936    -0.232877     1.195944     125.85
 O       4.608402     1.131999     1.413599     173.58
 H       4.061471     1.586612     2.130708      28.87
 H       4.629886    -0.862001     1.775460      31.69
 H       3.043375    -0.223980     1.648855      31.36
55
name = lig-Water-frame_810
 C      -1.639655     3.906325     2.724068      66.61
 H      -2.112997     4.754506     2.326340      26.07
 C      -1.090603     1.438511     2.711601      40.59
 H      -1.375657     0.552063     2.089735      26.51
 C      -0.017044     1.638931     3.594099      -4.31
 O       0.712591     0.598804     4.165343     170.89
 C       0.212541    -0.741303     4.033257     127.39
 H       0.766469    -1.507313     4.719970      25.87
 H       0.200878    -1.029084     2.968011      28.23
 H      -0.725352    -0.759301     4.266023      31.37
 C       0.163110     3.035723     4.188263      26.87
 O       1.126390     3.071426     5.190294     144.77
 H       0.859149     3.946645     5.795939      22.82
 C      -0.523423     4.044904     3.667000      68.99
 H      -0.469169     5.167303     3.958975      21.01
 C      -1.965181     2.558226     2.393497      -5.80
 C      -3.146438     2.102362     1.447312      94.66
 H      -3.909247     2.853084     1.448513      27.39
 O      -3.773695     0.865174     1.992481     169.82
 H      -4.674390     0.974433     1.699403      22.66
 C      -2.763721     1.994470    -0.053994      89.88
 H      -2.126030     2.880393    -0.287807      25.81
 C      -4.138974     2.027141    -0.912677      95.96
 O      -5.309727     1.273159    -0.263663     280.31
 H      -4.964718     0.371137    -0.523999      25.21
 H      -4.060334     1.718766    -1.893313      29.92
 H      -4.116790     3.087841    -1.274960      27.42
 C       1.437405     1.636529    -0.864758      52.41
 H       2.255426     2.382492    -0.360804      29.62
 C       1.023822    -0.490705    -2.062052      50.54
 H       1.474497    -1.437771    -2.835450      22.27
 C      -0.276573    -0.324208    -1.577258      17.41
 O      -1.375474    -1.229909    -1.840840     191.84
 C      -0.877504    -2.663485    -1.713492      76.81
 H      -0.322427    -2.695101    -0.647585      26.76
 H      -1.927644    -3.429907    -1.865601      24.31
 H       0.073697    -2.738715    -2.416772      24.61
 C      -0.776575     0.714225    -0.725946      25.78
 O      -2.137013     0.716882    -0.341765     136.19
 C       0.062903     1.766277    -0.574854      60.47
 H      -0.468251     2.746705    -0.083526      25.16
 C       1.992729     0.384862    -1.396744      -0.71
 C       3.538696     0.039283    -1.397361      56.36
 H       3.761450    -0.356248    -2.607944      26.65
 O       4.333445     1.338214    -1.596451       0.76
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 H       4.216880     1.945086    -0.628357      28.73
 C       4.112151    -0.845363    -0.177168      92.10
 H       3.461043    -1.744289    -0.184146      29.29
 O       5.449562    -1.143630    -0.597639     111.33
 H       5.683802    -2.098021    -0.374418      24.41
 C       4.022948    -0.215567     1.252654      98.07
 O       4.596424     1.134877     1.418228     170.37
 H       4.017832     1.577459     2.089374      30.85
 H       4.856960    -0.823096     1.831517      26.08
 H       2.844854    -0.125391     1.567665      26.73
55
name = lig-Water-frame_811
 C      -1.628645     3.816074     2.691774      55.66
 H      -2.219195     4.773791     2.245460      22.67
 C      -1.122599     1.534584     2.727501      58.53
 H      -1.375315     0.563717     2.310020      24.17
 C       0.010576     1.648347     3.607258      39.42
 O       0.711786     0.637336     4.170636     166.70
 C       0.280990    -0.760698     4.111508      93.85
 H       0.819037    -1.522761     4.632632      25.09
 H       0.233434    -1.211817     3.051835      25.90
 H      -1.022958    -0.544196     4.182031      21.30
 C       0.132120     2.926214     4.196322      19.15
 O       1.112299     3.038325     5.182931     135.04
 H       1.034031     3.860865     5.575465      31.48
 C      -0.540888     4.123714     3.708656      58.28
 H      -0.345657     5.128693     3.846699      21.93
 C      -1.937649     2.513761     2.327560      53.58
 C      -3.109689     2.117721     1.508765      83.96
 H      -3.965604     2.992219     1.587878      24.78
 O      -3.762242     0.896015     1.979334     151.70
 H      -4.860758     0.725337     1.814084      19.28
 C      -2.790510     2.005253    -0.062858      71.02
 H      -2.136786     2.847866    -0.266147      25.70
 C      -4.230463     2.047070    -0.944361      79.10
 O      -5.309033     1.319161    -0.257689     254.62
 H      -5.214299     0.418272    -0.675514      26.73
 H      -4.033278     1.491326    -2.048180      24.70
 H      -4.356238     3.121240    -1.148286      27.01
 C       1.411645     1.656109    -0.842157      70.36
 H       2.263519     2.160091    -0.660639      26.65
 C       1.049270    -0.491606    -2.031540      46.16
 H       1.400724    -1.119655    -2.664662      22.47
 C      -0.360600    -0.332315    -1.590205      11.62
 O      -1.366968    -1.255704    -1.845876     241.11
 C      -0.919909    -2.613711    -1.654830     121.33
 H      -0.449406    -3.067733    -0.721707      27.33
 H      -1.685947    -3.142027    -1.826416      30.16
 H      -0.183077    -2.814692    -2.455597      26.31
 C      -0.773073     0.724469    -0.754949      30.05
 O      -2.069084     0.666954    -0.327266     129.57
 C       0.119080     1.753981    -0.576906      78.34
 H      -0.217406     2.636776    -0.215905      27.52
 C       1.969735     0.416292    -1.388710      14.92
 C       3.480005     0.026615    -1.485205      69.47
 H       3.720443    -0.311358    -2.388610      28.96
 O       4.363918     1.354691    -1.599355     111.76
 H       4.356743     1.849237    -0.849566      34.64
 C       4.022879    -0.827860    -0.177607      73.41
 H       3.345036    -1.695293    -0.131678      26.82
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 O       5.481443    -1.199264    -0.562215     127.74
 H       5.616755    -2.136272    -0.204051      25.29
 C       4.043660    -0.196198     1.307053     113.57
 O       4.590101     1.131775     1.403008     238.98
 H       3.920422     1.722705     1.959082      26.80
 H       4.538474    -0.885765     1.927952      28.31
 H       3.029040    -0.253110     1.543762      29.07
55
name = lig-Water-frame_812
 C      -1.589738     3.799060     2.705631      57.85
 H      -2.162809     4.507457     2.309076      30.59
 C      -1.092413     1.530678     2.767420      60.29
 H      -1.306460     0.477615     2.595347      20.92
 C      -0.032398     1.668440     3.612709      32.51
 O       0.757905     0.654403     4.187091     206.37
 C       0.240140    -0.752702     4.122204     115.56
 H       0.887998    -1.344496     4.868320      24.93
 H       0.448844    -1.200775     3.152453      27.05
 H      -0.690622    -0.782574     4.429688      28.56
 C       0.118809     2.875597     4.200316      28.04
 O       1.112469     2.998475     5.178278      92.28
 H       1.150816     3.995201     5.557626      28.67
 C      -0.617418     4.123184     3.676215      81.74
 H      -0.097731     5.157227     3.961620      15.41
 C      -1.928099     2.508838     2.258454      47.49
 C      -3.155333     2.150386     1.520499     102.96
 H      -3.765866     2.991359     1.649918      26.94
 O      -3.748073     0.912561     1.986286     249.24
 H      -4.612951     0.690532     1.809176      27.01
 C      -2.863307     1.985345    -0.063269      57.62
 H      -2.168823     2.830843    -0.461547      24.16
 C      -4.256810     2.049116    -0.980821      89.81
 O      -5.305427     1.384063    -0.277291     254.40
 H      -5.424564     0.444125    -0.575056      29.16
 H      -3.982193     1.495438    -1.837126      27.50
 H      -4.827050     3.037948    -0.932778      24.89
 C       1.508124     1.589857    -0.847342      53.86
 H       2.266542     2.534581    -0.729003      21.88
 C       1.027474    -0.436836    -1.924853     115.67
 H       1.399229    -1.305084    -2.791073      20.97
 C      -0.403566    -0.359346    -1.613867      26.09
 O      -1.352257    -1.290408    -1.839726     242.34
 C      -0.927562    -2.573003    -1.627566      93.38
 H      -0.647113    -3.131004    -0.642083      24.55
 H      -2.025293    -3.279103    -1.971667      22.81
 H      -0.338757    -2.994727    -2.525860      23.52
 C      -0.772214     0.711031    -0.823271      46.85
 O      -2.033110     0.650739    -0.299272     146.00
 C       0.136558     1.784578    -0.552833      69.83
 H      -0.069592     2.967908    -0.097486      19.25
 C       1.930525     0.432240    -1.417184      45.73
 C       3.432929     0.115539    -1.488830      47.18
 H       3.741709    -0.737745    -2.469632      22.50
 O       4.379726     1.328408    -1.631058     104.44
 H       4.441349     1.819311    -0.708719      25.54
 C       3.970200    -0.782196    -0.208500      59.71
 H       3.352874    -1.754587    -0.069439      24.10
 O       5.481962    -1.260052    -0.523821     105.80
 H       5.533756    -2.141870    -0.075518      26.90
 C       4.056120    -0.183913     1.302764      87.05
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 O       4.585865     1.133955     1.384454     244.17
 H       3.924524     1.726597     1.792433      26.88
 H       4.367716    -1.045967     2.066903      24.53
 H       2.867404    -0.273052     1.715315      22.65
55
name = lig-Water-frame_813
 C      -1.563649     3.817714     2.720864      41.31
 H      -2.276797     4.687584     2.252213      22.75
 C      -1.079305     1.433587     2.778495      49.82
 H      -1.350220     0.354185     2.711165      22.60
 C      -0.065193     1.665974     3.655944      25.12
 O       0.803491     0.652913     4.196298     153.40
 C       0.256261    -0.738759     4.143373     101.60
 H       0.856853    -0.997227     5.039614      24.32
 H       0.620211    -1.200808     3.146009      24.43
 H      -0.879088    -1.063497     4.729751      22.51
 C       0.109401     2.962067     4.205733      21.70
 O       1.122211     2.979343     5.177258     125.44
 H       1.105650     3.922255     5.580783      24.60
 C      -0.630680     4.041638     3.660917      27.20
 H      -0.238446     4.930950     3.999945      20.66
 C      -1.883737     2.496082     2.237015       8.72
 C      -3.215111     2.158694     1.462273      84.40
 H      -3.882787     3.191397     1.642627      24.39
 O      -3.695422     0.926247     2.021000     197.84
 H      -4.670525     0.780283     1.630725      20.88
 C      -2.936341     1.981432    -0.080629      72.54
 H      -2.354106     2.703950    -0.536539      28.70
 C      -4.251711     2.047407    -0.943948      92.66
 O      -5.340419     1.425396    -0.292052     277.43
 H      -5.383516     0.463899    -0.388854      29.45
 H      -3.960388     1.613086    -2.057897      25.19
 H      -4.749001     3.012084    -1.058428      26.58
 C       1.601103     1.605972    -0.826142      62.27
 H       1.983765     2.550843    -0.733468      25.14
 C       0.952013    -0.463758    -1.872701      77.01
 H       1.255215    -1.263541    -2.441618      26.70
 C      -0.362108    -0.361403    -1.628901      14.84
 O      -1.349584    -1.314031    -1.833595     237.38
 C      -1.014277    -2.671146    -1.664657     117.44
 H      -0.737053    -2.785142    -0.585284      26.80
 H      -1.855398    -3.086677    -1.836844      29.06
 H      -0.264928    -3.131156    -2.424111      25.03
 C      -0.775140     0.761201    -0.869694      24.83
 O      -2.053592     0.666490    -0.258706     125.64
 C       0.171488     1.854054    -0.523153      55.38
 H      -0.077651     2.682365    -0.112676      21.93
 C       1.964187     0.437405    -1.465146      46.47
 C       3.453105     0.168154    -1.482175      96.65
 H       3.575550    -0.548167    -2.127321      29.73
 O       4.366794     1.279051    -1.671448     150.18
 H       4.533594     1.576870    -0.608002      22.04
 C       3.966268    -0.741848    -0.215171      81.78
 H       3.418795    -1.628934    -0.170923      28.58
 O       5.436130    -1.300361    -0.489771     132.85
 H       5.523986    -2.221670    -0.030153      25.19
 C       3.980700    -0.211572     1.280135     107.17
 O       4.601369     1.127736     1.355844     219.10
 H       3.879770     1.694869     1.858087      25.71
 H       4.522465    -0.875193     1.896848      27.20
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 H       3.021911    -0.043964     1.648589      27.84
55
name = lig-Water-frame_814
 C      -1.623079     3.830095     2.660314      57.25
 H      -2.080848     4.708801     2.403266      22.17
 C      -1.111701     1.320062     2.765335      39.38
 H      -1.446631     0.327444     2.572799      26.76
 C      -0.063979     1.658819     3.736373     -24.82
 O       0.805892     0.662571     4.191519     159.38
 C       0.291179    -0.729466     4.225806     129.92
 H       0.935571    -1.086030     5.045063      27.87
 H       0.535680    -1.245489     3.351251      30.79
 H      -0.666334    -0.961191     4.408379      30.67
 C       0.122627     3.006201     4.201735      44.70
 O       1.129371     2.998105     5.177817     273.75
 H       1.066623     3.791934     5.704222      22.43
 C      -0.586502     3.964117     3.690640      95.56
 H      -0.492608     5.082901     4.067756      21.20
 C      -1.837827     2.473100     2.249312     -41.64
 C      -3.228033     2.198591     1.401059     104.50
 H      -3.943960     2.933352     1.513560      26.38
 O      -3.660514     0.945321     2.052052     169.22
 H      -4.613069     0.844634     1.587234      19.81
 C      -2.999631     1.971872    -0.106600      80.39
 H      -2.336749     2.860089    -0.548123      25.50
 C      -4.222647     2.018799    -0.926921     106.57
 O      -5.409727     1.440212    -0.300321     320.54
 H      -5.139856     0.467252    -0.246610      27.40
 H      -4.135418     1.860200    -2.000608      26.76
 H      -4.286129     3.166129    -1.201388      26.44
 C       1.574246     1.673094    -0.794643      41.85
 H       2.273193     2.623809    -0.642615      25.37
 C       0.953133    -0.514377    -1.839174      70.68
 H       1.291702    -1.598088    -2.336604      24.09
 C      -0.376753    -0.332602    -1.598527      11.92
 O      -1.351319    -1.309772    -1.852282     194.29
 C      -1.059788    -2.786723    -1.683433      83.77
 H      -0.697749    -2.555745    -0.604322      25.49
 H      -2.255080    -3.344414    -1.752630      22.63
 H      -0.187769    -3.173983    -2.246072      25.07
 C      -0.779444     0.875226    -0.869379      29.41
 O      -2.103224     0.708510    -0.225770     108.86
 C       0.221155     1.818950    -0.546770      47.37
 H      -0.290805     2.798461     0.126246      22.20
 C       2.018103     0.463907    -1.489955      19.78
 C       3.503603     0.181043    -1.428288      85.58
 H       3.636405    -0.678875    -2.461214      24.64
 O       4.346862     1.229201    -1.687646     215.60
 H       4.620532     1.424577    -0.869166      33.08
 C       3.998971    -0.716563    -0.196534      83.99
 H       3.242087    -1.630140    -0.349452      27.17
 O       5.360847    -1.311373    -0.461325     138.11
 H       5.498210    -2.211218    -0.088472      24.69
 C       3.919910    -0.217252     1.210233     101.45
 O       4.617753     1.128515     1.321436     171.11
 H       4.056695     1.658470     1.947142      29.46
 H       4.688933    -0.840982     1.788675      26.28
 H       2.802141     0.088037     1.659340      24.99
55
name = lig-Water-frame_815
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 C      -1.625587     3.779588     2.639234      36.84
 H      -2.137469     4.799848     2.358940      21.80
 C      -1.130029     1.287743     2.782917      24.37
 H      -1.474942     0.298042     2.350085      28.59
 C      -0.101173     1.607354     3.762890      -0.92
 O       0.787976     0.676135     4.193334     122.44
 C       0.386930    -0.710825     4.315127     122.77
 H       0.950552    -1.406117     5.056384      28.62
 H       0.546252    -1.354894     3.315716      29.50
 H      -0.921484    -0.715331     4.307824      26.93
 C       0.185140     2.924541     4.218634      32.71
 O       1.144271     3.043799     5.184723     135.76
 H       1.006790     3.840404     5.928279      27.04
 C      -0.606098     4.022358     3.681505      38.62
 H      -0.708977     4.997171     4.133296      16.43
 C      -1.856334     2.459032     2.244242     -39.77
 C      -3.160003     2.202124     1.373185     102.05
 H      -4.151913     2.934516     1.498659      24.03
 O      -3.650828     0.972032     2.056896     203.28
 H      -4.511937     0.735627     1.855483      28.30
 C      -2.971842     1.976514    -0.132138     110.24
 H      -2.413122     2.794522    -0.385451      28.68
 C      -4.229043     2.043349    -0.940859     102.56
 O      -5.462358     1.446036    -0.319678     306.51
 H      -5.048201     0.558523    -0.161194      27.61
 H      -4.177945     1.648772    -2.060861      25.97
 H      -4.150460     3.105871    -0.938819      28.43
 C       1.562803     1.742413    -0.807634      58.35
 H       2.448810     2.265409    -0.484819      31.09
 C       1.059105    -0.566027    -1.825124      36.06
 H       1.284163    -1.626629    -2.072401      26.08
 C      -0.435849    -0.296531    -1.538551      -9.08
 O      -1.365335    -1.295833    -1.899015     146.90
 C      -1.132037    -2.853393    -1.644641     106.08
 H      -0.738246    -2.934974    -0.650276      31.09
 H      -1.904969    -3.395053    -1.704999      30.90
 H      -0.199445    -3.288048    -2.246807      26.57
 C      -0.806953     0.933009    -0.861355      18.49
 O      -2.140952     0.781044    -0.214720     131.54
 C       0.193874     1.828471    -0.530742      66.72
 H      -0.097030     2.544579     0.046155      33.15
 C       2.017644     0.502754    -1.465492     -15.15
 C       3.551828     0.077435    -1.442433     104.36
 H       3.731611    -0.440125    -2.281142      32.22
 O       4.339510     1.211939    -1.716987     114.89
 H       4.940851     1.555348    -0.819751      26.03
 C       3.991955    -0.759476    -0.218948     122.97
 H       3.241502    -1.452265    -0.294795      33.64
 O       5.283373    -1.284493    -0.446709     191.07
 H       5.393340    -2.218040    -0.069666      24.83
 C       3.878348    -0.168887     1.170453     130.97
 O       4.638424     1.130200     1.276517     144.87
 H       4.188029     1.694258     1.973983      29.04
 H       4.392873    -0.922351     1.796887      32.61
 H       2.939027    -0.202834     1.512888      34.03
55
name = lig-Water-frame_816
 C      -1.574941     3.747460     2.672319      62.56
 H      -2.280019     4.473174     2.220582      27.91
 C      -1.155161     1.334082     2.797594      68.44
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 H      -1.293172     0.392287     2.328753      35.78
 C      -0.161218     1.535730     3.737030     -32.57
 O       0.799341     0.661269     4.221864     124.36
 C       0.415375    -0.737394     4.346798     131.84
 H       0.802034    -1.304674     5.140012      30.10
 H       0.612503    -1.161897     3.434426      30.51
 H      -0.571335    -0.563533     4.512485      29.37
 C       0.184234     2.875815     4.210569     -37.09
 O       1.175126     3.109153     5.225280      87.96
 H       0.931637     3.843018     5.757565      29.77
 C      -0.648144     4.049062     3.659270      21.50
 H      -0.673141     5.024346     4.244551      17.86
 C      -1.911288     2.436717     2.227309      11.51
 C      -3.139990     2.187239     1.390446     104.50
 H      -3.778160     2.955064     1.520225      31.62
 O      -3.630947     0.987684     2.058423     127.16
 H      -4.684333     0.647762     2.062251      22.04
 C      -2.900803     1.971991    -0.121337     100.27
 H      -2.265006     2.930605    -0.449575      28.20
 C      -4.266246     2.074994    -0.974122      85.88
 O      -5.475333     1.459208    -0.349129     264.60
 H      -5.254750     0.549657    -0.080079      29.84
 H      -4.079325     1.463454    -1.902835      27.16
 H      -4.590595     3.183118    -0.857249      26.75
 C       1.577912     1.721204    -0.863583      63.13
 H       2.390652     2.232990    -0.270304      32.96
 C       1.104859    -0.535903    -1.763987      42.69
 H       1.428618    -1.640121    -1.985027      27.74
 C      -0.415733    -0.299305    -1.496053      -8.39
 O      -1.389349    -1.304393    -1.939201     125.69
 C      -1.107880    -2.846146    -1.592185      88.71
 H      -0.831084    -3.320845    -0.529575      27.95
 H      -2.183080    -3.586159    -1.861312      25.05
 H      -0.473727    -3.249961    -2.338903      28.51
 C      -0.867211     0.890424    -0.865583      17.88
 O      -2.140949     0.856846    -0.232146     165.75
 C       0.172351     1.861680    -0.507487      29.19
 H      -0.059086     2.819924     0.288551      30.71
 C       1.990773     0.490170    -1.418242       1.34
 C       3.562173     0.011215    -1.445810      79.19
 H       3.836384    -0.697182    -2.522781      27.10
 O       4.371681     1.242968    -1.730917     133.72
 H       4.983887     1.510347    -0.986701      28.73
 C       3.946199    -0.794215    -0.254056     105.36
 H       3.127661    -1.680729    -0.106988      30.17
 O       5.239880    -1.260970    -0.446385     171.41
 H       5.298531    -2.163487    -0.011785      26.63
 C       3.887546    -0.115664     1.141220     116.26
 O       4.650339     1.120369     1.232326     143.41
 H       4.159501     1.707852     1.912211      28.96
 H       4.163286    -0.958230     1.884449      31.45
 H       2.671092    -0.247094     1.458621      31.50
55
name = lig-Water-frame_817
 C      -1.568306     3.705973     2.683674      57.67
 H      -2.305577     4.380937     2.227138      27.15
 C      -1.192642     1.393169     2.778763      51.33
 H      -1.173262     0.342841     2.394819      34.95
 C      -0.158963     1.525375     3.738519    -111.77
 O       0.834399     0.640261     4.264353     104.70
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 C       0.425072    -0.746763     4.362868      85.82
 H       0.880194    -1.099547     5.416536      23.79
 H       0.702948    -1.252949     3.315936      25.80
 H      -0.808755    -0.768278     4.742966      22.49
 C       0.109082     2.895742     4.180863     -63.71
 O       1.191654     3.158286     5.239405      52.12
 H       0.892277     4.060400     5.678408      18.86
 C      -0.641445     4.005687     3.686682      69.42
 H      -0.487309     5.024212     4.184833      22.05
 C      -1.917460     2.414711     2.249946      51.75
 C      -3.131010     2.151445     1.419490      86.29
 H      -3.656524     3.283434     1.572537      28.25
 O      -3.640782     0.967851     2.073152     135.95
 H      -4.606918     0.922577     1.926004      26.60
 C      -2.857006     2.066231    -0.102940      94.63
 H      -2.316142     2.846978    -0.509005      31.32
 C      -4.307990     2.095513    -0.954552      89.95
 O      -5.474171     1.472251    -0.377008     250.06
 H      -5.465179     0.530442    -0.067042      30.45
 H      -4.007463     1.612215    -1.947452      28.70
 H      -4.881572     3.003912    -1.209788      26.34
 C       1.559675     1.674890    -0.886881      49.64
 H       2.128242     2.402733    -0.236765      33.30
 C       1.044381    -0.486141    -1.676135      59.17
 H       1.587330    -1.484769    -2.022862      27.77
 C      -0.342747    -0.356150    -1.486287      14.33
 O      -1.393006    -1.335824    -1.941700     158.11
 C      -1.136087    -2.867538    -1.554393     113.62
 H      -0.898290    -3.165523    -0.609100      31.34
 H      -2.038094    -3.083681    -1.873113      30.13
 H      -0.512623    -3.154542    -2.548127      25.93
 C      -0.882148     0.842938    -0.853767       3.16
 O      -2.107600     0.879447    -0.280919     161.70
 C       0.163336     1.913509    -0.474585      25.53
 H      -0.027425     2.733287     0.147015      31.09
 C       2.010369     0.428172    -1.380624      22.72
 C       3.540654    -0.007669    -1.519659     109.30
 H       3.671194    -0.673946    -2.242662      34.55
 O       4.401567     1.265349    -1.749201     139.94
 H       4.940453     1.381809    -0.989144      30.72
 C       3.856113    -0.834381    -0.241381     119.02
 H       3.316652    -1.690325    -0.089823      32.45
 O       5.241126    -1.260038    -0.457039     159.55
 H       5.367608    -2.122091     0.010337      27.47
 C       3.837173    -0.106366     1.125662     130.00
 O       4.645598     1.105408     1.199158     167.76
 H       4.088742     1.672589     1.757666      34.54
 H       4.190687    -0.793221     1.923762      32.32
 H       2.882074     0.255219     1.277107      34.78
55
name = lig-Water-frame_818
 C      -1.609548     3.683948     2.681350      75.47
 H      -2.199706     4.666472     2.381571      24.23
 C      -1.158060     1.354324     2.779834      58.60
 H      -1.326470     0.329143     2.446882      29.65
 C      -0.103685     1.590161     3.768089     -25.56
 O       0.839748     0.633791     4.294657     148.29
 C       0.392771    -0.759633     4.414856     133.28
 H       1.019257    -0.987835     5.196812      28.71
 H       0.667754    -1.404092     3.657966      31.63
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 H      -0.567546    -1.121308     4.580708      29.71
 C       0.056666     2.919639     4.192632       7.48
 O       1.162770     3.202606     5.208830     128.03
 H       1.041751     4.129764     5.679404      24.14
 C      -0.613806     3.945955     3.719704      99.61
 H      -0.387257     4.951971     3.982874      24.65
 C      -1.891294     2.419225     2.289774      51.62
 C      -3.114051     2.187551     1.456091      92.78
 H      -3.724299     2.977904     1.558877      29.94
 O      -3.679109     0.958367     2.073948     125.48
 H      -4.605535     1.023027     1.710241      25.03
 C      -2.888025     2.174200    -0.085848      69.06
 H      -2.280838     3.063792    -0.530691      26.41
 C      -4.333343     2.084930    -0.943731      98.77
 O      -5.488437     1.477794    -0.390435     257.97
 H      -5.373505     0.511985    -0.180839      29.31
 H      -3.963241     1.745229    -1.993979      27.43
 H      -4.695694     3.037430    -1.453005      26.69
 C       1.493573     1.657853    -0.842350      41.96
 H       2.128405     2.485937    -0.536016      31.48
 C       0.988688    -0.493464    -1.615619      67.00
 H       1.385299    -1.399087    -2.099205      29.29
 C      -0.343077    -0.415989    -1.478847      23.40
 O      -1.346887    -1.359687    -1.899207     219.22
 C      -1.156829    -2.823297    -1.619234      93.62
 H      -0.782979    -2.919605    -0.457311      26.82
 H      -2.385343    -2.990311    -1.834756      22.61
 H      -0.443893    -3.184762    -2.260262      27.60
 C      -0.791414     0.839258    -0.824718      28.05
 O      -2.092574     0.860094    -0.346733     131.50
 C       0.157442     1.863174    -0.515171      57.85
 H      -0.137442     2.860358     0.114997      27.80
 C       2.058675     0.408946    -1.345520      32.77
 C       3.476778     0.048371    -1.542798      86.59
 H       3.573319    -0.866554    -2.483809      28.72
 O       4.407441     1.250048    -1.776726      52.77
 H       4.907430     1.203817    -0.727278      28.42
 C       3.825821    -0.838403    -0.208776      93.55
 H       3.189801    -1.850635    -0.213192      28.99
 O       5.266865    -1.265144    -0.470063     102.49
 H       5.488515    -2.168238    -0.026179      23.13
 C       3.773034    -0.092478     1.104698     125.55
 O       4.654444     1.095940     1.160006     140.77
 H       4.060978     1.752098     1.655563      33.45
 H       4.134510    -0.707648     1.946502      32.16
 H       2.817944     0.612839     1.215292      30.35
55
name = lig-Water-frame_819
 C      -1.631907     3.756456     2.729039      19.58
 H      -2.060951     4.638692     2.473038      26.96
 C      -1.059630     1.278587     2.827740      46.01
 H      -1.488599     0.322331     2.508851      22.23
 C      -0.053645     1.621980     3.777904      27.38
 O       0.799000     0.649334     4.304859     178.08
 C       0.399822    -0.787178     4.472743      88.97
 H       1.200932    -1.162524     5.284470      22.82
 H       0.811111    -1.538267     3.620886      25.69
 H      -0.770849    -1.142668     4.604654      23.41
 C       0.102211     2.918098     4.290542      44.27
 O       1.118813     3.232143     5.145414     120.64
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 H       1.029009     3.990252     5.687245      34.26
 C      -0.651392     3.932039     3.682506      71.73
 H      -0.290937     5.064221     3.830876      18.64
 C      -1.875779     2.422685     2.317905      19.67
 C      -3.082396     2.211326     1.480304      87.15
 H      -4.090329     2.945281     1.687655      23.55
 O      -3.734542     0.969859     2.052702     120.17
 H      -4.699408     0.811075     1.524212      19.04
 C      -2.947090     2.238234    -0.090599      76.80
 H      -2.391056     3.130191    -0.366329      24.82
 C      -4.302689     2.097700    -0.976532      90.33
 O      -5.504474     1.474233    -0.397329     297.03
 H      -5.132019     0.570152    -0.369060      26.98
 H      -3.989997     1.485598    -1.876118      26.97
 H      -4.419483     3.178357    -1.192507      26.80
 C       1.488065     1.645932    -0.784116      63.08
 H       2.244393     2.509442    -0.984866      27.29
 C       1.016935    -0.559794    -1.592116      78.23
 H       1.105122    -1.553849    -2.336364      22.86
 C      -0.415581    -0.423250    -1.438075      10.53
 O      -1.274968    -1.356614    -1.846790     250.07
 C      -1.213898    -2.724520    -1.653604     116.76
 H      -0.882370    -2.766723    -0.697426      30.07
 H      -2.110886    -3.339061    -1.598356      25.99
 H      -0.330010    -3.433934    -2.123226      24.33
 C      -0.709593     0.819558    -0.790756      32.58
 O      -2.101010     0.852437    -0.420186     100.46
 C       0.134955     1.798942    -0.559160      66.66
 H      -0.272805     2.785156    -0.179897      21.77
 C       2.013455     0.455259    -1.306718      30.31
 C       3.431017     0.065030    -1.565575      98.78
 H       3.514761    -0.480928    -2.370312      31.93
 O       4.402895     1.186034    -1.760865     126.20
 H       4.703557     1.301133    -0.929391      33.43
 C       3.843853    -0.853321    -0.218308      99.17
 H       3.135030    -1.628407    -0.318728      29.96
 O       5.295842    -1.267634    -0.473597     160.15
 H       5.422045    -2.193712    -0.140700      25.45
 C       3.689635    -0.036420     1.091457     110.61
 O       4.683333     1.098936     1.111128     159.40
 H       4.199324     1.834407     1.566014      30.18
 H       3.821794    -0.733983     2.005262      28.45
 H       2.647693     0.179428     1.202803      30.00
55
name = lig-Water-frame_820
 C      -1.639061     3.795200     2.786731       7.81
 H      -2.242262     4.742253     2.276869      15.56
 C      -1.005687     1.284782     2.861681      58.02
 H      -1.422284     0.253140     2.679467      17.89
 C      -0.021930     1.586037     3.786344      38.50
 O       0.757086     0.648150     4.323631     221.95
 C       0.443113    -0.865738     4.516989     100.62
 H       0.883202    -1.209832     5.382661      24.84
 H       0.759114    -1.232568     3.603165      27.19
 H      -0.626564    -0.757218     4.738818      24.45
 C       0.116947     2.932276     4.343778      27.72
 O       1.121010     3.241372     5.095857      97.47
 H       0.800922     4.012022     5.826457      20.64
 C      -0.645562     3.980815     3.661680      14.66
 H      -0.350072     4.926297     3.846087      34.82
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 C      -1.849408     2.416561     2.360546      39.18
 C      -3.151390     2.219912     1.493061     102.92
 H      -3.788290     2.952912     1.751431      29.22
 O      -3.795114     0.975652     2.005205     255.37
 H      -4.549581     0.653374     1.643546      26.71
 C      -3.000400     2.218317    -0.076211      69.99
 H      -2.448366     3.139113    -0.326476      22.56
 C      -4.227962     2.139990    -0.997082      85.96
 O      -5.489030     1.472191    -0.408661     258.05
 H      -5.121101     0.548281    -0.493949      25.54
 H      -4.039025     1.303934    -1.780484      24.63
 H      -4.464985     3.199666    -1.048746      27.29
 C       1.553787     1.665712    -0.768084      77.25
 H       2.129181     2.464207    -1.080204      27.58
 C       1.018354    -0.660794    -1.615473      65.62
 H       1.219937    -1.445899    -2.248159      25.67
 C      -0.375909    -0.405861    -1.371509      11.16
 O      -1.255869    -1.324069    -1.837252     257.38
 C      -1.189579    -2.698127    -1.638376     104.19
 H      -0.878445    -2.827745    -0.450778      24.54
 H      -2.125138    -3.440722    -1.622345      23.16
 H      -0.544966    -3.269387    -2.190564      26.91
 C      -0.775054     0.734730    -0.757304      19.08
 O      -2.122440     0.879620    -0.492471     122.68
 C       0.146162     1.804137    -0.591375      64.20
 H      -0.355529     2.776900    -0.372186      17.52
 C       1.904968     0.460060    -1.291529      12.87
 C       3.415917     0.096584    -1.515375      67.54
 H       3.494529    -0.473833    -2.709240      24.99
 O       4.380004     1.108994    -1.760408      37.84
 H       4.657914     1.560595    -0.773306      23.23
 C       3.901653    -0.821637    -0.279765      96.70
 H       3.107773    -1.672263    -0.276864      26.65
 O       5.299951    -1.261426    -0.472508     165.66
 H       5.321759    -2.237639    -0.223481      24.93
 C       3.622610    -0.025016     1.081804      93.13
 O       4.689607     1.095380     1.060750     145.12
 H       4.306245     1.852831     1.542990      27.81
 H       3.722992    -0.665933     1.916002      28.98
 H       2.456051     0.052027     1.140849      25.51
55
name = lig-Water-frame_821
 C      -1.689709     3.784216     2.775972      49.18
 H      -2.230291     4.460388     2.307602      15.26
 C      -1.035085     1.352288     2.863351      60.77
 H      -1.191960     0.303087     2.779659      21.32
 C      -0.018010     1.565155     3.820305      32.17
 O       0.774195     0.614670     4.381610     177.13
 C       0.451354    -0.859308     4.544995      89.00
 H       0.820635    -1.261770     5.596243      22.49
 H       0.674368    -1.266648     3.471879      23.46
 H      -0.666980    -0.727154     4.753647      23.29
 C       0.036932     2.932401     4.263124      36.96
 O       1.177985     3.277226     5.124615     215.88
 H       0.840345     3.889838     5.737298      24.51
 C      -0.579070     4.022809     3.700065      13.01
 H      -0.326896     5.158853     4.077287      32.17
 C      -1.837210     2.408022     2.400914      16.83
 C      -3.219297     2.167888     1.499862      64.55
 H      -3.706051     3.328441     1.786899      24.83
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 O      -3.815299     0.984938     1.978541     194.51
 H      -4.772204     0.605647     1.567857      19.18
 C      -3.003284     2.154185    -0.045437      79.68
 H      -2.397698     3.070527    -0.378722      21.62
 C      -4.184677     2.151763    -0.976899      96.62
 O      -5.438540     1.474622    -0.426805     312.33
 H      -5.365968     0.489352    -0.494020      29.97
 H      -3.920238     1.685676    -1.911235      28.68
 H      -4.676626     3.144773    -1.310432      26.20
 C       1.552444     1.698399    -0.782197      50.80
 H       2.205238     2.673513    -0.919642      23.91
 C       1.000962    -0.676903    -1.610735      61.12
 H       1.627975    -1.589746    -2.242126      23.61
 C      -0.270850    -0.460453    -1.324802      23.24
 O      -1.295329    -1.281145    -1.858113     232.57
 C      -1.145718    -2.734826    -1.523601      94.40
 H      -0.858918    -2.979145    -0.573093      28.65
 H      -2.248108    -2.952136    -1.843463      23.24
 H      -0.427181    -3.100873    -2.477411      23.08
 C      -0.865419     0.724572    -0.700729       2.52
 O      -2.178203     0.921089    -0.554523     128.51
 C       0.157018     1.826810    -0.606833      61.00
 H      -0.377160     2.926838    -0.527038      18.73
 C       1.858775     0.371170    -1.313935      16.13
 C       3.403966     0.078957    -1.507627      97.20
 H       3.394753    -0.439650    -2.333365      33.07
 O       4.375949     1.065832    -1.742523      42.30
 H       4.401850     1.728033    -0.927095      24.96
 C       3.922521    -0.781566    -0.347803     115.49
 H       3.374096    -1.725624    -0.190508      28.88
 O       5.282280    -1.246886    -0.475039     148.37
 H       5.327220    -2.220116    -0.239190      24.95
 C       3.584174    -0.051053     1.031620      89.94
 O       4.654531     1.084553     1.016040     137.51
 H       4.306741     1.823214     1.617245      28.16
 H       3.950251    -0.690545     1.962909      27.10
 H       2.580464     0.446694     0.983760      27.12
55
name = lig-Water-frame_822
 C      -1.670622     3.716552     2.791522      53.02
 H      -2.413167     4.549899     2.277539      18.32
 C      -1.063952     1.400986     2.886087      52.68
 H      -1.160658     0.302961     2.562648      24.67
 C      -0.057127     1.576875     3.853178      38.24
 O       0.832742     0.580311     4.462645     149.10
 C       0.402886    -0.799250     4.562018     122.99
 H       0.969600    -1.217823     5.358749      26.49
 H       0.622328    -1.519272     3.774114      28.27
 H      -0.738960    -1.047373     4.632579      25.73
 C       0.036980     2.933496     4.198860       7.45
 O       1.230294     3.284672     5.146601     179.61
 H       0.961687     4.073753     5.839082      19.13
 C      -0.572586     4.100832     3.715823      11.13
 H      -0.367450     4.968651     4.166386      28.31
 C      -1.889625     2.409695     2.404796      30.28
 C      -3.247363     2.153585     1.516338      92.21
 H      -3.723711     3.025307     1.573170      30.11
 O      -3.849788     0.977387     1.968714     235.97
 H      -4.770311     0.949860     1.575929      24.08
 C      -2.955435     2.107536    -0.029987     106.40
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 H      -2.363746     2.923882    -0.305331      26.74
 C      -4.218358     2.144182    -0.966995      97.57
 O      -5.374559     1.480103    -0.452136     349.99
 H      -5.435558     0.519936    -0.539613      31.99
 H      -3.749699     2.021267    -2.040588      25.34
 H      -4.636670     3.061475    -1.305108      26.25
 C       1.498350     1.701453    -0.841746      57.80
 H       2.166648     2.479849    -0.614103      29.24
 C       1.083449    -0.690562    -1.622321      63.44
 H       1.476440    -1.495516    -1.970792      29.63
 C      -0.313580    -0.520017    -1.279280      -1.82
 O      -1.326857    -1.245763    -1.853617     176.37
 C      -1.124909    -2.748853    -1.521021     102.80
 H      -0.733758    -3.132600    -0.436189      26.56
 H      -2.137708    -2.870981    -1.813956      24.82
 H      -0.466911    -3.023792    -2.264609      27.93
 C      -0.833466     0.784169    -0.657387      -0.54
 O      -2.264081     0.945900    -0.605092     147.16
 C       0.106234     1.866182    -0.613537      57.91
 H      -0.200082     2.854563    -0.537163      24.97
 C       1.922904     0.347750    -1.318723      18.61
 C       3.374546     0.034685    -1.481349      84.30
 H       3.398984    -0.840966    -2.477093      24.19
 O       4.372503     1.072390    -1.742726      74.01
 H       4.262129     1.664545    -1.041804      34.09
 C       3.900767    -0.778533    -0.348833     118.87
 H       3.386332    -1.766393    -0.290877      29.43
 O       5.274717    -1.213858    -0.492738     148.97
 H       5.379611    -2.127071    -0.167955      26.26
 C       3.636763    -0.055861     0.966767     128.68
 O       4.597473     1.081884     0.981348     143.28
 H       4.222028     1.657219     1.687237      30.69
 H       3.867775    -0.642705     1.774894      33.25
 H       2.753699     0.590045     0.985395      29.43
55
name = lig-Water-frame_823
 C      -1.643793     3.724706     2.813017      39.77
 H      -2.301934     4.461938     2.541755      29.02
 C      -1.083396     1.363460     2.908782      52.05
 H      -1.268463     0.498786     2.336245      28.43
 C      -0.098808     1.592276     3.884526     -18.36
 O       0.866185     0.577483     4.520963     128.19
 C       0.331457    -0.779833     4.570684     119.51
 H       1.071415    -1.173518     5.378056      27.19
 H       0.739868    -1.552991     3.790344      29.13
 H      -0.697221    -1.045830     4.708924      29.94
 C       0.150024     2.987809     4.220241      -1.52
 O       1.248721     3.274857     5.157796     128.26
 H       1.137478     4.150288     5.681292      19.28
 C      -0.636874     4.087912     3.681651      29.84
 H      -0.403475     5.128209     4.234122      15.64
 C      -1.985235     2.410165     2.386228      13.49
 C      -3.183703     2.119946     1.507732      82.59
 H      -4.110350     3.057105     1.536390      24.38
 O      -3.894775     0.970157     1.979937     176.75
 H      -4.772087     1.065149     1.596603      25.37
 C      -2.912637     2.073454    -0.042522     104.36
 H      -2.255365     3.047511    -0.216521      25.08
 C      -4.238554     2.161228    -0.978829      86.44
 O      -5.328528     1.480203    -0.478323     289.62
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 H      -5.199081     0.507988    -0.671142      29.29
 H      -3.902747     1.702489    -1.860876      28.63
 H      -4.541222     3.310662    -0.915620      25.88
 C       1.425989     1.624917    -0.918100      83.78
 H       2.184595     2.335398    -0.414368      32.63
 C       1.095979    -0.665531    -1.593227      32.57
 H       1.371422    -1.881138    -1.948583      24.39
 C      -0.390456    -0.492738    -1.234924      -6.62
 O      -1.335912    -1.241732    -1.809010     169.65
 C      -1.122824    -2.728714    -1.535819      94.03
 H      -0.796211    -2.953305    -0.535171      30.60
 H      -2.198804    -3.412089    -1.660090      24.08
 H      -0.296751    -3.228980    -2.263973      25.95
 C      -0.777145     0.825162    -0.661460      10.65
 O      -2.310760     0.938782    -0.642310     142.60
 C       0.057587     1.884886    -0.621835      60.07
 H      -0.179867     3.087937    -0.328823      23.17
 C       2.014748     0.418033    -1.304979      19.04
 C       3.385071    -0.063988    -1.533141     102.14
 H       3.512875    -0.658458    -2.279521      29.96
 O       4.357094     1.080122    -1.778254     -14.47
 H       4.181865     1.747137    -0.865449      30.06
 C       3.859147    -0.833707    -0.302960     110.81
 H       3.148692    -1.729355    -0.405412      30.59
 O       5.281193    -1.164019    -0.525548     125.43
 H       5.421638    -2.059117    -0.033548      24.53
 C       3.727819    -0.024148     0.895228     142.68
 O       4.552852     1.096031     0.961689     111.37
 H       4.143721     1.566310     1.732696      29.51
 H       3.707039    -0.798190     1.837201      31.64
 H       2.573624     0.310333     1.065580      32.66
55
name = lig-Water-frame_824
 C      -1.662226     3.739725     2.820528      33.52
 H      -2.389175     4.662527     2.638116      23.35
 C      -1.138651     1.334212     2.902494      40.17
 H      -1.280745     0.364013     2.307612      27.17
 C      -0.098939     1.621958     3.923185     -45.95
 O       0.840772     0.613619     4.538597      97.18
 C       0.340807    -0.819661     4.590341      98.51
 H       0.808925    -1.148603     5.539732      28.14
 H       0.699539    -1.191642     3.619078      29.51
 H      -0.831975    -0.792385     4.917541      25.86
 C       0.275542     3.059676     4.271583      17.76
 O       1.252896     3.252671     5.142983     148.53
 H       1.114240     4.138100     5.554849      27.70
 C      -0.645893     4.028556     3.702841      55.44
 H      -0.616538     5.073129     3.933197      17.98
 C      -2.022702     2.412431     2.412253      27.74
 C      -3.166394     2.121694     1.474950     102.30
 H      -3.838167     2.810914     1.583556      31.53
 O      -3.921746     0.957372     2.011101     131.99
 H      -4.931462     0.925891     1.534701      19.94
 C      -2.879839     2.084683    -0.075404     107.36
 H      -2.340112     2.945117    -0.214724      29.37
 C      -4.212070     2.239053    -0.954500      86.24
 O      -5.321504     1.447383    -0.489034     265.87
 H      -4.910087     0.577248    -0.708478      27.73
 H      -4.068174     1.595264    -1.925724      24.15
 H      -4.391665     3.243488    -0.779936      27.76
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 C       1.402221     1.582102    -0.952687      60.35
 H       2.070818     2.293824    -0.496384      30.23
 C       1.020995    -0.661403    -1.531390      50.40
 H       1.243911    -1.546405    -1.850905      27.25
 C      -0.365665    -0.399019    -1.214057       9.11
 O      -1.357063    -1.293309    -1.747535     177.81
 C      -1.144162    -2.740425    -1.583721     117.79
 H      -0.790860    -2.707160    -0.434794      28.94
 H      -1.880566    -3.427497    -1.576384      29.50
 H      -0.357975    -3.242055    -2.148675      28.99
 C      -0.822020     0.813052    -0.712392      17.05
 O      -2.283552     0.908708    -0.661971     138.18
 C       0.055942     1.945400    -0.618475      65.75
 H      -0.212668     2.774642    -0.199444      28.00
 C       2.018599     0.417634    -1.333052      24.98
 C       3.458301    -0.077416    -1.557560      94.53
 H       3.627954    -0.760143    -2.678614      24.90
 O       4.323427     1.095988    -1.804477     125.03
 H       4.308686     1.590973    -1.012998      34.71
 C       3.828437    -0.904473    -0.307739     113.77
 H       3.127566    -1.720489    -0.213657      30.37
 O       5.281500    -1.136887    -0.554619     135.39
 H       5.471871    -1.966079    -0.046653      28.10
 C       3.731254    -0.050440     0.919457     153.16
 O       4.519813     1.132000     0.963339     123.58
 H       4.112006     1.666962     1.726967      28.15
 H       3.880006    -0.673209     1.719663      36.20
 H       2.643486     0.026469     0.963284      34.21
55
name = lig-Water-frame_825
 C      -1.741031     3.739208     2.815930      53.19
 H      -2.339462     4.639649     2.629581      25.02
 C      -1.182217     1.335786     2.904713      49.41
 H      -1.207258     0.296383     2.656650      23.47
 C      -0.076062     1.657517     3.942381     -30.44
 O       0.774327     0.679600     4.534770      84.79
 C       0.333067    -0.802408     4.635182     103.95
 H       0.713678    -1.299674     5.563446      27.07
 H       0.477150    -1.136584     3.570614      27.11
 H      -0.658930    -0.681690     4.768863      28.07
 C       0.285624     3.053915     4.253583      31.56
 O       1.284352     3.245820     5.142996     161.93
 H       1.089858     4.199674     5.657423      26.80
 C      -0.610003     3.966152     3.746000      94.87
 H      -0.611729     5.101608     3.833841      15.08
 C      -1.995727     2.404699     2.462144      39.30
 C      -3.162020     2.079177     1.441163      62.50
 H      -3.856720     3.205142     1.610877      23.85
 O      -3.945699     0.941035     2.038073     170.45
 H      -4.715408     0.712987     1.605802      27.32
 C      -2.881345     2.083333    -0.115597      95.77
 H      -2.213601     3.022166    -0.395277      24.00
 C      -4.153937     2.279797    -0.917797      96.47
 O      -5.321224     1.400228    -0.483472     291.15
 H      -4.901223     0.508053    -0.572514      28.60
 H      -3.995875     2.232086    -2.020970      26.92
 H      -4.495544     3.411970    -0.986387      26.80
 C       1.419423     1.622148    -0.936403      38.43
 H       2.114924     2.490343    -0.734723      25.68
 C       0.934272    -0.591088    -1.440615      73.65
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 H       1.273846    -1.680651    -1.975583      24.59
 C      -0.329047    -0.356999    -1.244969      19.73
 O      -1.387843    -1.346422    -1.692348     205.61
 C      -1.102270    -2.723595    -1.552421      93.54
 H      -0.734717    -2.738150    -0.500044      27.21
 H      -2.203076    -3.422405    -1.644233      23.35
 H      -0.251517    -3.130407    -2.243957      24.67
 C      -0.917634     0.841988    -0.780384      33.85
 O      -2.214077     0.872196    -0.662198     156.88
 C       0.067256     1.901210    -0.636623      60.68
 H      -0.299345     2.876640     0.095849      21.81
 C       1.939954     0.315449    -1.405107      32.20
 C       3.518488    -0.058077    -1.630496     112.76
 H       3.543988    -0.566859    -2.431445      32.55
 O       4.295877     1.093662    -1.845098     176.83
 H       4.430251     1.572192    -0.925322      26.24
 C       3.860352    -0.927662    -0.358199      98.18
 H       3.288255    -1.905845    -0.010293      26.75
 O       5.277371    -1.140517    -0.576160     150.26
 H       5.545126    -2.024021    -0.187642      27.08
 C       3.702858    -0.113976     0.970031      88.69
 O       4.482800     1.185790     0.975878     104.06
 H       4.040479     1.792803     1.611676      29.07
 H       4.263159    -0.696577     1.883979      27.50
 H       2.508903     0.104911     0.972477      26.83
55
name = lig-Water-frame_826
 C      -1.764816     3.710672     2.863736      51.48
 H      -2.395161     4.562873     2.506548      26.46
 C      -1.142528     1.365477     2.991802      70.95
 H      -1.323212     0.263909     2.923616      23.68
 C      -0.080963     1.670140     3.912049       5.60
 O       0.707960     0.742298     4.536564     145.52
 C       0.313860    -0.716490     4.652983      99.91
 H       0.864212    -1.422140     5.387954      25.77
 H       0.360599    -1.388085     3.711911      26.60
 H      -0.919598    -0.704464     4.666532      22.92
 C       0.226836     2.975367     4.210684      27.04
 O       1.330736     3.276240     5.164207     159.75
 H       1.161685     4.006262     5.715659      31.63
 C      -0.628036     3.966950     3.736059     115.33
 H      -0.289204     5.044370     4.023990       9.83
 C      -1.985689     2.368824     2.464099      -3.18
 C      -3.201977     2.090272     1.448369      79.94
 H      -3.617529     2.956582     1.435111      29.31
 O      -3.920547     0.942267     2.065912     161.21
 H      -4.754117     0.570842     1.513139      22.92
 C      -2.876315     2.101342    -0.151925      92.87
 H      -2.216444     2.853771    -0.433907      27.17
 C      -4.142253     2.346386    -0.904288      99.70
 O      -5.290255     1.366416    -0.488801     277.39
 H      -5.029400     0.400685    -0.450437      27.84
 H      -3.957981     2.432063    -1.906556      29.24
 H      -4.646890     3.281424    -0.838849      27.79
 C       1.476108     1.670455    -0.916409      48.87
 H       2.143728     2.559779    -1.088909      27.05
 C       0.934577    -0.632582    -1.415644      81.72
 H       1.120480    -1.544013    -1.877536      26.70
 C      -0.446505    -0.362983    -1.294868      17.64
 O      -1.410206    -1.358503    -1.640102     195.03
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 C      -1.069019    -2.738475    -1.501614     113.37
 H      -0.607409    -3.088722    -0.419350      26.30
 H      -1.953237    -3.068234    -1.716541      28.82
 H      -0.337457    -2.965773    -2.345160      26.01
 C      -0.907100     0.889047    -0.866141      35.13
 O      -2.207275     0.848563    -0.638288     180.01
 C       0.051616     1.849516    -0.614325      71.18
 H      -0.098701     2.652716    -0.080979      27.30
 C       1.886351     0.311717    -1.450742      20.71
 C       3.468930    -0.017722    -1.646080      87.62
 H       3.533252    -0.800547    -2.709741      24.33
 O       4.280271     1.104236    -1.879922     151.86
 H       4.581140     1.439927    -0.849870      23.26
 C       3.932611    -0.917797    -0.379609     105.79
 H       3.515958    -1.874037    -0.275994      28.46
 O       5.299803    -1.167689    -0.593735     174.18
 H       5.506224    -2.148310    -0.396973      27.05
 C       3.684851    -0.166649     1.033487     100.88
 O       4.438062     1.234533     0.977475     142.52
 H       3.844849     1.840143     1.534638      28.53
 H       4.222314    -0.661507     1.759979      30.78
 H       2.714443     0.129782     1.274378      29.36
55
name = lig-Water-frame_827
 C      -1.747524     3.677775     2.933026      26.42
 H      -2.432419     4.439443     2.372339      20.14
 C      -1.101894     1.370042     3.097145      66.91
 H      -1.528651     0.380116     2.994177      28.65
 C      -0.098657     1.642928     3.864638      49.35
 O       0.666140     0.753141     4.554681     220.98
 C       0.230107    -0.636473     4.626832     133.11
 H       0.915105    -1.080097     5.329926      27.90
 H       0.463861    -1.315129     3.762939      28.22
 H      -0.723362    -0.794550     4.901096      30.46
 C       0.182663     2.952144     4.217445       4.39
 O       1.360015     3.277871     5.142782      57.10
 H       1.072323     4.093548     5.829061      19.76
 C      -0.650207     4.009407     3.711435      40.62
 H      -0.224264     4.900904     4.114082      20.56
 C      -1.992824     2.331263     2.439231     -44.01
 C      -3.185371     2.065990     1.470518      49.07
 H      -3.948500     3.170928     1.447751      22.34
 O      -3.881675     0.952516     2.076704     130.83
 H      -4.725922     0.688857     1.507625      21.03
 C      -2.866251     2.086803    -0.148399      95.50
 H      -2.117144     2.946978    -0.358395      24.33
 C      -4.195620     2.373811    -0.873430      72.37
 O      -5.244151     1.354139    -0.506470     275.78
 H      -4.954501     0.408544    -0.527245      25.87
 H      -4.024142     2.133895    -2.060650      23.05
 H      -4.736843     3.289745    -0.363401      23.02
 C       1.514211     1.663642    -0.947353      68.87
 H       2.121186     2.501350    -1.192306      26.63
 C       0.890837    -0.712908    -1.426904      70.37
 H       1.156110    -1.815997    -1.858372      23.63
 C      -0.552726    -0.405546    -1.361862       9.56
 O      -1.427496    -1.337460    -1.562299     192.69
 C      -0.994052    -2.736156    -1.450949     106.96
 H      -0.629693    -3.390242    -0.622414      27.03
 H      -2.123098    -3.245542    -1.860935      24.11
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 H      -0.390426    -2.987624    -2.333867      27.02
 C      -0.849688     0.891783    -0.957730      31.64
 O      -2.276181     0.854593    -0.594119     177.28
 C       0.113919     1.806273    -0.603194      62.07
 H      -0.132267     2.905370    -0.084760      24.57
 C       1.900927     0.428296    -1.444302      24.95
 C       3.349919    -0.040035    -1.685428      94.43
 H       3.534919    -0.611309    -2.425186      30.43
 O       4.280044     1.122961    -1.891349     204.04
 H       4.533734     1.330632    -1.074978      31.54
 C       3.981196    -0.862660    -0.389601      96.21
 H       3.405079    -1.879570    -0.662041      24.56
 O       5.368543    -1.201053    -0.612639     193.02
 H       5.394555    -2.174146    -0.530369      27.97
 C       3.723287    -0.174621     1.039971      86.25
 O       4.382895     1.259468     0.970647     147.24
 H       3.715162     1.797468     1.498717      27.03
 H       4.219682    -0.862073     1.878400      26.69
 H       2.643706     0.020267     1.661603      25.22
55
name = lig-Water-frame_828
 C      -1.759051     3.639531     2.930842      61.20
 H      -2.332046     4.397486     2.517163      25.45
 C      -1.209268     1.334835     3.092866      55.71
 H      -1.558522     0.304787     3.008703      29.71
 C      -0.047857     1.635793     3.887947      26.05
 O       0.639543     0.730171     4.579387     173.18
 C       0.187282    -0.585893     4.603202     116.89
 H       0.959383    -0.723031     5.505110      22.93
 H       0.522686    -1.039570     3.587471      25.92
 H      -0.822889    -0.848794     5.222494      24.57
 C       0.168328     3.013523     4.254220      17.62
 O       1.343103     3.274710     5.101115     153.70
 H       1.083158     4.062991     5.581865      26.70
 C      -0.625522     4.014565     3.720700      56.31
 H      -0.427101     5.175161     4.107731      21.62
 C      -1.968671     2.335868     2.453951      -3.60
 C      -3.178119     2.101554     1.498615      91.77
 H      -3.849842     2.765916     1.672967      30.96
 O      -3.844228     0.960387     2.068757     177.66
 H      -4.633463     0.871785     1.592104      25.99
 C      -2.858486     2.081454    -0.102189     103.74
 H      -2.225310     2.962074    -0.194286      27.22
 C      -4.271965     2.344703    -0.846984     106.60
 O      -5.204570     1.344827    -0.515826     320.83
 H      -4.741530     0.492278    -0.772058      27.36
 H      -4.195405     2.257994    -1.834492      29.35
 H      -4.549231     3.246078    -0.326166      28.33
 C       1.511551     1.651440    -1.004049      63.22
 H       2.213995     2.581592    -1.045448      26.04
 C       0.837178    -0.750113    -1.481070      58.33
 H       1.299732    -1.767156    -1.625226      24.98
 C      -0.480603    -0.443484    -1.428526      19.50
 O      -1.484780    -1.362880    -1.462654     208.25
 C      -1.012359    -2.777004    -1.490388     116.43
 H      -0.606157    -3.292404    -0.505632      27.74
 H      -1.755484    -3.356771    -1.675246      31.02
 H      -0.254734    -3.009254    -2.389551      26.75
 C      -0.858434     0.876235    -1.007147       6.65
 O      -2.329087     0.880090    -0.556308     142.73
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 C       0.202110     1.837611    -0.587662      63.23
 H      -0.239094     2.756424    -0.321927      29.16
 C       1.896909     0.442055    -1.424107      37.07
 C       3.276143    -0.000041    -1.651465      76.73
 H       3.486588    -0.784744    -2.677800      25.16
 O       4.261799     1.128468    -1.935867      57.15
 H       4.565844     1.453432    -0.854400      23.37
 C       3.953282    -0.822924    -0.427948      95.65
 H       3.340951    -1.636838    -0.558107      29.38
 O       5.435281    -1.209596    -0.637242     176.18
 H       5.440903    -2.227936    -0.493836      25.18
 C       3.781880    -0.172583     1.066832     111.29
 O       4.317400     1.239812     0.959316     168.36
 H       3.739310     1.771760     1.588790      26.90
 H       4.312979    -0.844190     1.720498      30.19
 H       2.823507    -0.207986     1.409772      30.81
55
name = lig-Water-frame_829
 C      -1.741391     3.629109     2.906022      52.62
 H      -2.396854     4.609748     2.646460      23.65
 C      -1.308212     1.276501     3.074624      34.92
 H      -1.484340     0.195947     2.962404      29.93
 C      -0.061136     1.680962     3.906017      -9.12
 O       0.627422     0.742034     4.607873     179.37
 C       0.197249    -0.583747     4.649205     136.05
 H       0.846501    -1.018789     5.371914      27.60
 H       0.298194    -0.985236     3.654972      26.95
 H      -0.770262    -0.746841     5.031021      28.11
 C       0.200555     3.059478     4.290368      28.38
 O       1.299156     3.264784     5.042188     115.76
 H       1.215819     4.223000     5.477992      27.19
 C      -0.619251     4.048450     3.748097      59.73
 H      -0.698950     5.038719     3.917946      25.80
 C      -1.952506     2.358126     2.479493      28.92
 C      -3.129712     2.106641     1.538842      70.30
 H      -3.977504     3.050911     1.864457      25.11
 O      -3.802516     0.940407     2.061467      81.36
 H      -4.801381     0.936423     1.576232      19.69
 C      -2.903530     2.105758    -0.021431     104.84
 H      -2.276654     2.999453    -0.208444      27.39
 C      -4.289847     2.320433    -0.775964      98.11
 O      -5.184891     1.310239    -0.511668     309.57
 H      -4.742374     0.515535    -0.931750      27.85
 H      -4.195561     2.683092    -1.998831      24.81
 H      -4.600264     3.396898    -0.510839      27.04
 C       1.517552     1.699130    -1.053396      53.09
 H       2.218825     2.421480    -0.817325      29.09
 C       0.903368    -0.711266    -1.542815      73.72
 H       1.323971    -1.717308    -1.530051      26.48
 C      -0.422550    -0.456469    -1.461234       8.41
 O      -1.546227    -1.435786    -1.367343     160.85
 C      -1.001586    -2.826026    -1.538356      96.27
 H      -0.524700    -2.743861    -0.484216      26.88
 H      -1.962397    -3.673623    -1.634848      24.62
 H      -0.248346    -2.897066    -2.250695      28.82
 C      -0.872647     0.875527    -0.995251      -1.16
 O      -2.312335     0.896307    -0.543370     124.25
 C       0.174437     1.839371    -0.622238      50.40
 H      -0.257735     2.879436    -0.358378      27.17
 C       1.844502     0.321346    -1.415345      25.34
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 C       3.327424     0.030749    -1.649148     112.67
 H       3.209824    -0.537376    -2.429692      30.91
 O       4.233642     1.132410    -1.953450     151.73
 H       4.409683     1.541425    -1.125182      30.93
 C       3.921764    -0.777864    -0.451763      80.02
 H       3.277542    -1.789159    -0.197099      27.15
 O       5.456002    -1.197771    -0.672260     124.50
 H       5.602328    -2.141467    -0.328400      24.11
 C       3.877245    -0.164935     1.017715      96.69
 O       4.250282     1.193537     0.953959     162.40
 H       3.839681     1.725025     1.738237      25.76
 H       4.595137    -0.775832     1.675178      28.78
 H       2.628039    -0.344728     1.120682      27.07
55
name = lig-Water-frame_830
 C      -1.689097     3.710397     2.901650      41.22
 H      -2.372155     4.406573     2.671618      24.27
 C      -1.289865     1.248233     3.106830      37.97
 H      -1.476676     0.217296     2.824281      27.13
 C      -0.175385     1.716839     3.901519      -1.31
 O       0.641312     0.785411     4.648319     141.98
 C       0.224957    -0.613317     4.696640     118.46
 H       0.830817    -1.530948     5.183180      24.24
 H       0.020898    -1.159016     3.639229      25.54
 H      -0.926347    -0.619295     4.884736      25.43
 C       0.203449     3.066113     4.273503      37.97
 O       1.281950     3.279336     5.022033     133.40
 H       1.449342     4.250515     5.358040      31.85
 C      -0.665473     4.043001     3.745711      51.42
 H      -0.747952     5.278443     3.961620      20.41
 C      -1.974399     2.349250     2.482820       5.39
 C      -3.138450     2.149561     1.607743     100.60
 H      -3.603779     3.013103     1.661027      30.25
 O      -3.793431     0.906901     2.045915     111.97
 H      -4.643708     0.826573     1.629237      23.00
 C      -2.966180     2.161374     0.051347      88.79
 H      -2.310690     3.019891    -0.323797      25.62
 C      -4.252629     2.385959    -0.743000     106.41
 O      -5.190570     1.268892    -0.511611     334.70
 H      -4.901362     0.388141    -0.845603      27.91
 H      -4.068955     2.617805    -1.693260      30.50
 H      -4.881527     3.279541    -0.440788      26.82
 C       1.483281     1.675786    -1.088315      47.10
 H       2.338131     2.346061    -0.639317      28.48
 C       1.005963    -0.685901    -1.610799      63.86
 H       1.310187    -1.863466    -1.579636      23.14
 C      -0.495534    -0.442954    -1.438287      -8.51
 O      -1.570947    -1.492811    -1.312021     140.27
 C      -1.025356    -2.860162    -1.519487     104.72
 H      -0.412759    -2.832517    -0.598945      28.03
 H      -1.748668    -3.537449    -1.581490      28.96
 H      -0.181922    -2.833993    -2.402339      25.63
 C      -0.882021     0.860731    -0.945002      15.64
 O      -2.242453     0.906491    -0.546552     139.45
 C       0.070454     1.853808    -0.705867      48.56
 H      -0.100614     2.897552    -0.252803      25.04
 C       1.831363     0.293783    -1.390728      20.60
 C       3.401024     0.049071    -1.607048     105.75
 H       3.248491    -0.644394    -2.673590      25.92
 O       4.190451     1.132901    -1.989804     103.98
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 H       4.333921     1.713234    -1.141815      27.74
 C       3.935076    -0.801071    -0.428011     112.22
 H       3.519204    -1.692236    -0.169169      29.88
 O       5.440603    -1.165812    -0.717778     127.31
 H       5.612748    -2.032988    -0.231954      26.93
 C       3.918316    -0.177967     0.908594     129.03
 O       4.200400     1.171489     0.953746     225.83
 H       3.826435     1.576006     1.783700      26.39
 H       4.617385    -0.685416     1.627215      29.08
 H       2.969843    -0.302540     1.204307      31.61
55
name = lig-Water-frame_831
 C      -1.664856     3.731242     2.869840      32.99
 H      -2.532464     4.472496     2.521775      24.85
 C      -1.235097     1.289875     3.128134      82.13
 H      -1.458874     0.285175     2.770560      26.86
 C      -0.268420     1.700628     3.942536      -2.30
 O       0.670895     0.812038     4.685815     102.27
 C       0.194305    -0.690399     4.684292     119.25
 H       0.786167    -1.389127     5.123630      30.83
 H       0.072891    -1.046124     3.689135      29.65
 H      -0.845131    -0.540011     5.086014      28.27
 C       0.138585     3.063263     4.202726      -7.22
 O       1.314526     3.296696     5.032388     184.27
 H       1.364187     4.196476     5.250504      25.76
 C      -0.699284     4.098786     3.762814      48.18
 H      -0.488501     4.991641     4.109680      20.48
 C      -1.969793     2.347201     2.517836      11.34
 C      -3.148303     2.147920     1.633169      55.86
 H      -3.774613     3.297348     1.635050      23.97
 O      -3.788436     0.885602     2.042688      80.69
 H      -4.637003     0.702105     1.496030      21.79
 C      -2.970828     2.222616     0.086254      87.17
 H      -2.364794     3.026630    -0.202701      25.93
 C      -4.248939     2.421435    -0.676397      77.07
 O      -5.217903     1.247776    -0.514122     245.87
 H      -4.838231     0.300466    -0.659053      25.21
 H      -3.854815     2.408585    -1.859769      23.43
 H      -4.953258     3.123101    -0.191995      25.31
 C       1.404657     1.607515    -1.076676      67.44
 H       2.135432     2.244866    -0.699497      31.07
 C       0.949853    -0.754184    -1.663540      43.74
 H       1.330972    -1.676234    -1.806251      26.50
 C      -0.550950    -0.452127    -1.384507      -4.72
 O      -1.559206    -1.514466    -1.288091     154.42
 C      -0.973451    -2.823007    -1.489610     107.01
 H      -0.255503    -3.453052    -0.689251      26.65
 H      -1.902942    -3.665188    -1.576552      25.47
 H      -0.543048    -2.899212    -2.418806      30.06
 C      -0.919290     0.828524    -0.884140      20.63
 O      -2.188145     0.927452    -0.542371     124.46
 C       0.035795     1.897858    -0.810466      66.05
 H      -0.163614     2.754878    -0.211051      25.87
 C       1.929296     0.389930    -1.368786      10.48
 C       3.412051    -0.012993    -1.610158     104.26
 H       3.646804    -0.552955    -2.424468      30.30
 O       4.162234     1.151290    -2.019504      63.39
 H       4.234012     1.890644    -1.173980      27.92
 C       4.039004    -0.839176    -0.431723      98.11
 H       3.471138    -1.921969    -0.419940      28.32
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 O       5.409825    -1.121292    -0.769335     117.82
 H       5.548413    -2.008179    -0.291850      27.21
 C       3.947161    -0.194732     0.843830     120.98
 O       4.186490     1.199090     0.937302     214.22
 H       3.642049     1.519801     1.743842      26.07
 H       4.591429    -0.785612     1.533529      30.94
 H       2.918552    -0.369519     1.567136      27.98
55
name = lig-Water-frame_832
 C      -1.728803     3.729482     2.802921      85.64
 H      -2.350608     4.490997     2.445564      31.36
 C      -1.227766     1.345112     3.092601      65.10
 H      -1.421507     0.294433     2.867938      22.56
 C      -0.230370     1.668268     4.070431       6.67
 O       0.684072     0.804042     4.704876      80.08
 C       0.134591    -0.699393     4.658876      90.66
 H       1.003708    -1.200192     5.366337      26.10
 H       0.176298    -0.916970     3.480528      24.52
 H      -0.700656    -0.725232     5.326173      27.92
 C       0.086604     3.049795     4.161773       5.42
 O       1.328617     3.291057     5.022983     136.64
 H       1.161735     4.332532     5.298404      20.95
 C      -0.691334     4.126803     3.784473      49.83
 H      -0.234561     5.168802     4.293057      15.58
 C      -1.951611     2.394967     2.567054      49.66
 C      -3.187226     2.162749     1.620578      89.41
 H      -3.866488     2.859896     1.857101      28.39
 O      -3.795784     0.886155     2.045799     151.17
 H      -4.553328     0.648425     1.313718      20.21
 C      -2.924851     2.251489     0.116601      77.72
 H      -2.262903     3.224116    -0.010992      22.75
 C      -4.264102     2.369590    -0.647473      90.37
 O      -5.246841     1.234225    -0.510188     300.31
 H      -4.622839     0.447982    -0.514241      26.93
 H      -4.033410     2.429132    -1.663379      28.28
 H      -4.809012     3.269793    -0.159630      25.97
 C       1.333315     1.567732    -1.031908      50.10
 H       2.001289     2.490169    -0.776543      25.02
 C       0.826789    -0.731493    -1.664061      47.97
 H       1.361495    -1.740296    -2.196842      22.47
 C      -0.515779    -0.513825    -1.328821      19.72
 O      -1.509174    -1.519394    -1.261401     183.75
 C      -0.954545    -2.868869    -1.459824     121.97
 H      -0.314160    -3.462237    -0.877332      28.59
 H      -1.892223    -3.377654    -1.473803      27.57
 H      -0.738546    -2.938182    -2.655413      25.57
 C      -0.920710     0.821744    -0.844230      10.00
 O      -2.212760     0.965843    -0.510909     142.68
 C       0.018045     1.900966    -0.914591      63.60
 H      -0.355472     2.766110    -0.162581      20.23
 C       1.977711     0.366394    -1.407800      19.72
 C       3.414956    -0.046994    -1.597741      79.07
 H       3.771110    -0.808799    -2.547187      24.52
 O       4.156009     1.204508    -2.027342     132.14
 H       4.110850     1.756816    -1.370507      35.74
 C       4.100036    -0.903387    -0.496814     110.61
 H       3.501637    -1.735597    -0.650671      31.17
 O       5.403902    -1.089918    -0.821955     150.35
 H       5.619250    -1.993810    -0.512085      28.31
 C       3.924284    -0.226685     0.923819     117.12
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 O       4.191721     1.240145     0.908912     225.18
 H       3.536857     1.645716     1.563384      26.46
 H       4.767605    -0.837416     1.447480      28.33
 H       3.075449    -0.482172     1.356190      30.94
55
name = lig-Water-frame_833
 C      -1.748474     3.789572     2.802407      73.62
 H      -2.339532     4.621130     2.288557      27.66
 C      -1.194915     1.375519     3.097558      53.49
 H      -1.500657     0.347920     2.938897      21.13
 C      -0.168133     1.647535     4.162249      16.95
 O       0.664072     0.762081     4.716976     142.62
 C       0.160240    -0.659018     4.652570     122.38
 H       0.994764    -0.984754     5.149124      29.31
 H       0.115396    -0.985170     3.708523      29.36
 H      -0.747783    -1.012343     5.363953      26.65
 C       0.104774     3.032749     4.209377      33.72
 O       1.300736     3.306166     4.990513     240.91
 H       1.144504     4.139020     5.491807      27.68
 C      -0.677413     4.140151     3.776672      45.08
 H      -0.433656     5.105759     3.986833      15.73
 C      -1.983521     2.443690     2.563749      24.89
 C      -3.194030     2.120985     1.631745      74.22
 H      -4.151227     2.808601     2.059150      21.58
 O      -3.805614     0.881451     2.031982     220.38
 H      -4.440747     0.699674     1.433762      26.59
 C      -2.863270     2.266633     0.133313     101.78
 H      -2.343073     3.134978     0.026674      24.30
 C      -4.297063     2.320746    -0.601777      96.78
 O      -5.247186     1.242058    -0.487496     340.56
 H      -4.630717     0.445238    -0.566780      26.63
 H      -4.200834     2.607035    -1.815332      23.27
 H      -4.638531     3.320529    -0.359417      26.81
 C       1.376988     1.575450    -0.987923      46.40
 H       1.858489     2.539617    -0.947205      23.99
 C       0.808725    -0.686704    -1.673366      68.61
 H       0.941284    -1.460070    -2.269527      25.70
 C      -0.471971    -0.550348    -1.253077      21.16
 O      -1.428763    -1.522762    -1.223094     181.53
 C      -1.007391    -2.915895    -1.523774      95.59
 H      -0.034511    -3.223789    -0.743270      23.44
 H      -2.078688    -3.425381    -1.303857      23.21
 H      -0.723737    -2.981407    -2.495886      27.81
 C      -0.899787     0.817041    -0.838974      10.20
 O      -2.283869     1.017232    -0.454904     189.80
 C      -0.065371     1.869026    -0.955373      61.49
 H      -0.305573     2.740808    -0.510220      20.98
 C       1.891061     0.261832    -1.469519      15.14
 C       3.454199    -0.052184    -1.651610      93.67
 H       3.374093    -0.689492    -2.463926      28.27
 O       4.156829     1.227189    -2.045019      79.77
 H       3.978493     1.870646    -1.154292      24.90
 C       4.074291    -0.884801    -0.543300      89.66
 H       3.441798    -1.913814    -0.622564      25.63
 O       5.460009    -1.080661    -0.886104     151.10
 H       5.743525    -2.034259    -0.723836      27.71
 C       3.962958    -0.273317     0.989706      81.49
 O       4.198107     1.254277     0.870382     163.13
 H       3.586172     1.780764     1.459150      26.45
 H       4.792208    -0.635104     1.524609      27.50
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 H       2.787013    -0.608313     1.308365      24.39
55
name = lig-Water-frame_834
 C      -1.724172     3.886933     2.852932      29.01
 H      -2.298866     4.636334     2.252231      20.92
 C      -1.151735     1.411546     3.160538      55.13
 H      -1.605996     0.426146     2.950791      21.51
 C      -0.177845     1.673001     4.135842      31.61
 O       0.627695     0.697746     4.738857     187.09
 C       0.210050    -0.615442     4.698887     120.43
 H       1.207684    -1.241941     5.007170      25.58
 H      -0.021729    -1.177584     3.606602      24.94
 H      -0.666495    -0.921510     5.128974      28.89
 C       0.153229     3.046450     4.317325      44.97
 O       1.271728     3.322258     4.964840     123.05
 H       1.172776     4.083855     5.617570      31.69
 C      -0.697400     4.087427     3.702317      30.08
 H      -0.517145     5.270330     3.778794      18.57
 C      -2.027415     2.459194     2.541396      -2.90
 C      -3.222214     2.097981     1.697712      99.06
 H      -3.861342     2.901773     1.762149      28.27
 O      -3.789100     0.851151     2.028262     141.33
 H      -4.674192     0.682673     1.419260      17.93
 C      -2.876515     2.227696     0.127045      82.28
 H      -2.277471     3.216254    -0.138214      21.08
 C      -4.299009     2.330944    -0.624152      92.86
 O      -5.224929     1.259071    -0.442693     324.49
 H      -4.868238     0.352553    -0.722155      26.52
 H      -4.190711     2.519109    -1.678863      27.18
 H      -4.810216     3.352614    -0.273195      25.74
 C       1.411113     1.562803    -0.997786      63.81
 H       2.071826     2.466881    -1.035306      21.66
 C       0.845282    -0.651890    -1.691575      52.43
 H       0.780906    -1.611309    -2.458486      19.11
 C      -0.474730    -0.504289    -1.149055      27.94
 O      -1.358582    -1.540551    -1.188707     209.46
 C      -1.067914    -2.940106    -1.536114     103.73
 H      -0.250831    -2.998326    -0.935122      27.60
 H      -1.880044    -3.634529    -1.125108      24.38
 H      -0.639558    -3.131719    -2.641979      24.39
 C      -0.956777     0.775303    -0.829752      15.89
 O      -2.332068     1.051313    -0.399026     228.33
 C      -0.063824     1.819697    -0.959681      35.99
 H      -0.350455     3.016729    -0.915095      16.45
 C       1.781150     0.234940    -1.489960      25.41
 C       3.429591    -0.004004    -1.724505      80.77
 H       3.244101    -0.647036    -2.741299      24.45
 O       4.146356     1.231686    -2.033327     125.50
 H       3.964371     1.769218    -1.142946      25.15
 C       4.030301    -0.865097    -0.542503      82.99
 H       3.654825    -1.843741    -0.426391      26.23
 O       5.540913    -1.083036    -0.954185     128.87
 H       5.668294    -2.062836    -0.803178      30.16
 C       3.962322    -0.295918     0.982103      89.09
 O       4.204288     1.238192     0.822612     171.46
 H       3.651072     1.711556     1.538221      25.23
 H       4.772117    -0.555809     1.806923      25.40
 H       3.032360    -0.463965     1.348654      27.61
55
name = lig-Water-frame_835
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 C      -1.744913     3.877421     2.854572     -14.23
 H      -2.229795     4.726347     2.411401      14.31
 C      -1.198513     1.469997     3.194487      62.23
 H      -1.509297     0.449961     3.021430      20.60
 C      -0.192265     1.723012     4.076878      34.75
 O       0.596215     0.673221     4.761764     213.57
 C       0.295547    -0.677570     4.688831     112.74
 H       1.000633    -1.426705     4.944354      24.28
 H       0.030574    -0.913621     3.737501      28.37
 H      -0.760809    -0.753003     5.292143      22.37
 C       0.115331     3.072523     4.379818      28.77
 O       1.299131     3.350486     4.982955      56.30
 H       1.172077     4.225600     5.606698      20.04
 C      -0.657401     4.069133     3.658252      61.36
 H      -0.351217     5.115228     3.810849      36.74
 C      -2.016020     2.473958     2.570037      27.50
 C      -3.209884     2.105162     1.718180      80.93
 H      -3.837329     3.154255     1.629745      25.51
 O      -3.791095     0.800941     2.024747     142.22
 H      -4.708528     0.780157     1.579882      20.83
 C      -2.935413     2.203705     0.105691      99.67
 H      -2.351119     3.032923    -0.172153      26.68
 C      -4.290760     2.383442    -0.636940      83.17
 O      -5.214374     1.267673    -0.383295     336.64
 H      -4.932991     0.423301    -0.816633      25.82
 H      -4.011662     2.418476    -1.826930      24.16
 H      -4.926337     3.089269    -0.155292      25.80
 C       1.373986     1.543349    -1.049431      43.96
 H       2.279730     2.210896    -1.063136      21.57
 C       0.793294    -0.716190    -1.733156      49.79
 H       1.050703    -1.551080    -2.316883      19.48
 C      -0.475083    -0.468080    -1.076129      22.22
 O      -1.354328    -1.566854    -1.162274     201.96
 C      -1.084320    -2.938458    -1.549844      98.82
 H       0.005039    -3.207184    -0.877233      22.21
 H      -1.797745    -3.699745    -1.131602      24.08
 H      -0.916402    -3.222005    -2.572843      25.55
 C      -1.058754     0.779810    -0.789294       6.97
 O      -2.339091     1.025798    -0.369772     232.40
 C       0.026490     1.834936    -0.942616      60.15
 H      -0.378234     2.712800    -1.249578      24.83
 C       1.795271     0.320764    -1.473798      30.75
 C       3.322432     0.033419    -1.813415      76.52
 H       3.566230    -0.495829    -2.749168      25.50
 O       4.121518     1.213181    -2.000974     181.49
 H       4.099825     1.688527    -1.211629      31.15
 C       4.058035    -0.835361    -0.519813      68.41
 H       3.662268    -1.922930    -0.404924      23.62
 O       5.594587    -1.090780    -1.003689     115.11
 H       5.586989    -2.043097    -0.803922      29.93
 C       4.002788    -0.245979     0.924622      99.85
 O       4.203578     1.204977     0.785290     196.46
 H       3.757147     1.532753     1.591105      25.85
 H       4.586863    -0.672172     1.661359      27.78
 H       2.888122    -0.376587     1.518197      22.50
55
name = lig-Water-frame_836
 C      -1.772234     3.799997     2.833260      62.48
 H      -2.276123     4.816833     2.575101      20.58
 C      -1.301028     1.506838     3.197258      67.13
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 H      -1.404280     0.430005     3.052070      22.73
 C      -0.167475     1.741308     4.063407      11.68
 O       0.593861     0.724889     4.783321     133.05
 C       0.274753    -0.761744     4.676715      99.53
 H       1.092873    -1.501337     5.112662      23.22
 H       0.005126    -0.815730     3.499174      22.26
 H      -0.460840    -0.846801     5.374013      25.83
 C       0.038992     3.093092     4.381010      30.04
 O       1.352842     3.404733     5.043673     157.32
 H       1.179394     4.272703     5.389255      25.52
 C      -0.565579     4.074084     3.665404      65.52
 H      -0.124709     5.082469     3.914776      26.75
 C      -2.006192     2.496286     2.611446      48.39
 C      -3.188861     2.159511     1.668689      91.09
 H      -3.929060     2.872267     1.927236      27.98
 O      -3.802311     0.776879     2.035112     140.49
 H      -4.655386     0.787412     1.620648      23.97
 C      -3.002256     2.185564     0.105748     100.13
 H      -2.300978     3.083541    -0.105590      24.49
 C      -4.281770     2.388979    -0.658706      89.63
 O      -5.213612     1.271049    -0.329515     340.14
 H      -4.805168     0.482596    -0.776511      27.01
 H      -4.004182     2.478357    -1.741662      26.78
 H      -4.938461     3.255421    -0.196443      25.03
 C       1.365860     1.547764    -1.115043      61.59
 H       2.127922     2.273561    -1.049248      27.88
 C       0.766278    -0.715845    -1.719055      59.33
 H       1.236069    -1.710418    -2.180284      20.73
 C      -0.484357    -0.516390    -1.071809      11.91
 O      -1.409969    -1.599232    -1.132222     203.03
 C      -1.013362    -2.944737    -1.503572      99.93
 H      -0.155640    -3.404228    -1.170960      28.70
 H      -1.954957    -3.593321    -1.073717      23.68
 H      -1.138361    -3.108031    -2.681241      24.69
 C      -1.054941     0.856731    -0.742445       4.65
 O      -2.338145     0.943734    -0.364171     202.62
 C       0.036444     1.831173    -0.908705      63.46
 H      -0.398421     2.829621    -1.368344      24.49
 C       1.830800     0.317203    -1.495638      39.05
 C       3.236150     0.062422    -1.834263      76.94
 H       3.619221    -0.562199    -2.731621      26.45
 O       4.089452     1.192522    -1.985029      76.91
 H       4.358674     1.742899    -1.005100      22.73
 C       4.108249    -0.828899    -0.525233      62.83
 H       3.614643    -1.812831    -0.550856      27.76
 O       5.596555    -1.092892    -1.020214     105.14
 H       5.702235    -2.083604    -0.783374      26.46
 C       3.984306    -0.174269     0.842506     121.74
 O       4.212144     1.173497     0.769040     133.84
 H       3.838694     1.582279     1.619661      25.41
 H       4.735464    -0.904545     1.476298      27.13
 H       3.050770    -0.338216     1.247993      27.32
55
name = lig-Water-frame_837
 C      -1.715403     3.824406     2.871086      54.53
 H      -2.388789     4.547117     2.560196      24.55
 C      -1.323663     1.467845     3.247159      61.83
 H      -1.546520     0.431735     2.925876      28.27
 C      -0.172683     1.707747     4.076240      17.89
 O       0.601121     0.801507     4.798534     104.35
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 C       0.246857    -0.814862     4.635014      88.76
 H       1.238622    -1.146707     5.000585      25.20
 H       0.021741    -1.091052     3.649425      26.62
 H      -0.575604    -1.131183     5.445294      24.09
 C       0.068291     3.088905     4.387473      19.96
 O       1.374825     3.442549     5.098365      45.74
 H       1.208248     4.493854     5.345554      21.62
 C      -0.533551     4.106382     3.657798      49.28
 H      -0.065790     5.171622     3.868192      26.05
 C      -2.066631     2.494052     2.589514      18.41
 C      -3.194907     2.165639     1.625870      92.32
 H      -4.111035     2.727289     2.102618      24.21
 O      -3.792464     0.779637     2.058858      31.22
 H      -4.735100     0.726933     1.458888      17.48
 C      -3.016265     2.199664     0.126991     102.35
 H      -2.321359     3.032161    -0.045133      25.20
 C      -4.314460     2.385609    -0.641918      99.66
 O      -5.207543     1.276412    -0.298923     344.35
 H      -4.730029     0.434878    -0.585480      27.43
 H      -4.138992     2.548716    -1.815650      25.25
 H      -4.643813     3.393338    -0.472731      26.93
 C       1.391891     1.568194    -1.182386      36.56
 H       1.912011     2.617305    -1.081921      27.80
 C       0.800536    -0.687194    -1.668352      73.00
 H       1.071459    -1.768100    -1.847140      24.52
 C      -0.517699    -0.580964    -1.111154      11.43
 O      -1.465144    -1.615434    -1.082553     181.52
 C      -1.021272    -2.961925    -1.490638     101.28
 H       0.084422    -3.600150    -1.316987      25.22
 H      -1.857636    -3.442351    -1.060805      27.64
 H      -1.250869    -2.837233    -2.549777      28.17
 C      -0.934797     0.882785    -0.717854      18.99
 O      -2.351678     0.859191    -0.361591     155.69
 C      -0.068403     1.863614    -0.887950      58.16
 H      -0.205566     2.929938    -1.009829      26.13
 C       1.806427     0.249035    -1.546162      35.74
 C       3.256449     0.054674    -1.789153     102.56
 H       3.269218    -0.709959    -2.681108      29.43
 O       4.070735     1.214489    -1.971210     133.68
 H       4.374212     1.447516    -1.119501      31.21
 C       4.141084    -0.827348    -0.610805      87.30
 H       3.595406    -1.788449    -0.586067      31.16
 O       5.550276    -1.092015    -1.003728     163.73
 H       5.846368    -1.997369    -0.778829      26.46
 C       3.998842    -0.190549     0.747602     118.39
 O       4.243839     1.193838     0.777040     112.38
 H       3.884051     1.692266     1.539650      27.63
 H       4.741758    -0.703293     1.251054      33.92
 H       2.837146    -0.453109     1.092502      27.48
55
name = lig-Water-frame_838
 C      -1.643489     3.865035     2.917223      46.29
 H      -2.456079     4.535896     2.423077      22.77
 C      -1.319189     1.399893     3.282322      51.82
 H      -1.671223     0.470024     2.915163      32.11
 C      -0.211905     1.685560     4.114231      20.72
 O       0.587660     0.833710     4.797622     102.51
 C       0.239329    -0.811395     4.649313      86.57
 H       1.299578    -0.998331     4.818138      26.37
 H      -0.007539    -1.322164     3.590783      26.74
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 H      -0.550570    -1.232678     5.214136      28.14
 C       0.187799     3.086019     4.388239      12.94
 O       1.353768     3.473177     5.133376      30.70
 H       1.229050     4.345056     5.517787      28.56
 C      -0.534972     4.153119     3.653502      50.42
 H      -0.254417     5.158604     3.702142      28.18
 C      -2.094372     2.473166     2.578377     -63.99
 C      -3.261875     2.122449     1.652366      86.98
 H      -4.084468     2.884764     1.761686      28.16
 O      -3.788032     0.788486     2.067163      79.67
 H      -4.491721     0.677515     1.495784      25.45
 C      -2.989600     2.203402     0.127037      87.06
 H      -2.296273     3.025181    -0.128416      26.34
 C      -4.327836     2.374486    -0.645034      86.82
 O      -5.206717     1.291718    -0.276333     353.43
 H      -4.757133     0.442972    -0.441170      29.85
 H      -4.254591     2.299972    -1.810461      25.96
 H      -4.625121     3.506562    -0.478206      25.24
 C       1.353325     1.616251    -1.238612      26.65
 H       1.886578     2.495802    -1.257863      30.84
 C       0.788092    -0.729458    -1.574302      72.44
 H       1.025729    -1.783634    -1.718218      29.12
 C      -0.535588    -0.569936    -1.160272      18.78
 O      -1.477791    -1.601568    -1.006878     179.74
 C      -1.039626    -2.980036    -1.511655      98.62
 H      -0.112991    -3.265804    -1.316520      31.91
 H      -1.862830    -3.754064    -0.914861      25.64
 H      -1.207799    -2.873818    -2.624394      28.99
 C      -0.896433     0.770454    -0.704760       9.23
 O      -2.346546     0.811094    -0.353752      93.58
 C      -0.073251     1.932748    -0.888136      54.68
 H      -0.260113     2.989536    -0.486781      25.52
 C       1.781733     0.282789    -1.565048      42.71
 C       3.334261    -0.024145    -1.732431     122.73
 H       3.183788    -0.654458    -2.685147      31.32
 O       4.046391     1.236861    -1.993251      59.25
 H       4.401499     1.375580    -0.984322      29.02
 C       4.130040    -0.836357    -0.748434     122.37
 H       3.608753    -1.849022    -0.529355      31.34
 O       5.491189    -1.068012    -0.984455     177.18
 H       5.764692    -1.982264    -0.731020      26.53
 C       3.978379    -0.238993     0.665070     119.68
 O       4.294467     1.249974     0.776925      68.86
 H       3.794627     1.660642     1.535126      28.95
 H       4.782588    -0.638138     1.446882      31.48
 H       2.979381    -0.502627     0.983610      32.30
55
name = lig-Water-frame_839
 C      -1.670407     3.835488     2.891961      55.87
 H      -2.098006     4.730392     2.450000      23.24
 C      -1.344280     1.387966     3.266728      54.33
 H      -1.616622     0.308396     3.094785      29.25
 C      -0.246208     1.728103     4.167429     -44.34
 O       0.553158     0.787576     4.790670      71.89
 C       0.267804    -0.773011     4.629525      96.63
 H       1.365136    -1.213663     4.857494      28.01
 H       0.033473    -1.074851     3.593980      31.98
 H      -0.537524    -1.149119     5.332383      28.60
 C       0.280612     3.121606     4.339767      -0.59
 O       1.326056     3.457378     5.157009     -85.04
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 H       1.048746     4.353749     5.759320      23.37
 C      -0.512846     4.151800     3.687541      42.70
 H      -0.342942     5.374595     3.648561      19.33
 C      -2.043744     2.459505     2.635589      -3.53
 C      -3.315224     2.084738     1.684134      80.11
 H      -4.048301     3.030652     1.590793      28.01
 O      -3.766901     0.808492     2.078543      88.57
 H      -4.569310     0.587527     1.425065      22.49
 C      -2.943093     2.164139     0.096547      78.05
 H      -2.245228     3.030461    -0.210267      26.79
 C      -4.306276     2.355282    -0.669257      94.31
 O      -5.229566     1.315237    -0.238440     297.07
 H      -4.796496     0.455180    -0.517746      29.78
 H      -4.146356     2.152161    -1.795302      27.43
 H      -4.837118     3.209456    -0.342067      27.55
 C       1.255791     1.660589    -1.290637      59.16
 H       2.174975     2.403767    -1.453874      30.09
 C       0.778687    -0.795314    -1.469658      55.04
 H       1.230469    -1.879691    -1.767043      26.55
 C      -0.549702    -0.527418    -1.191575      42.27
 O      -1.463117    -1.594501    -0.932501     165.10
 C      -1.138962    -2.981016    -1.524689     105.19
 H       0.082241    -2.973028    -1.119576      27.07
 H      -1.585511    -3.756940    -1.096247      31.46
 H      -1.134177    -3.151605    -2.683099      29.76
 C      -0.949928     0.674111    -0.704776     -10.24
 O      -2.316026     0.798856    -0.338736      81.65
 C      -0.019492     1.960830    -0.880261      56.76
 H      -0.389774     2.660302    -0.083509      27.55
 C       1.762678     0.356293    -1.539887      22.94
 C       3.367892    -0.089214    -1.750417     103.58
 H       3.437598    -0.499282    -2.854748      30.88
 O       4.030073     1.241843    -2.003960       1.17
 H       4.376675     1.607464    -1.005975      26.55
 C       4.080776    -0.880465    -0.795677     133.27
 H       3.616339    -1.837108    -0.680438      32.84
 O       5.463564    -1.038451    -0.991784     177.46
 H       5.568522    -1.995244    -0.689241      27.96
 C       3.998155    -0.259927     0.629553     123.47
 O       4.338615     1.294192     0.765466      55.03
 H       3.697604     1.560596     1.490461      30.46
 H       4.529041    -0.716556     1.418583      35.79
 H       2.881054    -0.448459     1.061219      34.06
55
name = lig-Water-frame_840
 C      -1.675274     3.787542     2.866166      69.94
 H      -1.930857     4.760364     2.415611      21.47
 C      -1.338156     1.419084     3.272280      54.58
 H      -1.459726     0.386202     3.282790      25.92
 C      -0.263718     1.787765     4.200425     -32.61
 O       0.515849     0.699541     4.788101      33.47
 C       0.327177    -0.706741     4.619804     122.81
 H       1.135371    -1.306089     4.935874      30.51
 H       0.021920    -0.786471     3.519210      31.64
 H      -0.410363    -0.927053     5.437141      28.68
 C       0.288644     3.160250     4.259208      22.68
 O       1.309828     3.439360     5.207141     176.90
 H       0.941037     4.223096     5.668817      22.57
 C      -0.505957     4.146334     3.706622      51.95
 H      -0.257109     5.087601     3.830559      19.80
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 C      -2.022625     2.453602     2.679530      41.61
 C      -3.283210     2.100452     1.679951      82.76
 H      -4.036772     2.924916     1.830315      30.16
 O      -3.766246     0.823553     2.081771      84.66
 H      -4.622188     0.561024     1.522137      23.51
 C      -2.894146     2.103796     0.068297      97.93
 H      -2.269526     2.914099    -0.158227      29.94
 C      -4.263176     2.293473    -0.684518      85.84
 O      -5.257018     1.310294    -0.199607     280.72
 H      -4.999068     0.470110    -0.665307      30.38
 H      -3.983410     2.284934    -1.872577      26.17
 H      -4.941914     3.155588    -0.356385      24.99
 C       1.247234     1.708510    -1.353428      83.95
 H       2.076962     2.327890    -1.489083      32.64
 C       0.864810    -0.811843    -1.396808      64.33
 H       1.231016    -1.684063    -1.715996      29.56
 C      -0.566690    -0.566608    -1.201056       6.25
 O      -1.465237    -1.616209    -0.886123     155.19
 C      -1.133943    -2.921572    -1.522515     119.48
 H      -0.233556    -3.052326    -1.215880      33.57
 H      -1.680971    -3.955206    -0.962015      26.55
 H      -1.160599    -3.128980    -2.578626      30.94
 C      -1.007870     0.725454    -0.724533       0.44
 O      -2.285657     0.807549    -0.317939     140.41
 C      -0.047532     1.878724    -0.815542      61.31
 H      -0.291639     2.583836    -0.067659      30.17
 C       1.713764     0.332226    -1.502817       2.92
 C       3.332264    -0.034272    -1.875304      94.85
 H       3.585359    -0.488273    -2.841657      28.89
 O       4.032022     1.246180    -1.995894     131.63
 H       4.201428     1.669559    -1.235185      33.48
 C       4.025937    -0.919978    -0.732798      97.56
 H       3.498324    -1.983727    -0.870471      28.96
 O       5.465764    -1.031834    -1.022547     160.48
 H       5.651676    -1.951612    -0.749410      28.71
 C       3.961801    -0.246029     0.634636     112.30
 O       4.366940     1.288368     0.744998      99.58
 H       3.732199     1.624032     1.411986      31.97
 H       4.564278    -0.935725     1.359191      31.12
 H       2.908950    -0.147340     1.006191      32.41
55
name = lig-Water-frame_841
 C      -1.611289     3.787347     2.873810      52.45
 H      -2.173796     4.567937     2.224318      24.81
 C      -1.265309     1.476729     3.347332      52.63
 H      -1.503941     0.409974     3.278131      26.03
 C      -0.247519     1.793425     4.195610       1.85
 O       0.509560     0.685453     4.802604      77.55
 C       0.333190    -0.627343     4.611105     124.45
 H       1.240840    -1.359325     4.933093      28.06
 H      -0.057317    -0.856250     3.528817      31.97
 H      -0.496488    -0.925185     5.273190      29.87
 C       0.263915     3.130465     4.228105      30.09
 O       1.290944     3.405793     5.243688     153.73
 H       1.032535     4.364736     5.652816      21.44
 C      -0.541428     4.100317     3.683771      56.70
 H      -0.098655     5.214697     4.021109      14.25
 C      -2.067313     2.450693     2.654604      35.21
 C      -3.182141     2.125580     1.666314      82.28
 H      -4.057761     2.874871     1.985369      28.47
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 O      -3.778735     0.822411     2.092074      58.22
 H      -4.539517     0.692462     1.624682      29.95
 C      -2.887523     2.044208     0.080161     102.40
 H      -2.161648     2.960274    -0.143265      26.41
 C      -4.226415     2.235476    -0.683993     100.96
 O      -5.275636     1.275822    -0.188046     278.53
 H      -5.279443     0.443543    -0.688761      30.80
 H      -4.057905     2.336697    -1.808595      28.30
 H      -4.551284     3.262825    -0.550719      28.87
 C       1.261065     1.671323    -1.396037      47.34
 H       1.934932     2.639999    -1.456273      27.39
 C       0.905910    -0.763120    -1.335656      66.24
 H       1.311218    -1.881679    -1.706738      25.44
 C      -0.554586    -0.621032    -1.167367     -10.97
 O      -1.479224    -1.650224    -0.870856     149.62
 C      -1.143581    -2.909250    -1.466121     108.74
 H       0.069235    -3.351147    -1.247394      25.48
 H      -1.780917    -3.487387    -1.020261      30.61
 H      -1.357704    -2.805875    -2.669057      27.66
 C      -0.997324     0.799253    -0.786423      22.82
 O      -2.286427     0.826311    -0.284173     159.02
 C      -0.105340     1.756616    -0.729504      59.97
 H      -0.167812     2.845054    -0.271743      25.44
 C       1.702468     0.290096    -1.503738      17.84
 C       3.268344     0.084463    -1.959189      85.73
 H       3.510748    -0.640665    -2.914523      26.39
 O       4.040276     1.238940    -2.027813      62.03
 H       3.999091     1.777861    -0.968520      22.45
 C       3.961505    -0.927871    -0.699684      87.31
 H       3.526627    -1.858012    -0.743381      30.99
 O       5.466767    -1.040709    -1.061103     145.13
 H       5.865518    -1.932594    -0.839003      27.02
 C       3.907511    -0.211650     0.679018     104.30
 O       4.391848     1.234919     0.711428     121.68
 H       3.863170     1.757546     1.382469      30.68
 H       4.567224    -0.870193     1.249624      30.24
 H       2.827832    -0.073725     1.001725      30.87
55
name = lig-Water-frame_842
 C      -1.604041     3.797503     2.828466      28.57
 H      -2.258840     4.403312     2.302834      22.39
 C      -1.248419     1.516065     3.394028      56.65
 H      -1.586854     0.493912     3.197155      28.46
 C      -0.166223     1.743425     4.190105      28.15
 O       0.541152     0.783374     4.835404     160.74
 C       0.287868    -0.640924     4.597261     123.34
 H       1.219129    -1.039459     4.774209      31.31
 H       0.026306    -1.014756     3.556125      30.68
 H      -0.645928    -1.115122     5.054804      29.08
 C       0.248270     3.061795     4.286719      34.18
 O       1.252265     3.382483     5.260755     143.15
 H       1.274174     4.368632     5.519613      33.61
 C      -0.536010     4.110561     3.673654      19.73
 H      -0.318770     5.079874     3.844390      14.13
 C      -2.051191     2.454214     2.636976      20.15
 C      -3.104823     2.125581     1.666366      87.82
 H      -3.923692     2.923576     1.776381      29.04
 O      -3.768395     0.820353     2.121843     -49.44
 H      -4.672241     0.829506     1.468968      18.99
 C      -2.890307     2.043921     0.114576     114.32
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 H      -2.291208     2.828600    -0.156243      27.95
 C      -4.190044     2.184647    -0.666631      83.68
 O      -5.287300     1.258604    -0.189383     252.58
 H      -5.382761     0.419748    -0.716624      28.85
 H      -4.176276     2.048509    -1.898099      25.80
 H      -4.294872     3.320078    -0.532088      26.48
 C       1.239788     1.587954    -1.378514      54.60
 H       1.566565     2.617430    -1.437413      26.29
 C       0.848730    -0.806728    -1.305325      71.05
 H       1.260297    -1.681021    -1.458667      28.94
 C      -0.510151    -0.622389    -1.087583      13.44
 O      -1.455942    -1.652247    -0.864761     184.99
 C      -1.110394    -2.903849    -1.445959     119.47
 H      -0.261802    -3.381505    -1.374424      30.48
 H      -2.165231    -3.485831    -0.975734      23.47
 H      -1.382908    -2.669052    -2.413246      29.01
 C      -1.009053     0.746618    -0.847684       6.11
 O      -2.293278     0.824706    -0.250236     122.50
 C      -0.040799     1.755582    -0.681753      59.54
 H      -0.311861     2.761669    -0.621476      24.35
 C       1.788988     0.352609    -1.563628      31.77
 C       3.203503     0.128268    -1.974319      98.62
 H       3.209298    -0.425615    -2.848864      27.82
 O       4.044502     1.264096    -2.040375     188.15
 H       3.940822     1.507257    -1.181377      31.04
 C       3.936698    -0.855747    -0.717222      69.22
 H       3.454461    -1.952920    -0.471377      26.60
 O       5.451910    -1.047906    -1.101146     134.23
 H       5.797361    -1.960128    -0.846259      27.58
 C       3.851363    -0.166173     0.713394     103.40
 O       4.412884     1.169895     0.668525     195.48
 H       4.006817     1.733416     1.379507      29.45
 H       4.500216    -0.701025     1.445623      29.37
 H       2.717164    -0.269669     1.118559      29.10
55
name = lig-Water-frame_843
 C      -1.628493     3.781085     2.766790      58.22
 H      -2.291391     4.723156     2.403795      21.60
 C      -1.303153     1.511600     3.375691      76.80
 H      -1.551282     0.506902     3.208128      32.46
 C      -0.089026     1.708097     4.170068      37.02
 O       0.585601     0.863929     4.882534     195.45
 C       0.211389    -0.679169     4.565356      90.36
 H       1.347537    -0.959118     4.866591      24.48
 H       0.273103    -0.876528     3.385097      25.92
 H      -0.570410    -1.126328     5.118869      27.20
 C       0.223949     3.066819     4.380570      41.01
 O       1.227701     3.354171     5.259619     121.07
 H       1.210012     4.305879     5.411208      31.97
 C      -0.517862     4.087534     3.660031      80.00
 H      -0.398830     5.294064     3.758452      25.94
 C      -1.941443     2.467100     2.655204      58.38
 C      -3.079591     2.089829     1.668012      75.02
 H      -3.830066     3.060802     1.621611      24.48
 O      -3.775467     0.841344     2.136326      78.02
 H      -4.474753     0.784752     1.475216      24.01
 C      -2.886050     2.035754     0.147608      98.66
 H      -2.275128     2.984920    -0.260149      22.84
 C      -4.177694     2.132813    -0.670041      96.24
 O      -5.296278     1.270264    -0.183474     298.59
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 H      -5.212719     0.456719    -0.736077      28.92
 H      -4.050465     1.823723    -1.713436      27.95
 H      -4.548462     3.141664    -0.479306      27.21
 C       1.180637     1.549089    -1.309107      72.20
 H       1.689258     2.510600    -1.575591      28.15
 C       0.821294    -0.800695    -1.305851      45.49
 H       1.303340    -1.934157    -1.249170      24.27
 C      -0.488166    -0.600482    -0.984901      38.94
 O      -1.392286    -1.610836    -0.835772     197.66
 C      -1.211278    -2.917528    -1.423209     106.86
 H      -0.105627    -3.535006    -1.247266      24.83
 H      -1.887360    -3.596985    -1.175825      28.54
 H      -1.323412    -2.777428    -2.675809      25.16
 C      -1.021597     0.672835    -0.841914       6.12
 O      -2.276963     0.778410    -0.235604     125.59
 C       0.016387     1.758019    -0.712338      67.69
 H      -0.534111     2.772891    -0.756846      22.75
 C       1.825257     0.388921    -1.615202      32.21
 C       3.182509     0.104806    -1.925149      91.46
 H       3.026662    -0.346566    -3.101194      24.20
 O       4.036772     1.283956    -2.075359      45.24
 H       4.119287     1.654137    -1.003319      22.31
 C       3.937285    -0.797781    -0.731535      92.90
 H       3.525345    -1.688577    -0.506379      30.07
 O       5.407287    -1.051473    -1.136280     176.43
 H       5.469843    -1.967775    -0.795205      29.12
 C       3.810322    -0.149872     0.736222     113.96
 O       4.417291     1.122688     0.627961     175.47
 H       4.079422     1.661755     1.379977      29.74
 H       4.343159    -0.672409     1.597808      29.45
 H       2.756094    -0.269937     1.122680      30.25
55
name = lig-Water-frame_844
 C      -1.611529     3.837663     2.752062      49.52
 H      -2.080188     4.680929     2.499847      24.06
 C      -1.288582     1.451781     3.378265      69.86
 H      -1.552325     0.387299     3.206443      30.52
 C      -0.107820     1.755470     4.106169       7.55
 O       0.627795     0.854515     4.940937     124.32
 C       0.252356    -0.681083     4.526077     105.15
 H       1.023479    -1.170851     5.013191      29.31
 H       0.249231    -0.645014     3.474502      28.35
 H      -0.596340    -1.027435     5.247127      25.52
 C       0.159740     3.118589     4.423449      27.99
 O       1.229752     3.336431     5.264434      87.05
 H       1.048152     4.380213     5.506177      23.99
 C      -0.516893     4.080040     3.636033      53.44
 H      -0.307630     5.141526     3.828204      28.60
 C      -1.883684     2.466426     2.616015      30.59
 C      -3.086580     2.067071     1.683301      92.98
 H      -3.687577     3.010488     1.745745      29.06
 O      -3.772034     0.886752     2.148471     115.28
 H      -4.470908     0.621424     1.436184      21.92
 C      -2.846233     2.032984     0.148201     105.76
 H      -2.349143     2.874942    -0.156944      29.05
 C      -4.209627     2.088965    -0.639518      85.48
 O      -5.293546     1.276391    -0.180597     306.58
 H      -5.051534     0.424564    -0.600176      29.01
 H      -3.711337     1.732024    -1.761882      24.82
 H      -4.821694     3.015724    -0.654862      25.66
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 C       1.216668     1.599023    -1.270734      60.51
 H       1.987190     2.319080    -1.669802      29.02
 C       0.912292    -0.785465    -1.334142      70.65
 H       1.115383    -1.785813    -1.153265      28.97
 C      -0.469130    -0.600885    -0.907345      16.32
 O      -1.351459    -1.602074    -0.786480     199.55
 C      -1.241075    -2.939011    -1.478616     108.77
 H      -0.358358    -3.264929    -1.077358      29.06
 H      -2.036210    -3.842852    -1.097812      24.68
 H      -1.180738    -2.959209    -2.478100      30.46
 C      -0.993736     0.684687    -0.751537      30.37
 O      -2.249267     0.711784    -0.237595     163.79
 C      -0.096640     1.740937    -0.776535      80.98
 H      -0.463313     2.771408    -0.703991      27.32
 C       1.721288     0.317758    -1.598628      28.04
 C       3.233565     0.062912    -1.899895     107.02
 H       3.269931    -0.358893    -2.820445      32.20
 O       4.012670     1.306075    -2.084846      31.70
 H       4.467974     1.760147    -1.274340      25.04
 C       3.957497    -0.730221    -0.748816      95.54
 H       3.392750    -1.830552    -0.755180      29.40
 O       5.325178    -1.055428    -1.154780     164.15
 H       5.351352    -1.997682    -0.804333      26.99
 C       3.799042    -0.171668     0.733981     126.38
 O       4.410084     1.114485     0.606090     144.95
 H       4.121478     1.699346     1.359313      28.43
 H       4.279547    -0.837559     1.459149      32.82
 H       2.614840     0.026702     0.961316      30.58
55
name = lig-Water-frame_845
 C      -1.535681     3.859135     2.784672      40.85
 H      -2.142518     4.778753     2.286291      20.75
 C      -1.224194     1.390595     3.363674      54.06
 H      -1.543072     0.401104     3.196565      30.17
 C      -0.148845     1.801747     4.098005       6.24
 O       0.641877     0.801332     4.965874     111.91
 C       0.317835    -0.629900     4.575008     109.05
 H       0.988707    -1.508002     5.016064      26.98
 H       0.070858    -0.595155     3.352344      26.70
 H      -0.689689    -0.759599     4.932236      28.87
 C       0.091468     3.142509     4.405036      28.97
 O       1.224619     3.374679     5.278124     155.19
 H       1.133656     4.202345     5.732739      26.50
 C      -0.511483     4.097914     3.635258      49.00
 H      -0.157703     5.146186     3.921098      29.11
 C      -1.892102     2.445431     2.541525     -10.91
 C      -3.075324     2.065843     1.697603      85.16
 H      -3.844278     3.024222     1.920627      27.02
 O      -3.768841     0.932921     2.166346     113.39
 H      -4.473510     0.506269     1.473072      21.96
 C      -2.845880     1.997169     0.159883     101.58
 H      -2.175286     2.912653    -0.143729      26.92
 C      -4.217361     2.062545    -0.639598     101.64
 O      -5.280625     1.240784    -0.183939     327.96
 H      -5.047174     0.270525    -0.330407      30.65
 H      -3.837670     1.832067    -1.627120      29.13
 H      -4.624009     3.065636    -0.932300      27.62
 C       1.288891     1.631943    -1.272511      33.99
 H       2.002679     2.389923    -1.500374      28.75
 C       0.922553    -0.793806    -1.333342      83.83
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 H       1.286092    -1.889342    -1.288640      27.67
 C      -0.396631    -0.610723    -0.887737      18.99
 O      -1.364153    -1.639805    -0.736221     162.27
 C      -1.261055    -2.975073    -1.470135      89.73
 H      -0.227652    -3.316535    -0.916261      25.75
 H      -2.109757    -3.454634    -1.049859      27.21
 H      -1.076516    -2.955362    -2.724167      25.88
 C      -0.951537     0.694378    -0.618206      32.12
 O      -2.245445     0.669507    -0.234612     186.54
 C      -0.192386     1.784858    -0.871640      76.63
 H      -0.426895     2.801680    -0.580871      24.98
 C       1.651046     0.257353    -1.551163      35.52
 C       3.296745     0.071426    -1.825844      83.89
 H       3.677666    -0.695825    -2.790625      28.99
 O       3.995367     1.339511    -2.120998      45.13
 H       4.473833     1.623722    -1.406697      30.36
 C       3.922945    -0.740248    -0.767680     117.25
 H       3.386356    -1.574988    -0.939712      34.50
 O       5.240278    -1.064389    -1.158051     161.70
 H       5.542339    -1.982456    -0.924709      24.72
 C       3.768141    -0.179426     0.672435     146.27
 O       4.416233     1.131647     0.611570     163.40
 H       4.115430     1.740842     1.328958      26.62
 H       4.232678    -1.029060     1.319194      31.59
 H       2.740073     0.079993     0.818180      30.50
55
name = lig-Water-frame_846
 C      -1.515562     3.833297     2.766873      33.35
 H      -2.006679     4.517011     2.155579      17.72
 C      -1.188200     1.399667     3.273805      54.73
 H      -1.475297     0.369843     3.185768      28.38
 C      -0.156132     1.774562     4.178941       7.33
 O       0.640506     0.752774     4.954134     177.99
 C       0.344090    -0.557617     4.607114     143.01
 H       0.946751    -1.385598     4.825350      29.10
 H       0.279631    -0.744728     3.582462      31.66
 H      -0.778757    -0.656983     4.736913      27.97
 C       0.095729     3.138943     4.401750      24.31
 O       1.202329     3.414673     5.277594     144.12
 H       1.141076     4.256240     5.883335      20.14
 C      -0.485819     4.176269     3.672557      27.21
 H      -0.052162     5.261419     3.894748      31.07
 C      -1.877398     2.424965     2.521927       2.18
 C      -3.092832     2.116124     1.691108      98.86
 H      -3.862408     2.870214     1.851173      29.69
 O      -3.767502     0.938171     2.205307     193.76
 H      -4.401020     0.734607     1.610810      29.47
 C      -2.872999     1.974972     0.167357     108.22
 H      -2.179012     2.708001    -0.148636      30.04
 C      -4.183585     2.055666    -0.662301      88.37
 O      -5.272015     1.186344    -0.180104     348.09
 H      -5.010940     0.244207    -0.205340      31.41
 H      -4.024924     1.662685    -1.873770      24.64
 H      -4.373118     3.133104    -0.834576      27.44
 C       1.273336     1.609784    -1.282646      41.49
 H       1.898924     2.585974    -1.251913      28.74
 C       0.852346    -0.916723    -1.297872      73.48
 H       1.487442    -1.777204    -1.678289      26.96
 C      -0.369273    -0.642734    -0.879017      20.81
 O      -1.384381    -1.680946    -0.702675     177.83
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 C      -1.198395    -2.963644    -1.440075     109.95
 H      -0.425415    -3.663067    -1.070054      29.18
 H      -2.282624    -3.365056    -1.074709      24.91
 H      -1.174545    -2.848692    -2.415252      32.04
 C      -0.900843     0.660980    -0.502162       7.88
 O      -2.268350     0.657468    -0.209855     160.25
 C      -0.150997     1.877125    -0.978562      56.19
 H      -0.505553     2.883766    -0.474798      21.63
 C       1.747249     0.329867    -1.522475      25.47
 C       3.340945     0.089979    -1.821734     111.48
 H       3.564124    -0.552591    -2.537106      37.08
 O       3.963836     1.366427    -2.175403      22.08
 H       4.513972     1.494638    -1.170100      24.83
 C       3.872597    -0.768563    -0.757095     111.47
 H       3.133603    -1.740003    -0.842308      30.05
 O       5.205729    -1.073630    -1.164071     173.03
 H       5.568899    -1.954343    -0.968425      23.34
 C       3.765392    -0.190587     0.579269     130.46
 O       4.441532     1.147757     0.631583     101.40
 H       4.036934     1.695765     1.351080      27.26
 H       4.121258    -0.875301     1.302931      34.31
 H       2.542274    -0.064469     0.878954      30.82
55
name = lig-Water-frame_847
 C      -1.494337     3.760462     2.734626      59.88
 H      -1.970840     4.521980     2.006836      27.62
 C      -1.149103     1.438746     3.178593      55.70
 H      -1.386944     0.359731     3.082747      23.37
 C      -0.161118     1.707078     4.270861      -8.31
 O       0.640962     0.766772     4.928829      87.66
 C       0.293994    -0.514313     4.592256     118.21
 H       1.091799    -1.218673     5.125893      28.40
 H       0.694478    -0.789817     3.425688      28.58
 H      -0.727871    -0.870367     4.875095      28.38
 C       0.160752     3.140628     4.432479      12.78
 O       1.182525     3.451448     5.281854     129.79
 H       0.937228     4.386269     5.669544      23.51
 C      -0.473131     4.250843     3.700706      35.87
 H      -0.134942     5.237335     3.777710      13.26
 C      -1.833435     2.433231     2.550608      48.26
 C      -3.119703     2.144000     1.673385      75.11
 H      -3.912808     3.107804     1.723315      26.22
 O      -3.749873     0.930770     2.265987      98.17
 H      -4.655403     0.934936     1.596082      20.93
 C      -2.902856     1.927618     0.148532     111.81
 H      -2.219901     2.736951    -0.245655      27.40
 C      -4.136495     2.016060    -0.740683      96.46
 O      -5.262830     1.154612    -0.163364     316.15
 H      -4.854358     0.261662    -0.329514      29.14
 H      -4.017518     1.665919    -1.706843      29.59
 H      -4.455300     3.088613    -0.518563      28.00
 C       1.217598     1.622393    -1.286363      62.78
 H       1.797106     2.476808    -1.177909      30.14
 C       0.908483    -0.961836    -1.318304      45.90
 H       1.236784    -1.806633    -1.896001      25.96
 C      -0.445313    -0.709255    -0.838876      -2.76
 O      -1.377872    -1.711765    -0.675533     182.95
 C      -1.185326    -2.950629    -1.344485     104.61
 H      -0.479338    -3.870334    -1.111835      26.09
 H      -2.192259    -3.520102    -1.353892      25.03
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 H      -1.222438    -2.651344    -2.579381      26.21
 C      -0.840072     0.675852    -0.456413       8.38
 O      -2.277198     0.653945    -0.164753     166.52
 C      -0.096497     1.895364    -1.007580      68.85
 H      -0.397968     2.815998    -0.716354      22.30
 C       1.862331     0.373197    -1.495116       8.35
 C       3.290386     0.143661    -1.852755     107.15
 H       3.234299    -0.542892    -2.963679      26.36
 O       3.955170     1.376564    -2.171410     156.02
 H       4.363919     1.637756    -1.369379      29.87
 C       3.818537    -0.842555    -0.747279     116.43
 H       3.225263    -1.668099    -0.574266      30.12
 O       5.210742    -1.085518    -1.174362     176.65
 H       5.393162    -2.041452    -0.855004      26.99
 C       3.728858    -0.178069     0.552239     128.30
 O       4.465276     1.148573     0.652393     117.96
 H       3.953902     1.604759     1.377620      29.35
 H       4.181069    -0.731413     1.480488      30.81
 H       2.732866    -0.162159     0.805499      31.78
55
name = lig-Water-frame_848
 C      -1.436652     3.764344     2.719813      52.29
 H      -1.922536     4.535405     2.076000      27.39
 C      -1.057424     1.427566     3.170356      55.52
 H      -1.345880     0.445554     2.861970      22.60
 C      -0.192999     1.719123     4.290255      13.80
 O       0.629135     0.831375     4.905895      80.05
 C       0.313209    -0.590090     4.552555     128.84
 H       0.910149    -0.841832     5.429419      27.74
 H       0.678275    -0.679963     3.637917      30.98
 H      -0.643865    -1.001118     4.890300      28.54
 C       0.201310     3.141746     4.437117      23.45
 O       1.174972     3.508745     5.310113     138.53
 H       0.961155     4.474075     5.471618      28.53
 C      -0.500062     4.196736     3.692889      63.09
 H      -0.195036     5.415279     3.675294      15.03
 C      -1.831259     2.456977     2.549361      32.22
 C      -3.143035     2.160584     1.669614      83.04
 H      -3.654231     3.117844     1.669022      27.95
 O      -3.764798     0.949781     2.293416     124.78
 H      -4.682216     0.949393     1.937622      26.40
 C      -2.895680     1.885342     0.105392     117.86
 H      -2.355814     2.797360    -0.266858      26.60
 C      -4.138847     1.990243    -0.733253      86.40
 O      -5.227123     1.123315    -0.154712     302.93
 H      -4.872844     0.244166    -0.491326      26.85
 H      -3.831771     1.766582    -2.006403      23.18
 H      -4.652150     2.897609    -0.539947      26.57
 C       1.227951     1.622668    -1.298218      57.58
 H       1.952291     2.522801    -1.329570      26.09
 C       0.988842    -0.891303    -1.356367      57.31
 H       0.881917    -1.903736    -1.970467      19.44
 C      -0.457346    -0.745225    -0.802989      -8.97
 O      -1.370599    -1.740520    -0.626849     210.26
 C      -1.211666    -2.959938    -1.347372     118.70
 H      -0.340503    -3.631687    -1.000996      27.03
 H      -2.101979    -3.580432    -1.298790      26.35
 H      -1.002088    -2.694213    -2.275408      32.02
 C      -0.824490     0.699319    -0.479759      30.50
 O      -2.243386     0.652686    -0.111521     198.29
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 C      -0.105771     1.794730    -0.954245      56.86
 H      -0.386870     2.982937    -1.016975      18.79
 C       1.850615     0.354212    -1.456937      23.27
 C       3.186962     0.143320    -1.947751     105.09
 H       3.049381    -0.202287    -2.854267      29.63
 O       3.951932     1.373561    -2.160226     161.27
 H       4.348155     1.866542    -1.359266      24.98
 C       3.830200    -0.866776    -0.779031      88.97
 H       3.224276    -1.895362    -0.573129      24.78
 O       5.219679    -1.127582    -1.169456     200.45
 H       5.337073    -2.030612    -0.806498      29.07
 C       3.753785    -0.153082     0.612325      97.74
 O       4.466706     1.139492     0.667259     154.39
 H       3.984088     1.602569     1.400754      28.04
 H       4.209942    -0.726994     1.350463      29.98
 H       2.492786     0.008010     0.822914      24.53
55
name = lig-Water-frame_849
 C      -1.393149     3.815513     2.709338      50.20
 H      -1.913248     4.617818     2.199951      26.14
 C      -0.992862     1.418218     3.187958      50.90
 H      -1.234201     0.416536     2.773452      22.66
 C      -0.213748     1.812568     4.241938      25.09
 O       0.595592     0.891914     4.888797      43.74
 C       0.368092    -0.650940     4.608925      98.32
 H       0.923171    -1.016431     5.491035      28.24
 H       0.759038    -0.866018     3.429783      26.07
 H      -0.773849    -0.945534     4.642405      26.19
 C       0.181532     3.155462     4.406131      22.55
 O       1.183221     3.565516     5.351781     133.02
 H       1.165138     4.633025     5.515531      26.38
 C      -0.502708     4.112417     3.674292      61.18
 H      -0.277625     5.047138     3.750327      18.90
 C      -1.839824     2.451920     2.524156       9.73
 C      -3.100550     2.137984     1.661878      75.79
 H      -3.738877     3.181275     1.760245      25.40
 O      -3.793010     1.001394     2.322429     136.70
 H      -4.721174     0.847201     2.070012      26.49
 C      -2.878940     1.890744     0.083965     106.92
 H      -2.308435     2.758519    -0.239870      26.28
 C      -4.180163     1.952654    -0.727930     106.33
 O      -5.169278     1.073286    -0.179243     360.45
 H      -5.097878     0.142662    -0.500902      28.97
 H      -3.895994     1.922083    -1.738499      29.09
 H      -4.701017     2.983715    -0.781753      26.36
 C       1.299428     1.604733    -1.303550      56.93
 H       1.897303     2.432549    -1.622890      27.79
 C       0.950121    -0.801510    -1.379564      78.06
 H       1.118662    -1.692481    -1.859998      22.85
 C      -0.353096    -0.697248    -0.786818       7.84
 O      -1.374649    -1.754020    -0.562177     190.69
 C      -1.201005    -2.974624    -1.345904      73.40
 H      -0.223200    -3.391667    -0.819092      24.35
 H      -2.201089    -3.686508    -1.057791      21.81
 H      -0.773299    -2.763669    -2.496987      24.76
 C      -0.881844     0.642283    -0.529768      25.57
 O      -2.173581     0.654477    -0.064375     206.45
 C      -0.122304     1.734608    -0.881533      73.34
 H      -0.545693     2.608204    -1.152430      26.87
 C       1.720933     0.309890    -1.425218      38.47
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 C       3.133498     0.138402    -1.969548      67.31
 H       3.060335    -0.242700    -3.202107      24.09
 O       3.953072     1.359653    -2.161667      75.93
 H       4.202264     1.919807    -1.203602      23.50
 C       3.857877    -0.860309    -0.830384      94.57
 H       3.362889    -1.795425    -0.855674      26.04
 O       5.222466    -1.178007    -1.153921     216.29
 H       5.525774    -2.078260    -0.828453      27.17
 C       3.744497    -0.124921     0.657863     103.40
 O       4.459309     1.133225     0.678440     124.61
 H       4.095481     1.662829     1.448064      27.27
 H       4.209495    -0.958197     1.364342      27.38
 H       2.816953     0.114787     0.880079      30.42
55
name = lig-Water-frame_850
 C      -1.429257     3.812424     2.662669      58.63
 H      -1.984394     4.788806     2.298289      26.72
 C      -1.028669     1.449651     3.147248      64.77
 H      -1.012176     0.368348     2.965367      23.99
 C      -0.170900     1.873478     4.184368      17.67
 O       0.562867     0.906133     4.886639      46.63
 C       0.413571    -0.662383     4.640539     123.34
 H       0.951568    -1.376086     5.331415      28.05
 H       0.808506    -1.027879     3.803104      30.76
 H      -0.605461    -0.787809     4.500170      26.98
 C       0.173276     3.194342     4.417104      21.17
 O       1.196285     3.603058     5.377246     185.38
 H       1.089528     4.527253     5.657436      28.27
 C      -0.472889     4.041297     3.658696      67.24
 H      -0.169012     5.237861     3.980972      15.26
 C      -1.810714     2.439625     2.497896      23.27
 C      -3.061880     2.128500     1.650507      89.77
 H      -3.798895     2.929274     1.797860      26.77
 O      -3.810768     1.065212     2.364328      98.33
 H      -4.769846     0.784551     1.859862      22.07
 C      -2.868806     1.938929     0.108550      91.68
 H      -2.135326     2.749544    -0.247841      22.99
 C      -4.231568     1.936956    -0.696252      92.62
 O      -5.133165     1.012208    -0.213014     319.80
 H      -5.154801     0.086045    -0.560815      27.26
 H      -3.921159     1.729632    -1.958868      24.86
 H      -4.545713     2.963892    -0.762641      27.57
 C       1.279412     1.594358    -1.278971      56.43
 H       1.818159     2.390510    -1.842817      27.03
 C       0.830495    -0.771775    -1.376694      83.10
 H       1.582290    -1.654871    -1.748835      19.89
 C      -0.295368    -0.650738    -0.762327      32.02
 O      -1.361861    -1.730363    -0.520244     192.45
 C      -1.141575    -2.993335    -1.326883     112.74
 H      -0.250759    -3.396170    -0.730368      25.60
 H      -1.934667    -3.557302    -1.124921      28.48
 H      -1.015987    -2.966287    -2.346416      29.61
 C      -0.927681     0.545593    -0.582246      15.51
 O      -2.119458     0.648246    -0.022259     179.25
 C      -0.079474     1.696596    -0.840426      92.36
 H      -0.839034     2.582622    -1.135973      22.06
 C       1.668838     0.305083    -1.449859      37.65
 C       3.136508     0.110359    -1.994957      88.80
 H       3.189854    -0.322038    -2.865599      30.12
 O       3.943595     1.348505    -2.150699     155.19
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 H       3.994618     1.593838    -1.319000      33.40
 C       3.886919    -0.811800    -0.891358      92.52
 H       3.245066    -1.789866    -0.985207      25.79
 O       5.242694    -1.209495    -1.146642     222.89
 H       5.591666    -2.107631    -0.826811      25.58
 C       3.779388    -0.157144     0.655310      90.81
 O       4.470912     1.134838     0.687132     164.79
 H       4.150069     1.635698     1.502568      26.96
 H       4.101164    -0.898447     1.327870      29.24
 H       2.596418     0.154027     1.106643      25.69
55
name = lig-Water-frame_851
 C      -1.490911     3.801418     2.637117      53.06
 H      -2.020461     4.602526     2.316007      25.34
 C      -1.071730     1.494808     3.118286      69.97
 H      -1.037092     0.426623     3.072303      24.89
 C      -0.093218     1.848390     4.120242       3.89
 O       0.559592     0.869329     4.906649     125.87
 C       0.452372    -0.629284     4.672803     104.30
 H       0.801224    -1.328836     5.438008      25.10
 H       1.108138    -1.019932     3.663535      24.26
 H      -0.734856    -0.814599     4.553367      21.09
 C       0.226040     3.207062     4.496456      -5.38
 O       1.200966     3.592851     5.378856      43.51
 H       0.823367     4.574253     5.802796      20.72
 C      -0.453047     4.129053     3.616678      49.86
 H      -0.259525     5.037781     3.905547      27.53
 C      -1.790099     2.446243     2.441339      41.24
 C      -3.048304     2.114363     1.648148      78.64
 H      -3.792843     3.059938     1.715547      25.46
 O      -3.837181     1.107065     2.393934     189.48
 H      -4.404868     0.922073     1.708701      28.82
 C      -2.841992     1.979186     0.144088     104.08
 H      -2.246687     2.754093    -0.206831      27.61
 C      -4.197604     1.911586    -0.729418      96.45
 O      -5.145373     0.945720    -0.226353     311.07
 H      -4.910179     0.104933    -0.755633      25.47
 H      -4.018185     1.575784    -1.718314      28.85
 H      -4.625736     2.961530    -0.567284      26.60
 C       1.189097     1.619773    -1.257554      65.50
 H       1.714161     2.417934    -1.831068      27.46
 C       0.849229    -0.820149    -1.415610      67.61
 H       1.394903    -1.721349    -1.421983      25.23
 C      -0.409055    -0.713343    -0.707709      23.88
 O      -1.323000    -1.697008    -0.514226     197.54
 C      -1.046115    -2.983666    -1.240071      78.28
 H      -0.197050    -3.624616    -0.846789      24.96
 H      -2.120343    -3.743004    -1.064372      22.76
 H      -1.131333    -2.936233    -2.469930      24.42
 C      -0.896345     0.554370    -0.618104      25.91
 O      -2.122605     0.633413     0.024791     154.71
 C      -0.084498     1.684200    -0.835737      77.27
 H      -0.633517     2.603212    -0.919977      26.80
 C       1.716553     0.328771    -1.529444      15.18
 C       3.183191     0.089882    -1.957577      87.88
 H       3.283628    -0.685625    -2.991207      25.32
 O       3.912401     1.318701    -2.161670      30.08
 H       4.004562     1.552223    -1.037443      23.68
 C       3.882228    -0.782739    -0.912936      97.31
 H       3.187083    -1.632409    -0.843058      27.75
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 O       5.277319    -1.207302    -1.160904     225.29
 H       5.408998    -2.104824    -0.770580      26.32
 C       3.755444    -0.181105     0.621694      99.12
 O       4.497942     1.124539     0.689686     185.20
 H       4.118370     1.593127     1.501708      26.96
 H       4.234513    -0.900017     1.425531      27.18
 H       2.838138    -0.108006     0.938696      31.27
55
name = lig-Water-frame_852
 C      -1.494740     3.795240     2.677699      40.02
 H      -2.245509     4.578648     2.111808      22.45
 C      -1.050856     1.519312     3.143890      52.13
 H      -1.396535     0.442297     2.941615      28.47
 C      -0.008300     1.806437     4.070452       9.41
 O       0.582043     0.804556     4.941750     134.84
 C       0.459809    -0.592260     4.650123     139.08
 H       0.703140    -0.934401     5.725132      24.96
 H       1.052498    -0.711088     3.865925      30.78
 H      -0.494854    -0.933655     4.571956      28.55
 C       0.243309     3.193001     4.494204      -8.20
 O       1.189173     3.590219     5.403504      89.69
 H       0.972067     4.479521     5.724194      27.79
 C      -0.453887     4.191861     3.573442      39.20
 H      -0.327040     5.438612     3.775796      24.77
 C      -1.799667     2.470447     2.368025      22.55
 C      -3.072817     2.152449     1.672943      93.75
 H      -3.499594     3.181788     1.598786      28.62
 O      -3.839732     1.149287     2.397313     157.69
 H      -4.422015     0.801855     1.539315      20.68
 C      -2.835298     1.944019     0.166820     101.13
 H      -2.300490     2.935236    -0.213663      26.01
 C      -4.136558     1.914977    -0.704991      85.82
 O      -5.164612     0.869285    -0.237542     277.65
 H      -4.825407     0.112846    -0.755719      26.66
 H      -3.923132     1.562891    -1.946857      24.37
 H      -4.753003     2.781484    -0.580647      26.36
 C       1.159585     1.626122    -1.295672      65.06
 H       1.616469     2.566859    -1.560819      29.62
 C       0.897561    -0.857501    -1.407315      50.04
 H       1.152430    -2.057578    -1.311204      24.45
 C      -0.474924    -0.787756    -0.725032      12.06
 O      -1.291554    -1.724840    -0.517339     199.80
 C      -1.029085    -3.011173    -1.160487     111.35
 H      -0.102212    -3.725393    -1.062449      26.58
 H      -1.798984    -3.509439    -0.929421      30.47
 H      -1.026570    -2.698456    -2.162541      30.66
 C      -0.882321     0.617082    -0.596057      31.34
 O      -2.153909     0.634669     0.060585     163.13
 C      -0.144346     1.701328    -0.831495      69.16
 H      -0.432682     2.800053    -0.683435      26.29
 C       1.754331     0.323953    -1.621092       5.84
 C       3.244627     0.036495    -1.961534     128.32
 H       3.265278    -0.505471    -2.762440      32.65
 O       3.878125     1.290079    -2.137820      76.95
 H       4.245220     1.684743    -1.321899      27.57
 C       3.879454    -0.769584    -0.846287     100.30
 H       3.230209    -1.692201    -0.704810      29.55
 O       5.287536    -1.175696    -1.191784     214.07
 H       5.353450    -2.066982    -0.735560      25.25
 C       3.804727    -0.221782     0.563136     101.22
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 O       4.511834     1.094507     0.682013     174.14
 H       4.106382     1.671156     1.407676      26.92
 H       4.389027    -0.818772     1.235629      29.83
 H       2.524360    -0.223146     0.811462      28.36
55
name = lig-Water-frame_853
 C      -1.498197     3.835856     2.708101      42.32
 H      -2.060345     4.480459     2.191388      23.84
 C      -1.033992     1.507655     3.150811      38.68
 H      -1.558537     0.621771     2.957135      28.09
 C       0.065762     1.777586     4.059979       5.84
 O       0.596654     0.795865     4.967632     112.15
 C       0.463787    -0.548436     4.691408     115.04
 H       0.822795    -0.789695     5.684901      25.13
 H       1.281935    -0.798597     3.778026      26.35
 H      -0.596885    -1.095159     4.385964      24.57
 C       0.215516     3.201704     4.379593      -5.54
 O       1.178744     3.554882     5.433142      42.22
 H       1.154200     4.671337     5.653714      19.24
 C      -0.451429     4.251013     3.573195      39.22
 H      -0.389869     5.281104     3.577048      28.72
 C      -1.768366     2.482920     2.370535       6.98
 C      -3.092350     2.220472     1.681892      86.01
 H      -3.589997     3.300401     1.664575      26.68
 O      -3.847061     1.196745     2.349458     184.25
 H      -4.505781     0.607729     1.832709      22.56
 C      -2.853146     1.895425     0.172026     113.66
 H      -2.325962     2.719283    -0.149949      29.31
 C      -4.099529     1.883518    -0.695811     101.25
 O      -5.160423     0.811328    -0.249400     296.38
 H      -4.984623    -0.124608    -0.704321      24.91
 H      -3.810756     1.836027    -1.706191      29.49
 H      -4.743663     2.809607    -0.714689      26.52
 C       1.184561     1.586896    -1.380540      23.63
 H       1.681512     2.623581    -1.220578      25.98
 C       0.897334    -0.904827    -1.338477      68.58
 H       1.118619    -1.964473    -1.525016      23.92
 C      -0.389311    -0.712220    -0.832724       8.45
 O      -1.290317    -1.812030    -0.484288     195.68
 C      -0.990655    -3.029790    -1.114664      76.44
 H      -0.031885    -3.516638    -0.941616      27.36
 H      -2.058790    -3.736905    -0.670281      21.76
 H      -0.964412    -2.640205    -2.251338      25.94
 C      -0.942076     0.600715    -0.520794      22.10
 O      -2.185022     0.657168     0.077129     189.07
 C      -0.181534     1.776595    -0.842941      50.00
 H      -0.348682     2.807319    -0.312743      23.52
 C       1.739590     0.286814    -1.684061      16.21
 C       3.267393     0.024882    -1.913885      92.44
 H       3.351369    -0.545526    -3.090893      28.83
 O       3.876456     1.285993    -2.150019     102.84
 H       4.365780     1.671828    -1.412588      27.87
 C       3.898181    -0.800192    -0.765115     102.58
 H       3.401142    -1.823116    -0.710243      27.68
 O       5.268251    -1.127202    -1.225313     177.70
 H       5.611769    -1.974762    -0.798278      25.34
 C       3.831341    -0.226911     0.524631     129.97
 O       4.511386     1.058858     0.658325     198.14
 H       4.090222     1.712226     1.290701      25.96
 H       4.427586    -0.974188     1.157532      28.15
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 H       2.895525    -0.181266     0.734604      32.72
55
name = lig-Water-frame_854
 C      -1.473174     3.859847     2.723849      53.96
 H      -2.018627     4.801852     2.189618      21.67
 C      -1.023281     1.500896     3.135244      40.09
 H      -1.484171     0.438760     3.145524      26.54
 C       0.079954     1.780314     4.053549     -17.99
 O       0.593223     0.870421     4.973206     117.71
 C       0.497666    -0.571005     4.699478     124.95
 H       0.917298    -1.178589     5.579110      27.09
 H       1.185777    -0.966689     4.068897      31.45
 H      -0.405018    -0.869524     4.380012      29.58
 C       0.227091     3.237726     4.261747      -2.04
 O       1.154106     3.522970     5.439026     118.70
 H       1.049157     4.438378     5.599521      24.26
 C      -0.459975     4.231825     3.580689      31.53
 H      -0.236023     5.404031     3.677955      24.57
 C      -1.713723     2.505395     2.455963      24.39
 C      -3.113727     2.288849     1.654287      85.97
 H      -3.833629     3.144656     1.799615      25.65
 O      -3.856113     1.234364     2.328899     217.14
 H      -4.500432     0.754605     1.889890      29.41
 C      -2.907337     1.871870     0.200776      92.23
 H      -2.145253     2.649895    -0.265653      23.90
 C      -4.134697     1.824965    -0.667462      91.68
 O      -5.139243     0.777515    -0.269327     318.37
 H      -5.014494    -0.084702    -0.728606      26.88
 H      -3.582135     1.887531    -1.850088      24.57
 H      -4.588433     2.840164    -0.631543      27.06
 C       1.185636     1.550390    -1.435156      32.76
 H       1.916988     2.277230    -1.207533      28.55
 C       0.904860    -0.896250    -1.297543      77.78
 H       1.314526    -1.906950    -1.736657      25.02
 C      -0.350345    -0.623536    -0.917616       3.24
 O      -1.270997    -1.849351    -0.429144     183.59
 C      -1.012526    -3.075895    -1.103631     117.13
 H       0.043114    -3.319652    -0.598049      26.26
 H      -1.626045    -3.737796    -0.872900      30.05
 H      -1.028200    -3.130276    -2.203276      29.27
 C      -0.980350     0.601569    -0.463897       8.62
 O      -2.207755     0.650228     0.088875     176.78
 C      -0.167820     1.804069    -0.839446      39.67
 H      -0.377990     2.651138    -0.225655      25.84
 C       1.697680     0.231812    -1.702668      23.03
 C       3.246757     0.012414    -1.920540      98.39
 H       3.449534    -0.447212    -2.744433      36.16
 O       3.895981     1.301127    -2.189848      58.91
 H       4.465243     1.513276    -1.233714      25.40
 C       3.943761    -0.887764    -0.793080     116.48
 H       3.442304    -1.847894    -0.714820      30.39
 O       5.261430    -1.068399    -1.261283     201.02
 H       5.762537    -1.825091    -0.891406      25.58
 C       3.914198    -0.217756     0.566026     122.16
 O       4.518773     1.030145     0.617028     146.05
 H       4.017173     1.629840     1.232826      27.68
 H       4.274884    -1.055323     1.231186      30.58
 H       2.703518    -0.061089     0.994723      30.03
55
name = lig-Water-frame_855
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 C      -1.452407     3.918445     2.699869      69.22
 H      -1.942952     4.745564     2.301555      28.77
 C      -0.998699     1.462115     3.142955      78.93
 H      -1.236808     0.452412     3.227549      27.11
 C       0.024732     1.829700     4.022739     -13.68
 O       0.601754     0.950354     4.974113      28.35
 C       0.562490    -0.605482     4.736534      92.36
 H       0.681211    -1.326051     5.566621      28.06
 H       1.358578    -0.978735     3.863419      28.25
 H      -0.589470    -0.736249     4.397374      24.14
 C       0.313443     3.224798     4.222905      13.36
 O       1.106128     3.466456     5.397898     116.70
 H       0.864081     4.525409     5.731129      12.14
 C      -0.448810     4.233693     3.595080      89.86
 H      -0.030514     5.228735     3.962851      15.58
 C      -1.731604     2.545151     2.530592      24.02
 C      -3.128051     2.311196     1.654315      88.03
 H      -3.827281     3.205295     1.751153      27.39
 O      -3.852651     1.259008     2.353272     125.89
 H      -4.635425     0.992155     1.581314      22.74
 C      -2.927374     1.907177     0.215579     101.80
 H      -2.347139     2.581436    -0.327625      29.20
 C      -4.171464     1.775145    -0.678630     112.26
 O      -5.115170     0.790469    -0.291122     315.68
 H      -4.764503    -0.027468    -0.893972      23.81
 H      -3.813669     1.598600    -1.650297      30.89
 H      -4.618706     2.762177    -0.480652      27.91
 C       1.155576     1.501929    -1.439548      58.71
 H       2.143372     2.115636    -1.457132      29.12
 C       0.954581    -0.866525    -1.326951      69.40
 H       1.376940    -1.873706    -1.767026      25.75
 C      -0.445231    -0.617355    -0.916511      -6.42
 O      -1.250962    -1.821982    -0.399765     149.58
 C      -0.951137    -3.113450    -1.076782      99.15
 H      -0.068220    -3.417164    -0.634462      29.86
 H      -1.730173    -4.181871    -0.736722      24.03
 H      -0.986543    -3.371009    -2.235055      27.35
 C      -0.943765     0.651029    -0.473543      18.56
 O      -2.224565     0.597150     0.111396     160.63
 C      -0.115578     1.736398    -0.828517      53.00
 H      -0.360293     2.783695    -0.235005      27.94
 C       1.670945     0.203485    -1.684187      31.16
 C       3.197838     0.019123    -1.912118      74.22
 H       3.497556    -0.742639    -2.932731      27.51
 O       3.939707     1.314148    -2.197259     124.64
 H       4.323815     1.402607    -1.389956      32.97
 C       3.964580    -0.940022    -0.852376      93.96
 H       3.353900    -1.939848    -0.717112      28.00
 O       5.293660    -1.001400    -1.313380     173.88
 H       5.685273    -1.837109    -0.874876      26.47
 C       3.909609    -0.259903     0.658190     127.19
 O       4.548335     1.025949     0.573424     154.40
 H       4.024749     1.582949     1.210202      30.68
 H       4.333750    -0.926232     1.462755      32.17
 H       3.002302    -0.095113     0.970271      35.85
55
name = lig-Water-frame_856
 C      -1.414389     3.957186     2.689742      44.84
 H      -2.116947     4.762814     2.215107      24.57
 C      -0.984571     1.466725     3.147749      64.96
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 H      -1.227211     0.360496     3.054448      24.54
 C      -0.022791     1.877348     4.010743      10.24
 O       0.630771     0.994497     4.977433      -9.02
 C       0.587803    -0.622397     4.719635     119.10
 H       0.574706    -1.076056     5.739823      27.51
 H       1.217984    -0.684271     3.911373      30.59
 H      -0.398455    -0.749207     4.438118      28.04
 C       0.398684     3.187267     4.229895      33.80
 O       1.046940     3.447152     5.353445     161.21
 H       0.894061     4.300121     5.719463      24.61
 C      -0.373114     4.230413     3.642389      94.56
 H      -0.083754     5.211662     3.980969      19.41
 C      -1.820822     2.573494     2.554254      11.37
 C      -3.111951     2.314848     1.711010      86.20
 H      -3.563152     3.392424     1.579104      27.07
 O      -3.879522     1.269896     2.358103     196.14
 H      -4.532875     1.174161     1.704963      30.61
 C      -2.929615     1.918287     0.202558      83.76
 H      -2.424585     2.800372    -0.394677      25.17
 C      -4.204811     1.777887    -0.649829      90.21
 O      -5.099287     0.786577    -0.319242     303.67
 H      -4.729037    -0.019060    -0.735340      26.68
 H      -4.021374     1.343946    -1.849375      23.54
 H      -4.817188     2.735706    -0.599892      25.68
 C       1.169005     1.466724    -1.420891      79.72
 H       1.806323     2.275191    -1.755813      28.34
 C       0.904610    -0.880968    -1.373280      64.85
 H       1.248915    -1.905478    -1.595016      25.34
 C      -0.526561    -0.704282    -0.871340       2.17
 O      -1.232493    -1.774234    -0.416217     153.01
 C      -0.921516    -3.219333    -1.019923      96.30
 H       0.157883    -3.688095    -0.736502      26.01
 H      -1.614214    -3.695981    -0.589961      29.32
 H      -0.899604    -3.128239    -2.152452      28.49
 C      -0.912314     0.653589    -0.514256      16.12
 O      -2.217916     0.555330     0.134637     151.27
 C      -0.043148     1.700599    -0.790911      84.09
 H      -0.222578     2.651781    -0.550958      28.90
 C       1.699454     0.229592    -1.657677      39.04
 C       3.179138    -0.015879    -1.966973     100.23
 H       3.205778    -0.564739    -2.771925      30.15
 O       3.960889     1.291737    -2.207539      84.00
 H       4.408799     1.504095    -1.236646      22.98
 C       3.935138    -0.931123    -0.859520      91.29
 H       3.499244    -1.891183    -0.875007      28.55
 O       5.346064    -0.962379    -1.357083     204.16
 H       5.589972    -1.823913    -0.964428      29.42
 C       3.924817    -0.348723     0.705558      82.19
 O       4.577840     1.030308     0.538848     142.61
 H       4.152969     1.684857     1.171538      29.33
 H       4.563670    -0.753492     1.564458      26.88
 H       2.695599    -0.144318     1.003869      27.26
55
name = lig-Water-frame_857
 C      -1.382518     3.957956     2.707951      37.38
 H      -2.104422     4.689720     2.271316      21.91
 C      -1.040144     1.513292     3.112073      68.06
 H      -1.300736     0.505183     2.801970      26.98
 C      -0.011898     1.855269     4.047914       4.55
 O       0.656798     1.004584     4.968539     -12.53
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 C       0.568731    -0.552288     4.722457     109.55
 H       0.843839    -0.764967     5.818511      26.94
 H       1.407616    -0.696031     3.900897      29.00
 H      -0.488568    -0.907266     4.316457      25.19
 C       0.397423     3.192442     4.209109      40.93
 O       1.042636     3.419315     5.360295      70.64
 H       0.931283     4.457372     5.603441      19.76
 C      -0.291217     4.217794     3.650580     101.63
 H      -0.244608     5.430792     3.866810      19.13
 C      -1.883130     2.586116     2.557845      16.06
 C      -3.060215     2.326531     1.750616      90.03
 H      -3.498048     3.353603     1.623961      28.71
 O      -3.910975     1.298652     2.371133     143.57
 H      -4.743527     1.062333     1.779450      25.03
 C      -2.909516     1.916680     0.169784      84.26
 H      -2.393026     2.771434    -0.231473      28.09
 C      -4.236350     1.803400    -0.680274     115.25
 O      -5.124073     0.754384    -0.306140     325.27
 H      -4.814029    -0.196239    -0.563027      26.02
 H      -3.925465     1.700564    -1.690341      29.66
 H      -4.819024     2.697525    -0.817114      27.88
 C       1.217125     1.485050    -1.414607      57.96
 H       1.426090     2.495780    -1.907009      28.39
 C       0.764437    -0.900203    -1.411656      64.04
 H       1.163034    -2.073499    -1.322229      24.41
 C      -0.489277    -0.775624    -0.839228      25.75
 O      -1.222944    -1.768772    -0.448680     158.70
 C      -0.838358    -3.257400    -0.960525      76.57
 H       0.066918    -3.687036    -0.768581      28.51
 H      -1.952695    -3.610425    -0.304904      22.15
 H      -0.947907    -2.969396    -2.047281      27.40
 C      -0.929879     0.569718    -0.542973      15.35
 O      -2.186523     0.571033     0.141749     159.18
 C       0.010576     1.660916    -0.753372      40.19
 H      -0.307116     2.876270    -0.789847      27.63
 C       1.746436     0.223155    -1.622549      29.90
 C       3.184477    -0.006636    -1.976219      83.67
 H       3.095735    -0.611334    -3.123054      25.27
 O       3.969812     1.234887    -2.205712      83.56
 H       4.345131     1.584127    -1.270762      25.86
 C       3.924966    -0.868849    -0.843969      91.11
 H       3.630407    -2.008390    -1.039531      26.65
 O       5.379008    -0.946588    -1.377323     151.50
 H       5.724876    -1.861839    -1.138724      27.97
 C       3.912781    -0.387398     0.705259     103.08
 O       4.583007     1.021898     0.511919     119.47
 H       4.221160     1.698050     1.147882      30.12
 H       4.562240    -0.856393     1.386208      30.84
 H       2.946780    -0.367317     0.999262      32.87
55
name = lig-Water-frame_858
 C      -1.365570     3.906627     2.758044      53.71
 H      -1.932722     4.783463     2.393790      21.40
 C      -1.106781     1.584400     3.079748      72.14
 H      -1.377395     0.595898     2.714765      29.74
 C      -0.004096     1.797250     4.058327     -31.72
 O       0.660594     0.984403     4.934588      95.63
 C       0.563988    -0.422157     4.719092     146.27
 H       0.992726    -0.780265     5.625243      30.80
 H       1.415089    -0.874293     4.190482      30.68
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 H      -0.318822    -0.990165     4.427335      27.91
 C       0.350499     3.192832     4.205994     -12.43
 O       1.085219     3.427287     5.422916     117.42
 H       1.105954     4.450218     5.399021      14.68
 C      -0.290257     4.271991     3.562303      33.85
 H      -0.149849     5.203221     3.805515      19.20
 C      -1.843968     2.609349     2.578911      59.60
 C      -3.058473     2.316698     1.717443      83.39
 H      -3.742751     3.274412     1.763455      28.04
 O      -3.949257     1.337924     2.396842     105.26
 H      -4.800284     0.968305     1.852073      23.91
 C      -2.889803     1.907868     0.180345      84.69
 H      -2.175433     2.697255    -0.231969      28.17
 C      -4.244312     1.815684    -0.714786      92.93
 O      -5.171225     0.720088    -0.273448     214.06
 H      -4.782463    -0.194470    -0.582768      25.50
 H      -3.598024     1.941252    -1.798278      25.18
 H      -4.840113     2.821679    -0.722243      26.73
 C       1.260728     1.539729    -1.417602      37.98
 H       1.485403     2.468977    -1.972209      27.44
 C       0.727214    -0.925710    -1.443840      79.02
 H       1.090536    -1.861808    -1.307223      28.62
 C      -0.416878    -0.764110    -0.812877      29.64
 O      -1.230722    -1.828246    -0.463254     197.95
 C      -0.865275    -3.222023    -0.874207     105.36
 H       0.166579    -3.701408    -0.544221      27.89
 H      -1.607732    -3.793791    -0.542657      30.13
 H      -1.088994    -3.178836    -2.040250      27.42
 C      -0.950631     0.502191    -0.547501      18.11
 O      -2.147389     0.627069     0.128056     182.64
 C      -0.020415     1.638508    -0.730494      39.00
 H      -0.456935     2.511268    -0.781829      31.32
 C       1.742715     0.173632    -1.582363      10.13
 C       3.209178    -0.006224    -2.003340     108.93
 H       3.294093    -0.464142    -2.879492      33.19
 O       3.964354     1.171556    -2.211061     168.24
 H       4.199974     1.461019    -1.386256      31.30
 C       3.965651    -0.856823    -0.865122     101.88
 H       3.612078    -1.813044    -0.927134      33.14
 O       5.396766    -0.937047    -1.373784     160.39
 H       5.799048    -1.848492    -1.287988      26.68
 C       3.945047    -0.376184     0.614299      99.13
 O       4.555209     0.989748     0.501170     168.10
 H       4.135198     1.576553     1.203090      28.74
 H       4.596539    -1.226973     1.188420      29.01
 H       2.817136    -0.421012     1.180304      29.72
55
name = lig-Water-frame_859
 C      -1.386399     3.907851     2.794249      72.34
 H      -1.846876     4.901006     2.392855      21.73
 C      -1.107588     1.585775     3.104939      70.05
 H      -1.453490     0.553623     2.806849      27.67
 C      -0.036448     1.808346     4.004873      29.56
 O       0.646420     0.958493     4.885653     161.82
 C       0.613618    -0.355623     4.745849     145.83
 H       0.857715    -0.968545     5.734854      26.39
 H       1.426931    -0.820519     4.031318      27.60
 H      -0.384531    -0.829127     4.539353      25.32
 C       0.305525     3.167490     4.263100     -10.92
 O       1.139608     3.452807     5.453890      80.83
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 H       1.259977     4.396686     5.564697      24.78
 C      -0.292421     4.263203     3.467190      46.16
 H       0.125977     5.399428     3.825657      23.07
 C      -1.804375     2.642614     2.566402      45.28
 C      -3.131156     2.309810     1.665086      86.44
 H      -3.755974     3.185496     1.699620      28.25
 O      -3.984751     1.362533     2.440687     171.18
 H      -4.581421     1.099428     1.823979      31.88
 C      -2.861864     1.914799     0.214310     105.15
 H      -2.188206     2.631841    -0.300101      25.41
 C      -4.198291     1.847733    -0.741246     100.18
 O      -5.191126     0.707228    -0.264154     229.26
 H      -4.773267    -0.054739    -0.700581      27.91
 H      -3.839592     1.713801    -1.700868      29.36
 H      -4.745441     2.695372    -0.467774      27.88
 C       1.249737     1.543300    -1.400954      53.30
 H       1.882775     2.343723    -1.893490      26.84
 C       0.840872    -0.900290    -1.480053      52.96
 H       1.300776    -2.110383    -1.523830      21.99
 C      -0.436217    -0.764062    -0.766567      14.98
 O      -1.242309    -1.907787    -0.461598     217.68
 C      -0.879319    -3.164896    -0.831790     103.79
 H       0.047866    -3.448979    -0.405323      29.76
 H      -1.689311    -4.205619    -0.446018      23.81
 H      -0.949803    -3.468080    -1.927482      27.58
 C      -0.930303     0.516826    -0.527121      36.95
 O      -2.128197     0.675786     0.113125     238.07
 C      -0.067778     1.565866    -0.754632      53.50
 H      -0.738943     2.609260    -0.638668      24.03
 C       1.700715     0.157832    -1.567234      15.55
 C       3.237807    -0.026986    -1.971217      88.73
 H       3.466008    -0.740952    -3.024366      27.42
 O       3.951624     1.128762    -2.243927      80.89
 H       4.178011     1.523380    -1.178695      23.25
 C       4.025987    -0.862048    -0.922433      99.64
 H       3.420518    -1.909674    -0.777737      28.90
 O       5.407542    -0.926926    -1.357167     204.25
 H       5.677577    -1.856918    -1.285146      26.27
 C       3.979663    -0.377431     0.504688     127.87
 O       4.500382     0.935799     0.517004     214.35
 H       4.095808     1.459061     1.260290      27.27
 H       4.534517    -1.135692     0.932587      31.29
 H       3.110029    -0.343084     1.078399      31.27
55
name = lig-Water-frame_860
 C      -1.445965     4.011262     2.773802      52.73
 H      -1.977729     4.758476     2.279239      25.02
 C      -1.094062     1.525129     3.140601      73.74
 H      -1.438322     0.543942     3.026389      29.38
 C      -0.060631     1.865538     3.966687      24.02
 O       0.633029     0.990077     4.848291     114.73
 C       0.665375    -0.451772     4.774983     151.46
 H       0.735462    -0.813987     5.742381      28.12
 H       1.210183    -0.592222     3.820428      26.84
 H      -0.451107    -0.542740     4.508273      23.53
 C       0.280151     3.196794     4.342296       1.96
 O       1.187502     3.451791     5.437043      32.62
 H       1.163348     4.495459     5.804483      21.17
 C      -0.198244     4.232722     3.490874      47.48
 H       0.122290     5.174080     3.523080      28.60
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 C      -1.835243     2.634568     2.502059     -10.08
 C      -3.181626     2.313548     1.667446      78.25
 H      -3.710781     3.396338     1.477219      26.91
 O      -3.999246     1.388654     2.482850      98.92
 H      -4.620750     1.033125     1.625541      22.92
 C      -2.846952     1.912583     0.205861     102.15
 H      -2.370014     2.816613    -0.263508      27.73
 C      -4.141726     1.840134    -0.681670      84.14
 O      -5.168728     0.727813    -0.274458     165.42
 H      -4.821682    -0.126328    -0.830879      24.43
 H      -4.218919     1.449590    -1.880358      23.80
 H      -4.742208     2.800403    -0.394674      25.63
 C       1.198286     1.487419    -1.369981      91.33
 H       2.114774     2.154713    -1.481813      32.13
 C       0.938758    -0.949288    -1.457795      48.74
 H       1.297455    -1.784496    -1.810629      24.89
 C      -0.442962    -0.835490    -0.763365       3.12
 O      -1.276246    -1.928486    -0.451936     184.55
 C      -0.914205    -3.214131    -0.798007     108.48
 H       0.133767    -3.311455    -0.277595      28.24
 H      -1.510072    -3.819418    -0.289627      28.31
 H      -0.597538    -3.565818    -1.887878      27.20
 C      -0.897184     0.529011    -0.487002      27.65
 O      -2.135855     0.695786     0.113776     223.26
 C      -0.098469     1.592825    -0.831555      86.53
 H      -0.464463     2.491966    -0.502014      27.13
 C       1.712230     0.203736    -1.595817       8.04
 C       3.255604    -0.117220    -1.978123     118.74
 H       3.270850    -0.733089    -2.772864      31.63
 O       3.947632     1.131429    -2.248396     137.32
 H       4.169868     1.536822    -1.468805      30.27
 C       4.024234    -0.904327    -0.980857     129.71
 H       3.585457    -1.821363    -0.884176      31.84
 O       5.416580    -0.934659    -1.337007     203.45
 H       5.615636    -1.911530    -1.194254      26.34
 C       4.027792    -0.383648     0.393314     110.84
 O       4.459127     0.908914     0.539743     197.87
 H       4.141062     1.432788     1.312287      26.00
 H       4.805149    -1.083119     1.049824      27.54
 H       2.925008    -0.402505     0.942668      27.71
55
name = lig-Water-frame_861
 C      -1.472525     4.047559     2.735318      35.96
 H      -2.149914     4.811502     2.098986      21.94
 C      -1.121008     1.512253     3.133765      59.76
 H      -1.419711     0.397274     3.200512      26.28
 C      -0.048085     1.904535     4.005170      13.65
 O       0.641231     1.055803     4.834761      85.78
 C       0.621918    -0.515184     4.735090     112.04
 H       0.937684    -0.809448     5.853148      22.67
 H       1.199571    -0.785244     3.838374      26.48
 H      -0.378998    -0.747744     4.495682      24.92
 C       0.281837     3.270900     4.406499      15.36
 O       1.224163     3.459731     5.408665     142.77
 H       0.848152     4.293397     5.732081      21.73
 C      -0.158392     4.185198     3.522898      48.76
 H       0.283932     5.321849     3.397500      26.00
 C      -1.885492     2.619971     2.453951     -21.92
 C      -3.184047     2.360377     1.703572      88.36
 H      -3.635652     3.294922     1.486982      29.80
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 O      -4.025445     1.418162     2.466827     157.26
 H      -4.616786     0.877819     1.910659      27.55
 C      -2.856756     1.913923     0.157977      91.87
 H      -2.453832     2.936907    -0.127782      28.33
 C      -4.154278     1.789815    -0.633064     123.81
 O      -5.115319     0.749334    -0.286524     293.62
 H      -4.910442    -0.073304    -0.682823      30.42
 H      -4.100026     1.739347    -1.619284      30.56
 H      -4.610914     2.741872    -0.603870      29.90
 C       1.199579     1.415327    -1.327664      58.36
 H       1.866855     2.238012    -1.081233      23.43
 C       0.930164    -0.980277    -1.374116      99.94
 H       1.341276    -1.915833    -2.194758      22.38
 C      -0.400710    -0.911732    -0.803758       5.77
 O      -1.326842    -1.879698    -0.455722     200.04
 C      -0.831286    -3.282726    -0.759873      71.17
 H       0.092593    -3.379918    -0.217386      29.28
 H      -1.775135    -3.893695     0.001619      22.74
 H      -0.600493    -3.424001    -1.816135      27.60
 C      -0.866936     0.488733    -0.456200      12.20
 O      -2.142772     0.688271     0.122422     178.82
 C      -0.100019     1.652385    -0.906690      44.12
 H      -0.255387     2.734140    -0.399467      25.87
 C       1.760161     0.214356    -1.638753      34.41
 C       3.223831    -0.141406    -1.981363      87.46
 H       3.077738    -0.817593    -3.066217      27.02
 O       3.940984     1.129249    -2.289442      87.93
 H       4.255406     1.631428    -1.416489      24.87
 C       4.023862    -0.938477    -1.010477     112.54
 H       3.682858    -2.100190    -1.069419      26.23
 O       5.440372    -0.972015    -1.334836     168.99
 H       5.758740    -1.883224    -1.085492      29.44
 C       4.041976    -0.428691     0.405157     119.87
 O       4.447495     0.935166     0.541124     253.81
 H       4.121591     1.390851     1.381539      24.53
 H       4.666818    -0.935497     0.990579      30.96
 H       3.003333    -0.688166     0.584862      30.09
55
name = lig-Water-frame_862
 C      -1.463709     3.982115     2.682454      54.47
 H      -1.872044     4.808409     2.242034      23.92
 C      -1.150089     1.555407     3.128961      59.60
 H      -1.388658     0.541033     3.160794      26.19
 C      -0.065019     1.931430     4.066401       4.74
 O       0.670128     1.072994     4.835653     120.37
 C       0.562566    -0.518421     4.698911      99.18
 H       1.105234    -0.819874     5.520947      24.66
 H       1.346072    -1.055858     4.030466      25.44
 H      -0.448630    -1.152503     4.615491      23.09
 C       0.290392     3.276089     4.415036      18.84
 O       1.245522     3.480106     5.380596      35.24
 H       0.840835     4.363075     5.836859      18.43
 C      -0.217181     4.249113     3.486199      47.82
 H       0.392053     5.154250     3.519524      27.33
 C      -1.903577     2.628377     2.472879      13.46
 C      -3.157134     2.365651     1.713756      74.05
 H      -3.833276     3.391267     1.655358      24.73
 O      -4.048243     1.449203     2.457909     194.98
 H      -4.639272     0.873099     1.964552      29.16
 C      -2.890298     1.932511     0.153356      81.96
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 H      -2.295086     2.772583    -0.220917      26.81
 C      -4.183634     1.743694    -0.602836     106.41
 O      -5.068129     0.777502    -0.276315     333.92
 H      -4.747354    -0.128674    -0.651247      27.75
 H      -3.605280     1.918892    -1.794363      23.00
 H      -4.696771     2.790316    -0.593829      26.51
 C       1.255769     1.396525    -1.275549      27.84
 H       1.666239     2.415747    -0.947068      22.03
 C       0.912563    -1.028923    -1.356100      89.93
 H       1.076549    -1.801575    -1.887153      26.90
 C      -0.363895    -0.913094    -0.835130       3.17
 O      -1.351256    -1.836849    -0.481089     191.77
 C      -0.781305    -3.338798    -0.647414      88.26
 H       0.164239    -3.554830    -0.105446      27.48
 H      -1.620466    -3.894302    -0.376299      26.82
 H      -0.877280    -3.380010    -1.830203      24.79
 C      -0.835284     0.480941    -0.463662       7.08
 O      -2.129835     0.653801     0.128189     176.72
 C      -0.133267     1.671603    -0.920206      36.41
 H      -0.158706     2.682337    -0.490330      24.85
 C       1.781685     0.136667    -1.647367      39.03
 C       3.176110    -0.115111    -2.053565     100.98
 H       3.142472    -0.530078    -2.984696      29.73
 O       3.933794     1.121056    -2.340955      88.41
 H       4.256314     1.509704    -1.363133      24.81
 C       4.063002    -1.021250    -1.022151     108.67
 H       3.715432    -2.000774    -1.117751      29.31
 O       5.487076    -1.015094    -1.360659     182.12
 H       5.849802    -1.848276    -0.989521      31.05
 C       4.005576    -0.480013     0.427712      82.87
 O       4.439802     0.973281     0.524769     182.48
 H       4.034095     1.353632     1.347884      25.29
 H       4.686559    -1.217721     1.172479      26.30
 H       2.875613    -0.759148     0.711285      25.47
55
name = lig-Water-frame_863
 C      -1.377531     3.898689     2.657072      59.41
 H      -1.747337     4.930105     2.223609      21.80
 C      -1.144171     1.656925     3.161073      78.37
 H      -1.450665     0.575611     2.970526      27.42
 C      -0.125129     1.946960     4.108734      12.29
 O       0.697497     1.009563     4.831987      87.77
 C       0.531615    -0.528103     4.663195     111.98
 H       1.136508    -0.808028     5.645462      25.86
 H       1.221963    -0.896714     3.932062      30.83
 H      -0.346571    -1.047825     4.765101      28.83
 C       0.267912     3.263468     4.334711      13.42
 O       1.249897     3.529672     5.372232      40.27
 H       1.253088     4.426707     5.820075      20.72
 C      -0.312993     4.287205     3.462286      58.54
 H       0.297794     5.275882     3.553936      19.96
 C      -1.891191     2.636787     2.540213      44.11
 C      -3.170536     2.373265     1.689882      91.80
 H      -3.721424     3.236284     1.745189      27.37
 O      -4.058541     1.471505     2.471616     199.52
 H      -4.698688     1.000845     1.681853      23.93
 C      -2.903875     1.944438     0.219561      84.94
 H      -2.182062     2.550048    -0.437361      25.57
 C      -4.145986     1.807252    -0.671045     117.96
 O      -5.033866     0.758734    -0.270287     338.34
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 H      -4.533535    -0.076059    -0.591646      28.28
 H      -3.697269     1.652229    -1.514232      33.46
 H      -4.779230     2.635313    -0.468213      27.68
 C       1.292763     1.417506    -1.215688      33.90
 H       1.948649     2.275803    -1.237968      25.34
 C       0.896168    -1.033041    -1.366619      67.46
 H       1.062300    -2.284723    -1.740419      20.53
 C      -0.389932    -0.828554    -0.817910       7.60
 O      -1.327624    -1.834545    -0.509975     170.62
 C      -0.766661    -3.321087    -0.594364      80.54
 H       0.196946    -3.667760    -0.078857      26.27
 H      -1.790153    -4.168763    -0.365032      24.21
 H      -0.791884    -3.520933    -1.590137      28.30
 C      -0.837839     0.520736    -0.500510      27.25
 O      -2.109029     0.598419     0.133947     179.76
 C      -0.122554     1.599317    -0.900752      56.38
 H      -0.402912     2.650615    -0.542302      26.42
 C       1.748878     0.065614    -1.598113      25.77
 C       3.195474    -0.064859    -2.111447      93.53
 H       3.256053    -0.608776    -3.255497      26.02
 O       3.927311     1.115763    -2.363369     180.16
 H       4.144889     1.356019    -1.545345      34.44
 C       4.113691    -1.058642    -1.033444      85.77
 H       3.595641    -2.133808    -1.058786      26.54
 O       5.535755    -1.053930    -1.400826     198.53
 H       5.844103    -1.909577    -0.929953      28.45
 C       3.952835    -0.563077     0.470848     103.14
 O       4.424674     0.961968     0.495570     146.49
 H       3.924804     1.446863     1.232548      27.72
 H       4.493244    -1.158972     1.057655      32.70
 H       2.981175    -0.447743     1.011651      29.77
55
name = lig-Water-frame_864
 C      -1.291525     3.930355     2.615713      54.31
 H      -1.833469     4.646062     2.050988      24.79
 C      -1.136000     1.695215     3.221542      67.37
 H      -1.402510     0.720277     2.841167      25.82
 C      -0.161483     1.924687     4.152934      -6.41
 O       0.694653     0.920934     4.809005      43.47
 C       0.576137    -0.510110     4.685614     118.42
 H       0.965256    -0.806548     5.620102      29.70
 H       0.947018    -0.668973     3.560298      28.78
 H      -0.601784    -0.788033     4.789476      26.35
 C       0.255726     3.310360     4.257614      18.03
 O       1.252291     3.556026     5.346885     169.64
 H       1.329547     4.567644     5.507944      20.27
 C      -0.344297     4.277605     3.502608      65.74
 H      -0.167821     5.446128     3.484215      15.58
 C      -1.895772     2.644401     2.585585      35.38
 C      -3.156195     2.362315     1.692098      75.61
 H      -3.684297     3.499753     1.625229      25.20
 O      -4.075688     1.471007     2.450135     222.83
 H      -4.617169     1.243808     1.765257      30.91
 C      -2.868998     1.927990     0.269789     109.48
 H      -2.303220     2.610291    -0.283236      25.04
 C      -4.103950     1.879599    -0.690265      72.27
 O      -4.991152     0.705486    -0.267129     332.62
 H      -4.517598    -0.062029    -0.485313      29.31
 H      -3.877203     1.395884    -1.901340      21.73
 H      -4.797002     2.777592    -0.583224      25.46
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 C       1.312002     1.400264    -1.186058      65.72
 H       2.183513     2.015684    -1.635899      26.45
 C       0.859169    -1.085440    -1.399618      47.88
 H       1.190485    -2.004640    -1.402738      20.69
 C      -0.431422    -0.747058    -0.786570      18.39
 O      -1.273208    -1.872837    -0.529524     196.54
 C      -0.824212    -3.295223    -0.555751     102.48
 H       0.054701    -3.517085    -0.005114      30.11
 H      -1.561014    -3.942330    -0.128376      27.55
 H      -0.433157    -3.708478    -1.679216      24.98
 C      -0.901426     0.524823    -0.535611      28.54
 O      -2.104227     0.545406     0.147844     188.77
 C      -0.023998     1.567549    -0.851713      61.52
 H      -0.724051     2.495852    -0.741979      22.16
 C       1.723902     0.051858    -1.532272      26.81
 C       3.250872    -0.092024    -2.184325      92.21
 H       3.229975    -0.688906    -3.056541      29.80
 O       3.914527     1.121551    -2.380511      58.01
 H       4.217237     1.478719    -1.328144      22.90
 C       4.108352    -1.065252    -1.049892      89.11
 H       3.666680    -2.055223    -1.059208      28.14
 O       5.561064    -1.102984    -1.422345     208.48
 H       5.834187    -1.986922    -1.054035      28.16
 C       3.899162    -0.567194     0.488056      77.32
 O       4.412969     0.905262     0.460185     145.24
 H       3.857183     1.534291     1.024256      28.59
 H       4.676710    -1.245273     1.213817      26.27
 H       2.945972    -0.364554     1.032382      26.72
55
name = lig-Water-frame_865
 C      -1.308282     3.954669     2.532414      57.64
 H      -1.894175     4.607854     1.825508      23.09
 C      -1.159637     1.648789     3.274618      57.45
 H      -1.312021     0.617767     2.934115      26.64
 C      -0.130679     1.896179     4.204297      -5.63
 O       0.681388     0.897970     4.786726      81.15
 C       0.544037    -0.473012     4.665316     144.01
 H       1.097484    -1.061726     5.519492      29.09
 H       0.694601    -0.779770     3.677024      31.98
 H      -0.479424    -0.542643     4.677762      30.45
 C       0.300232     3.322778     4.276061      22.17
 O       1.246055     3.569670     5.279206     125.97
 H       1.109888     4.572178     5.271708      18.33
 C      -0.347932     4.321964     3.547581      68.33
 H      -0.353419     5.371213     3.611927      18.93
 C      -1.893749     2.691736     2.592469      28.88
 C      -3.131255     2.390820     1.737044      86.87
 H      -3.520987     3.300709     1.467135      30.64
 O      -4.070954     1.488048     2.418975     144.09
 H      -4.880040     1.201213     1.733898      22.70
 C      -2.826371     1.882800     0.258128      88.42
 H      -2.232905     2.909776     0.019401      23.54
 C      -4.086717     1.860635    -0.729764     101.69
 O      -4.951836     0.679015    -0.252933     334.29
 H      -4.441371    -0.199296    -0.472673      27.92
 H      -3.973808     1.756871    -1.677918      30.72
 H      -4.579830     2.830398    -0.832586      27.37
 C       1.365770     1.336478    -1.215772      63.60
 H       1.945546     2.024658    -1.802244      27.77
 C       0.806284    -1.035978    -1.389795      67.82
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 H       1.399945    -2.163888    -1.267391      21.09
 C      -0.436232    -0.792220    -0.789151      25.27
 O      -1.232749    -1.917408    -0.539384     212.97
 C      -0.817944    -3.238550    -0.572611      94.52
 H       0.023687    -3.210220     0.286377      28.15
 H      -1.790099    -3.866912     0.102234      24.09
 H      -0.438406    -3.636837    -1.395175      30.59
 C      -0.955935     0.504869    -0.562293      23.65
 O      -2.133090     0.532182     0.172578     171.72
 C       0.031232     1.586374    -0.786177      61.83
 H      -0.479234     2.508347    -0.926907      27.01
 C       1.734574     0.036638    -1.489226      25.17
 C       3.285640    -0.170741    -2.149308      79.54
 H       3.188484    -0.834814    -3.184462      27.71
 O       3.912476     1.150847    -2.358900      63.69
 H       4.223215     1.425711    -1.504805      29.84
 C       4.075551    -1.028684    -1.065281      93.51
 H       3.701757    -2.116240    -1.167323      28.77
 O       5.553145    -1.150618    -1.426890     162.59
 H       5.816393    -2.102929    -1.198942      26.73
 C       3.913165    -0.526248     0.498539     109.34
 O       4.409414     0.832835     0.416455     192.98
 H       3.819155     1.454744     0.897164      30.28
 H       4.514566    -1.039735     1.098497      32.57
 H       2.766273    -0.657695     0.815555      27.91
55
name = lig-Water-frame_866
 C      -1.369666     3.974328     2.472011      87.48
 H      -1.725059     4.807180     1.804995      27.24
 C      -1.191471     1.585792     3.327576      51.50
 H      -1.349165     0.483268     3.159629      24.64
 C      -0.088999     1.887179     4.204216      16.22
 O       0.705384     0.953513     4.786643     116.05
 C       0.462448    -0.463099     4.636758     127.04
 H       1.160193    -1.136184     5.151929      28.66
 H       0.764040    -1.045031     3.617087      28.24
 H      -0.687160    -0.710545     4.814405      25.53
 C       0.328706     3.269319     4.323182      16.66
 O       1.244356     3.594636     5.193915     175.67
 H       1.081796     4.568607     5.556505      20.69
 C      -0.369615     4.345784     3.536810     106.28
 H      -0.195999     5.531619     3.974181      15.52
 C      -1.871401     2.699248     2.586831      42.13
 C      -3.107831     2.362584     1.758760      71.49
 H      -3.668945     3.408867     1.388779      24.74
 O      -4.073742     1.518490     2.386734     167.94
 H      -4.853614     1.186401     1.826172      25.48
 C      -2.781247     1.877730     0.221953      94.61
 H      -2.106328     2.641147     0.088917      28.11
 C      -4.066543     1.803767    -0.703266      85.07
 O      -4.910903     0.685143    -0.242955     294.58
 H      -4.437707    -0.143371    -0.549107      28.55
 H      -3.663100     1.830907    -1.967918      24.92
 H      -4.570492     2.807179    -0.683166      26.34
 C       1.379736     1.288031    -1.276425      41.07
 H       1.740580     2.265190    -1.727538      23.63
 C       0.827322    -0.998232    -1.341074      64.57
 H       1.178554    -1.987646    -1.385690      22.89
 C      -0.439788    -0.899011    -0.816502      36.71
 O      -1.243725    -1.907809    -0.556159     239.09
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 C      -0.785198    -3.197200    -0.466854     110.33
 H      -0.102818    -3.202531     0.298833      31.36
 H      -1.750357    -3.652538    -0.178508      26.45
 H      -0.468416    -3.740446    -1.532815      26.01
 C      -0.945000     0.493453    -0.570577      22.76
 O      -2.174139     0.562866     0.192354     167.47
 C       0.030980     1.579281    -0.727160      61.35
 H      -0.033828     2.773493    -1.011951      24.58
 C       1.797754    -0.011776    -1.494006      43.88
 C       3.283887    -0.255449    -2.060711      75.31
 H       3.228406    -0.634597    -3.104776      29.15
 O       3.899406     1.152491    -2.348726      49.88
 H       4.287689     1.409867    -1.461504      27.31
 C       4.056139    -1.016535    -1.068704     106.26
 H       3.647107    -2.064493    -1.206764      28.33
 O       5.524223    -1.180817    -1.433189     154.01
 H       5.693651    -2.152222    -1.189007      27.23
 C       3.903042    -0.491480     0.419509     112.09
 O       4.405546     0.781727     0.381461     229.98
 H       3.780129     1.374597     0.908666      26.97
 H       4.583291    -1.165488     1.243107      26.67
 H       2.889077    -0.766863     0.597499      27.68
55
name = lig-Water-frame_867
 C      -1.374622     4.036635     2.502269      36.92
 H      -1.675018     4.865650     1.906937      26.98
 C      -1.210537     1.566633     3.381644      71.09
 H      -1.555112     0.576289     3.329370      27.92
 C      -0.079849     1.901339     4.137441      26.82
 O       0.757442     0.990603     4.805386     146.02
 C       0.352933    -0.502050     4.562243     118.13
 H       1.166989    -0.965965     5.215657      27.49
 H       0.629445    -0.767539     3.606175      28.47
 H      -0.520400    -0.893152     5.037054      28.13
 C       0.254155     3.249222     4.290389      14.97
 O       1.292402     3.640590     5.164893     248.17
 H       1.089334     4.422317     5.759338      22.83
 C      -0.386833     4.325674     3.526219      19.24
 H      -0.054716     5.173372     3.847276      13.91
 C      -1.855786     2.625528     2.575864      18.36
 C      -3.122434     2.351408     1.694412      89.83
 H      -3.615515     3.245231     1.631494      26.01
 O      -4.079186     1.546954     2.389431     252.65
 H      -4.676303     1.261088     1.735146      31.02
 C      -2.760420     1.873088     0.219816      89.29
 H      -1.847332     2.502622    -0.269434      23.77
 C      -4.006209     1.773400    -0.697320     110.42
 O      -4.866493     0.712992    -0.254283     340.56
 H      -4.519702    -0.072984    -0.600418      31.19
 H      -3.564021     1.607350    -1.556188      30.68
 H      -4.701670     2.586161    -0.403084      25.43
 C       1.325560     1.283925    -1.333574      58.19
 H       1.856446     2.257483    -1.480956      22.05
 C       0.880620    -1.002019    -1.286110      35.49
 H       1.122875    -2.196295    -1.590627      20.68
 C      -0.444598    -0.886813    -0.847355      22.41
 O      -1.306853    -1.867639    -0.576937     231.89
 C      -0.743136    -3.204729    -0.404794      94.34
 H       0.070206    -3.447039     0.454075      25.92
 H      -1.902022    -3.878630    -0.213276      23.48
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 H      -0.512993    -3.611715    -1.301139      28.89
 C      -0.899005     0.481949    -0.543631      22.35
 O      -2.187120     0.591343     0.190212     182.83
 C       0.048883     1.559266    -0.724501      76.10
 H      -0.029515     2.558368    -0.692921      27.73
 C       1.883457    -0.032924    -1.533679      47.73
 C       3.252301    -0.239262    -1.984144      90.22
 H       3.270862    -0.688516    -3.069517      28.24
 O       3.873391     1.115251    -2.328020       8.32
 H       4.376986     1.445617    -1.376081      23.65
 C       4.082189    -1.062080    -1.052435     115.25
 H       3.536702    -2.050346    -1.067588      28.41
 O       5.477053    -1.197321    -1.447536     204.70
 H       5.651993    -2.094439    -1.029904      27.55
 C       3.938054    -0.559987     0.319236     115.12
 O       4.396211     0.789134     0.368698     200.50
 H       3.851332     1.374245     0.943613      26.87
 H       4.374104    -1.154993     1.018946      29.61
 H       2.738442    -0.583623     0.617261      24.16
55
name = lig-Water-frame_868
 C      -1.350188     4.040996     2.606697      36.14
 H      -1.849426     4.852329     1.936787      24.61
 C      -1.246731     1.607404     3.391943      67.59
 H      -1.776497     0.624048     3.464019      29.61
 C      -0.061256     1.910303     4.079301       4.58
 O       0.776122     0.993078     4.815210      89.09
 C       0.315929    -0.521059     4.539604      96.17
 H       1.149206    -0.793633     5.224050      26.03
 H       0.342061    -0.518097     3.340112      25.08
 H      -0.607487    -0.883045     5.097325      26.15
 C       0.168118     3.290847     4.240937      17.44
 O       1.357150     3.656550     5.152995      70.23
 H       0.958993     4.521501     5.621979      24.09
 C      -0.406912     4.229093     3.504825      10.64
 H       0.211050     5.377099     3.597896      23.31
 C      -1.841252     2.566048     2.552294     -34.80
 C      -3.089024     2.349360     1.627010      80.95
 H      -3.586394     3.464517     1.709664      23.68
 O      -4.092619     1.566963     2.401928     179.03
 H      -4.646387     1.177196     1.509258      25.33
 C      -2.719721     1.899698     0.220982     112.59
 H      -2.188253     2.525874    -0.406000      29.03
 C      -3.959615     1.767915    -0.617049      87.19
 O      -4.833773     0.726956    -0.267208     244.89
 H      -4.631051    -0.221273    -0.658193      25.48
 H      -3.528367     1.442102    -1.825236      24.94
 H      -4.661775     2.629282    -0.545100      25.62
 C       1.285843     1.290353    -1.366210      50.69
 H       2.073312     2.043362    -1.362588      26.36
 C       0.955623    -1.092087    -1.253759     113.33
 H       1.096469    -2.065099    -1.759468      28.04
 C      -0.428249    -0.774458    -0.866048       0.49
 O      -1.378028    -1.855457    -0.584820     182.28
 C      -0.766670    -3.245870    -0.319512      92.55
 H      -0.042478    -3.422815     0.376500      31.08
 H      -1.553420    -3.964124    -0.164149      27.93
 H      -0.294427    -3.605050    -1.399076      25.29
 C      -0.853025     0.471592    -0.483644      30.94
 O      -2.150464     0.578363     0.170700     186.81
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 C       0.068919     1.485308    -0.755078      58.70
 H      -0.338431     2.549413    -0.192713      24.76
 C       1.863898     0.002046    -1.555823      30.20
 C       3.256775    -0.170196    -1.992189     122.33
 H       3.281728    -0.890166    -2.908265      29.60
 O       3.860101     1.062141    -2.280116     105.12
 H       4.207110     1.374289    -1.541744      33.29
 C       4.097697    -1.137355    -1.052023     120.95
 H       3.503447    -2.128184    -0.926378      30.26
 O       5.424393    -1.217888    -1.463734     190.10
 H       5.822526    -1.999633    -0.907840      26.09
 C       3.911667    -0.611404     0.268836     105.53
 O       4.406937     0.827181     0.365663     130.87
 H       3.877421     1.360114     1.009042      29.29
 H       4.460154    -1.368020     1.092200      27.74
 H       2.952273    -0.455206     0.545676      30.62
55
name = lig-Water-frame_869
 C      -1.416565     3.943944     2.653216      53.16
 H      -1.893046     4.670501     2.113977      26.02
 C      -1.293301     1.644788     3.370476      59.48
 H      -1.721311     0.690823     3.551856      31.24
 C      -0.032829     1.916382     4.070471      -2.67
 O       0.736426     0.987332     4.798694     138.88
 C       0.320812    -0.481375     4.533363     116.16
 H       1.182318    -1.062624     4.914315      27.68
 H       0.082227    -0.587931     3.514628      28.58
 H      -0.702162    -0.642938     4.942257      26.55
 C       0.208713     3.280109     4.271669      11.21
 O       1.368987     3.667136     5.125728      26.50
 H       1.106885     4.605592     5.359397      25.51
 C      -0.358732     4.277699     3.486250      47.73
 H       0.055190     5.112410     3.326244      29.86
 C      -1.831730     2.594094     2.518816      22.04
 C      -3.029897     2.408686     1.640465      89.66
 H      -3.395816     3.334876     1.427407      29.14
 O      -4.119420     1.585523     2.352726     188.01
 H      -4.617944     1.063761     1.770020      32.71
 C      -2.713661     1.908932     0.211324      78.08
 H      -2.274250     2.894799    -0.364339      26.81
 C      -3.928971     1.750786    -0.624145     122.29
 O      -4.831423     0.706254    -0.261792     280.99
 H      -4.654646    -0.186644    -0.665065      28.04
 H      -3.754605     1.640918    -1.590648      30.40
 H      -4.378447     2.763615    -0.856570      27.04
 C       1.301698     1.299314    -1.376723      63.98
 H       2.175945     2.056363    -1.331928      26.86
 C       0.990491    -1.135891    -1.254615     114.60
 H       1.206884    -2.165491    -1.788521      26.46
 C      -0.389315    -0.772548    -0.867393      -5.85
 O      -1.417612    -1.856221    -0.582888     141.11
 C      -0.782525    -3.260997    -0.330014      67.83
 H       0.023485    -3.137292     0.598488      26.97
 H      -1.687301    -4.081284    -0.080489      24.76
 H      -0.161359    -3.507954    -1.147548      27.31
 C      -0.829308     0.471258    -0.416570      29.78
 O      -2.070262     0.555687     0.146958     155.96
 C       0.032020     1.482422    -0.737813      69.53
 H      -0.221096     2.200413    -0.127624      31.48
 C       1.749056     0.019422    -1.560104      22.40
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 C       3.277247    -0.172399    -2.033031     114.33
 H       3.238272    -0.819402    -2.979951      30.60
 O       3.862941     1.015826    -2.269360      45.67
 H       4.165411     1.438463    -1.253406      21.81
 C       4.047000    -1.194106    -1.067529     121.84
 H       3.599371    -2.195065    -1.057014      30.72
 O       5.400251    -1.245062    -1.483916     234.91
 H       5.907228    -1.907198    -0.996477      28.36
 C       3.932829    -0.629160     0.332795      91.36
 O       4.437169     0.857256     0.363625     156.63
 H       3.868443     1.304573     1.065652      29.43
 H       4.446697    -1.229738     1.026010      30.84
 H       2.704536    -0.535320     0.578036      27.89
55
name = lig-Water-frame_870
 C      -1.479867     3.848627     2.683336      52.86
 H      -2.013259     4.702375     2.113592      22.35
 C      -1.275771     1.658780     3.364330      68.06
 H      -1.640567     0.652797     3.474177      31.03
 C      -0.051616     1.920392     4.080013      13.59
 O       0.677290     0.959922     4.766280     181.15
 C       0.323387    -0.401534     4.542114     133.26
 H       1.003418    -1.350978     4.532514      26.59
 H       0.050509    -0.694747     3.417975      29.40
 H      -0.612664    -0.515262     5.055372      26.45
 C       0.350035     3.277276     4.326921      13.85
 O       1.346616     3.662883     5.079063       1.61
 H       1.353495     4.675467     5.307369      29.88
 C      -0.330257     4.301971     3.459970      44.03
 H       0.149683     5.480843     3.205235      23.56
 C      -1.853758     2.635622     2.506547      52.41
 C      -2.997502     2.419294     1.655810      75.05
 H      -3.453779     3.463002     1.205131      24.43
 O      -4.127294     1.636364     2.303910     155.49
 H      -4.657492     0.969671     1.721884      27.34
 C      -2.701845     1.922944     0.187292      77.41
 H      -2.138356     2.767634    -0.058600      28.53
 C      -3.940448     1.749788    -0.664074      93.73
 O      -4.855630     0.685800    -0.238392     291.93
 H      -4.516636    -0.075290    -0.709731      29.70
 H      -3.564561     1.576285    -1.917421      26.05
 H      -4.330584     2.767310    -0.759561      26.69
 C       1.319148     1.331916    -1.340874      62.05
 H       1.929448     2.165705    -1.421411      30.10
 C       0.939125    -1.135933    -1.283598     103.65
 H       1.394782    -2.200546    -1.566503      24.95
 C      -0.361802    -0.915142    -0.844706       8.61
 O      -1.414800    -1.864082    -0.587578     196.18
 C      -0.776473    -3.218766    -0.306585      79.57
 H      -0.347248    -2.919676     0.562260      31.41
 H      -1.770006    -3.906401    -0.151073      25.69
 H      -0.083079    -3.594887    -1.149288      25.50
 C      -0.792435     0.436549    -0.393932      23.57
 O      -1.995808     0.561944     0.138815     149.82
 C       0.026540     1.509044    -0.710082      41.22
 H      -0.041279     2.592795    -0.048381      28.97
 C       1.691703    -0.009834    -1.588268      34.88
 C       3.234564    -0.267705    -2.070487      90.56
 H       3.166421    -0.558859    -3.217351      27.81
 O       3.915616     1.021449    -2.247463      67.82
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 H       3.981994     1.294980    -1.294683      29.94
 C       3.981861    -1.202031    -1.075909     100.08
 H       3.589610    -2.300418    -1.275613      25.68
 O       5.396473    -1.251061    -1.522684     184.05
 H       5.826681    -2.057862    -1.084825      28.11
 C       3.908219    -0.595832     0.408129     106.86
 O       4.459453     0.855261     0.369251     127.19
 H       3.936128     1.335307     1.045959      30.42
 H       4.568378    -1.185568     1.253927      29.05
 H       2.953521    -0.724107     0.655156      32.34
55
name = lig-Water-frame_871
 C      -1.459452     3.945887     2.719950      38.38
 H      -2.045896     4.648133     2.158306      23.06
 C      -1.214428     1.648505     3.360058      97.82
 H      -1.558277     0.580659     3.232297      31.33
 C      -0.099920     1.946250     4.097261       2.39
 O       0.653765     0.928673     4.737423     225.22
 C       0.275548    -0.380833     4.489733     136.97
 H       1.012390    -1.136866     4.650434      30.19
 H      -0.024270    -0.440978     3.464049      30.00
 H      -0.489598    -0.669190     5.332629      26.34
 C       0.414009     3.334678     4.260847      12.24
 O       1.386341     3.653939     5.072724      28.88
 H       1.322873     4.582103     5.351607      29.11
 C      -0.297005     4.296492     3.430583      43.61
 H      -0.007010     5.260257     3.453026      29.79
 C      -1.905074     2.570839     2.545946     -42.47
 C      -3.065825     2.400307     1.595657      95.59
 H      -3.449664     3.348129     1.468740      28.14
 O      -4.127359     1.702127     2.269094     189.99
 H      -4.509810     1.107996     1.450937      24.35
 C      -2.671034     1.888046     0.196092      81.51
 H      -1.799497     2.619208    -0.148531      27.31
 C      -3.941991     1.759397    -0.768289     100.00
 O      -4.871182     0.683135    -0.226326     269.19
 H      -4.385091    -0.128877    -0.698273      27.18
 H      -3.486053     1.440929    -1.601164      30.00
 H      -4.600934     2.657398    -0.564661      24.77
 C       1.292322     1.332184    -1.277907     -14.83
 H       1.802992     2.349478    -1.647355      27.18
 C       0.873912    -1.145114    -1.321539      80.05
 H       1.369982    -2.113378    -1.372625      27.29
 C      -0.400042    -1.040787    -0.784224      22.05
 O      -1.375779    -1.881240    -0.616180     242.19
 C      -0.809452    -3.138322    -0.299242     114.62
 H      -0.406322    -3.003615     0.839602      27.43
 H      -1.749280    -3.821399    -0.220487      26.94
 H      -0.148084    -3.714323    -1.044425      28.06
 C      -0.712207     0.383326    -0.424790       4.97
 O      -1.968390     0.585378     0.159676     157.04
 C       0.077462     1.587019    -0.646673      59.86
 H       0.002873     2.575754    -0.434813      30.38
 C       1.724616    -0.017110    -1.635763      11.08
 C       3.145267    -0.330070    -2.132384     100.54
 H       3.152621    -0.640635    -3.170008      28.14
 O       3.967112     1.020567    -2.225260      41.69
 H       4.023306     1.331757    -1.274771      29.42
 C       3.956019    -1.203051    -1.099158      99.74
 H       3.518456    -2.140635    -1.178123      30.11
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 O       5.390108    -1.255418    -1.553106     190.77
 H       5.582696    -2.206694    -1.254548      28.20
 C       3.934291    -0.569271     0.460557     101.15
 O       4.456275     0.820650     0.384575     134.01
 H       4.000598     1.451654     1.020523      30.23
 H       4.610193    -1.059908     1.181260      31.16
 H       2.785654    -0.716699     0.965770      29.52
55
name = lig-Water-frame_872
 C      -1.439242     4.022875     2.732892      19.42
 H      -2.006695     4.808648     2.206966      20.92
 C      -1.188884     1.604319     3.307624      91.69
 H      -1.406309     0.611947     3.096299      32.15
 C      -0.101106     1.999066     4.140715     -43.51
 O       0.661963     0.945325     4.720185      17.91
 C       0.196033    -0.416791     4.468370     121.19
 H       1.293387    -0.791022     4.805113      28.99
 H      -0.246390    -0.400632     3.426445      29.65
 H      -0.421592    -0.815318     5.214553      34.78
 C       0.377100     3.352125     4.107558      51.08
 O       1.480620     3.644793     5.101333     261.13
 H       1.150532     4.551698     5.529673      12.11
 C      -0.276472     4.255714     3.427577      48.32
 H       0.000136     5.445585     3.696563      20.54
 C      -1.926861     2.565444     2.618809     -79.70
 C      -3.116855     2.372399     1.558792      84.86
 H      -3.481367     3.523298     1.545557      22.96
 O      -4.143649     1.736683     2.214931     222.92
 H      -4.530100     1.285939     1.493431      32.17
 C      -2.613916     1.854829     0.190538     102.77
 H      -1.930733     2.474007    -0.349135      29.09
 C      -3.947651     1.773482    -0.778857      77.32
 O      -4.851251     0.673700    -0.243811     273.43
 H      -4.517257    -0.220062    -0.406700      30.62
 H      -3.489309     1.358929    -1.893387      25.88
 H      -4.711729     2.563742    -0.755260      25.18
 C       1.303560     1.325695    -1.264819      49.18
 H       1.778693     2.076360    -1.743728      30.63
 C       0.848179    -1.140540    -1.369310      71.10
 H       1.361354    -2.284331    -1.291447      20.98
 C      -0.413563    -0.983691    -0.728668      30.15
 O      -1.355557    -1.924977    -0.654809     279.88
 C      -0.861847    -3.110123    -0.225112     136.51
 H      -0.412068    -3.327094     0.709515      32.49
 H      -1.829361    -3.924730    -0.323649      26.97
 H      -0.172830    -3.582043    -0.932142      30.53
 C      -0.661143     0.377473    -0.448530      17.97
 O      -1.970468     0.586663     0.199279     180.67
 C       0.144525     1.571023    -0.602098      59.52
 H      -0.259440     2.744738    -0.584090      26.95
 C       1.742473    -0.001180    -1.662532      32.27
 C       3.091315    -0.304525    -2.157994      88.16
 H       3.222311    -1.005781    -3.169380      27.04
 O       3.994379     0.990112    -2.227118     -13.94
 H       4.174635     1.372163    -1.175028      24.92
 C       3.957602    -1.158629    -1.111467      90.33
 H       3.415792    -2.230534    -0.885858      27.76
 O       5.349887    -1.281477    -1.564142     187.63
 H       5.555677    -2.222336    -1.456721      29.53
 C       3.923790    -0.544168     0.478027     105.95
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 O       4.438399     0.784027     0.408806     154.53
 H       3.972033     1.455152     0.991676      30.49
 H       4.740493    -1.193990     1.110669      29.27
 H       3.075681    -0.487543     0.989959      31.56
55
name = lig-Water-frame_873
 C      -1.464190     4.011589     2.715316      37.88
 H      -1.922240     4.983530     2.320504      21.03
 C      -1.176218     1.594161     3.245850      15.96
 H      -1.370539     0.492367     3.034879      27.59
 C      -0.090130     2.010784     4.150334      -2.74
 O       0.660007     1.009695     4.713654     -55.79
 C       0.192413    -0.453507     4.473029     118.51
 H       1.162218    -0.780738     4.510731      33.32
 H      -0.219265    -0.758596     3.450782      32.28
 H      -0.628474    -0.892264     5.188756      29.85
 C       0.412433     3.277195     4.058913      15.60
 O       1.541803     3.650897     5.107543     310.92
 H       1.092854     4.326439     5.700430      11.74
 C      -0.284721     4.341351     3.414324      38.23
 H       0.002545     5.334292     3.776277      18.10
 C      -1.929545     2.663366     2.660123      16.42
 C      -3.083542     2.432537     1.577334      91.40
 H      -3.365252     3.400159     1.240342      31.24
 O      -4.185308     1.731622     2.170641     143.28
 H      -4.932342     1.237210     1.497914      23.70
 C      -2.615836     1.832816     0.142782      98.52
 H      -2.100314     2.700158    -0.432044      30.54
 C      -3.925584     1.710237    -0.788981     106.89
 O      -4.829982     0.670479    -0.261492     297.12
 H      -4.497507    -0.241655    -0.230271      31.23
 H      -3.822215     1.590169    -1.840012      29.39
 H      -4.535092     2.634527    -1.030611      27.57
 C       1.362790     1.286251    -1.305625      48.82
 H       2.061307     2.094851    -1.821044      27.84
 C       0.876699    -1.139679    -1.395346      46.97
 H       1.182456    -2.094974    -1.501350      23.07
 C      -0.357366    -0.843200    -0.722623      19.28
 O      -1.368889    -1.939223    -0.677776     244.64
 C      -0.928630    -3.217248    -0.173344     108.29
 H      -0.423882    -3.332027     0.891615      29.37
 H      -1.802413    -3.891672    -0.324185      27.52
 H      -0.067043    -3.452108    -0.976232      26.84
 C      -0.697692     0.442937    -0.413210      30.22
 O      -1.970688     0.559477     0.244305     203.32
 C       0.175617     1.528662    -0.573566      71.79
 H      -0.451399     2.390927    -0.610609      32.61
 C       1.694339    -0.012891    -1.654361      35.96
 C       3.141709    -0.269609    -2.156755     112.28
 H       3.181417    -0.875609    -2.980111      32.40
 O       3.999043     0.946609    -2.243907     108.79
 H       4.209565     1.101347    -1.405744      35.18
 C       3.926819    -1.128594    -1.061406     110.59
 H       3.575683    -2.040473    -0.848060      33.81
 O       5.285284    -1.311061    -1.567278     181.55
 H       5.619958    -2.254501    -1.546736      27.29
 C       3.967501    -0.536640     0.446307     119.61
 O       4.436306     0.783869     0.437754     108.77
 H       3.843157     1.324793     0.987966      31.41
 H       4.632673    -1.340205     0.865662      31.07
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 H       2.909976    -0.453199     1.080296      29.58
55
name = lig-Water-frame_874
 C      -1.473572     4.031524     2.712033      48.77
 H      -2.003940     4.842085     2.354992      25.17
 C      -1.169758     1.640763     3.200035      54.50
 H      -1.435784     0.628768     3.037877      28.45
 C      -0.108659     1.946853     4.077760     -28.49
 O       0.643827     1.045578     4.717979       0.09
 C       0.199263    -0.487472     4.481004     101.76
 H       1.176977    -1.196305     4.403694      27.85
 H      -0.088259    -0.843878     3.474018      31.13
 H      -0.529658    -0.715640     5.193023      30.42
 C       0.493381     3.270594     4.091298     -17.26
 O       1.560540     3.640244     5.079600     147.32
 H       1.167476     4.261606     5.724559      15.96
 C      -0.292358     4.388193     3.426709      39.76
 H       0.043324     5.490369     3.671258      16.36
 C      -1.940768     2.745433     2.642139      49.24
 C      -3.024491     2.485562     1.576214      69.22
 H      -3.389305     3.483256     1.043152      28.68
 O      -4.247736     1.706266     2.146686     139.92
 H      -4.864077     1.455858     1.489045      31.75
 C      -2.671304     1.840941     0.083798      88.61
 H      -2.169334     2.755007    -0.293449      30.35
 C      -3.918542     1.632472    -0.783789     109.61
 O      -4.831427     0.681134    -0.274965     268.48
 H      -4.238643    -0.188940    -0.251884      28.59
 H      -3.737790     1.445724    -2.004312      26.41
 H      -4.295209     2.679953    -0.815152      28.31
 C       1.419249     1.280932    -1.362369      56.58
 H       2.128286     2.032816    -1.561427      25.65
 C       0.883255    -1.084354    -1.381666      29.56
 H       1.076311    -2.232807    -1.958429      21.48
 C      -0.306159    -0.806207    -0.759008      15.76
 O      -1.377436    -1.902268    -0.675270     195.58
 C      -0.916359    -3.324905    -0.153973      87.32
 H      -0.702182    -3.097873     0.893832      27.93
 H      -1.983863    -4.017546    -0.378419      24.85
 H      -0.170946    -3.654754    -0.760556      30.05
 C      -0.770374     0.511853    -0.332561      38.77
 O      -1.961803     0.546211     0.278646     213.77
 C       0.193601     1.470901    -0.588967      70.57
 H      -0.371680     2.497266    -0.519342      31.15
 C       1.694372    -0.045502    -1.653302      45.33
 C       3.219538    -0.238587    -2.089141      99.20
 H       3.141253    -0.767730    -3.241425      27.12
 O       3.979386     0.894275    -2.305179      77.10
 H       4.389352     1.017969    -1.258671      26.76
 C       3.892080    -1.089927    -0.995505     117.09
 H       3.430845    -2.223819    -0.936922      26.20
 O       5.233577    -1.328046    -1.573551     152.21
 H       5.507156    -2.273883    -1.417239      29.30
 C       3.964038    -0.559130     0.389475     124.19
 O       4.457484     0.816614     0.476958     152.17
 H       3.712507     1.303039     0.978856      27.93
 H       4.666587    -1.368829     0.923713      28.22
 H       3.054224    -0.729894     0.814674      31.96
55
name = lig-Water-frame_875
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 C      -1.447757     4.099623     2.740011      31.88
 H      -2.224137     4.826352     2.228908      20.90
 C      -1.194469     1.730945     3.158313     107.30
 H      -1.592415     0.707958     3.021029      29.88
 C      -0.097385     1.916901     3.963425     -98.81
 O       0.630681     0.996915     4.726901      49.96
 C       0.270262    -0.519774     4.476612     100.89
 H       0.996898    -1.254660     4.757625      28.57
 H      -0.190194    -0.528673     3.385444      29.97
 H      -0.476295    -0.606681     5.332654      27.70
 C       0.524197     3.355399     4.139270     -14.82
 O       1.550616     3.605329     5.022039      12.28
 H       1.266934     4.427487     5.613312      18.67
 C      -0.262979     4.369894     3.489544      59.47
 H       0.045112     5.507818     3.336220      19.72
 C      -1.948896     2.755751     2.575974      46.02
 C      -3.030891     2.516257     1.524171      70.02
 H      -3.464560     3.504272     1.330899      29.99
 O      -4.268169     1.709138     2.153218     102.76
 H      -4.794005     1.573133     1.267906      28.13
 C      -2.725141     1.846351     0.091266      82.12
 H      -1.997291     2.590021    -0.355922      30.18
 C      -3.901358     1.600640    -0.814178     116.02
 O      -4.833372     0.671848    -0.286898     310.33
 H      -4.242443    -0.068179    -0.315821      33.53
 H      -3.462051     1.215957    -1.740684      29.59
 H      -4.338381     2.589203    -0.598534      28.13
 C       1.408812     1.270276    -1.362970      45.47
 H       2.173008     2.117328    -1.355760      26.50
 C       0.865439    -1.101460    -1.402411      64.18
 H       0.933589    -1.852718    -1.984151      29.50
 C      -0.352047    -0.847976    -0.780015      10.69
 O      -1.353991    -1.854925    -0.666103     178.10
 C      -0.959148    -3.359335    -0.158581      84.67
 H      -0.876552    -3.111062     0.902119      27.11
 H      -1.815613    -3.905880    -0.342075      27.91
 H      -0.011458    -4.071945    -0.621873      24.61
 C      -0.760711     0.487423    -0.285388      42.22
 O      -1.977428     0.571606     0.311987     217.06
 C       0.184021     1.491950    -0.641513      64.96
 H       0.226850     2.607150    -0.309884      29.38
 C       1.806891    -0.023123    -1.674040      50.43
 C       3.226830    -0.271254    -2.069094     118.46
 H       3.222077    -0.685286    -2.966946      32.00
 O       3.982389     0.876109    -2.331149     129.31
 H       4.487346     1.243830    -1.583095      30.68
 C       3.867707    -1.129712    -0.997488     140.59
 H       3.265090    -1.952531    -1.018313      33.87
 O       5.202685    -1.347839    -1.576273     188.75
 H       5.386338    -2.217830    -1.181892      31.25
 C       3.985413    -0.614978     0.346743     105.79
 O       4.464862     0.844868     0.524664     165.69
 H       3.743748     1.409579     0.891287      31.37
 H       4.715117    -1.103762     1.085266      27.95
 H       2.879492    -0.865710     0.772306      27.46
55
name = lig-Water-frame_876
 C      -1.456211     4.134059     2.758802      54.72
 H      -1.956891     4.912029     2.289419      31.99
 C      -1.238930     1.775520     3.117996      65.16
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 H      -1.719663     0.779207     3.031279      32.37
 C      -0.009662     1.964282     3.886950    -141.31
 O       0.623502     0.916951     4.720798      93.65
 C       0.295988    -0.495810     4.496412     122.60
 H       1.152107    -1.145970     4.946235      25.19
 H      -0.138734    -0.454172     3.572942      26.93
 H      -0.542411    -0.652602     5.191605      25.73
 C       0.468778     3.403115     4.157666       0.43
 O       1.533669     3.584932     4.972665      66.23
 H       1.465817     4.493803     5.300252      27.08
 C      -0.238772     4.366478     3.523209      89.82
 H       0.130835     5.362998     3.345760      26.29
 C      -1.930032     2.794196     2.481608     -35.29
 C      -3.094711     2.522075     1.493429      81.25
 H      -3.562451     3.577995     1.490251      27.02
 O      -4.254878     1.735482     2.153329     108.14
 H      -4.775987     1.479709     1.224802      24.74
 C      -2.710689     1.862574     0.159950      95.49
 H      -1.937795     2.332329    -0.525042      29.33
 C      -3.873815     1.614854    -0.809573     102.11
 O      -4.839945     0.645592    -0.299809     238.83
 H      -4.437173    -0.280152    -0.299352      30.38
 H      -3.348623     1.213161    -1.798382      28.43
 H      -4.577886     2.538126    -0.964504      26.54
 C       1.389990     1.260251    -1.323482      78.19
 H       2.077463     2.131076    -1.265785      32.95
 C       0.858820    -1.062856    -1.431213     119.63
 H       0.905270    -2.130164    -2.198065      23.88
 C      -0.436888    -0.895561    -0.781641      16.89
 O      -1.312651    -1.841805    -0.659258     195.19
 C      -0.955373    -3.341019    -0.174537      76.32
 H      -0.904973    -3.275562     0.989568      27.17
 H      -2.109052    -3.908514    -0.493174      24.61
 H      -0.183660    -3.874816    -0.417860      29.53
 C      -0.684901     0.428481    -0.287501      -4.63
 O      -2.010413     0.610190     0.353829     155.29
 C       0.187129     1.553263    -0.682081      49.98
 H       0.415873     2.493326    -0.125403      34.47
 C       1.880349     0.015374    -1.675894      39.85
 C       3.211921    -0.297317    -2.039733     112.20
 H       3.331961    -1.081364    -3.067752      28.78
 O       4.008409     0.905487    -2.376710      72.74
 H       4.463339     1.356216    -1.677792      32.11
 C       3.887629    -1.169871    -1.068231     122.68
 H       3.087211    -2.099735    -1.007610      29.72
 O       5.179867    -1.396208    -1.570419     171.71
 H       5.563479    -2.161848    -1.005339      27.37
 C       3.974804    -0.629382     0.395896     116.31
 O       4.459226     0.851282     0.558256     135.97
 H       3.731639     1.451014     0.859868      36.16
 H       4.705398    -1.106050     1.069537      31.14
 H       3.014836    -0.646783     0.829506      33.47
55
name = lig-Water-frame_877
 C      -1.449858     4.132385     2.767845      61.60
 H      -1.706046     5.185860     2.317419      24.20
 C      -1.239185     1.778875     3.108552      17.62
 H      -1.690194     0.812451     3.069208      30.71
 C       0.062623     2.020050     3.846808     -26.51
 O       0.623502     0.888581     4.697620      47.65
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 C       0.289817    -0.446335     4.563152     128.55
 H       1.300429    -0.912267     4.751615      26.21
 H       0.045739    -0.830551     3.378255      26.63
 H      -0.647493    -0.820630     5.066015      25.78
 C       0.391251     3.335709     4.160133      24.70
 O       1.527425     3.577859     4.928914     127.16
 H       1.682665     4.558676     5.090462      26.49
 C      -0.278719     4.391639     3.500562      52.27
 H       0.370543     5.477837     3.617403      23.34
 C      -1.902323     2.868934     2.392248       1.32
 C      -3.175338     2.551063     1.517024      97.18
 H      -3.625957     3.570980     1.256274      28.21
 O      -4.221552     1.763563     2.131070     173.44
 H      -4.757695     1.313415     1.518813      30.62
 C      -2.664412     1.889487     0.196922      94.80
 H      -2.048663     2.519072    -0.449892      29.46
 C      -3.869069     1.627526    -0.816086     103.35
 O      -4.850729     0.612949    -0.310442     251.09
 H      -4.641880    -0.388305    -0.363502      28.49
 H      -3.433583     1.323828    -1.836154      28.36
 H      -4.473767     2.353057    -1.348287      27.74
 C       1.406325     1.281463    -1.271554      58.34
 H       2.077620     2.121379    -1.351068      29.16
 C       0.857202    -1.044089    -1.517062      59.22
 H       0.992768    -1.921861    -1.869620      27.91
 C      -0.416031    -0.884197    -0.799607      16.20
 O      -1.302912    -1.904317    -0.644003     239.12
 C      -1.045312    -3.277323    -0.167662     109.32
 H      -0.924752    -3.311197     0.847424      30.44
 H      -1.829319    -3.709469    -0.536285      29.24
 H       0.075243    -3.723789    -0.680511      25.11
 C      -0.647066     0.418625    -0.298764     -16.36
 O      -2.014742     0.623166     0.399277     141.32
 C       0.174355     1.565989    -0.689209      38.57
 H       0.118480     2.418689     0.162595      31.68
 C       1.815458     0.008714    -1.651196      30.98
 C       3.254534    -0.328069    -2.096622     114.99
 H       3.259977    -0.929371    -2.848443      34.07
 O       4.034759     0.933662    -2.449516      29.43
 H       4.334592     1.334897    -1.434503      26.37
 C       3.900024    -1.229312    -1.078528     116.92
 H       3.382904    -2.124380    -0.963943      32.55
 O       5.182883    -1.478733    -1.560999     243.87
 H       5.781856    -2.021925    -1.023131      27.94
 C       3.962539    -0.579676     0.460379      96.33
 O       4.453984     0.835519     0.572434     130.65
 H       3.640597     1.340835     0.922527      31.95
 H       4.703049    -1.420346     1.003020      28.19
 H       2.966493    -0.503062     1.037059      29.83
55
name = lig-Water-frame_878
 C      -1.420249     4.209118     2.736277      60.15
 H      -1.757330     5.145135     2.290116      25.36
 C      -1.191269     1.814205     3.101061      29.90
 H      -1.588893     0.739888     3.091688      27.84
 C       0.034597     1.982492     3.820512      -4.22
 O       0.621911     0.945292     4.658358     100.43
 C       0.277426    -0.448874     4.545375     135.16
 H       1.257687    -0.910500     4.769268      26.34
 H       0.338657    -0.921753     3.613466      29.08
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 H      -0.572776    -0.917284     5.107519      25.92
 C       0.363208     3.288892     4.159045      15.90
 O       1.523260     3.566570     4.884642     122.39
 H       1.743992     4.547188     4.945752      27.03
 C      -0.291085     4.417374     3.502415      61.04
 H       0.124763     5.305828     3.755495      26.12
 C      -1.889137     2.891360     2.359851      -8.85
 C      -3.225095     2.596821     1.521983      94.32
 H      -3.661621     3.537817     1.013553      27.17
 O      -4.174928     1.798974     2.143845     130.75
 H      -4.757792     1.075995     1.536647      22.39
 C      -2.658378     1.924251     0.182759      78.15
 H      -2.110580     2.903610    -0.168736      27.55
 C      -3.867584     1.587534    -0.838567      85.84
 O      -4.873791     0.595816    -0.315045     295.92
 H      -4.541283    -0.250257    -0.624936      29.12
 H      -3.339571     1.139201    -1.824785      26.63
 H      -4.409802     2.497630    -1.314713      26.03
 C       1.437922     1.332303    -1.214576      39.00
 H       2.207349     2.161150    -1.524357      27.33
 C       0.823973    -1.001218    -1.568972      56.99
 H       1.259854    -2.212561    -1.767802      23.66
 C      -0.329940    -0.855360    -0.827917      11.66
 O      -1.321780    -1.959105    -0.630647     206.64
 C      -1.031120    -3.189710    -0.203265     101.08
 H      -0.929607    -3.313363     0.993741      25.38
 H      -1.957576    -3.999645    -0.772708      23.60
 H      -0.267655    -3.425886    -0.744930      30.33
 C      -0.686600     0.450627    -0.313768       5.28
 O      -1.968796     0.623136     0.433024     145.14
 C       0.133729     1.535415    -0.613940      50.52
 H      -0.188278     2.347380    -0.020920      30.98
 C       1.731348    -0.015725    -1.638356       6.82
 C       3.280440    -0.305288    -2.146399      82.41
 H       3.128262    -0.907232    -3.289489      26.97
 O       4.052516     0.936334    -2.476847      94.76
 H       4.182796     1.202461    -1.622593      35.12
 C       3.932901    -1.247359    -1.001045      89.48
 H       3.424884    -2.311968    -0.894633      27.35
 O       5.222110    -1.556834    -1.572535     223.55
 H       5.821394    -2.051257    -0.977567      28.32
 C       3.951361    -0.548515     0.510048     119.54
 O       4.441872     0.800256     0.575703     180.93
 H       3.710015     1.244778     1.044503      31.83
 H       4.553737    -1.333063     0.970756      31.11
 H       3.002805    -0.637283     1.101143      29.99
55
name = lig-Water-frame_879
 C      -1.405394     4.281345     2.657951      41.23
 H      -2.016268     5.088772     2.189477      22.98
 C      -1.162758     1.841546     3.059262      80.76
 H      -1.499130     0.858298     3.003404      28.21
 C      -0.047888     1.909385     3.826499     -37.05
 O       0.611275     1.028612     4.604382     175.56
 C       0.310311    -0.483706     4.524904      92.36
 H       1.154254    -0.957442     5.235583      22.13
 H       0.365788    -0.849021     3.340640      22.66
 H      -0.502952    -0.757531     5.180751      22.58
 C       0.378967     3.316745     4.128807      -1.85
 O       1.524286     3.540983     4.843378      93.29
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 H       1.615875     4.486114     4.895891      29.91
 C      -0.285646     4.369618     3.535624      61.82
 H      -0.118901     5.599048     3.946528      22.97
 C      -1.883830     2.898824     2.395852     -17.42
 C      -3.209460     2.622650     1.480087      85.30
 H      -3.700226     3.572800     1.035574      27.03
 O      -4.159485     1.812828     2.189540     179.80
 H      -4.399848     1.262178     1.452519      28.82
 C      -2.704772     1.970883     0.162642      79.01
 H      -2.087880     2.788913    -0.087077      26.09
 C      -3.849938     1.549168    -0.878893      88.86
 O      -4.878392     0.600843    -0.324168     298.77
 H      -4.479982    -0.170304    -0.873594      24.29
 H      -3.282955     0.898202    -1.631181      25.86
 H      -4.295328     2.503702    -0.998149      26.81
 C       1.445582     1.366371    -1.171071      55.93
 H       2.091323     2.098197    -1.480730      28.58
 C       0.803676    -1.068904    -1.601678      70.59
 H       1.243183    -1.940113    -1.707767      25.09
 C      -0.318312    -0.850320    -0.825453       8.18
 O      -1.363115    -1.896768    -0.640402     213.12
 C      -1.039953    -3.196009    -0.238077     120.86
 H      -0.928980    -3.303440     0.761975      30.28
 H      -1.676518    -3.856405    -0.543764      28.67
 H       0.029642    -3.605315    -0.887470      24.06
 C      -0.775654     0.453964    -0.333601      18.71
 O      -1.886375     0.640289     0.440987     159.72
 C       0.134739     1.497129    -0.516123      41.32
 H      -0.396737     2.630242    -0.420276      24.74
 C       1.742424     0.045583    -1.654676       1.80
 C       3.238744    -0.306626    -2.223721      80.48
 H       3.176493    -0.658829    -3.120433      30.78
 O       4.048145     0.895984    -2.486580      55.22
 H       4.277505     1.385059    -1.574867      29.66
 C       3.963568    -1.245067    -0.931690      80.37
 H       3.321537    -2.134618    -0.823264      28.32
 O       5.276915    -1.618692    -1.582214     194.16
 H       5.712724    -2.235460    -0.897132      27.60
 C       3.935259    -0.566223     0.509586     107.70
 O       4.425921     0.762398     0.578240     160.15
 H       3.827398     1.345309     1.171439      28.76
 H       4.726616    -1.230317     1.239534      27.16
 H       2.942896    -0.754882     0.981445      27.59
55
name = lig-Water-frame_880
 C      -1.409528     4.264903     2.571638      49.38
 H      -2.155211     5.095618     2.228537      20.95
 C      -1.189917     1.833543     2.980863      74.37
 H      -1.640850     0.800980     2.770284      23.68
 C      -0.107534     1.951698     3.866006      -3.80
 O       0.610589     1.059783     4.558928     103.57
 C       0.382680    -0.507961     4.519348     109.32
 H       1.020301    -0.845381     5.272371      27.46
 H       0.273969    -0.707975     3.551287      30.64
 H      -0.696158    -0.481214     4.981603      26.24
 C       0.396313     3.315698     4.062968      12.89
 O       1.535395     3.509429     4.814083     150.77
 H       1.520188     4.506737     5.020153      21.90
 C      -0.320050     4.412357     3.566547      68.97
 H      -0.198061     5.289270     3.915136      24.70
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 C      -1.881594     2.956626     2.440845      14.81
 C      -3.134196     2.636826     1.463553      83.07
 H      -3.652861     3.655578     1.257943      24.14
 O      -4.141626     1.829345     2.226129     119.27
 H      -4.381262     1.224889     1.458081      27.17
 C      -2.762212     1.965456     0.157670      62.90
 H      -1.937811     2.592550    -0.426761      22.72
 C      -3.804729     1.515066    -0.861936      89.23
 O      -4.850462     0.616710    -0.349423     294.09
 H      -4.761995    -0.319948    -0.791859      25.46
 H      -3.292489     1.022327    -1.729964      26.72
 H      -4.341779     2.556605    -1.086451      24.59
 C       1.391822     1.335245    -1.132509      46.84
 H       2.038488     2.329680    -1.338609      24.75
 C       0.818852    -1.065057    -1.593779      35.31
 H       1.253204    -2.232602    -1.872899      21.16
 C      -0.402894    -0.869796    -0.800932      15.27
 O      -1.404437    -1.782912    -0.665719     188.43
 C      -0.941598    -3.221332    -0.317659      83.26
 H      -0.786666    -3.255671     0.877988      24.81
 H      -1.983850    -4.041427    -0.560746      22.31
 H      -0.109456    -3.639528    -0.603640      28.83
 C      -0.812873     0.442502    -0.362506      11.53
 O      -1.834653     0.675380     0.443902     134.58
 C       0.157522     1.528211    -0.466260      67.56
 H      -0.136542     2.458526    -0.661904      26.89
 C       1.792319     0.113364    -1.690610      24.60
 C       3.179314    -0.267618    -2.183579      68.91
 H       3.215659    -0.908845    -3.318145      24.64
 O       4.039981     0.846231    -2.473308      67.95
 H       4.363624     1.543075    -1.718887      26.69
 C       3.988329    -1.212185    -0.935701      66.56
 H       3.254219    -2.073508    -0.784197      26.64
 O       5.313668    -1.672853    -1.552449     208.35
 H       5.563789    -2.459648    -1.011828      28.76
 C       3.960890    -0.627039     0.510299     113.01
 O       4.408749     0.747658     0.581445     183.91
 H       3.867713     1.355155     1.152865      28.68
 H       4.613402    -1.135965     1.243053      28.36
 H       2.832777    -0.746244     0.778377      26.00
55
name = lig-Water-frame_881
 C      -1.412744     4.238757     2.548428      68.60
 H      -1.939209     5.066998     2.314502      25.86
 C      -1.242058     1.793973     2.914349      56.67
 H      -1.702454     0.890905     2.609455      24.73
 C      -0.163422     2.049764     3.879709      11.73
 O       0.640454     1.044294     4.533293      33.47
 C       0.367964    -0.427683     4.548124      98.36
 H       1.215023    -0.942818     5.292854      25.17
 H       0.380240    -0.908399     3.375727      27.01
 H      -0.661370    -0.480452     4.685027      28.70
 C       0.386599     3.310355     3.983285      18.52
 O       1.551706     3.492416     4.797150     147.79
 H       1.502497     4.388701     5.266975      21.61
 C      -0.402411     4.430880     3.532462      55.81
 H      -0.006036     5.588752     4.044648      18.99
 C      -1.896905     2.980545     2.431471      37.45
 C      -3.045041     2.660648     1.497394      87.10
 H      -3.537116     3.701684     1.416675      25.28
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 O      -4.105544     1.844859     2.226186      67.12
 H      -4.678631     1.084696     1.712178      23.13
 C      -2.737791     1.928633     0.123461      88.76
 H      -2.196817     2.433464    -0.594689      29.05
 C      -3.789527     1.505424    -0.834059     111.08
 O      -4.823259     0.630304    -0.370640     330.27
 H      -4.856202    -0.260496    -0.594421      30.37
 H      -3.329807     1.358394    -1.943122      24.77
 H      -4.310819     2.298846    -1.312821      26.84
 C       1.361056     1.323008    -1.116659      60.83
 H       1.860080     2.200652    -1.116239      28.19
 C       0.866821    -1.027210    -1.545948      82.00
 H       0.926482    -1.955726    -2.044057      24.18
 C      -0.460409    -0.858619    -0.813633      14.83
 O      -1.441445    -1.734109    -0.690801     211.26
 C      -0.939310    -3.246626    -0.335258      91.12
 H      -0.788239    -3.112626     0.677053      28.20
 H      -1.703445    -3.680521    -0.615958      28.15
 H       0.182502    -3.690346    -0.815747      24.39
 C      -0.757029     0.470958    -0.387978      26.40
 O      -1.852329     0.709766     0.463067     156.03
 C       0.186997     1.514433    -0.474984      53.36
 H      -0.052942     2.753316    -0.591253      25.61
 C       1.798339     0.098237    -1.715513      37.17
 C       3.170919    -0.246267    -2.117289     112.02
 H       3.171175    -0.936154    -2.819731      29.83
 O       4.048468     0.821885    -2.479523     132.16
 H       4.194231     1.354453    -1.791944      36.56
 C       4.000415    -1.189450    -0.990891      78.45
 H       3.355128    -2.135544    -0.887759      27.21
 O       5.315653    -1.712676    -1.496897     207.10
 H       5.452344    -2.642310    -1.153734      28.01
 C       3.969315    -0.655131     0.477062     111.97
 O       4.408193     0.746801     0.577837     167.59
 H       3.700934     1.241622     1.080354      28.89
 H       4.476275    -1.421917     1.353359      26.91
 H       2.931227    -0.669039     0.700269      28.99
55
name = lig-Water-frame_882
 C      -1.398497     4.253634     2.599471      55.10
 H      -1.887305     5.288272     2.166847      23.27
 C      -1.270557     1.802414     2.906691      63.86
 H      -1.666218     0.803674     2.631982      25.14
 C      -0.219037     2.056132     3.844350      -5.65
 O       0.679753     1.031262     4.511938      51.76
 C       0.352691    -0.340043     4.513004     145.85
 H       0.990281    -0.828799     5.100448      32.48
 H       0.697815    -0.874536     3.684554      32.18
 H      -0.754187    -0.711872     4.754062      28.05
 C       0.364587     3.371981     3.939237       5.85
 O       1.554276     3.481365     4.783906     172.07
 H       1.433855     4.236048     5.364535      24.27
 C      -0.422137     4.478323     3.509722      68.16
 H      -0.077168     5.331062     3.693055      21.64
 C      -1.909590     2.902832     2.377234      45.38
 C      -3.016379     2.673737     1.509770      93.10
 H      -3.480837     3.667194     1.260341      26.30
 O      -4.065671     1.854260     2.226252     116.03
 H      -4.650435     1.340013     1.765723      29.09
 C      -2.670717     1.877717     0.100228      84.10
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 H      -2.180379     2.700761    -0.641186      26.62
 C      -3.813313     1.498573    -0.859675     104.90
 O      -4.818218     0.659870    -0.367830     289.85
 H      -4.598800    -0.362421    -0.598834      25.96
 H      -3.286014     1.217017    -1.821464      27.56
 H      -4.420586     2.415685    -1.272871      26.18
 C       1.386884     1.296719    -1.131082      55.78
 H       2.116470     2.235339    -1.075065      26.22
 C       0.848100    -0.945459    -1.477748     135.62
 H       0.855112    -1.890141    -2.238726      26.02
 C      -0.428904    -0.772570    -0.868811      18.04
 O      -1.466417    -1.760326    -0.715492     200.42
 C      -0.879985    -3.207067    -0.362744      74.79
 H      -0.806325    -3.105100     0.783760      24.64
 H      -1.954915    -3.838985    -0.865120      23.10
 H      -0.113170    -3.371855    -1.026059      28.37
 C      -0.705886     0.517843    -0.366589      21.79
 O      -1.898344     0.739546     0.467710     176.89
 C       0.174252     1.552652    -0.523288      51.38
 H      -0.068644     2.435591    -0.119417      26.66
 C       1.748433     0.048887    -1.686113      41.41
 C       3.229269    -0.253878    -2.001050     101.35
 H       3.111252    -1.133177    -2.889046      27.02
 O       4.060223     0.806613    -2.515703      65.54
 H       4.070060     1.350736    -1.531952      27.70
 C       4.002925    -1.208233    -1.031118     103.83
 H       3.409986    -2.115308    -1.028432      28.40
 O       5.297716    -1.722108    -1.446042     241.54
 H       5.345263    -2.683583    -1.155204      28.26
 C       3.978484    -0.678990     0.435734     107.64
 O       4.418237     0.737938     0.575023     197.09
 H       3.597697     1.178900     0.978289      28.58
 H       4.365948    -1.448488     1.139081      28.85
 H       2.826542    -0.612454     0.752245      28.15
55
name = lig-Water-frame_883
 C      -1.456196     4.275978     2.628781      49.21
 H      -1.826411     5.015882     2.075079      25.14
 C      -1.271420     1.794439     2.952596      94.04
 H      -1.539779     0.725751     2.839575      31.18
 C      -0.208089     2.025217     3.796797     -53.92
 O       0.690333     1.063263     4.482420      90.47
 C       0.303218    -0.293997     4.458054     120.94
 H       0.954353    -0.750275     5.496085      28.55
 H       0.933079    -0.795534     3.550414      31.38
 H      -0.598884    -0.686159     4.786784      31.09
 C       0.338625     3.410694     3.958879       1.36
 O       1.529795     3.472980     4.756984      67.61
 H       1.332204     4.262085     5.400520      23.19
 C      -0.378129     4.482110     3.485837      70.11
 H       0.051513     5.729677     3.475838      15.09
 C      -1.883683     2.876353     2.324321      19.25
 C      -3.073266     2.647191     1.443369      95.98
 H      -3.498856     3.639245     0.942211      28.64
 O      -4.003255     1.879381     2.236679      94.08
 H      -4.659178     1.562016     1.440195      25.31
 C      -2.613769     1.899644     0.078858      96.18
 H      -2.044212     2.686277    -0.284257      31.57
 C      -3.848427     1.549158    -0.913802      89.20
 O      -4.830831     0.648443    -0.353410     322.43
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 H      -4.313571    -0.153226    -0.578043      29.88
 H      -3.270158     0.793643    -1.643942      26.73
 H      -4.296199     2.483338    -1.031584      28.65
 C       1.466887     1.324115    -1.154300      48.71
 H       2.299793     1.959862    -1.172877      30.78
 C       0.763033    -0.941348    -1.458480     108.58
 H       0.993381    -1.776897    -2.177166      29.01
 C      -0.417243    -0.686913    -0.909889      20.61
 O      -1.438583    -1.793574    -0.739325     207.24
 C      -0.942115    -3.118493    -0.418630     118.84
 H      -0.707360    -3.367304     0.648084      30.19
 H      -1.536529    -3.829323    -0.664552      32.08
 H      -0.029332    -3.232462    -1.221861      25.62
 C      -0.717571     0.544319    -0.307398      18.48
 O      -1.917742     0.750465     0.436831     169.67
 C       0.164336     1.597783    -0.570749      42.80
 H      -0.062844     2.365594     0.417894      29.91
 C       1.748449     0.050940    -1.605005      26.58
 C       3.290336    -0.353365    -1.976191     102.67
 H       3.114251    -0.793180    -2.916262      31.58
 O       4.059342     0.812335    -2.506314      47.18
 H       4.253426     1.395952    -1.713069      32.01
 C       3.990881    -1.243189    -1.019056     109.70
 H       3.201034    -2.154918    -1.059023      28.41
 O       5.278930    -1.704825    -1.411989     234.00
 H       5.354999    -2.608708    -1.060589      29.28
 C       3.926297    -0.674459     0.382771     114.13
 O       4.432099     0.707568     0.567350     178.18
 H       3.724148     1.286272     0.938210      32.16
 H       4.586008    -1.493304     1.092730      28.38
 H       2.960620    -0.707533     0.710650      32.78
55
name = lig-Water-frame_884
 C      -1.527133     4.210880     2.638572      45.72
 H      -2.006858     5.026019     1.892982      21.33
 C      -1.258101     1.754015     3.019430      57.51
 H      -1.560007     0.736920     2.953923      34.74
 C      -0.112364     2.039878     3.775456      24.38
 O       0.658216     1.135178     4.445078     101.38
 C       0.359627    -0.313526     4.449980     134.46
 H       0.715435    -0.503192     5.349831      29.21
 H       0.706242    -0.706942     3.576008      27.35
 H      -0.817262    -0.517931     4.589505      24.37
 C       0.319069     3.382879     4.017174       7.60
 O       1.480677     3.487076     4.737182     113.63
 H       1.369885     4.304254     5.273225      27.92
 C      -0.304534     4.554972     3.438020      47.03
 H       0.043220     5.478075     3.436379      26.46
 C      -1.858887     2.930427     2.285263     -51.07
 C      -3.114668     2.617075     1.335753      94.04
 H      -3.564292     3.558281     0.943646      31.18
 O      -3.961520     1.890800     2.196988      89.03
 H      -4.684101     1.737421     1.467080      26.08
 C      -2.626109     1.955969     0.093546      73.27
 H      -1.753912     2.692055    -0.238833      28.48
 C      -3.821873     1.583035    -0.934990      94.24
 O      -4.836406     0.643013    -0.325908     303.97
 H      -4.382039    -0.213120    -0.446595      30.59
 H      -3.431353     1.039560    -1.736794      30.37
 H      -4.259427     2.654372    -1.212225      26.91
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 C       1.522265     1.366685    -1.157664      43.37
 H       2.443267     2.034975    -1.209407      30.52
 C       0.744281    -0.957224    -1.507696      74.45
 H       0.992768    -1.948710    -2.006591      25.09
 C      -0.503154    -0.670050    -0.900438      15.53
 O      -1.394705    -1.786973    -0.753801     247.95
 C      -0.935976    -3.018240    -0.504700     114.79
 H      -0.522222    -3.336096     0.501247      29.49
 H      -1.693971    -4.054335    -0.764724      25.05
 H       0.020552    -3.305724    -1.011027      26.57
 C      -0.752574     0.575375    -0.267625      17.73
 O      -1.903156     0.725305     0.389444     167.94
 C       0.181848     1.659106    -0.541317      49.96
 H       0.232092     2.291526     0.223808      34.28
 C       1.804416     0.056677    -1.503504      17.40
 C       3.298306    -0.400700    -2.032036      92.82
 H       3.167223    -0.834874    -3.142177      29.64
 O       4.062961     0.822563    -2.477897      53.05
 H       4.466608     1.429021    -1.842920      32.51
 C       3.940654    -1.308871    -0.987851     131.32
 H       3.237185    -2.091037    -0.926875      32.49
 O       5.263031    -1.677276    -1.390798     231.18
 H       5.530415    -2.572676    -0.960906      25.84
 C       3.910040    -0.669051     0.368360     116.97
 O       4.454048     0.663536     0.546454     157.05
 H       3.836158     1.335674     0.963613      31.27
 H       4.608449    -1.296775     0.992142      30.87
 H       2.798131    -0.850487     0.827962      28.82
55
name = lig-Water-frame_885
 C      -1.544708     4.198794     2.618447      55.11
 H      -2.074247     4.957793     2.109337      23.38
 C      -1.238700     1.769995     3.059197      48.03
 H      -1.704685     0.733726     2.930332      27.03
 C      -0.046905     2.072580     3.745376      31.23
 O       0.638744     1.187952     4.427216     104.58
 C       0.346293    -0.291034     4.440056     107.72
 H       0.825975    -0.669715     5.571984      21.66
 H       0.654913    -0.892981     3.442667      23.06
 H      -0.687565    -0.251518     4.246143      24.41
 C       0.289471     3.403544     4.042918      20.29
 O       1.444797     3.516817     4.743736     142.89
 H       1.476057     4.413099     5.147293      25.17
 C      -0.297258     4.516430     3.366382      44.27
 H       0.231174     5.697699     3.518646      22.60
 C      -1.865883     2.917706     2.273024      -4.79
 C      -3.075701     2.628088     1.286059      95.93
 H      -3.695931     3.632998     1.105883      26.60
 O      -3.960560     1.881997     2.121379     144.28
 H      -4.797024     1.605429     1.764186      26.31
 C      -2.639645     2.000060     0.071999      92.14
 H      -1.923312     2.567215    -0.436358      28.65
 C      -3.782128     1.638037    -0.924177      96.74
 O      -4.823659     0.675826    -0.299731     267.81
 H      -4.577139    -0.346356    -0.338011      25.58
 H      -3.469308     1.422386    -2.120162      24.89
 H      -4.314215     2.429706    -1.371997      27.49
 C       1.540441     1.402125    -1.129479      38.50
 H       2.259999     2.260292    -1.160730      24.80
 C       0.767559    -0.932358    -1.562747      58.98
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 H       0.898235    -2.113623    -1.677840      18.05
 C      -0.553414    -0.703838    -0.893685      13.19
 O      -1.380964    -1.719518    -0.766807     240.15
 C      -0.883521    -3.061958    -0.571014     116.10
 H      -0.572547    -2.987371     0.524452      26.51
 H      -1.718446    -3.535897    -0.931683      26.18
 H       0.095513    -3.388603    -1.136707      23.90
 C      -0.740316     0.613131    -0.291210      18.73
 O      -1.911766     0.693936     0.361153     188.05
 C       0.260552     1.661473    -0.510919      38.93
 H       0.382596     2.751988     0.142245      25.98
 C       1.867220     0.015738    -1.450637      51.42
 C       3.258662    -0.382325    -2.120335      83.24
 H       3.235442    -1.040442    -3.034706      31.23
 O       4.061612     0.820800    -2.462346      84.76
 H       4.693153     1.323259    -1.662873      25.78
 C       3.893149    -1.346518    -0.981977      98.15
 H       3.246292    -2.373677    -0.775231      25.58
 O       5.258685    -1.657958    -1.372763     212.14
 H       5.637822    -2.481392    -0.988156      27.67
 C       3.869191    -0.664816     0.411829      99.42
 O       4.479594     0.630906     0.514887     208.94
 H       3.798858     1.234179     0.951061      29.14
 H       4.679131    -1.334227     1.089110      26.45
 H       2.977812    -0.784753     0.864847      26.85
55
name = lig-Water-frame_886
 C      -1.496394     4.230337     2.597220      54.21
 H      -2.131148     5.096992     2.263849      24.66
 C      -1.244296     1.834693     3.032946      73.67
 H      -1.662406     0.898274     2.891830      28.46
 C      -0.072319     2.099834     3.698060       7.09
 O       0.679886     1.179922     4.449680     136.52
 C       0.334950    -0.249090     4.418942     128.87
 H       0.636632    -0.749275     5.194982      29.44
 H       0.826922    -0.819170     3.690456      28.00
 H      -0.799300    -0.277234     4.275520      24.71
 C       0.272696     3.476509     4.015392      18.30
 O       1.433414     3.560855     4.781064     118.03
 H       1.555376     4.553052     5.048067      24.61
 C      -0.323275     4.469186     3.301154      69.75
 H       0.071773     5.401070     3.571910      24.58
 C      -1.889042     2.838702     2.298599      10.43
 C      -3.043584     2.696838     1.330644      91.91
 H      -3.517787     3.624118     1.128376      30.02
 O      -3.973481     1.843873     2.066806      96.90
 H      -4.931955     1.418466     1.796193      20.82
 C      -2.657240     1.980208    -0.021359      88.59
 H      -2.040484     2.683800    -0.722573      27.50
 C      -3.769940     1.659191    -0.952917     106.38
 O      -4.798322     0.735508    -0.287850     275.99
 H      -4.503725    -0.174386    -0.426574      29.17
 H      -3.360393     1.413415    -1.850689      30.36
 H      -4.578664     2.507209    -1.129918      25.71
 C       1.534715     1.393522    -1.084400      49.69
 H       2.111529     2.297521    -1.151621      25.80
 C       0.777980    -0.900185    -1.544073      75.92
 H       1.012165    -1.890492    -1.659632      24.67
 C      -0.459859    -0.670798    -0.918612      19.48
 O      -1.392035    -1.652548    -0.786530     204.09
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 C      -0.803834    -3.085086    -0.599991      97.09
 H      -0.745816    -3.017753     0.466519      26.98
 H      -1.892611    -3.562533    -1.007080      24.88
 H      -0.019216    -3.452927    -1.402853      23.99
 C      -0.687106     0.628123    -0.360628      12.34
 O      -1.950350     0.694845     0.349056     177.04
 C       0.365509     1.673518    -0.442479      57.79
 H       0.102076     2.679034    -0.368541      30.19
 C       1.895312    -0.009537    -1.477809      50.31
 C       3.222731    -0.360739    -2.133754      97.20
 H       3.151951    -1.019024    -3.002928      31.24
 O       4.069065     0.813022    -2.442099     200.89
 H       4.473888     0.862809    -1.630017      33.23
 C       3.853539    -1.377981    -0.973683     108.68
 H       3.395132    -2.248218    -0.882938      31.40
 O       5.263789    -1.629076    -1.364582     205.61
 H       5.533689    -2.526413    -1.027062      28.46
 C       3.892847    -0.695390     0.469464     108.31
 O       4.491970     0.616944     0.482760     186.69
 H       3.783039     1.178475     0.837497      30.50
 H       4.495104    -1.454909     1.122608      28.83
 H       2.814688    -0.628916     1.050053      25.81
55
name = lig-Water-frame_887
 C      -1.469404     4.226111     2.534930      58.26
 H      -2.102173     5.172335     2.354407      24.39
 C      -1.261007     1.881415     2.966237      94.14
 H      -1.575264     0.795429     2.843443      31.00
 C      -0.093059     2.132513     3.710525     -26.10
 O       0.732328     1.157350     4.478820     132.94
 C       0.286365    -0.181164     4.360478     103.68
 H       0.538892    -0.840837     5.449811      22.13
 H       1.034126    -0.658225     3.581238      25.44
 H      -0.781099    -0.510819     4.411191      22.79
 C       0.309082     3.467574     3.968751       6.03
 O       1.426031     3.628843     4.823550      91.85
 H       1.522205     4.556898     5.053443      30.38
 C      -0.364893     4.441143     3.264966      63.94
 H      -0.047328     5.612123     3.562474      21.07
 C      -1.915677     2.864194     2.336025       7.18
 C      -3.031528     2.712724     1.377266      68.55
 H      -3.356833     3.856460     1.055350      26.79
 O      -4.008723     1.784408     2.056614      67.63
 H      -4.644592     1.526210     1.353526      25.28
 C      -2.652334     1.975486    -0.099129      91.31
 H      -2.095307     2.690067    -0.684681      30.06
 C      -3.860364     1.686756    -0.944904     101.52
 O      -4.761629     0.799899    -0.299755     251.29
 H      -4.295184    -0.084067    -0.541309      26.27
 H      -3.244018     1.073265    -1.864933      25.53
 H      -4.378791     2.607460    -0.881114      27.89
 C       1.570455     1.334095    -1.050993      48.79
 H       2.283120     2.227055    -1.304477      25.18
 C       0.836037    -0.862003    -1.491607      59.02
 H       1.230617    -1.938789    -1.970099      22.11
 C      -0.340361    -0.588776    -0.933121      24.21
 O      -1.376184    -1.612661    -0.813030     183.67
 C      -0.823605    -3.073358    -0.668267     108.41
 H      -0.653586    -3.396542     0.483175      26.58
 H      -1.636698    -3.814411    -0.803679      27.79
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 H      -0.090985    -3.409875    -1.384218      26.91
 C      -0.641701     0.634756    -0.413784      15.85
 O      -1.966937     0.734911     0.305688     152.51
 C       0.376386     1.643895    -0.388604      59.72
 H      -0.181177     2.703244    -0.610025      30.68
 C       1.864326     0.045467    -1.544164      41.40
 C       3.199309    -0.364223    -2.087124      90.36
 H       2.958145    -0.906428    -3.161085      27.97
 O       4.055084     0.773245    -2.419003     158.41
 H       4.473840     0.740527    -1.441753      28.58
 C       3.864164    -1.333368    -0.969741      90.35
 H       3.217766    -2.408287    -1.063138      25.32
 O       5.270147    -1.601270    -1.354211     195.05
 H       5.379683    -2.582613    -1.121461      27.55
 C       3.884365    -0.744022     0.529496     119.95
 O       4.504020     0.601198     0.451809     129.88
 H       3.784871     1.285995     0.708844      28.94
 H       4.343682    -1.608678     1.228004      28.44
 H       2.964326    -0.533657     0.906479      29.70
55
name = lig-Water-frame_888
 C      -1.487107     4.215280     2.458099      55.11
 H      -2.029680     5.038496     2.207094      18.93
 C      -1.237650     1.844784     2.923825      32.68
 H      -1.478348     0.816383     2.768917      27.02
 C      -0.083386     2.140057     3.776234     -22.16
 O       0.739635     1.168910     4.490852     100.47
 C       0.286687    -0.198655     4.358450     125.56
 H       0.530816    -0.474382     5.257621      31.24
 H       0.828273    -0.538864     3.503830      32.10
 H      -0.775107    -0.467038     4.226746      27.09
 C       0.389274     3.421643     3.928178      12.09
 O       1.412448     3.692925     4.852160      82.03
 H       1.341244     4.654761     5.201055      24.27
 C      -0.354961     4.494787     3.285207      51.22
 H      -0.265254     5.614411     3.402535      22.19
 C      -1.957454     2.978384     2.337966      38.32
 C      -3.045261     2.698095     1.381382      89.31
 H      -3.389658     3.656445     1.151126      30.83
 O      -4.040641     1.750227     2.033018      88.76
 H      -4.387363     1.510437     1.103369      25.04
 C      -2.638209     1.994976    -0.083775      92.77
 H      -1.949366     2.709800    -0.621182      28.75
 C      -3.908874     1.703659    -0.942423     113.37
 O      -4.736453     0.829380    -0.323736     293.47
 H      -4.286037    -0.101535    -0.445875      25.76
 H      -3.678855     1.244042    -1.807954      31.46
 H      -4.228341     2.830188    -1.157004      27.35
 C       1.636764     1.321865    -1.029078      59.60
 H       2.379459     1.959206    -1.336770      26.70
 C       0.969213    -0.900703    -1.489596     113.80
 H       1.046422    -1.690407    -2.070421      27.36
 C      -0.305902    -0.584981    -0.921730      11.53
 O      -1.314594    -1.608826    -0.839061     216.64
 C      -0.879832    -3.053455    -0.688739      94.40
 H      -0.377427    -3.384468     0.181607      28.97
 H      -1.698145    -3.897349    -0.894503      25.77
 H       0.099198    -3.268210    -1.442603      24.58
 C      -0.639539     0.664531    -0.400822      26.05
 O      -1.937727     0.791479     0.212981     195.42
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 C       0.319502     1.627378    -0.389259      58.84
 H      -0.053351     2.654218    -0.487151      30.30
 C       1.833496     0.141119    -1.604574      37.34
 C       3.177992    -0.376299    -2.061172     104.19
 H       2.974985    -0.832465    -2.974064      30.00
 O       4.039564     0.711456    -2.362874     162.89
 H       4.622889     1.119279    -1.559726      25.93
 C       3.866444    -1.308315    -0.979797     105.73
 H       3.288557    -2.098614    -1.077858      31.94
 O       5.263973    -1.581899    -1.338290     246.91
 H       5.422132    -2.537565    -1.248649      29.95
 C       3.865320    -0.792052     0.538564      96.96
 O       4.525513     0.577348     0.427566     166.50
 H       3.873400     1.275330     0.631334      31.05
 H       4.383622    -1.500276     1.274333      28.43
 H       2.725641    -0.563139     0.848745      27.93
55
name = lig-Water-frame_889
 C      -1.459964     4.262840     2.433801      46.66
 H      -2.080447     5.111065     1.805672      20.80
 C      -1.174411     1.842172     2.913154      47.33
 H      -1.514837     0.823244     2.652977      27.41
 C      -0.077901     2.086802     3.825715     -12.48
 O       0.701022     1.218654     4.480040     109.31
 C       0.288892    -0.216172     4.341845     106.01
 H       0.746943    -0.604274     5.451474      25.81
 H       0.736942    -0.727174     3.401628      29.87
 H      -0.816958    -0.171860     4.032219      27.45
 C       0.450207     3.469010     3.891058      -1.09
 O       1.406875     3.756262     4.876511     145.87
 H       1.024811     4.601937     5.366684      18.88
 C      -0.346153     4.526225     3.303723      51.82
 H      -0.157322     5.684485     3.436318      21.47
 C      -1.976751     2.973969     2.325271      38.82
 C      -3.071289     2.638259     1.366766      88.40
 H      -3.809565     3.615550     1.141507      27.28
 O      -4.058324     1.747697     1.987640      77.22
 H      -4.492528     1.072573     1.203461      20.03
 C      -2.617703     2.053476    -0.030731      98.31
 H      -1.922148     2.754416    -0.545045      30.01
 C      -3.883918     1.800513    -0.961643     100.86
 O      -4.761798     0.825928    -0.320032     283.51
 H      -4.431893    -0.047139    -0.384215      29.73
 H      -3.847108     1.458595    -2.194836      25.93
 H      -4.366917     2.665908    -1.385083      27.95
 C       1.637001     1.381960    -0.984379      52.71
 H       2.548949     2.126553    -1.181957      26.79
 C       1.000330    -0.929002    -1.478294     108.72
 H       0.930079    -1.861595    -2.288672      23.51
 C      -0.280855    -0.671012    -0.910152      10.15
 O      -1.245895    -1.630428    -0.855899     224.91
 C      -0.884075    -3.030268    -0.745690     102.05
 H      -0.188864    -3.106258     0.198896      27.66
 H      -1.828456    -3.607589    -1.153516      25.61
 H      -0.161466    -3.153486    -1.476489      29.08
 C      -0.674917     0.668371    -0.354738      29.88
 O      -1.886386     0.832063     0.102398     203.46
 C       0.333362     1.648035    -0.447929      56.32
 H       0.149078     2.799205    -0.150125      28.32
 C       1.858553     0.168731    -1.653326      38.32
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 C       3.196242    -0.340334    -2.003788     101.98
 H       3.138793    -1.079717    -3.028819      27.43
 O       4.054199     0.690406    -2.331353     192.94
 H       4.466805     1.150386    -1.723484      35.59
 C       3.881343    -1.278261    -0.968296      95.27
 H       3.200123    -2.337321    -0.986795      26.54
 O       5.251439    -1.554373    -1.329002     213.45
 H       5.541830    -2.500380    -1.301444      27.64
 C       3.802867    -0.788424     0.486897     106.56
 O       4.555337     0.536545     0.414508     162.75
 H       3.892078     1.206755     0.699105      34.21
 H       4.510249    -1.309691     1.309407      28.21
 H       2.794684    -0.776736     0.813085      31.61
55
name = lig-Water-frame_890
 C      -1.444851     4.334819     2.415172      55.85
 H      -1.800807     4.987454     1.752266      25.53
 C      -1.126483     1.876219     2.911793      72.44
 H      -1.555838     0.890062     2.613679      26.50
 C      -0.081062     2.095430     3.806021      -9.02
 O       0.667855     1.233694     4.470288     127.97
 C       0.305341    -0.219782     4.339167     132.28
 H       0.564819    -0.832310     5.101660      31.83
 H       0.766341    -0.795541     3.540228      30.95
 H      -0.734733    -0.128257     4.279456      30.06
 C       0.440352     3.538875     3.865234       6.38
 O       1.397269     3.814848     4.902793     191.74
 H       1.016149     4.577751     5.440470      20.99
 C      -0.340879     4.552495     3.299714      62.47
 H       0.212140     5.596751     3.569494      17.25
 C      -1.932624     2.907804     2.320143      -2.52
 C      -3.161382     2.587744     1.331823     104.56
 H      -3.735472     3.388915     1.102609      30.39
 O      -4.077958     1.716602     1.952980     178.85
 H      -4.495203     1.088130     1.461939      27.86
 C      -2.608317     2.142906    -0.015861      90.18
 H      -2.001642     2.925033    -0.467714      29.42
 C      -3.844970     1.874056    -1.044706      83.62
 O      -4.815959     0.843442    -0.308759     240.63
 H      -4.434840    -0.148143    -0.601171      24.68
 H      -3.545971     1.563087    -1.937060      31.35
 H      -4.678489     2.717651    -1.106465      25.56
 C       1.638533     1.456147    -0.978331      51.91
 H       2.282388     2.254622    -0.807324      25.91
 C       0.936633    -0.954825    -1.505538      89.44
 H       1.107373    -1.768796    -2.088881      25.69
 C      -0.250497    -0.732243    -0.882536      16.43
 O      -1.215996    -1.645583    -0.866092     237.67
 C      -0.851810    -2.975959    -0.808447     103.38
 H      -0.471788    -3.092653     0.173794      28.15
 H      -1.862947    -3.458056    -1.042060      25.86
 H      -0.240615    -3.320121    -1.885863      23.79
 C      -0.614533     0.632614    -0.359166      24.95
 O      -1.887341     0.851851     0.017993     182.85
 C       0.370264     1.723639    -0.513670      48.44
 H       0.365621     2.530836     0.298489      25.95
 C       1.891410     0.148900    -1.652961      29.81
 C       3.255501    -0.337477    -1.984848     117.83
 H       3.270767    -0.967469    -2.762122      31.65
 O       4.094574     0.703664    -2.367486     116.38
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 H       4.366470     1.197086    -1.390440      24.99
 C       3.864934    -1.334321    -0.928359     115.86
 H       3.407782    -2.232110    -0.897573      32.20
 O       5.246979    -1.509258    -1.332586     240.78
 H       5.571086    -2.461132    -1.207170      27.48
 C       3.803708    -0.762102     0.426880     106.39
 O       4.564318     0.502095     0.413411     185.53
 H       3.941243     1.183087     0.852499      29.83
 H       4.353239    -1.359817     1.125677      29.87
 H       2.705085    -0.778570     0.877879      28.35
55
name = lig-Water-frame_891
 C      -1.426405     4.311525     2.423141      48.09
 H      -1.710006     5.202508     1.646414      21.02
 C      -1.135712     1.902976     2.894156      77.98
 H      -1.449612     0.899872     2.755449      24.85
 C      -0.060163     2.206333     3.741453      -1.59
 O       0.669108     1.196508     4.482465     100.50
 C       0.302422    -0.200940     4.320205     114.29
 H       0.539684    -0.976459     5.272261      26.89
 H       0.800835    -0.632489     3.408025      29.17
 H      -0.871677    -0.381105     4.503659      26.21
 C       0.381790     3.548990     3.888905      21.72
 O       1.386759     3.839728     4.907309     152.93
 H       1.169009     4.781338     5.423780      17.10
 C      -0.304433     4.592528     3.279020      61.45
 H       0.253595     5.539762     3.494160      15.85
 C      -1.862800     2.914555     2.298728     -23.83
 C      -3.201690     2.526612     1.316523      69.01
 H      -3.649233     3.690887     1.028803      24.86
 O      -4.092080     1.684628     1.985174     112.66
 H      -4.620613     0.983930     1.158902      15.34
 C      -2.629039     2.210635    -0.060725      90.56
 H      -2.018271     3.145879    -0.377384      27.59
 C      -3.850877     1.951042    -1.045413      48.28
 O      -4.845386     0.848424    -0.336122     273.04
 H      -4.540299     0.048387    -0.752970      27.01
 H      -3.152560     1.491441    -1.986428      22.82
 H      -4.545444     2.721801    -0.806164      24.23
 C       1.646655     1.467420    -1.025827      40.97
 H       2.295851     2.347557    -0.646348      22.01
 C       0.921399    -0.902754    -1.552107      56.99
 H       1.330725    -1.962505    -1.958701      19.45
 C      -0.246537    -0.700335    -0.834765      20.15
 O      -1.237399    -1.633747    -0.875528     250.38
 C      -0.829116    -2.973390    -0.937156     131.75
 H      -0.541488    -3.416534     0.130272      25.39
 H      -1.892491    -3.529773    -0.661035      23.69
 H      -0.344751    -3.400167    -1.686398      29.05
 C      -0.487094     0.609774    -0.414723      27.89
 O      -1.924768     0.861904    -0.045970     146.81
 C       0.370245     1.748251    -0.510229      50.79
 H       0.299332     2.403897     0.390492      26.27
 C       1.900525     0.134936    -1.591080      39.55
 C       3.312964    -0.355850    -1.976652      85.65
 H       3.228732    -1.071976    -3.025217      27.04
 O       4.173820     0.761342    -2.384203     135.22
 H       4.208138     1.094661    -1.447348      30.13
 C       3.871461    -1.367725    -0.905643     107.47
 H       3.310813    -2.462755    -0.915449      23.88
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 O       5.257881    -1.466937    -1.339838     249.75
 H       5.563083    -2.342967    -1.045751      29.85
 C       3.816172    -0.734514     0.418143     106.67
 O       4.550298     0.487684     0.425915     169.46
 H       4.085418     1.137660     0.966552      29.68
 H       4.233017    -1.711801     1.086168      26.31
 H       2.799021    -0.509236     0.792161      28.03
55
name = lig-Water-frame_892
 C      -1.387486     4.282242     2.415797      58.30
 H      -1.778039     5.089534     1.893196      24.55
 C      -1.149560     1.922971     2.889174      38.48
 H      -1.375514     0.802303     2.918634      24.71
 C      -0.012200     2.279453     3.688018       3.74
 O       0.671367     1.170487     4.499649     119.30
 C       0.260280    -0.224091     4.338771     115.44
 H       0.806628    -0.564652     5.173295      23.18
 H       0.628107    -0.427809     3.307815      24.99
 H      -0.731525    -0.506713     4.335883      25.77
 C       0.339005     3.558002     3.978581      10.97
 O       1.379365     3.843761     4.890252     -42.04
 H       1.154444     4.741181     5.247260      29.72
 C      -0.276838     4.608182     3.234386      66.67
 H       0.116145     5.811146     3.251846      23.78
 C      -1.842986     2.973996     2.232377      -4.70
 C      -3.174065     2.559019     1.336331      86.24
 H      -3.537245     3.502671     1.218972      28.82
 O      -4.121438     1.627376     2.000059     174.09
 H      -4.434934     1.312208     1.134041      22.79
 C      -2.666409     2.231736    -0.110404      92.10
 H      -2.073129     3.064086    -0.366603      28.04
 C      -3.822013     1.984004    -0.991659      88.92
 O      -4.854024     0.891349    -0.391538     273.88
 H      -4.519024    -0.097789    -0.756663      20.79
 H      -3.505765     1.691434    -1.925101      29.92
 H      -4.404650     2.976793    -1.066200      26.11
 C       1.654668     1.464536    -1.070254      42.98
 H       2.546451     2.099849    -0.967547      22.80
 C       0.971377    -0.843236    -1.603203      68.29
 H       1.293232    -1.873486    -1.677128      21.48
 C      -0.240898    -0.651874    -0.826738      24.56
 O      -1.277490    -1.607989    -0.881037     204.21
 C      -0.886948    -3.040476    -0.948709     105.51
 H      -0.218093    -3.419336    -0.194493      27.74
 H      -1.778051    -3.573383    -0.844844      26.29
 H      -0.191265    -3.551886    -1.940991      23.77
 C      -0.465650     0.649795    -0.461310      25.82
 O      -1.936810     0.868531    -0.109218     156.48
 C       0.380350     1.702487    -0.474661      50.31
 H       0.023913     2.613541     0.251950      25.90
 C       1.929669     0.142445    -1.522369      38.78
 C       3.328525    -0.405802    -2.053086      95.04
 H       3.167319    -0.844887    -2.908043      32.93
 O       4.244004     0.803330    -2.377437      78.54
 H       4.384678     1.304779    -1.562147      30.72
 C       3.885828    -1.378857    -0.944545     122.87
 H       3.313744    -2.288185    -0.977466      28.41
 O       5.274962    -1.444060    -1.338615     287.70
 H       5.694765    -2.275754    -0.921455      27.43
 C       3.825122    -0.757827     0.471767     117.62
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 O       4.555311     0.481560     0.443590     151.54
 H       4.117455     1.104052     1.085230      28.52
 H       4.163701    -1.527321     1.138031      28.71
 H       2.772347    -0.387701     0.714469      26.16
55
name = lig-Water-frame_893
 C      -1.339196     4.267162     2.406721      47.29
 H      -2.027434     5.111290     1.978331      25.38
 C      -1.133852     1.949095     2.903474      48.62
 H      -1.457489     0.953642     2.898964      30.43
 C       0.017360     2.232513     3.665860     -11.78
 O       0.648579     1.206580     4.504476      74.33
 C       0.254714    -0.215908     4.325466     109.26
 H       1.095113    -0.545862     5.101839      22.01
 H       0.550671    -0.535148     3.303865      26.40
 H      -0.908111    -0.527809     4.311142      23.41
 C       0.330679     3.625807     4.062441      -3.72
 O       1.378704     3.822056     4.857457      77.58
 H       1.088828     4.769548     5.332630      20.58
 C      -0.255633     4.629068     3.184598      58.89
 H      -0.067285     5.639024     3.173227      28.35
 C      -1.863582     2.969797     2.164601      23.41
 C      -3.070907     2.614792     1.403275      68.00
 H      -3.837881     3.632024     1.377965      24.67
 O      -4.113479     1.595553     2.007121      47.51
 H      -4.615298     1.316159     1.038101      19.55
 C      -2.686685     2.183457    -0.106045      87.76
 H      -2.005748     3.027942    -0.566614      26.28
 C      -3.868704     2.015374    -0.939879     108.09
 O      -4.837174     0.965977    -0.475989     282.45
 H      -4.417613     0.069949    -0.493394      26.20
 H      -3.796168     1.722321    -2.151324      25.19
 H      -4.251531     2.950144    -1.389750      27.02
 C       1.679561     1.448715    -1.100926      59.29
 H       2.610282     1.998496    -1.317518      23.21
 C       0.985921    -0.804633    -1.575107      69.41
 H       1.262479    -1.882900    -1.706944      24.50
 C      -0.218727    -0.643957    -0.897827      15.30
 O      -1.302287    -1.595869    -0.880606     173.60
 C      -0.891184    -3.118676    -0.982403      91.83
 H       0.036690    -3.198819    -0.308281      26.46
 H      -1.972509    -3.778105    -1.162217      23.39
 H      -0.512968    -3.215735    -1.936511      28.78
 C      -0.600216     0.712993    -0.477865      10.05
 O      -1.920286     0.880604    -0.169402     151.63
 C       0.430560     1.692468    -0.429129      73.08
 H       0.025770     2.673513    -0.206812      31.29
 C       1.998436     0.159110    -1.502063      39.98
 C       3.330370    -0.361914    -2.072712      77.98
 H       3.128623    -0.853821    -3.235635      26.13
 O       4.293992     0.805413    -2.377487       6.23
 H       4.651404     1.536350    -1.611337      24.83
 C       3.929546    -1.330209    -1.005554     105.76
 H       3.306650    -2.360151    -1.056995      25.82
 O       5.303733    -1.446815    -1.328634     273.59
 H       5.768697    -2.238968    -0.947455      27.11
 C       3.798017    -0.774850     0.501645      98.83
 O       4.587231     0.483921     0.472899     169.48
 H       4.070973     1.091425     1.100888      28.48
 H       4.237364    -1.358870     1.508921      26.60
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 H       2.669901    -0.558103     0.666605      27.14
55
name = lig-Water-frame_894
 C      -1.358123     4.270027     2.350001      52.97
 H      -2.081389     5.070063     2.083655      28.30
 C      -1.115274     1.982721     2.900894      69.27
 H      -1.617409     0.966034     2.784945      34.54
 C       0.025386     2.188507     3.694427     -14.64
 O       0.604302     1.270406     4.490770     111.29
 C       0.273035    -0.197103     4.298206     127.64
 H       0.920230    -0.872322     4.912337      27.84
 H       0.547443    -0.653335     3.312491      29.02
 H      -0.686140    -0.360745     4.656773      27.30
 C       0.309634     3.651283     4.037371       4.57
 O       1.391359     3.832794     4.865528     181.36
 H       1.248466     4.567716     5.492606      23.55
 C      -0.236755     4.593391     3.166590      53.03
 H      -0.055678     5.892582     3.334683      23.52
 C      -1.828453     2.932811     2.177846      42.17
 C      -3.047119     2.684424     1.443192      76.33
 H      -3.674156     3.424008     1.359257      32.12
 O      -4.074496     1.581466     1.990165      92.76
 H      -4.692636     1.294004     1.383583      29.53
 C      -2.654960     2.149343    -0.087367      90.19
 H      -2.109818     2.833918    -0.635949      30.48
 C      -3.955143     2.009518    -1.008658     107.38
 O      -4.834617     1.087937    -0.538428     320.71
 H      -4.281320     0.231938    -0.485017      29.10
 H      -3.621757     1.607972    -1.936362      30.51
 H      -4.450417     3.002604    -1.154906      27.33
 C       1.729090     1.422367    -1.115870      24.78
 H       2.377883     2.325887    -1.492699      27.01
 C       0.994238    -0.821129    -1.493191      69.87
 H       1.235620    -1.838133    -2.032204      29.34
 C      -0.262271    -0.624551    -0.984402      14.36
 O      -1.309267    -1.602735    -0.872976     168.29
 C      -0.908139    -3.144640    -1.047288      99.70
 H      -0.109844    -3.232205    -0.315362      30.08
 H      -1.699017    -3.723052    -0.980198      30.54
 H      -0.708857    -2.873970    -2.247727      24.96
 C      -0.701639     0.752998    -0.499941      -6.99
 O      -1.931186     0.896738    -0.209424     131.69
 C       0.469504     1.695677    -0.408642      44.06
 H       0.212991     2.868075    -0.749379      34.17
 C       2.055415     0.157884    -1.532265      60.52
 C       3.347509    -0.255205    -2.091603     109.66
 H       3.293778    -0.706401    -2.956380      32.97
 O       4.340209     0.801239    -2.398504      55.93
 H       4.594830     1.257206    -1.639057      33.30
 C       3.982175    -1.303270    -1.036307     101.47
 H       3.479658    -2.291975    -1.158643      30.36
 O       5.349536    -1.450305    -1.326886     237.51
 H       5.630639    -2.374590    -1.030587      24.41
 C       3.778255    -0.779269     0.522807     125.60
 O       4.607823     0.483695     0.516885     155.35
 H       4.077539     1.166005     0.963561      32.56
 H       4.131785    -1.306181     1.352881      35.04
 H       2.685265    -0.708831     0.715503      33.79
55
name = lig-Water-frame_895
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 C      -1.397209     4.278022     2.299277      61.29
 H      -2.006542     5.112262     2.009920      25.63
 C      -1.106380     1.944668     2.888717      94.08
 H      -1.543694     0.975763     2.771300      33.92
 C      -0.014544     2.229574     3.730583      16.28
 O       0.585035     1.290575     4.489331     142.40
 C       0.308495    -0.181516     4.274728     124.59
 H       0.873615    -0.920304     4.955759      27.19
 H       0.339916    -0.491186     3.222255      29.88
 H      -0.693757    -0.257900     4.899223      24.49
 C       0.316435     3.600666     3.956138      -2.84
 O       1.418298     3.838878     4.889260     170.38
 H       1.269305     4.592933     5.631378      17.99
 C      -0.249249     4.614685     3.164819      51.02
 H      -0.015747     5.500264     3.453781      28.21
 C      -1.758500     2.949439     2.248226      34.24
 C      -3.064931     2.639629     1.403965      58.63
 H      -3.681401     3.769952     1.192366      25.42
 O      -3.981423     1.592650     2.016373      87.67
 H      -4.834328     1.347951     1.384982      23.97
 C      -2.658020     2.152499    -0.079003      86.79
 H      -2.013458     2.963596    -0.644601      29.17
 C      -3.982502     2.042155    -1.084245      82.47
 O      -4.878541     1.180913    -0.564211     245.33
 H      -4.440296     0.225773    -0.658599      26.49
 H      -3.307038     1.611666    -2.053770      26.86
 H      -4.569728     2.953383    -0.840418      25.84
 C       1.754989     1.435800    -1.116161      35.69
 H       2.068387     2.388051    -1.376462      29.27
 C       1.032674    -0.870310    -1.437070      56.16
 H       1.161871    -1.667182    -2.107989      28.92
 C      -0.369602    -0.584649    -1.034964       4.84
 O      -1.311920    -1.616773    -0.853258     155.82
 C      -0.903354    -3.048804    -1.179196      97.99
 H      -0.134181    -3.452372    -0.442794      29.05
 H      -1.814473    -3.819411    -0.611100      25.07
 H      -0.691752    -3.150426    -2.154535      30.41
 C      -0.631871     0.765597    -0.553062       1.20
 O      -2.010291     0.906642    -0.215309     146.79
 C       0.465054     1.729896    -0.476085      47.53
 H       0.342297     2.691297    -0.745006      37.91
 C       2.057305     0.152685    -1.579350      27.32
 C       3.428208    -0.151664    -2.064943      99.34
 H       3.353240    -0.862563    -3.118032      27.62
 O       4.370925     0.791265    -2.436694      91.89
 H       4.557036     1.085823    -1.418589      28.27
 C       4.028897    -1.266190    -1.028409      89.83
 H       3.484741    -2.287525    -1.224590      29.08
 O       5.413342    -1.459881    -1.327194     227.40
 H       5.501831    -2.463405    -1.173693      22.74
 C       3.781278    -0.759280     0.481662     111.11
 O       4.607888     0.474630     0.565916     115.25
 H       4.052912     1.298124     0.840087      31.01
 H       4.234913    -1.680462     1.223942      29.11
 H       2.634272    -0.618588     0.780826      32.15
55
name = lig-Water-frame_896
 C      -1.381761     4.321360     2.305785      87.91
 H      -1.967097     5.190728     1.719789      25.44
 C      -1.083758     1.875858     2.889181      73.70
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 H      -1.404740     0.831673     2.814712      27.13
 C      -0.086000     2.273902     3.755836      11.35
 O       0.610371     1.270716     4.510668      61.53
 C       0.291826    -0.148739     4.293221     139.87
 H       1.167441    -0.645974     4.890916      30.13
 H       0.051769    -0.275597     3.216810      31.68
 H      -0.694204    -0.327882     4.675274      33.22
 C       0.377704     3.553679     3.891104      19.55
 O       1.434164     3.839610     4.913024     150.37
 H       1.068350     4.632231     5.357427      16.47
 C      -0.309713     4.582735     3.153244      55.42
 H       0.165943     5.750620     3.612642      14.26
 C      -1.776976     2.980801     2.270530       6.91
 C      -3.092165     2.596863     1.324946      92.70
 H      -3.435730     3.497960     1.207410      31.65
 O      -3.878781     1.622278     2.053757     200.76
 H      -4.595602     1.579197     1.376963      30.15
 C      -2.686255     2.218031    -0.108821      99.38
 H      -2.042010     3.008494    -0.366742      31.54
 C      -3.911192     2.109513    -1.118175     102.19
 O      -4.960245     1.194646    -0.583277     287.64
 H      -4.793182     0.264880    -0.754140      30.70
 H      -3.522076     1.997469    -2.120029      31.05
 H      -4.393620     3.056830    -1.107319      29.52
 C       1.711734     1.452145    -1.089598      62.49
 H       2.303682     2.484325    -1.333934      29.09
 C       1.039815    -0.880033    -1.403753      49.85
 H       1.143673    -1.841812    -2.150869      26.41
 C      -0.404833    -0.559068    -1.060825       6.56
 O      -1.305168    -1.630500    -0.840677     150.93
 C      -0.935478    -2.967703    -1.220535     119.48
 H       0.016291    -3.398298    -0.798033      29.53
 H      -1.697332    -3.398872    -0.860592      32.09
 H      -0.699446    -3.534483    -2.351562      25.97
 C      -0.561525     0.762345    -0.601469      21.97
 O      -2.066894     0.899865    -0.208177     151.65
 C       0.442108     1.714315    -0.604061      51.06
 H       0.126433     2.965885    -0.388261      27.75
 C       2.024534     0.167560    -1.617271      10.04
 C       3.501315    -0.197433    -2.099791     117.11
 H       3.328111    -0.744922    -2.903817      32.68
 O       4.405221     0.821533    -2.436638      76.42
 H       4.766002     1.135933    -1.477086      26.17
 C       4.050970    -1.211131    -1.011645     101.83
 H       3.389853    -2.133296    -1.214117      29.72
 O       5.468408    -1.469977    -1.324236     254.80
 H       5.713119    -2.442006    -1.230827      22.09
 C       3.817014    -0.773167     0.431762     131.91
 O       4.597099     0.462635     0.613620     192.08
 H       4.016853     1.231751     0.832096      32.65
 H       4.219551    -1.583141     0.920213      34.12
 H       2.842121    -0.520569     0.721518      32.72
55
name = lig-Water-frame_897
 C      -1.368837     4.372587     2.315226      53.29
 H      -1.790491     5.023906     1.676948      24.64
 C      -1.098101     1.860096     2.877380      57.46
 H      -1.348336     0.771595     2.798106      27.54
 C      -0.117537     2.231317     3.799563     -37.69
 O       0.642959     1.263455     4.538132      40.03
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 C       0.265870    -0.084634     4.306177     155.57
 H       1.222516    -0.525788     4.610397      31.88
 H       0.152308    -0.290001     3.220022      32.07
 H      -0.775816    -0.519287     4.706634      29.03
 C       0.455166     3.565171     3.852155       4.12
 O       1.411165     3.838616     4.903579     139.72
 H       1.018028     4.747009     5.170433      15.76
 C      -0.301709     4.602040     3.208332      58.73
 H      -0.028910     5.497731     3.281832      24.25
 C      -1.850292     2.952540     2.227934       2.43
 C      -3.030554     2.545795     1.296900      88.30
 H      -3.698328     3.681511     1.245372      26.33
 O      -3.785656     1.667553     2.079341     192.49
 H      -4.521581     1.505525     1.436542      29.49
 C      -2.723750     2.255397    -0.153728      89.19
 H      -1.983981     3.136769    -0.313583      26.56
 C      -3.849949     2.195852    -1.103390      87.87
 O      -5.039855     1.224815    -0.609828     192.21
 H      -4.869683     0.186041    -0.847737      25.71
 H      -3.692409     2.053315    -2.327362      26.53
 H      -4.241433     3.211062    -1.426977      27.71
 C       1.694215     1.497519    -1.094800      59.88
 H       2.519901     2.093806    -1.178678      33.51
 C       1.005282    -0.876135    -1.440386      66.77
 H       1.186427    -1.800430    -1.805229      30.12
 C      -0.327428    -0.579550    -1.072948      15.98
 O      -1.281689    -1.606822    -0.853271     176.16
 C      -0.913708    -2.933304    -1.298056     105.40
 H       0.085212    -3.116278    -0.886281      29.35
 H      -2.054184    -3.488956    -0.909989      24.55
 H      -1.036825    -3.202669    -2.275386      29.93
 C      -0.613909     0.739964    -0.629918       6.83
 O      -2.059704     0.895377    -0.203480     114.85
 C       0.369216     1.774232    -0.716650      68.50
 H       0.075475     2.525930    -0.139569      31.52
 C       1.992605     0.185368    -1.628393       4.17
 C       3.524468    -0.277574    -2.100784      88.01
 H       3.336096    -0.880204    -3.190295      27.57
 O       4.450264     0.880568    -2.416027      54.45
 H       4.889358     1.260120    -1.726857      30.86
 C       4.063214    -1.165573    -1.033255     110.37
 H       3.389064    -2.081347    -1.132859      30.52
 O       5.507635    -1.459363    -1.321017     219.68
 H       5.856569    -2.398032    -1.088571      19.86
 C       3.889933    -0.758552     0.357919     128.87
 O       4.601352     0.448453     0.655673     144.65
 H       3.966975     1.121166     0.983620      33.66
 H       4.352746    -1.677360     1.096880      29.38
 H       2.717780    -0.563058     0.680746      31.26
55
name = lig-Water-frame_898
 C      -1.366309     4.302462     2.345008      47.11
 H      -1.767172     5.185769     1.585218      22.30
 C      -1.147349     1.897077     2.864500      69.71
 H      -1.443623     0.899399     2.709299      30.09
 C      -0.089890     2.189239     3.832219     -19.43
 O       0.651236     1.283142     4.565501      90.81
 C       0.237988    -0.053624     4.293739     146.74
 H       1.184010    -0.792135     4.458712      29.68
 H       0.329454    -0.302911     3.219391      32.03
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 H      -0.501044    -0.535826     4.917114      31.18
 C       0.485397     3.569316     3.846649       7.34
 O       1.358750     3.852359     4.867290     138.14
 H       1.318009     4.811034     5.248845      20.01
 C      -0.279235     4.589289     3.250486      64.53
 H       0.045574     5.862406     3.053021      18.55
 C      -1.871844     2.927706     2.167920      37.13
 C      -2.988430     2.610157     1.315454     114.74
 H      -3.638970     3.329486     1.232919      31.12
 O      -3.726247     1.687993     2.092905     180.71
 H      -4.544556     1.170285     1.618708      25.45
 C      -2.701486     2.266994    -0.192102      84.11
 H      -2.046443     3.046741    -0.553213      26.73
 C      -3.860089     2.266322    -1.149801      82.16
 O      -5.088849     1.283888    -0.647636     244.01
 H      -4.629068     0.457357    -0.803075      30.05
 H      -3.642849     1.649124    -2.059318      28.83
 H      -4.251661     3.271615    -1.259654      28.32
 C       1.690332     1.489470    -1.144224      21.65
 H       2.740624     2.049080    -0.935153      28.13
 C       0.989029    -0.826870    -1.517856      67.06
 H       1.364363    -2.000948    -1.522720      24.18
 C      -0.251750    -0.615823    -1.057136      29.00
 O      -1.250878    -1.547451    -0.883226     216.25
 C      -0.971422    -2.920393    -1.335345     100.92
 H       0.038977    -3.143143    -0.877148      28.09
 H      -1.567943    -3.582500    -0.933323      30.43
 H      -1.206201    -2.710397    -2.580568      25.24
 C      -0.730357     0.723475    -0.669563      -0.10
 O      -1.999114     0.896642    -0.209587     124.15
 C       0.271018     1.804013    -0.800382      33.76
 H       0.062504     2.573458     0.207652      26.89
 C       1.971547     0.185278    -1.621903      14.68
 C       3.500147    -0.304963    -2.127433      92.31
 H       3.561585    -0.725090    -3.068767      31.71
 O       4.461799     0.918235    -2.425672      23.66
 H       4.985758     1.429005    -1.571791      24.83
 C       4.105500    -1.186084    -1.087144     111.36
 H       3.515379    -2.216383    -1.027898      28.75
 O       5.534601    -1.428666    -1.322870     233.43
 H       5.690132    -2.337305    -0.880455      25.43
 C       3.945908    -0.754600     0.368501     150.16
 O       4.618502     0.448278     0.693873     174.13
 H       3.979938     1.058340     1.214202      29.62
 H       4.272898    -1.464984     1.020207      34.99
 H       2.933957    -0.783657     0.522977      32.55
55
name = lig-Water-frame_899
 C      -1.367174     4.215978     2.356034      68.88
 H      -1.719753     5.025353     1.902662      28.30
 C      -1.175739     1.954521     2.883099      66.64
 H      -1.622304     0.923418     2.663323      30.06
 C      -0.058926     2.214283     3.796770     -11.47
 O       0.645220     1.295390     4.597618     100.64
 C       0.293874    -0.101089     4.270511     129.66
 H       1.067664    -0.788232     4.596102      31.49
 H       0.071194    -0.186244     3.170109      30.80
 H      -0.507241    -0.422328     5.026621      30.00
 C       0.441141     3.566813     3.878114       1.29
 O       1.340821     3.868469     4.847639     156.54
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 H       1.430827     4.731787     5.197195      22.80
 C      -0.270572     4.622870     3.213576      63.98
 H       0.147003     5.498226     3.214673      21.40
 C      -1.792802     2.961422     2.151425      65.23
 C      -2.985241     2.659541     1.296313      86.85
 H      -3.784439     3.651028     1.132818      26.57
 O      -3.705555     1.646585     2.123109     208.80
 H      -4.334301     1.169160     1.645196      32.08
 C      -2.644906     2.250885    -0.213284      83.08
 H      -1.984235     2.963774    -0.793935      24.87
 C      -3.921747     2.253137    -1.167692      73.89
 O      -5.090928     1.380686    -0.688871     274.88
 H      -4.504046     0.561902    -0.654547      29.37
 H      -3.445982     1.541587    -2.005570      28.14
 H      -4.269988     3.249651    -1.217596      28.87
 C       1.677874     1.464661    -1.193403      47.03
 H       2.361541     2.150415    -0.836466      31.26
 C       1.039907    -0.835057    -1.604790      87.55
 H       1.397903    -1.748680    -1.482003      28.04
 C      -0.265888    -0.603111    -1.019326      20.53
 O      -1.237807    -1.502511    -0.893991     206.06
 C      -1.004246    -2.858616    -1.417673     102.97
 H      -0.036492    -3.312401    -1.211973      28.87
 H      -1.572652    -3.860101    -0.796144      25.36
 H      -1.020332    -2.641046    -2.411918      30.00
 C      -0.765528     0.740438    -0.750660      13.73
 O      -1.956998     0.902180    -0.217140     157.31
 C       0.194259     1.810577    -0.793629      29.14
 H       0.178477     2.564136    -0.177384      30.97
 C       1.996740     0.181233    -1.634964      15.58
 C       3.473176    -0.233278    -2.119399      93.74
 H       3.584864    -0.740766    -3.216240      26.13
 O       4.458498     0.947287    -2.426600     120.80
 H       4.677154     1.276697    -1.533066      32.06
 C       4.172218    -1.247309    -1.105697     109.85
 H       3.692638    -2.269606    -1.129872      29.40
 O       5.551293    -1.397310    -1.326606     207.16
 H       5.666989    -2.292770    -0.929270      27.44
 C       3.990826    -0.750300     0.376673     115.76
 O       4.635302     0.471860     0.736249     139.47
 H       4.083943     1.041596     1.282080      31.46
 H       4.427408    -1.684110     1.130718      29.02
 H       2.756756    -0.813186     0.494938      30.06
55
name = lig-Water-frame_900
 C      -1.314046     4.233395     2.386325      72.45
 H      -2.003354     5.121215     1.937055      27.30
 C      -1.161990     1.966032     2.931447      44.36
 H      -1.626441     1.039195     2.833498      32.95
 C      -0.045789     2.260146     3.723056     -11.05
 O       0.633696     1.295331     4.617082     102.28
 C       0.330879    -0.154946     4.266626     117.53
 H       1.265949    -0.763110     4.738060      25.44
 H      -0.172134    -0.177838     3.320666      26.42
 H      -0.650408    -0.240944     4.821497      25.77
 C       0.340219     3.590582     3.919733      20.68
 O       1.366420     3.854596     4.846586      32.23
 H       1.263457     4.890056     5.075575      25.80
 C      -0.270247     4.560867     3.160438      62.90
 H       0.325862     5.704196     3.381118      20.23
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 C      -1.720596     2.973998     2.143325      -0.20
 C      -3.021642     2.721224     1.253026      91.89
 H      -3.457967     3.588585     1.210833      32.64
 O      -3.683414     1.603726     2.145403     192.45
 H      -4.323475     1.227027     1.441674      29.32
 C      -2.609014     2.229447    -0.222311      97.68
 H      -1.927354     2.925840    -0.759125      27.73
 C      -3.963861     2.159142    -1.153712      96.13
 O      -5.044954     1.485358    -0.728990     260.98
 H      -4.805256     0.497746    -0.422766      28.14
 H      -3.404486     1.933458    -2.156271      29.56
 H      -4.216197     3.221048    -1.507276      28.64
 C       1.567368     1.454521    -1.218540      68.86
 H       2.175994     2.423725    -0.954513      30.91
 C       1.049764    -0.829806    -1.649383      65.78
 H       1.486627    -1.972758    -1.691902      24.81
 C      -0.265739    -0.544550    -1.025754      14.40
 O      -1.252514    -1.507161    -0.876511     193.09
 C      -1.011766    -2.840553    -1.452043     105.07
 H       0.052241    -3.252759    -1.536243      26.47
 H      -1.764458    -3.447039    -1.079548      28.64
 H      -1.082456    -2.863198    -2.726177      25.67
 C      -0.702804     0.786131    -0.842666      33.03
 O      -1.978602     0.910010    -0.213644     187.03
 C       0.222451     1.743791    -0.806893      48.74
 H       0.098128     2.982928    -0.462835      26.99
 C       2.072257     0.194374    -1.673981      16.67
 C       3.483858    -0.146802    -2.133223     108.70
 H       3.274496    -0.697674    -3.068458      28.27
 O       4.416159     0.949269    -2.407549     150.37
 H       4.476482     1.274689    -1.485100      33.49
 C       4.213960    -1.260628    -1.086293     100.90
 H       3.721031    -2.323448    -1.340016      28.55
 O       5.587567    -1.370466    -1.340929     167.20
 H       5.950644    -2.326445    -1.161513      22.26
 C       3.988880    -0.814053     0.411727     135.40
 O       4.658858     0.491957     0.763939     127.25
 H       4.026809     1.114440     1.235009      33.32
 H       4.413757    -1.547335     0.959918      35.37
 H       3.024554    -0.651951     0.621816      32.50
55
name = lig-Water-frame_901
 C      -1.313868     4.362560     2.353534      46.48
 H      -2.041043     5.016613     1.992173      26.52
 C      -1.130210     1.957140     2.965748      48.71
 H      -1.590057     0.929819     3.059145      31.22
 C      -0.022630     2.262501     3.697944      14.46
 O       0.616936     1.301375     4.601285      84.37
 C       0.329758    -0.161159     4.313883     127.15
 H       1.143038    -0.703733     4.561899      30.97
 H       0.048151    -0.376088     3.199790      28.92
 H      -0.622301    -0.394764     4.838264      27.03
 C       0.280167     3.595418     3.977833      23.14
 O       1.388760     3.860531     4.845166     100.68
 H       1.108068     4.772290     5.068401      27.61
 C      -0.196554     4.568875     3.156079      74.81
 H       0.004293     5.564730     3.367322      25.39
 C      -1.707750     2.948818     2.122559     -10.85
 C      -2.959009     2.707882     1.256816      78.11
 H      -3.566056     3.829110     1.270628      25.41
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 O      -3.671671     1.583467     2.116861     132.69
 H      -4.436597     1.334566     1.413552      27.19
 C      -2.636933     2.209244    -0.224055     107.62
 H      -1.979976     3.006079    -0.574409      27.60
 C      -3.888039     2.133994    -1.178953     103.78
 O      -5.035385     1.540184    -0.736931     282.21
 H      -5.068538     0.674698    -0.459694      33.93
 H      -3.623082     1.825854    -2.306624      28.32
 H      -4.201645     3.080704    -1.476562      29.52
 C       1.498335     1.487253    -1.232630      66.32
 H       2.117615     2.360504    -1.420125      28.97
 C       1.061702    -0.836477    -1.644713      60.88
 H       1.242504    -1.788244    -2.072515      26.15
 C      -0.231014    -0.520999    -1.100582      10.33
 O      -1.258658    -1.532130    -0.862968     176.46
 C      -0.994439    -2.805030    -1.575865     105.06
 H       0.017302    -3.127318    -1.390052      26.82
 H      -2.073891    -3.358583    -1.145640      23.45
 H      -1.395865    -2.936086    -2.528313      27.60
 C      -0.693988     0.800221    -0.877228       8.45
 O      -2.004447     0.914804    -0.217386     152.51
 C       0.313313     1.772836    -0.822896      80.14
 H      -0.085935     2.672954    -0.925185      33.00
 C       2.094959     0.229019    -1.692403      17.72
 C       3.507249    -0.103040    -2.132684     106.98
 H       3.187219    -0.669534    -3.106479      26.68
 O       4.353355     0.941299    -2.375490     119.09
 H       4.451012     1.557691    -1.431411      27.55
 C       4.207117    -1.242929    -1.075322      96.59
 H       3.709232    -2.164808    -1.320047      30.53
 O       5.659400    -1.342879    -1.364089     176.46
 H       6.024075    -2.253498    -1.392133      25.34
 C       3.997293    -0.849474     0.421031      96.34
 O       4.686088     0.497829     0.778162     148.49
 H       3.917919     1.131532     1.000031      32.05
 H       4.560921    -1.726077     1.156311      27.56
 H       2.875007    -0.587756     0.842893      28.11
55
name = lig-Water-frame_902
 C      -1.334241     4.397052     2.292845      35.23
 H      -2.004073     5.267199     1.892891      25.48
 C      -1.125982     1.930764     2.950731      54.81
 H      -1.490395     0.928416     3.134652      31.77
 C       0.013621     2.226615     3.748971      20.73
 O       0.599660     1.297826     4.558098     107.28
 C       0.279759    -0.126401     4.329400     131.40
 H       1.294403    -0.813344     4.581535      26.55
 H       0.447022    -0.417003     3.305544      30.23
 H      -0.479048    -0.705828     5.009860      25.93
 C       0.309784     3.568858     4.032371      13.60
 O       1.385047     3.875003     4.841843     114.60
 H       1.191604     4.740350     5.354922      25.40
 C      -0.174871     4.621394     3.153386      36.14
 H      -0.040125     5.842055     3.439932      18.89
 C      -1.704883     2.971580     2.121499      23.48
 C      -2.894466     2.676335     1.306214      97.77
 H      -3.562249     3.419188     1.248877      31.72
 O      -3.677751     1.592068     2.041527     194.45
 H      -4.470218     1.428870     1.635739      29.93
 C      -2.690311     2.201464    -0.225101     100.53
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 H      -2.034875     3.113026    -0.494476      25.81
 C      -3.751651     2.145531    -1.251851      92.27
 O      -5.085196     1.586628    -0.715407     204.36
 H      -4.983181     0.546034    -0.550104      27.74
 H      -3.780650     1.412346    -2.122734      25.82
 H      -4.157032     3.226767    -1.294903      26.78
 C       1.618220     1.511740    -1.315801      46.36
 H       2.216130     2.306147    -1.752160      29.03
 C       1.083957    -0.793055    -1.637411      74.67
 H       1.093937    -1.721436    -2.364366      24.95
 C      -0.234530    -0.536555    -1.194262       9.52
 O      -1.231909    -1.539096    -0.881141     173.50
 C      -1.063444    -2.784867    -1.646823     109.80
 H      -0.127608    -3.240645    -1.204174      26.37
 H      -1.693166    -3.438497    -1.077407      28.27
 H      -1.478826    -2.709492    -2.799208      26.17
 C      -0.717150     0.774938    -0.837295      -2.31
 O      -1.994087     0.911056    -0.239666     128.55
 C       0.274732     1.814843    -0.845187      14.37
 H      -0.220287     2.895564    -1.144236      29.77
 C       2.020317     0.246654    -1.668451      38.92
 C       3.499399    -0.129041    -2.104730     100.95
 H       3.512540    -0.588732    -3.171477      27.41
 O       4.311174     0.985851    -2.336022     138.81
 H       4.454750     1.547277    -1.675570      35.01
 C       4.198983    -1.181054    -1.075026      82.99
 H       3.605527    -2.258062    -1.240586      27.94
 O       5.722743    -1.296657    -1.390207     157.49
 H       5.847972    -2.275251    -1.444352      26.53
 C       4.021092    -0.860626     0.478300     122.40
 O       4.695306     0.477255     0.775125     205.94
 H       3.990941     1.125694     0.803576      35.11
 H       4.426178    -1.545062     1.051829      33.64
 H       3.041725    -0.898953     0.750263      32.44
55
name = lig-Water-frame_903
 C      -1.325509     4.374927     2.256078      56.65
 H      -1.695849     5.302271     1.761752      23.51
 C      -1.102870     1.940686     2.918824      73.44
 H      -1.528520     0.931424     2.925607      29.32
 C      -0.001689     2.204040     3.800690      18.50
 O       0.596026     1.259343     4.533700     163.97
 C       0.311472    -0.146177     4.361689     132.95
 H       1.169736    -0.497164     4.807014      28.09
 H       0.417641    -0.345410     3.233213      27.07
 H      -0.425353    -0.625677     4.920764      27.79
 C       0.370638     3.594805     4.023984     -11.84
 O       1.388789     3.895042     4.868032     152.17
 H       1.251774     4.619053     5.592176      20.61
 C      -0.228904     4.690437     3.158562      35.31
 H       0.112902     5.707687     3.503349      21.10
 C      -1.690562     3.021744     2.153726      33.39
 C      -2.897964     2.561791     1.331717      99.03
 H      -3.717193     3.479457     1.210259      25.96
 O      -3.667552     1.604688     1.978876     190.01
 H      -4.668955     1.574055     1.639961      23.82
 C      -2.666840     2.211049    -0.207771      94.50
 H      -2.036929     2.984869    -0.580356      28.76
 C      -3.725470     2.156276    -1.287120      86.58
 O      -5.136227     1.609643    -0.673026     243.85
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 H      -4.741763     0.683138    -0.719851      26.46
 H      -3.430287     1.417691    -2.046997      28.04
 H      -3.899060     3.205936    -1.493450      27.99
 C       1.720497     1.567381    -1.403673      33.69
 H       2.417460     2.371699    -1.837013      23.57
 C       1.056975    -0.773999    -1.656778      74.75
 H       1.225485    -1.598350    -2.399317      26.21
 C      -0.289208    -0.552881    -1.247783      18.44
 O      -1.189348    -1.529764    -0.932966     200.91
 C      -1.141840    -2.778983    -1.679797     116.90
 H      -0.193708    -3.322334    -1.558007      28.10
 H      -1.764832    -3.686079    -1.039240      24.16
 H      -1.090358    -2.537198    -2.737894      29.79
 C      -0.707145     0.761589    -0.756532      19.60
 O      -1.961660     0.896005    -0.273071     148.26
 C       0.201679     1.868677    -0.928039      33.86
 H       0.000803     2.918008    -0.976335      26.29
 C       1.979268     0.221997    -1.651174      30.73
 C       3.485303    -0.172879    -2.060643      82.12
 H       3.652795    -0.639551    -3.075994      28.03
 O       4.289302     1.050225    -2.334847      23.86
 H       4.464203     1.671678    -1.458056      27.44
 C       4.191739    -1.129289    -1.063741      88.06
 H       3.777848    -2.083993    -1.180552      29.90
 O       5.740563    -1.253315    -1.410822     140.02
 H       5.733962    -2.270622    -1.360959      27.49
 C       4.071934    -0.817237     0.480763      91.61
 O       4.687018     0.426899     0.766583     192.10
 H       4.046110     1.211241     0.736510      30.05
 H       4.677574    -1.726462     1.168852      25.05
 H       2.876362    -1.045267     0.672509      25.84
55
name = lig-Water-frame_904
 C      -1.254130     4.367449     2.253691      74.10
 H      -1.617276     5.123141     1.560176      26.89
 C      -1.061623     1.987552     2.892074      83.21
 H      -1.549918     1.017140     2.581833      28.09
 C      -0.063732     2.234231     3.820527     -24.05
 O       0.606837     1.225934     4.542110      97.70
 C       0.389008    -0.174244     4.364722     109.35
 H       1.295944    -0.458924     5.121186      25.92
 H       0.209795    -0.398072     3.336460      30.69
 H      -0.759943    -0.388642     4.787686      27.95
 C       0.389567     3.658734     3.943689      19.06
 O       1.423103     3.903102     4.929297     196.86
 H       1.073454     4.619778     5.499643      20.93
 C      -0.282612     4.670816     3.206327      67.25
 H       0.195145     5.741504     3.455608      14.30
 C      -1.697922     3.028117     2.186645      33.19
 C      -2.966451     2.521187     1.292002      99.65
 H      -3.417834     3.473011     1.223013      30.31
 O      -3.683878     1.573540     1.949825     193.11
 H      -4.614655     1.768669     1.546978      24.86
 C      -2.587171     2.204884    -0.177295      86.16
 H      -1.833406     2.931942    -0.671886      25.50
 C      -3.776655     2.163894    -1.263701      68.44
 O      -5.123134     1.631240    -0.658901     311.03
 H      -4.843066     0.711250    -0.666673      28.43
 H      -3.039629     1.637246    -2.060172      25.36
 H      -3.786361     3.097860    -1.888812      26.34
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 C       1.699066     1.624629    -1.463174      35.33
 H       2.470600     2.297555    -1.561630      21.24
 C       0.972631    -0.786561    -1.696540      67.00
 H       1.389049    -1.688426    -2.239788      24.14
 C      -0.324804    -0.538191    -1.256917      29.01
 O      -1.174871    -1.540226    -0.990724     233.89
 C      -1.166803    -2.808781    -1.670823     130.87
 H      -0.129819    -3.252673    -1.849137      25.98
 H      -2.067524    -3.465659    -1.497979      27.15
 H      -1.097199    -2.580920    -2.806124      29.28
 C      -0.639523     0.788497    -0.700531      31.04
 O      -1.945010     0.870651    -0.295563     150.89
 C       0.236723     1.877891    -1.051393      63.36
 H       0.039262     2.998092    -0.714283      23.11
 C       2.028973     0.222170    -1.661928      20.97
 C       3.483666    -0.173032    -2.013132      77.66
 H       3.501735    -0.820895    -3.022297      26.48
 O       4.273502     1.126048    -2.328190      39.51
 H       4.403058     1.523575    -1.347033      27.34
 C       4.231021    -1.062974    -1.023119      88.88
 H       3.850334    -2.242483    -1.224727      25.21
 O       5.705436    -1.221831    -1.419585     143.71
 H       5.939492    -2.153602    -1.234246      29.94
 C       4.114408    -0.829774     0.465933     128.55
 O       4.672945     0.394248     0.769611     250.61
 H       4.052916     1.172168     0.794222      30.34
 H       4.666889    -1.478605     0.912700      30.59
 H       3.116896    -0.857070     0.718871      30.35
55
name = lig-Water-frame_905
 C      -1.197438     4.350719     2.251209      59.61
 H      -1.658593     4.978858     1.377718      22.72
 C      -1.048879     2.022352     2.850750      78.09
 H      -1.327933     1.059439     2.523116      27.74
 C      -0.096370     2.287870     3.833662      -2.29
 O       0.629536     1.251594     4.553280      58.06
 C       0.411054    -0.191377     4.413457     127.90
 H       1.053290    -0.779646     4.962789      30.99
 H       0.366287    -0.645013     3.342649      28.63
 H      -0.562756    -0.241867     4.683917      30.51
 C       0.399337     3.664509     3.892221      13.20
 O       1.438313     3.905436     4.978438     142.13
 H       0.984743     4.797230     5.357086      19.41
 C      -0.287032     4.650162     3.284508      80.09
 H       0.135082     5.768839     3.165329      17.06
 C      -1.729207     3.009215     2.188070      27.20
 C      -2.933570     2.576020     1.233713      78.14
 H      -3.477045     3.631765     1.170642      27.22
 O      -3.742633     1.524864     1.936166     200.36
 H      -4.558968     1.631437     1.527134      28.37
 C      -2.512112     2.198379    -0.183598      99.05
 H      -1.813687     2.899610    -0.500003      27.28
 C      -3.787184     2.169115    -1.215864      82.90
 O      -5.045223     1.662443    -0.683299     333.08
 H      -5.104951     0.617823    -0.493432      26.98
 H      -3.340008     1.499040    -1.937683      27.94
 H      -4.020073     3.009690    -1.927511      25.31
 C       1.601334     1.607300    -1.494982      56.66
 H       2.435375     2.395728    -1.219549      21.80
 C       0.946435    -0.777119    -1.761056      51.78
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 H       1.327190    -1.905846    -1.819524      23.25
 C      -0.306532    -0.502032    -1.240614      12.12
 O      -1.215418    -1.573809    -1.029283     209.19
 C      -1.139046    -2.808660    -1.753039     116.32
 H      -0.159442    -3.356939    -1.596279      25.83
 H      -2.276086    -3.318504    -1.663874      23.64
 H      -1.494469    -2.640593    -2.833393      27.25
 C      -0.552900     0.821333    -0.711511      17.86
 O      -1.935752     0.849790    -0.295982     146.31
 C       0.338546     1.889179    -1.158841      75.67
 H       0.046808     2.736643    -0.485450      23.94
 C       2.058557     0.255046    -1.686508      20.64
 C       3.492611    -0.135147    -1.999875      92.92
 H       3.349714    -0.722250    -2.898182      30.07
 O       4.247159     1.164866    -2.303652     110.14
 H       4.457982     1.487150    -1.491583      32.80
 C       4.290052    -1.084394    -1.007865     118.17
 H       3.866807    -1.994785    -1.172127      31.34
 O       5.656060    -1.182600    -1.415546     174.35
 H       6.091682    -2.006540    -1.076902      28.24
 C       4.136931    -0.828224     0.415442     102.07
 O       4.685789     0.421723     0.793365     187.05
 H       3.957126     1.038150     0.943092      30.16
 H       4.873512    -1.740084     0.984894      25.14
 H       3.041810    -0.794653     0.900893      25.12
55
name = lig-Water-frame_906
 C      -1.205345     4.297489     2.230119      71.98
 H      -1.535861     5.034907     1.587854      26.94
 C      -1.043156     2.012284     2.828024      52.26
 H      -1.092097     0.877063     2.659529      24.32
 C      -0.078417     2.317545     3.832306      13.61
 O       0.671735     1.312283     4.560220      42.40
 C       0.390290    -0.195804     4.409487     107.95
 H       1.003644    -1.034121     5.020860      25.82
 H       0.709579    -0.618182     3.466103      27.58
 H      -0.755514    -0.409628     4.834659      24.20
 C       0.450346     3.599175     3.957747      13.72
 O       1.403860     3.918080     4.987807     121.38
 H       1.297301     4.855366     5.362212      26.07
 C      -0.282529     4.689165     3.277484      57.41
 H       0.097111     5.686795     3.186212      16.67
 C      -1.766538     3.015290     2.148323      45.85
 C      -2.866706     2.671882     1.214374      79.51
 H      -3.662921     3.434235     1.067674      26.27
 O      -3.788250     1.503314     1.920836     112.96
 H      -4.724123     1.355956     1.383697      22.83
 C      -2.495251     2.186458    -0.212746      90.83
 H      -1.742483     3.050068    -0.460438      24.05
 C      -3.760558     2.125855    -1.177615      96.67
 O      -4.976409     1.695248    -0.695425     311.71
 H      -5.049074     0.762706    -0.473623      30.92
 H      -3.757280     1.163167    -1.887575      22.12
 H      -4.138409     3.003772    -1.551852      24.96
 C       1.618267     1.561800    -1.512409      60.92
 H       2.173439     2.376471    -1.161834      20.94
 C       1.014445    -0.758552    -1.793568      60.04
 H       1.138516    -1.813484    -1.640864      21.98
 C      -0.264177    -0.489824    -1.218358       7.24
 O      -1.271881    -1.583229    -1.052442     178.93
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 C      -1.159173    -2.805563    -1.869699     115.86
 H      -0.426359    -3.518135    -1.428168      26.34
 H      -2.066489    -3.281178    -1.334010      25.82
 H      -1.408087    -2.676763    -2.920737      28.55
 C      -0.517797     0.818676    -0.794939      26.47
 O      -1.898158     0.856124    -0.281964     159.32
 C       0.330948     1.878575    -1.160751      68.61
 H       0.205324     2.785533    -0.574966      21.72
 C       2.010926     0.267258    -1.720697      27.87
 C       3.520948    -0.048013    -1.985702      72.45
 H       3.388229    -0.598091    -3.089299      26.58
 O       4.209359     1.154993    -2.298528     103.81
 H       4.679867     1.697594    -1.400591      23.40
 C       4.313374    -1.109162    -1.038216      97.45
 H       3.623315    -2.175942    -1.193299      26.16
 O       5.634320    -1.134215    -1.408188     165.73
 H       6.054164    -1.902778    -0.897089      27.66
 C       4.171101    -0.854964     0.453080     120.77
 O       4.714385     0.483413     0.827844     236.12
 H       3.897759     0.981296     1.176276      25.89
 H       4.615838    -1.595809     0.893884      31.65
 H       3.178030    -1.017420     0.811416      27.90
55
name = lig-Water-frame_907
 C      -1.219472     4.275060     2.249924      59.37
 H      -1.561281     5.301876     1.753389      26.20
 C      -1.022814     1.960851     2.837863      65.41
 H      -1.138678     0.918325     2.775883      28.01
 C      -0.030763     2.294135     3.807256       9.44
 O       0.716034     1.347260     4.573787       6.64
 C       0.341600    -0.214120     4.429660     112.25
 H       0.967248    -0.574076     5.219147      29.59
 H       0.778277    -0.387400     3.394956      28.61
 H      -0.595851    -0.519663     4.600588      29.61
 C       0.475619     3.620438     4.069686       7.43
 O       1.375191     3.902746     4.969873      96.39
 H       1.359757     4.847860     5.355682      26.81
 C      -0.260708     4.651600     3.217995      61.88
 H       0.186748     5.856855     3.422458      14.46
 C      -1.772419     2.999534     2.108965      51.70
 C      -2.872083     2.696477     1.192275      84.97
 H      -3.655867     3.392119     1.051460      27.15
 O      -3.824220     1.503588     1.901318     140.07
 H      -4.529266     1.280615     1.254384      26.11
 C      -2.491609     2.190720    -0.246325      98.90
 H      -1.874482     2.937058    -0.664511      26.76
 C      -3.704910     2.024549    -1.178793     108.99
 O      -4.983369     1.724677    -0.641491     325.32
 H      -4.831591     0.751819    -0.528405      29.88
 H      -3.504038     1.439034    -2.036517      29.79
 H      -3.844358     3.217712    -1.368368      25.75
 C       1.657000     1.543665    -1.508889      50.59
 H       2.390705     2.405398    -1.382921      20.35
 C       1.065385    -0.739112    -1.769322      72.94
 H       1.272530    -1.950173    -1.783319      24.13
 C      -0.210905    -0.525033    -1.226595      20.29
 O      -1.298029    -1.548174    -1.082448     154.57
 C      -1.211179    -2.797901    -1.907787     105.59
 H      -0.468626    -3.599116    -1.564450      26.51
 H      -2.115076    -3.417718    -1.255812      23.81
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 H      -1.012609    -2.815977    -3.109336      25.54
 C      -0.585562     0.796570    -0.897346      30.50
 O      -1.825416     0.890613    -0.259943     149.15
 C       0.263479     1.856271    -1.089969      69.33
 H       0.296114     3.031535    -0.897938      25.43
 C       1.996656     0.231451    -1.768408      43.81
 C       3.535676     0.017779    -2.007173     103.41
 H       3.608917    -0.405076    -2.990483      30.06
 O       4.205469     1.159786    -2.279567     180.91
 H       4.578619     1.707320    -1.608817      28.72
 C       4.222381    -1.129794    -1.078491      97.11
 H       3.802027    -2.035278    -1.242833      32.71
 O       5.653736    -1.099491    -1.396102     135.48
 H       5.993876    -1.821891    -0.869026      30.34
 C       4.196543    -0.845434     0.484379      99.47
 O       4.726167     0.531200     0.869832     165.44
 H       4.037724     1.044998     1.374123      27.40
 H       4.818258    -1.788820     1.145824      26.92
 H       3.059825    -1.088485     0.714991      27.00
55
name = lig-Water-frame_908
 C      -1.237693     4.334345     2.290018      50.09
 H      -1.743293     5.127644     1.868180      26.95
 C      -1.001742     1.938733     2.861482      58.57
 H      -1.426132     0.882131     2.758413      33.55
 C       0.044481     2.267068     3.784523     -18.12
 O       0.729021     1.346438     4.589757      76.88
 C       0.360447    -0.168274     4.440398     116.52
 H       0.997674    -0.255791     5.373831      22.76
 H       0.704076    -0.353755     3.428137      29.28
 H      -0.832335    -0.546602     4.346719      24.64
 C       0.384573     3.682904     4.082565      13.83
 O       1.398607     3.867831     4.973251      89.93
 H       1.117712     4.833662     5.346273      17.55
 C      -0.171383     4.586176     3.207413      60.36
 H       0.029921     5.545535     3.420204      31.61
 C      -1.721303     2.952065     2.104125      -9.11
 C      -2.931459     2.629725     1.160705      78.03
 H      -3.582159     3.666312     1.104866      25.90
 O      -3.823552     1.530549     1.875546     163.57
 H      -4.391522     1.379259     1.117596      29.00
 C      -2.500361     2.165792    -0.267228      91.91
 H      -1.886880     2.887952    -0.921652      26.41
 C      -3.643388     2.038659    -1.199846     112.48
 O      -5.000985     1.713634    -0.566841     256.19
 H      -4.880316     0.652568    -0.629488      27.58
 H      -3.144117     1.768252    -2.260952      28.28
 H      -3.549648     3.012439    -1.464063      30.42
 C       1.637155     1.568377    -1.470857      45.16
 H       2.508269     2.189694    -1.804290      23.55
 C       1.075821    -0.828577    -1.716277      76.25
 H       1.492640    -1.723025    -2.068955      29.40
 C      -0.194335    -0.583084    -1.259848      24.40
 O      -1.284537    -1.502911    -1.137982     182.20
 C      -1.251768    -2.819332    -1.887984     122.28
 H      -0.302816    -3.403078    -1.661385      26.67
 H      -2.242039    -3.397434    -1.835976      26.83
 H      -0.960631    -2.793531    -2.880894      29.62
 C      -0.692599     0.777908    -0.978118      18.89
 O      -1.752537     0.924725    -0.222755     125.29
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 C       0.299159     1.868845    -1.041803      72.65
 H      -0.011894     2.856680    -1.110134      29.21
 C       2.066128     0.230044    -1.813314      30.43
 C       3.513410     0.009223    -2.029344      87.78
 H       3.763072    -0.561924    -3.106470      25.68
 O       4.238320     1.203518    -2.281579     119.94
 H       4.484767     1.815637    -1.439361      25.46
 C       4.160327    -1.061676    -1.073568      68.36
 H       3.841899    -2.255039    -1.404897      28.06
 O       5.678267    -1.071054    -1.386161      94.60
 H       6.051374    -1.863180    -0.907819      25.00
 C       4.202795    -0.856140     0.531627     126.43
 O       4.726939     0.541040     0.907771     134.09
 H       4.133469     1.091175     1.446295      31.43
 H       4.793481    -1.446713     1.008932      35.59
 H       3.135756    -0.872858     0.792148      28.88
55
name = lig-Water-frame_909
 C      -1.266815     4.325510     2.339919      47.13
 H      -1.972075     5.106060     1.831605      23.53
 C      -0.993901     1.923817     2.878412      53.62
 H      -1.550268     1.001221     2.789081      31.73
 C       0.097265     2.260494     3.762235      25.85
 O       0.708482     1.335992     4.597285     114.75
 C       0.375047    -0.077659     4.445743     135.25
 H       0.866939    -0.597125     5.337520      27.82
 H       0.853679    -0.561792     3.532416      28.23
 H      -0.610723    -0.247384     4.428771      29.14
 C       0.295525     3.627714     4.047773      25.84
 O       1.416102     3.855623     4.986846     147.90
 H       1.182078     4.717119     5.488362      21.44
 C      -0.120678     4.540694     3.182112      57.49
 H      -0.006570     5.821234     3.417676      24.89
 C      -1.640679     2.933175     2.119141       0.01
 C      -2.967977     2.574041     1.178448      93.86
 H      -3.348919     3.493058     1.122698      31.55
 O      -3.791826     1.591189     1.827246     159.82
 H      -4.513287     1.443695     0.993085      21.15
 C      -2.495460     2.136134    -0.280084     110.63
 H      -1.849156     2.880325    -0.731840      26.52
 C      -3.597948     2.104276    -1.248057      76.08
 O      -4.976345     1.661180    -0.532682     249.52
 H      -5.158275     0.754168    -0.666523      32.22
 H      -3.338448     1.573133    -2.145910      29.74
 H      -3.836018     3.236209    -1.625102      26.19
 C       1.627073     1.561197    -1.464886      64.76
 H       2.265158     2.268908    -1.941418      26.36
 C       1.134227    -0.906190    -1.671652      55.28
 H       1.562861    -1.779801    -2.426304      25.05
 C      -0.247044    -0.622030    -1.300060      11.99
 O      -1.271971    -1.485439    -1.207435     157.81
 C      -1.246174    -2.825921    -1.864373      98.48
 H      -0.296709    -3.283194    -1.409246      24.43
 H      -2.352539    -3.360731    -2.095106      23.64
 H      -1.045821    -2.461291    -3.056815      26.32
 C      -0.667795     0.767644    -1.048310      -2.78
 O      -1.731031     0.935237    -0.155751     141.33
 C       0.354046     1.844346    -1.040290      66.79
 H      -0.330552     2.801963    -1.145570      22.74
 C       2.069319     0.253115    -1.808350       8.67
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 C       3.522080    -0.048924    -2.094772      92.26
 H       3.592381    -0.580797    -2.969914      30.03
 O       4.299261     1.264784    -2.278620     110.89
 H       4.260648     1.754858    -1.314508      25.25
 C       4.179313    -1.019415    -1.037552      89.35
 H       3.811985    -1.896174    -1.286550      32.42
 O       5.686515    -1.041701    -1.371432     113.51
 H       6.061532    -1.919074    -1.040089      24.53
 C       4.153000    -0.777453     0.533433     108.55
 O       4.737843     0.525529     0.933347     138.04
 H       4.013088     1.077420     1.415491      29.57
 H       4.998217    -1.614646     1.060404      26.35
 H       3.147266    -0.784233     1.066747      27.44
55
name = lig-Water-frame_910
 C      -1.304155     4.263516     2.366632      56.51
 H      -1.871305     5.056565     1.901048      25.34
 C      -0.987288     1.925270     2.885538      61.78
 H      -1.418017     0.924466     2.882642      29.73
 C       0.082583     2.221257     3.732585      44.45
 O       0.697622     1.322022     4.611406     166.04
 C       0.430454    -0.013175     4.450918     138.46
 H       0.656680    -0.801345     5.242055      28.18
 H       0.952605    -0.615629     3.691636      29.99
 H      -0.797839    -0.055606     4.545863      25.66
 C       0.335383     3.524222     4.061883       7.29
 O       1.400956     3.832907     4.982151     105.87
 H       1.332568     4.725765     5.528866      19.04
 C      -0.166072     4.637422     3.124440      42.31
 H       0.120393     5.511094     3.346553      26.93
 C      -1.590838     2.934108     2.132699      25.01
 C      -2.902381     2.526895     1.227711      86.32
 H      -3.475954     3.631982     1.052837      26.76
 O      -3.778807     1.650937     1.757294     219.37
 H      -4.471123     1.508568     1.177083      28.65
 C      -2.476986     2.133550    -0.252410     109.78
 H      -1.786450     3.034331    -0.405382      26.17
 C      -3.628599     2.178117    -1.299453      76.59
 O      -4.932021     1.624846    -0.521372     214.42
 H      -5.252237     0.688996    -0.771348      30.23
 H      -3.647659     1.243939    -2.058285      26.22
 H      -4.106733     3.057846    -1.539009      27.45
 C       1.646715     1.551392    -1.501743      74.38
 H       2.048789     2.582773    -1.830065      25.58
 C       1.207327    -0.938392    -1.681124      62.15
 H       1.292272    -1.755836    -2.267155      28.50
 C      -0.267336    -0.625485    -1.361168     -19.20
 O      -1.308147    -1.500559    -1.264940     181.43
 C      -1.199545    -2.771868    -1.900419     126.85
 H      -0.579872    -3.445998    -1.325164      28.29
 H      -2.273290    -3.251621    -1.891713      27.02
 H      -0.961292    -2.546826    -2.821416      31.97
 C      -0.551281     0.745239    -1.062995       6.45
 O      -1.736072     0.916692    -0.100365     127.35
 C       0.315026     1.787167    -1.081588      65.84
 H      -0.007412     2.785356    -0.993071      27.18
 C       2.016831     0.232189    -1.754842      10.85
 C       3.560587    -0.042741    -2.124498      70.07
 H       3.457920    -0.662646    -3.228152      27.49
 O       4.336032     1.278009    -2.272297     121.75
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 H       4.307615     1.688606    -1.480190      32.63
 C       4.258116    -0.939977    -0.980904      77.49
 H       3.581625    -2.039232    -1.125453      28.37
 O       5.674056    -1.019692    -1.349073     171.61
 H       5.968037    -1.912620    -1.168951      24.85
 C       4.135405    -0.695743     0.553724     136.80
 O       4.741668     0.511950     0.959615     207.68
 H       3.983529     1.041035     1.254009      32.08
 H       4.626890    -1.513043     0.807100      34.10
 H       3.220912    -0.926459     1.190593      29.70
55
name = lig-Water-frame_911
 C      -1.308521     4.240523     2.375945      58.77
 H      -1.830019     5.055355     1.847551      25.59
 C      -0.985369     1.904209     2.876289      71.28
 H      -1.190741     0.795645     2.863001      28.02
 C       0.053190     2.163892     3.738827      30.84
 O       0.724583     1.324421     4.641016     169.78
 C       0.410744    -0.038974     4.471243     121.40
 H       0.596628    -0.574169     5.474504      25.40
 H       0.894017    -0.418308     3.533462      29.55
 H      -0.631667    -0.123096     4.334155      27.89
 C       0.432577     3.545507     4.035830       8.18
 O       1.378733     3.790660     4.971983      66.39
 H       1.235735     4.752646     5.233884      22.92
 C      -0.232512     4.630335     3.133125      65.75
 H       0.388959     5.768106     3.339912      20.27
 C      -1.623308     2.887801     2.133270      39.78
 C      -2.809409     2.587416     1.239330     106.32
 H      -3.352651     3.395636     1.086680      31.81
 O      -3.773369     1.672067     1.753179     159.39
 H      -4.577437     1.558258     1.022844      19.40
 C      -2.438564     2.178440    -0.206374      96.10
 H      -1.777363     3.055125    -0.305090      26.79
 C      -3.702328     2.142572    -1.294014      84.64
 O      -4.908634     1.608495    -0.509438     234.04
 H      -4.961789     0.638585    -0.866335      27.41
 H      -3.674701     1.342692    -2.064590      27.97
 H      -4.036400     3.064981    -1.600759      27.49
 C       1.630818     1.573716    -1.549116      50.87
 H       2.179435     2.470707    -1.582650      27.16
 C       1.166744    -0.903441    -1.688609      77.22
 H       1.281082    -2.061065    -2.098575      24.11
 C      -0.210163    -0.611171    -1.428566       8.05
 O      -1.359444    -1.503165    -1.303249     195.89
 C      -1.154570    -2.724470    -1.907040     110.03
 H      -0.786769    -3.683396    -1.321195      26.03
 H      -2.329236    -3.183794    -1.752118      24.74
 H      -0.575430    -2.841618    -3.087624      25.54
 C      -0.509340     0.680819    -0.989985      15.87
 O      -1.733916     0.881538    -0.094712     110.03
 C       0.309310     1.748695    -1.151245      68.51
 H       0.265294     2.831500    -0.746338      24.04
 C       2.043010     0.188108    -1.716622      16.59
 C       3.583789    -0.000475    -2.135934      89.10
 H       3.606835    -0.409873    -3.042921      32.77
 O       4.346695     1.222264    -2.311101      87.16
 H       4.492783     1.854894    -1.371447      24.96
 C       4.269401    -0.899072    -0.968309     111.56
 H       3.839175    -1.776479    -0.935746      35.04
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 O       5.652277    -1.006162    -1.319863     170.22
 H       5.918893    -1.969115    -1.193364      25.34
 C       4.110311    -0.631475     0.551890     117.04
 O       4.745526     0.517790     1.000190     187.54
 H       4.034195     1.197161     1.189943      31.41
 H       4.740670    -1.714467     0.885214      26.21
 H       3.120664    -0.889858     0.970280      28.48
55
name = lig-Water-frame_912
 C      -1.305559     4.247548     2.358439      57.41
 H      -1.857106     5.017551     1.701525      19.06
 C      -0.973124     1.825856     2.860681      73.42
 H      -1.170851     0.822490     2.631101      28.72
 C       0.061825     2.189954     3.801437     -32.41
 O       0.754807     1.340402     4.668747      78.20
 C       0.382310    -0.106279     4.497986      98.00
 H       0.718776    -0.382506     5.482246      27.46
 H       0.889055    -0.318148     3.523462      29.86
 H      -0.756004    -0.319183     4.151666      24.79
 C       0.473434     3.588794     3.911592      35.35
 O       1.363865     3.766142     4.966516     109.19
 H       1.227728     4.774834     5.081095      25.34
 C      -0.202919     4.595327     3.246160      64.50
 H       0.088023     5.519320     3.127213      16.62
 C      -1.685612     2.841948     2.149145      -2.39
 C      -2.750549     2.630358     1.222059      78.64
 H      -3.334544     3.733796     1.097120      25.12
 O      -3.788439     1.661670     1.786104     147.73
 H      -4.314139     1.667286     0.977317      25.43
 C      -2.394188     2.223034    -0.181400      72.51
 H      -1.681977     2.975722    -0.647809      23.00
 C      -3.760390     2.073993    -1.205795      80.77
 O      -4.898755     1.596217    -0.521943     331.85
 H      -4.668957     0.656539    -0.601862      28.42
 H      -3.423653     1.503237    -2.245822      25.92
 H      -3.710910     3.188999    -1.734813      24.30
 C       1.620151     1.533280    -1.596746      40.18
 H       2.522463     2.245141    -1.441969      22.61
 C       1.086560    -0.906404    -1.723934      76.60
 H       1.502843    -1.833798    -1.731121      27.68
 C      -0.183501    -0.599087    -1.456874      20.52
 O      -1.358082    -1.469330    -1.343324     200.48
 C      -1.142218    -2.794700    -1.946057     132.32
 H      -0.683861    -3.471991    -1.252029      29.54
 H      -2.244423    -3.019869    -2.116042      27.40
 H      -0.647448    -2.939208    -2.738644      32.98
 C      -0.560933     0.638434    -0.863817       1.58
 O      -1.715360     0.841028    -0.133639      98.46
 C       0.341630     1.775085    -1.202295      70.16
 H       0.156369     2.634394    -0.523629      23.55
 C       2.131147     0.188857    -1.720247      26.64
 C       3.589652     0.059769    -2.047278      84.61
 H       3.798617    -0.476328    -3.190536      26.15
 O       4.352722     1.175237    -2.343036     167.65
 H       4.671572     1.770152    -1.667914      30.49
 C       4.253220    -0.836700    -0.982398      91.87
 H       3.838887    -2.070555    -1.016529      28.39
 O       5.653726    -1.005210    -1.295544     140.67
 H       5.905254    -1.954109    -1.125489      26.12
 C       4.118127    -0.650575     0.538839     113.37
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 O       4.749409     0.555857     1.061105     201.78
 H       4.125342     1.330421     1.223472      31.86
 H       4.661058    -1.297245     1.055762      30.41
 H       2.944871    -0.624351     0.643857      26.55
55
name = lig-Water-frame_913
 C      -1.288681     4.214683     2.346702      58.92
 H      -1.747801     4.941372     1.766763      23.85
 C      -0.939140     1.768995     2.852896      41.81
 H      -1.240401     0.740964     2.426514      25.78
 C       0.060525     2.238555     3.840591      -2.36
 O       0.754708     1.358554     4.679654      39.58
 C       0.351550    -0.143729     4.492122     104.71
 H       0.889937    -0.616603     5.439244      26.96
 H       1.043352    -0.525838     3.736644      30.37
 H      -0.713840    -0.424088     4.390571      27.53
 C       0.495172     3.556931     3.812677      39.27
 O       1.359256     3.778625     4.950356     162.62
 H       1.415382     4.720188     5.297478      25.29
 C      -0.227460     4.545650     3.296216      82.83
 H       0.000867     5.737872     3.133001      16.36
 C      -1.680770     2.858008     2.220244      32.42
 C      -2.778143     2.686230     1.195027      87.17
 H      -3.115877     3.618407     1.121189      31.07
 O      -3.775856     1.666832     1.816028     156.84
 H      -4.405660     1.631908     1.029216      24.65
 C      -2.366749     2.231997    -0.213004      64.63
 H      -1.744561     2.742672    -0.981262      25.63
 C      -3.708540     2.065143    -1.144168      98.95
 O      -4.894580     1.579717    -0.558483     283.18
 H      -4.657051     0.585492    -0.200818      26.16
 H      -3.252485     1.602823    -2.017965      29.94
 H      -3.790994     3.012469    -1.452376      30.80
 C       1.690085     1.456456    -1.631905      46.68
 H       2.507802     2.133005    -1.469808      25.32
 C       1.124455    -0.874910    -1.768015      84.14
 H       1.657471    -1.912034    -1.527777      26.13
 C      -0.273415    -0.587460    -1.421325      15.72
 O      -1.309982    -1.435389    -1.405189     159.82
 C      -1.175641    -2.871247    -1.937637      70.93
 H      -0.591126    -3.302137    -1.010010      25.31
 H      -2.278753    -3.186934    -2.451931      25.34
 H      -0.399796    -2.837525    -3.037692      24.70
 C      -0.563749     0.687878    -0.789981      15.78
 O      -1.712321     0.803504    -0.177433     144.74
 C       0.314048     1.770073    -1.170294      82.30
 H       0.055494     2.629470    -0.568541      25.69
 C       2.136729     0.209554    -1.757731      31.33
 C       3.610080     0.044875    -1.982025     112.33
 H       3.625644    -0.559460    -2.775559      32.32
 O       4.374776     1.161148    -2.399447     130.37
 H       4.740338     1.768474    -1.647096      25.48
 C       4.246382    -0.878484    -0.982991     119.63
 H       3.804936    -1.721461    -1.233850      34.84
 O       5.682775    -1.006263    -1.285863     149.29
 H       5.898429    -1.895482    -0.999448      28.21
 C       4.081347    -0.605377     0.506609     109.63
 O       4.758293     0.616627     1.122858     188.13
 H       4.075987     1.286560     1.268137      34.03
 H       4.582481    -1.424287     1.330341      25.78
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 H       3.049993    -0.456341     0.610611      28.75
55
name = lig-Water-frame_914
 C      -1.243442     4.158885     2.384634      76.09
 H      -1.745543     5.058608     1.803765      24.05
 C      -0.911068     1.773791     2.844175      73.29
 H      -1.147716     0.784560     2.587735      28.18
 C       0.029501     2.190231     3.814474      -1.81
 O       0.726407     1.349618     4.677313      52.34
 C       0.397399    -0.168585     4.525989     113.11
 H       0.751160    -0.721831     5.341431      30.25
 H       1.041926    -0.712953     3.761433      29.64
 H      -0.726426    -0.381831     4.591362      27.02
 C       0.546783     3.523236     3.838409       0.44
 O       1.379667     3.794247     4.928265     193.52
 H       1.382703     4.686378     5.364103      18.26
 C      -0.309910     4.584633     3.223159      62.39
 H       0.050815     5.585326     3.573305      19.89
 C      -1.638065     2.866523     2.283353      46.66
 C      -2.784023     2.683552     1.196769      66.62
 H      -3.317112     3.784288     1.051867      26.90
 O      -3.741030     1.698712     1.810999     134.36
 H      -4.686779     1.616740     1.337560      25.62
 C      -2.387511     2.170715    -0.276996     100.89
 H      -1.767473     2.774567    -0.919015      28.38
 C      -3.587619     2.078505    -1.065850      73.57
 O      -4.895592     1.548574    -0.584493     267.66
 H      -4.861812     0.638565    -0.234561      30.44
 H      -3.259645     1.349397    -1.987722      25.92
 H      -4.131294     3.203827    -1.218630      24.98
 C       1.703348     1.463635    -1.615695      54.54
 H       2.376170     2.355242    -1.629570      24.50
 C       1.193449    -0.849580    -1.776354     100.99
 H       1.396808    -1.875951    -1.661823      26.46
 C      -0.293066    -0.569516    -1.370290      12.20
 O      -1.296686    -1.441990    -1.485038     182.01
 C      -1.151743    -2.892723    -1.963598     119.70
 H      -0.834139    -3.419585    -1.147383      31.42
 H      -2.050278    -3.436480    -2.415088      27.85
 H      -0.511169    -2.765918    -2.631866      33.58
 C      -0.498422     0.746861    -0.810318      40.55
 O      -1.765513     0.793431    -0.190856     163.50
 C       0.317394     1.731749    -1.094297      85.70
 H       0.158455     2.881577    -0.856014      25.47
 C       2.087087     0.178572    -1.807418      34.94
 C       3.635291     0.009176    -1.935774      70.27
 H       3.483729    -0.829620    -2.867142      27.10
 O       4.408250     1.167100    -2.459481     105.95
 H       4.646121     1.757576    -1.560748      25.35
 C       4.296526    -0.908413    -0.940106      89.44
 H       3.567067    -1.895783    -1.329939      27.88
 O       5.716618    -1.013927    -1.284906     146.65
 H       5.988514    -1.891764    -0.851935      25.69
 C       4.072975    -0.550526     0.540167     119.83
 O       4.764652     0.669570     1.162342     185.29
 H       3.945582     1.233960     1.354255      30.36
 H       4.132113    -1.459263     1.043950      30.90
 H       2.927850    -0.363652     0.800118      28.00
55
name = lig-Water-frame_915
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 C      -1.254917     4.184625     2.387126      77.35
 H      -1.825235     4.878703     1.917892      26.29
 C      -0.901320     1.821166     2.843976     105.03
 H      -1.112644     0.717087     2.814850      31.63
 C       0.043206     2.119780     3.771204     -44.98
 O       0.691285     1.285858     4.670866      67.93
 C       0.463983    -0.183998     4.569854     115.47
 H       0.735454    -0.657652     5.639584      26.92
 H       0.772606    -0.606827     3.620754      31.09
 H      -0.725757    -0.210250     4.558088      26.66
 C       0.523148     3.540881     3.904257     -14.44
 O       1.424096     3.802807     4.912641     156.76
 H       1.156986     4.763547     5.186522      13.50
 C      -0.255319     4.590659     3.237235      60.00
 H      -0.040448     5.575100     3.714642      22.20
 C      -1.631708     2.821791     2.258813      52.60
 C      -2.786352     2.676115     1.214062      92.17
 H      -3.387308     3.506414     1.053439      33.65
 O      -3.709594     1.729525     1.803099     206.98
 H      -4.573112     1.825544     1.518478      33.63
 C      -2.394843     2.090806    -0.268264     109.49
 H      -1.701842     2.974806    -0.588112      28.61
 C      -3.559860     2.094220    -1.055864     115.10
 O      -4.912054     1.533284    -0.594157     303.64
 H      -4.825320     0.530716    -0.515372      29.77
 H      -3.511130     1.472622    -1.943454      29.67
 H      -3.917374     3.013318    -1.239446      31.80
 C       1.638371     1.546989    -1.556392      67.70
 H       2.185001     2.478681    -1.928517      27.05
 C       1.137385    -0.853012    -1.746049      71.62
 H       1.309285    -1.967109    -1.982307      25.23
 C      -0.174740    -0.552232    -1.345381      18.87
 O      -1.338113    -1.477300    -1.558891     173.68
 C      -1.114040    -2.870320    -1.953023      97.76
 H      -0.937038    -3.739215    -1.102737      27.12
 H      -2.134661    -3.406984    -2.367287      25.62
 H      -0.051813    -2.848680    -2.784453      25.02
 C      -0.518853     0.710612    -0.845584      28.80
 O      -1.823611     0.814553    -0.198404     173.65
 C       0.440900     1.786102    -1.041588      74.29
 H       0.216558     2.771969    -1.113883      30.39
 C       2.104658     0.166914    -1.839683      33.16
 C       3.640251    -0.065537    -2.005657      82.97
 H       3.718904    -0.553453    -2.871982      29.64
 O       4.425988     1.159502    -2.480872     129.28
 H       4.569414     1.738510    -1.813232      33.21
 C       4.318792    -0.936420    -0.898778     103.08
 H       3.889781    -1.844769    -0.865406      33.79
 O       5.742616    -1.044847    -1.271584     145.20
 H       6.130914    -1.831188    -0.805983      26.57
 C       4.019721    -0.479231     0.598096     126.27
 O       4.751951     0.690479     1.181367     174.93
 H       3.987133     1.249592     1.526455      32.32
 H       4.082844    -1.623669     1.112659      28.52
 H       3.016732    -0.284649     0.711573      30.95
55
name = lig-Water-frame_916
 C      -1.293480     4.202138     2.387393       5.14
 H      -2.079017     4.931708     1.892029      24.71
 C      -0.909525     1.807742     2.852144      70.90
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 H      -1.263594     0.770118     2.888294      29.94
 C       0.132341     2.128561     3.755352       7.68
 O       0.675803     1.205548     4.663385     142.49
 C       0.471762    -0.175054     4.638911     138.19
 H       0.876309    -0.488380     5.514826      28.39
 H       0.687307    -0.534604     3.589308      27.06
 H      -0.635916    -0.265059     4.543722      26.48
 C       0.437399     3.527797     3.965682      11.78
 O       1.461096     3.833992     4.901644      69.71
 H       1.228123     4.754020     5.130887      31.36
 C      -0.123119     4.554671     3.317771      63.77
 H      -0.253305     5.740883     3.563925      13.14
 C      -1.653685     2.829820     2.153421      17.02
 C      -2.778364     2.597887     1.235219      95.17
 H      -3.356694     3.624377     1.039370      27.59
 O      -3.677137     1.734045     1.820001     198.54
 H      -4.553732     2.052542     1.368743      26.44
 C      -2.361051     2.086784    -0.162883     117.62
 H      -1.715202     2.862161    -0.383547      28.12
 C      -3.648097     2.081370    -1.112475      78.47
 O      -4.927833     1.520499    -0.582198     309.32
 H      -4.629607     0.536458    -0.891864      24.17
 H      -3.465116     1.631573    -2.191802      26.89
 H      -3.709379     3.304889    -1.479802      25.75
 C       1.665269     1.582685    -1.553596      54.09
 H       2.130844     2.360615    -2.053996      26.44
 C       1.098129    -0.889232    -1.721519      76.81
 H       1.371529    -1.757399    -2.344910      26.56
 C      -0.113343    -0.566475    -1.327095      14.42
 O      -1.364269    -1.511817    -1.613301     159.67
 C      -1.024131    -2.880713    -1.958640     135.51
 H      -0.906455    -3.526052    -1.174451      30.76
 H      -2.051553    -2.951490    -2.491877      25.89
 H      -0.347758    -3.138703    -2.567222      31.80
 C      -0.573181     0.675364    -0.860437       2.55
 O      -1.827374     0.819743    -0.221548     156.67
 C       0.480310     1.838714    -0.970477      75.32
 H      -0.003659     2.915278    -1.153763      26.54
 C       2.141539     0.208893    -1.838752      22.11
 C       3.645079    -0.112824    -2.108845      69.88
 H       3.942755    -0.619699    -3.172492      25.01
 O       4.423832     1.116481    -2.494627      75.81
 H       4.565010     1.991296    -1.777991      24.38
 C       4.348651    -0.909030    -0.841466      78.10
 H       4.071942    -2.115214    -0.554718      27.44
 O       5.767933    -1.077643    -1.246917     127.13
 H       6.154132    -1.837078    -0.813456      28.26
 C       3.988084    -0.444546     0.659724     120.05
 O       4.723391     0.682235     1.195249     182.83
 H       4.149827     1.302091     1.661554      33.77
 H       4.290721    -1.188489     1.339989      30.38
 H       2.833798    -0.160473     0.528888      26.95
55
name = lig-Water-frame_917
 C      -1.311569     4.202729     2.409639      37.69
 H      -1.938798     4.999038     2.073091      25.83
 C      -0.923104     1.794920     2.866164      31.75
 H      -1.388863     0.831656     2.813015      26.10
 C       0.192838     2.135490     3.739229       9.92
 O       0.691553     1.192023     4.659165     127.16
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 C       0.422203    -0.161423     4.641576     125.28
 H       1.157886    -0.626018     5.480113      23.76
 H       0.926410    -0.654625     3.778557      25.43
 H      -0.708448    -0.613267     4.826664      23.54
 C       0.416313     3.487086     4.068952       7.19
 O       1.484850     3.863145     4.894223      96.36
 H       1.487985     4.819602     5.268583      26.38
 C      -0.137862     4.556927     3.307938      54.04
 H      -0.056804     5.536920     3.493769      19.89
 C      -1.616017     2.882813     2.081348      15.00
 C      -2.772270     2.539533     1.237898     112.70
 H      -3.053582     3.579242     1.041169      28.75
 O      -3.696849     1.715079     1.851094     238.91
 H      -4.514050     1.874079     1.222889      24.87
 C      -2.384956     2.123976    -0.080493      99.57
 H      -1.590644     2.850007    -0.547024      23.00
 C      -3.745716     2.138076    -1.214428      79.89
 O      -4.905415     1.509918    -0.601658     366.06
 H      -4.746855     0.600294    -0.768664      29.44
 H      -3.256701     1.715961    -2.139522      27.96
 H      -3.680292     3.154737    -1.406611      29.30
 C       1.759931     1.546459    -1.588747      54.38
 H       2.376387     2.427570    -2.111578      20.11
 C       1.195204    -0.879666    -1.752751      66.22
 H       1.386537    -1.663013    -2.482480      22.12
 C      -0.210081    -0.613283    -1.301742      -1.92
 O      -1.324156    -1.509061    -1.644352     158.58
 C      -1.012964    -2.868210    -1.962515      92.06
 H      -0.907918    -3.440377    -0.888639      23.95
 H      -1.968335    -3.017295    -2.646650      24.13
 H      -0.109198    -3.322731    -2.875530      22.01
 C      -0.570689     0.715815    -0.844310       9.50
 O      -1.783024     0.779955    -0.250749     167.29
 C       0.372197     1.858827    -0.903778      77.21
 H      -0.025779     2.805945    -0.935320      26.91
 C       2.144865     0.238222    -1.815813      25.88
 C       3.665768    -0.128724    -2.207559      72.01
 H       3.681926    -0.811271    -3.019542      26.49
 O       4.424011     1.085950    -2.489939     195.78
 H       4.430613     1.757042    -1.805013      28.81
 C       4.380172    -0.929483    -0.771158      80.73
 H       4.031676    -1.868470    -0.761584      29.54
 O       5.797410    -1.090604    -1.212966     148.44
 H       6.049222    -1.993738    -0.802771      29.48
 C       3.959249    -0.372478     0.686827     105.62
 O       4.710714     0.687649     1.206508     227.30
 H       4.142937     1.375563     1.701660      28.64
 H       4.277292    -1.133545     1.584424      23.57
 H       2.931063    -0.246922     0.572615      25.26
55
name = lig-Water-frame_918
 C      -1.270929     4.220069     2.462833      73.38
 H      -1.812913     5.146327     2.131114      25.61
 C      -0.922745     1.849023     2.863391      52.43
 H      -1.338916     0.789305     2.723257      25.51
 C       0.171444     2.098111     3.728493      -9.12
 O       0.722091     1.226294     4.662509     119.20
 C       0.403602    -0.238128     4.656285     132.61
 H       1.069723    -0.597995     5.362514      27.19
 H       0.944299    -0.742542     3.829512      26.05
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 H      -0.484799    -0.620923     4.959806      27.60
 C       0.443962     3.514346     4.144312      -6.03
 O       1.519166     3.876522     4.909882     107.65
 H       1.486531     4.820529     5.272297      24.01
 C      -0.251290     4.501288     3.259359      41.67
 H       0.358725     5.596620     3.557996      19.71
 C      -1.519666     2.884071     2.103557      36.78
 C      -2.736446     2.537018     1.251022      94.57
 H      -3.173242     3.582442     1.022562      27.79
 O      -3.757118     1.678165     1.873687     200.54
 H      -4.440415     1.483119     1.246526      26.39
 C      -2.421847     2.139377    -0.143701     105.85
 H      -1.803228     2.818890    -0.616270      26.78
 C      -3.753066     2.179974    -1.248897      57.04
 O      -4.879197     1.523938    -0.647039     310.76
 H      -4.814955     0.451649    -0.484184      24.66
 H      -3.309710     1.556838    -2.071098      26.71
 H      -4.057207     3.365018    -1.336760      25.23
 C       1.781696     1.550244    -1.594856      42.89
 H       2.457778     2.282072    -1.809622      21.22
 C       1.241443    -0.820585    -1.784069      70.82
 H       1.422053    -1.753671    -2.426934      21.36
 C      -0.254335    -0.665378    -1.321387       0.66
 O      -1.245668    -1.471963    -1.665169     210.39
 C      -1.001602    -2.894842    -1.998181     131.14
 H      -0.955842    -3.336578    -1.083957      30.63
 H      -1.849659    -3.502181    -2.547945      25.73
 H      -0.206794    -2.965284    -2.515731      31.16
 C      -0.516630     0.763383    -0.815051      28.34
 O      -1.759882     0.742694    -0.261771     182.46
 C       0.325497     1.793332    -0.907439      67.89
 H       0.032116     2.900465    -0.658614      25.58
 C       2.163991     0.226468    -1.802008      19.28
 C       3.659263    -0.105457    -2.195332      79.24
 H       3.521740    -0.938243    -2.958203      26.80
 O       4.425011     1.028637    -2.508764     160.06
 H       4.333072     1.568738    -1.646361      28.45
 C       4.402289    -0.914340    -0.752955      61.81
 H       3.724312    -1.956841    -0.994803      23.95
 O       5.827291    -1.108367    -1.148477     180.59
 H       5.918509    -2.060278    -0.902169      29.58
 C       3.983859    -0.357221     0.716661     113.02
 O       4.716718     0.741628     1.221944     235.49
 H       4.016640     1.359910     1.548521      29.17
 H       3.892066    -1.268219     1.325813      26.56
 H       2.807254    -0.232697     0.729682      23.79
55
name = lig-Water-frame_919
 C      -1.262591     4.255266     2.468029      62.75
 H      -1.777935     5.131565     1.963830      24.51
 C      -0.895366     1.882346     2.852421      82.00
 H      -1.113406     0.893593     2.666403      27.43
 C       0.126878     2.111669     3.781822     -32.53
 O       0.746717     1.234637     4.665481     116.46
 C       0.468952    -0.309003     4.658632      84.17
 H       1.101477    -0.580273     5.614647      20.77
 H       0.634846    -0.745068     3.626349      22.68
 H      -0.760718    -0.515149     5.007082      21.12
 C       0.444944     3.536390     4.111952      -6.29
 O       1.558115     3.885598     4.941747     111.46
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 H       1.270756     4.812875     5.194017      25.59
 C      -0.225259     4.472362     3.345442      59.91
 H       0.183869     5.343669     3.348701      28.78
 C      -1.474094     2.862712     2.155344      16.90
 C      -2.722113     2.579203     1.252433      74.80
 H      -3.446493     3.441536     1.149838      25.69
 O      -3.797337     1.639807     1.898686     122.73
 H      -4.354502     1.174742     1.130860      23.32
 C      -2.487042     2.114019    -0.281784      86.09
 H      -1.819311     2.980494    -0.708404      24.59
 C      -3.696617     2.199357    -1.202992      92.16
 O      -4.883844     1.518860    -0.686717     321.27
 H      -4.593635     0.599606    -0.413484      28.74
 H      -3.526076     1.582583    -2.170152      25.87
 H      -4.329202     3.099372    -1.368372      23.43
 C       1.707030     1.547852    -1.535571      42.45
 H       2.535155     2.409931    -1.451647      20.37
 C       1.168893    -0.798199    -1.805955      93.48
 H       1.539843    -1.727730    -2.157833      22.74
 C      -0.128510    -0.635273    -1.379442      21.50
 O      -1.215271    -1.449499    -1.690530     219.33
 C      -1.013269    -2.915945    -2.013352     107.70
 H      -0.851933    -3.515342    -0.961477      27.02
 H      -1.817961    -3.547325    -2.471802      24.55
 H       0.213120    -2.770752    -2.492042      20.63
 C      -0.490738     0.693162    -0.798443      22.89
 O      -1.779581     0.748081    -0.257077     162.98
 C       0.412949     1.769307    -0.975837      63.80
 H       0.232272     2.677540    -0.392683      24.91
 C       2.203185     0.229891    -1.801036      53.24
 C       3.624109    -0.103667    -2.092699      93.99
 H       3.655227    -0.864853    -2.983055      27.54
 O       4.429730     0.977949    -2.534552     112.61
 H       4.438913     1.512935    -1.559494      27.90
 C       4.359504    -0.898607    -0.806971      89.72
 H       3.814715    -1.747204    -0.880364      28.55
 O       5.833562    -1.135004    -1.057855     218.06
 H       5.942238    -2.102366    -0.993906      29.82
 C       3.973430    -0.399431     0.696989      92.69
 O       4.720498     0.799676     1.242382     173.17
 H       3.962448     1.411495     1.413170      29.40
 H       3.901222    -1.430905     1.282885      24.32
 H       2.979423     0.002308     0.704460      24.26
55
name = lig-Water-frame_920
 C      -1.265216     4.249171     2.437478      45.63
 H      -1.738102     4.978850     1.850539      22.42
 C      -0.815875     1.854786     2.869924      33.21
 H      -1.010155     0.758735     2.561349      26.44
 C       0.097778     2.173699     3.895210       4.31
 O       0.766447     1.209268     4.661901      82.53
 C       0.490112    -0.333822     4.680416     117.74
 H       1.083155    -0.676551     5.512967      28.76
 H       0.464651    -0.720795     3.691233      30.45
 H      -0.460113    -0.297407     4.822935      33.02
 C       0.469249     3.480395     4.057445      23.82
 O       1.565490     3.903137     4.965799     -26.64
 H       1.205467     4.836601     5.262393      25.56
 C      -0.174503     4.481261     3.446923      91.14
 H       0.115104     5.707614     3.299694      14.71
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 C      -1.540886     2.909086     2.161917      -8.47
 C      -2.764802     2.597257     1.224250      71.39
 H      -3.393050     3.471459     1.256951      25.97
 O      -3.802268     1.592972     1.912538     146.66
 H      -4.222581     1.213582     1.121527      27.92
 C      -2.504491     2.128783    -0.381107      75.89
 H      -1.796292     2.863902    -0.713325      23.54
 C      -3.689783     2.149600    -1.173013     113.04
 O      -4.896350     1.484581    -0.699295     359.72
 H      -4.538678     0.593706    -0.572049      31.37
 H      -3.514220     1.867283    -2.233166      27.19
 H      -4.032826     3.126900    -1.390484      26.39
 C       1.697964     1.544132    -1.453952      65.80
 H       2.276643     2.361488    -1.192800      24.12
 C       1.171542    -0.790334    -1.839326      73.24
 H       1.624948    -1.831675    -1.931751      22.55
 C      -0.046279    -0.551908    -1.431796      25.78
 O      -1.218760    -1.453346    -1.710867     174.49
 C      -0.917582    -2.914382    -1.971658     124.47
 H      -0.750408    -3.465626    -1.104277      30.37
 H      -1.859595    -3.227964    -2.671828      25.67
 H      -0.105681    -3.075628    -2.533471      30.52
 C      -0.472111     0.592116    -0.813825       5.56
 O      -1.812295     0.784118    -0.261662     116.04
 C       0.491581     1.730453    -1.012791      34.12
 H       0.364038     2.584251    -0.332127      25.34
 C       2.171483     0.257107    -1.795666      43.55
 C       3.626543    -0.140320    -1.988390     106.92
 H       3.734217    -0.750768    -2.842215      29.00
 O       4.438996     0.956401    -2.522663     169.60
 H       4.726228     1.569891    -1.932792      33.09
 C       4.318033    -0.848679    -0.857842      88.25
 H       3.816637    -2.019912    -0.750775      23.34
 O       5.808948    -1.153749    -0.960317     185.12
 H       5.961742    -2.158064    -1.024432      27.85
 C       3.970974    -0.435873     0.639738      88.12
 O       4.721904     0.821405     1.255802     147.66
 H       3.998619     1.539281     1.398281      29.68
 H       4.224779    -1.228449     1.389841      26.18
 H       2.966499     0.037985     0.561330      24.89
55
name = lig-Water-frame_921
 C      -1.215183     4.215175     2.450468      54.25
 H      -1.748361     5.061524     1.801736      22.93
 C      -0.758239     1.822678     2.869618      27.71
 H      -0.938370     0.823160     2.593686      28.78
 C       0.065708     2.149107     3.988078     -15.82
 O       0.806494     1.174440     4.669806       6.28
 C       0.496608    -0.284772     4.675889     105.18
 H       1.160188    -0.860300     5.381585      28.67
 H       0.689070    -0.837957     3.647030      29.19
 H      -0.777034    -0.254779     4.967057      26.91
 C       0.561844     3.477425     4.072358      -5.46
 O       1.539533     3.918181     4.981805     120.10
 H       1.344241     4.789652     5.365506      22.13
 C      -0.199222     4.587931     3.425867      56.24
 H       0.095169     5.558742     3.673831      21.25
 C      -1.631343     2.910505     2.163168       8.83
 C      -2.828983     2.581254     1.193630      68.66
 H      -3.285157     3.680588     1.188205      26.76
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 O      -3.762556     1.563455     1.906125     149.48
 H      -4.318296     1.321353     1.146937      28.30
 C      -2.452139     2.142320    -0.358853      66.47
 H      -1.686447     2.833858    -0.838545      25.67
 C      -3.753414     2.103578    -1.213827      82.24
 O      -4.891525     1.434472    -0.697677     290.23
 H      -4.745556     0.338447    -0.829005      26.54
 H      -3.396236     1.982225    -2.314917      27.17
 H      -3.595603     3.380171    -1.169864      22.79
 C       1.789245     1.523799    -1.388226      67.31
 H       2.433896     2.439859    -1.152308      26.40
 C       1.320357    -0.801330    -1.886222      84.79
 H       1.518945    -1.840301    -1.917501      25.26
 C      -0.136643    -0.534687    -1.482867      10.05
 O      -1.190548    -1.469498    -1.718961     148.13
 C      -0.874333    -2.870804    -1.954865     100.56
 H      -0.765304    -3.513970    -0.943910      27.49
 H      -1.702464    -3.017003    -2.576683      28.06
 H       0.047656    -3.319791    -2.901890      24.94
 C      -0.469969     0.614848    -0.835011      27.81
 O      -1.823922     0.812381    -0.287293     110.20
 C       0.420793     1.662469    -0.954947       8.01
 H       0.303814     2.683977    -0.403346      27.82
 C       2.126439     0.254465    -1.790800      42.54
 C       3.659677    -0.140885    -1.917063      94.44
 H       3.649433    -0.928816    -2.877130      27.82
 O       4.451931     0.943720    -2.521583      96.89
 H       5.011506     1.709668    -2.047518      21.81
 C       4.295762    -0.891145    -0.816400     118.86
 H       3.928811    -1.839405    -0.800626      31.16
 O       5.767928    -1.155003    -0.877063     197.31
 H       5.833100    -2.124312    -0.953662      29.12
 C       4.001048    -0.391706     0.580759     112.80
 O       4.720294     0.816281     1.247861     149.56
 H       4.077024     1.510747     1.430882      34.81
 H       4.346178    -1.070605     1.367757      29.04
 H       2.834802    -0.319610     0.596019      30.00
55
name = lig-Water-frame_922
 C      -1.174234     4.223540     2.460441      55.15
 H      -1.645461     5.026667     2.064083      25.87
 C      -0.769004     1.848041     2.853599      43.91
 H      -0.934132     0.749030     2.661489      30.03
 C       0.060241     2.090159     4.020065     -40.20
 O       0.868849     1.133912     4.698605      39.55
 C       0.438939    -0.229248     4.650190     147.46
 H       1.131041    -0.798527     5.329602      31.07
 H       0.775779    -0.674973     3.766805      33.33
 H      -0.424181    -0.484463     4.981496      35.02
 C       0.601254     3.575583     4.100597     -23.64
 O       1.522714     3.908015     5.007055     118.45
 H       1.358061     4.884855     5.374795      16.20
 C      -0.220865     4.599672     3.388185      55.54
 H       0.075302     5.656027     3.888564      19.17
 C      -1.656295     2.832428     2.198132      19.32
 C      -2.862303     2.580821     1.183159      92.25
 H      -3.336245     3.483451     1.010918      31.22
 O      -3.695264     1.564160     1.863142     138.85
 H      -4.595227     1.450469     1.283676      23.95
 C      -2.398450     2.121566    -0.280466      81.43
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 H      -1.769494     2.840044    -0.867358      27.16
 C      -3.743888     2.138755    -1.263765      91.16
 O      -4.881872     1.363531    -0.703796     343.12
 H      -4.904537     0.506269    -0.967941      34.87
 H      -3.567888     1.806716    -2.243372      29.10
 H      -3.962458     3.139747    -1.063759      28.37
 C       1.826678     1.535231    -1.297390      75.12
 H       2.671939     2.276630    -1.343154      27.35
 C       1.323836    -0.833865    -1.897419      76.91
 H       1.601165    -1.898612    -2.143649      26.60
 C      -0.192910    -0.599326    -1.564865       3.00
 O      -1.126633    -1.478787    -1.716731     178.78
 C      -0.804298    -2.853094    -1.983395     119.99
 H      -0.818950    -3.368408    -1.041561      30.02
 H      -1.909253    -3.242013    -2.454484      25.53
 H      -0.128754    -3.068655    -2.607134      32.95
 C      -0.543096     0.690928    -0.853080      21.16
 O      -1.805613     0.817389    -0.323999     172.86
 C       0.404442     1.663631    -0.860958      61.15
 H       0.056166     2.599555    -0.555830      30.75
 C       2.211579     0.245292    -1.778204      25.74
 C       3.691458    -0.124441    -1.941740     107.63
 H       3.612942    -0.840077    -2.638165      32.88
 O       4.474863     0.941488    -2.543186     125.27
 H       5.028157     1.495036    -1.830446      26.47
 C       4.330289    -0.926701    -0.717105      91.55
 H       3.701727    -2.036707    -0.831163      27.00
 O       5.723629    -1.141447    -0.815585     215.22
 H       5.800993    -2.126326    -0.794469      26.86
 C       4.014574    -0.324825     0.587740     129.05
 O       4.715487     0.795290     1.208776     165.21
 H       3.976216     1.470084     1.437362      32.17
 H       4.373994    -1.251246     1.268336      28.56
 H       2.968375    -0.503644     0.800243      31.33
55
name = lig-Water-frame_923
 C      -1.178813     4.200242     2.463516      35.46
 H      -1.823490     5.163439     2.138963      18.96
 C      -0.820499     1.851433     2.861866      60.33
 H      -1.007953     0.781677     2.711539      30.09
 C       0.109956     2.127069     3.988167     -69.33
 O       0.913830     1.124160     4.734117      15.49
 C       0.452860    -0.212454     4.633620     119.23
 H       1.115508    -0.617300     5.402737      29.83
 H       0.670224    -0.564902     3.509415      30.05
 H      -0.684123    -0.680248     5.019299      26.70
 C       0.531087     3.619938     4.103180      -0.33
 O       1.525446     3.913051     5.060623     178.80
 H       1.352622     4.862840     5.279426      18.97
 C      -0.168881     4.552394     3.410259      62.86
 H      -0.203922     5.700354     3.609895      21.92
 C      -1.612734     2.796410     2.246963       8.10
 C      -2.826796     2.546287     1.190848      90.48
 H      -3.578786     3.460427     0.917775      26.04
 O      -3.650541     1.577844     1.803760     201.96
 H      -4.520245     1.569107     1.481090      29.49
 C      -2.407813     2.091450    -0.233115      91.80
 H      -1.821549     2.916091    -0.653578      25.63
 C      -3.711566     2.156630    -1.243971      72.93
 O      -4.874653     1.322722    -0.703381     296.74
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 H      -4.810753     0.371862    -1.101614      29.23
 H      -3.665226     1.664180    -2.314601      25.39
 H      -4.617194     3.057018    -1.244687      20.39
 C       1.816934     1.510216    -1.216359      74.83
 H       2.587848     2.222317    -1.385098      28.15
 C       1.212726    -0.863659    -1.885742      68.25
 H       1.697180    -1.689616    -2.421309      27.20
 C      -0.119839    -0.596979    -1.615611      18.24
 O      -1.098662    -1.508764    -1.719150     224.10
 C      -0.859906    -2.851890    -1.995764      96.85
 H      -0.645066    -3.362995    -0.940857      27.98
 H      -1.672085    -3.374902    -2.297678      28.74
 H       0.312145    -2.933759    -2.792258      22.30
 C      -0.592903     0.685097    -0.923655       0.95
 O      -1.793748     0.807148    -0.355249     160.73
 C       0.478730     1.718567    -0.778244      60.48
 H      -0.129815     2.728796    -0.597746      30.05
 C       2.310557     0.245967    -1.730607       0.74
 C       3.728806    -0.103157    -1.977305      88.12
 H       3.712618    -1.043221    -2.839224      28.06
 O       4.513186     0.941144    -2.549029     164.51
 H       4.855433     1.222744    -1.769806      32.02
 C       4.326065    -0.951904    -0.660683     107.63
 H       3.686752    -1.754076    -0.680060      33.81
 O       5.699788    -1.138187    -0.774536     219.48
 H       5.951155    -2.120254    -0.559153      23.81
 C       4.036412    -0.344141     0.689398     132.46
 O       4.692671     0.785258     1.153079     164.61
 H       3.946129     1.408722     1.395160      31.68
 H       4.405225    -1.270598     1.217417      31.47
 H       2.905379    -0.313447     1.049725      30.32
55
name = lig-Water-frame_924
 C      -1.227981     4.170612     2.475568      54.28
 H      -1.881632     4.887439     2.140237      23.25
 C      -0.843406     1.809120     2.942404      24.01
 H      -1.120529     0.801072     2.716948      31.83
 C       0.184111     2.224925     3.905594      -6.63
 O       0.913367     1.178891     4.753265      69.60
 C       0.461276    -0.262638     4.611077     126.26
 H       1.180915    -0.737221     5.365413      25.13
 H       0.498705    -0.536734     3.630910      29.32
 H      -0.530035    -0.301603     4.796656      29.10
 C       0.472655     3.547867     4.154328      15.20
 O       1.517536     3.917205     5.101074    -167.83
 H       1.389795     4.928021     5.368966      31.64
 C      -0.168649     4.532257     3.388450      66.19
 H      -0.168281     5.628916     3.439983      16.94
 C      -1.569345     2.860143     2.250203     -31.52
 C      -2.782135     2.520108     1.203271     102.51
 H      -3.321447     3.379864     1.093802      30.08
 O      -3.615403     1.567463     1.786159     188.73
 H      -4.531913     1.621878     1.384469      24.00
 C      -2.468357     2.104200    -0.242239      86.74
 H      -1.727170     2.983493    -0.412147      25.41
 C      -3.767139     2.142949    -1.207449     106.19
 O      -4.868456     1.261800    -0.703039     322.74
 H      -4.484373     0.284542    -0.957669      25.44
 H      -3.420098     1.842835    -2.155233      29.48
 H      -4.253912     2.950244    -1.447703      28.28
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 C       1.823576     1.449739    -1.162538      50.86
 H       2.416559     2.491001    -1.233305      25.95
 C       1.209478    -0.816948    -1.883478      92.18
 H       1.517189    -1.569808    -2.608514      27.49
 C      -0.063787    -0.543827    -1.607357      15.03
 O      -1.125546    -1.534309    -1.729571     247.22
 C      -0.811254    -2.882740    -1.992280     118.22
 H      -0.296575    -3.297883    -1.119183      30.30
 H      -1.735288    -3.575380    -2.489499      24.83
 H      -0.092927    -2.912147    -2.579401      32.16
 C      -0.502834     0.673873    -1.023006      10.81
 O      -1.807871     0.781763    -0.381767     139.89
 C       0.489049     1.751827    -0.727164      49.76
 H       0.250991     2.733818    -0.541702      32.70
 C       2.282137     0.223667    -1.658741      24.15
 C       3.760282    -0.168993    -2.041218      97.91
 H       3.820002    -0.836026    -2.739952      33.91
 O       4.557922     0.935609    -2.542529      98.92
 H       4.940088     1.376349    -1.609677      27.01
 C       4.285419    -0.888783    -0.649606      86.25
 H       3.578299    -1.951810    -0.592900      29.44
 O       5.714919    -1.154619    -0.744478     188.33
 H       5.947070    -2.033872    -0.400554      25.97
 C       4.016434    -0.427739     0.833317     124.46
 O       4.678993     0.804633     1.102387     152.86
 H       4.020820     1.484787     1.357057      31.93
 H       4.505279    -1.265330     1.512621      29.33
 H       3.018629    -0.178605     1.031779      27.74
55
name = lig-Water-frame_925
 C      -1.261533     4.155360     2.514272      64.47
 H      -1.983873     4.901932     1.979722      24.12
 C      -0.847599     1.813297     3.033547      32.63
 H      -1.127624     0.742176     2.781894      29.81
 C       0.241784     2.208577     3.825785      17.17
 O       0.890208     1.264887     4.747475      55.20
 C       0.495048    -0.265072     4.603275      97.48
 H       1.075639    -0.959919     5.173752      27.12
 H       0.568686    -0.702829     3.468138      25.94
 H      -0.705218    -0.064981     4.865561      22.54
 C       0.473625     3.528467     4.237227      10.50
 O       1.489578     3.910647     5.118650      87.19
 H       1.312055     4.845714     5.481534      21.26
 C      -0.227878     4.512714     3.337832      53.40
 H       0.237420     5.683224     3.491050      19.74
 C      -1.541778     2.854159     2.221958       1.10
 C      -2.706623     2.493559     1.239201      80.58
 H      -3.133963     3.641618     1.243748      25.77
 O      -3.611819     1.527491     1.816510     177.73
 H      -4.432904     1.557552     1.150016      23.22
 C      -2.507838     2.156048    -0.266053      92.18
 H      -1.773240     2.860843    -0.556609      25.46
 C      -3.798486     2.084528    -1.154998      75.77
 O      -4.831458     1.183995    -0.715877     353.12
 H      -4.393020     0.363444    -0.628779      30.88
 H      -3.136145     1.809317    -2.095776      25.79
 H      -3.899144     3.367430    -1.428823      23.40
 C       1.839647     1.450574    -1.109190      62.36
 H       2.364861     2.295953    -1.015029      24.21
 C       1.321504    -0.735034    -1.915089      82.58
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 H       1.309431    -1.606104    -2.609431      19.34
 C      -0.114711    -0.525591    -1.568902      21.48
 O      -1.168033    -1.519193    -1.736914     160.37
 C      -0.780509    -2.940073    -1.971560      90.36
 H      -0.180442    -3.416645    -1.123462      26.45
 H      -1.555853    -3.389847    -2.367765      28.73
 H       0.149440    -3.024399    -3.130505      23.93
 C      -0.409767     0.735850    -1.052621      44.04
 O      -1.815312     0.752079    -0.424310     110.74
 C       0.490419     1.700772    -0.736244      50.34
 H       0.517855     2.818808    -0.345099      26.44
 C       2.214088     0.172659    -1.614945      35.29
 C       3.766950    -0.199769    -2.015068      66.93
 H       3.835970    -1.046397    -2.972950      25.98
 O       4.614417     0.927942    -2.495340     136.35
 H       4.914642     1.668393    -1.884764      26.93
 C       4.221655    -0.878863    -0.638339      93.52
 H       3.862853    -1.845215    -0.708436      28.35
 O       5.737138    -1.154194    -0.726235     172.51
 H       5.777467    -2.137563    -0.347514      26.51
 C       4.012032    -0.500343     0.950673     111.52
 O       4.691272     0.842088     1.062617     147.27
 H       4.022800     1.571100     1.365511      26.32
 H       4.376902    -1.196796     1.675774      29.57
 H       2.810686    -0.312475     1.027029      24.03
55
name = lig-Water-frame_926
 C      -1.315805     4.184924     2.522039      52.74
 H      -1.788005     4.969283     1.917186      23.78
 C      -0.864306     1.850880     3.055361      65.85
 H      -0.974812     0.823248     2.944468      28.36
 C       0.288930     2.122023     3.823651      -2.23
 O       0.881188     1.315687     4.723785     122.02
 C       0.478066    -0.213796     4.552475     115.20
 H       1.006674    -0.975168     5.224690      26.73
 H       0.625756    -0.568231     3.621530      28.85
 H      -0.517165    -0.282188     4.967842      26.40
 C       0.468969     3.584643     4.243979      -0.67
 O       1.452034     3.883912     5.124728     114.94
 H       1.180614     4.840989     5.509921      18.14
 C      -0.209469     4.513853     3.369531      48.15
 H       0.247815     5.412355     3.466243      24.40
 C      -1.513094     2.737557     2.215536      11.23
 C      -2.640871     2.518071     1.286937      92.64
 H      -3.116481     3.421851     1.253984      28.12
 O      -3.624792     1.488907     1.852083     223.96
 H      -4.225806     1.363415     1.160539      28.59
 C      -2.507278     2.169624    -0.257968      84.84
 H      -1.865646     2.869833    -0.998049      23.01
 C      -3.734650     2.083860    -1.137184     102.40
 O      -4.791385     1.135065    -0.736185     283.37
 H      -4.286214     0.256537    -0.332363      25.91
 H      -3.383456     1.611191    -2.020105      29.23
 H      -3.976554     3.040554    -1.106681      29.08
 C       1.842402     1.436341    -1.053634      58.87
 H       2.777113     2.168206    -0.785890      23.20
 C       1.281360    -0.730497    -1.972819      57.27
 H       1.521940    -1.678354    -2.466778      20.68
 C      -0.135577    -0.538659    -1.545208      18.88
 O      -1.181042    -1.498459    -1.739443     167.56
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 C      -0.650091    -2.944724    -2.027127     108.47
 H      -0.220050    -3.524867    -1.126225      27.25
 H      -1.796346    -3.436146    -2.227357      25.35
 H      -0.265725    -3.084650    -2.821472      32.29
 C      -0.460177     0.773397    -1.010543      27.53
 O      -1.802261     0.746733    -0.478554     139.16
 C       0.564723     1.694130    -0.762405      63.81
 H       0.297936     2.537563    -0.153205      25.77
 C       2.260635     0.187728    -1.609477      46.91
 C       3.753317    -0.191766    -1.940481      91.21
 H       3.763450    -0.856442    -2.654828      32.02
 O       4.662563     0.906964    -2.459070     126.82
 H       4.698152     1.720383    -1.953654      32.63
 C       4.239875    -0.910335    -0.607126      78.58
 H       3.810795    -2.062267    -0.853642      24.36
 O       5.742488    -1.146026    -0.704821     188.32
 H       5.751150    -2.122149    -0.542849      27.11
 C       3.963606    -0.479825     0.968733     103.33
 O       4.695449     0.862268     1.040683     140.75
 H       3.996879     1.456633     1.401053      27.44
 H       4.302523    -1.332719     1.782000      27.03
 H       2.951603    -0.540733     1.159934      26.84
55
name = lig-Water-frame_927
 C      -1.315541     4.169286     2.518080      40.77
 H      -1.653769     5.022152     1.902088      23.68
 C      -0.835320     1.839962     3.053784      56.57
 H      -1.004149     0.731914     2.996151      23.22
 C       0.292847     2.151413     3.879104      16.67
 O       0.894005     1.283448     4.708070     147.42
 C       0.477723    -0.147597     4.553711     102.42
 H       1.127887    -0.578430     5.297963      25.83
 H       0.629064    -0.421254     3.375888      24.03
 H      -0.625989    -0.440649     4.933221      24.57
 C       0.451333     3.568990     4.160210      23.49
 O       1.408229     3.866895     5.134429     149.59
 H       1.276130     4.822825     5.469627      20.24
 C      -0.191598     4.489400     3.429189      49.63
 H       0.182089     5.747868     3.415167      20.50
 C      -1.494956     2.712537     2.234483      11.06
 C      -2.626343     2.495291     1.298499      77.03
 H      -3.347305     3.450553     1.241986      23.54
 O      -3.610800     1.462282     1.897106     206.29
 H      -4.248269     1.149154     1.133874      23.48
 C      -2.427800     2.141202    -0.272502     100.59
 H      -2.025492     2.840856    -0.912270      27.57
 C      -3.669844     2.025292    -1.103266      82.90
 O      -4.750845     1.090908    -0.726106     273.26
 H      -4.328929     0.250134    -0.448003      28.25
 H      -3.558705     1.668249    -2.207127      24.90
 H      -4.469888     3.096441    -1.039751      22.94
 C       1.953076     1.407569    -1.010892      36.48
 H       2.755242     1.883933    -0.578165      23.31
 C       1.168374    -0.763616    -2.013790      84.31
 H       1.738436    -1.674787    -2.319645      18.33
 C      -0.117676    -0.541554    -1.549390      19.15
 O      -1.144235    -1.494528    -1.738893     177.74
 C      -0.658759    -2.929765    -2.017505      94.21
 H      -0.153764    -3.401481    -1.193029      28.04
 H      -1.547578    -3.378487    -1.937129      28.93
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 H      -0.082789    -3.161563    -3.337062      21.59
 C      -0.554323     0.728674    -0.955831      18.31
 O      -1.782610     0.782390    -0.526050     187.71
 C       0.574533     1.714076    -0.755815      38.32
 H       0.098574     2.442672    -0.027919      21.14
 C       2.326453     0.236843    -1.638804      52.89
 C       3.735485    -0.110087    -1.791411      67.96
 H       3.741330    -0.998793    -2.692481      25.70
 O       4.700544     0.863541    -2.423942      92.16
 H       4.314731     1.737630    -1.852497      30.17
 C       4.302524    -1.009247    -0.563139      88.79
 H       3.707206    -1.865224    -0.735968      27.36
 O       5.725279    -1.119028    -0.688811     228.84
 H       5.976726    -2.132909    -0.676547      24.83
 C       3.957852    -0.456317     0.916190     103.19
 O       4.666890     0.837904     1.040215     148.99
 H       3.981426     1.477303     1.450035      25.98
 H       4.394750    -1.213737     1.508926      29.37
 H       2.793257    -0.440657     1.293670      22.92
55
name = lig-Water-frame_928
 C      -1.228764     4.115665     2.530418      68.53
 H      -1.683015     4.970621     1.879041      23.22
 C      -0.759489     1.766258     3.050390      27.83
 H      -1.144610     0.767346     2.930590      23.15
 C       0.223404     2.232645     3.929325      27.86
 O       0.910008     1.224773     4.704926     191.65
 C       0.492726    -0.081626     4.555161     131.99
 H       1.321551    -0.405189     5.228718      26.54
 H       0.633982    -0.352690     3.567746      30.01
 H      -0.587728    -0.387613     4.738228      28.51
 C       0.493716     3.512914     4.105554      29.12
 O       1.369903     3.840386     5.132885      -4.77
 H       1.326568     4.844694     5.416010      21.49
 C      -0.233338     4.554649     3.419860      18.94
 H      -0.079337     5.484758     3.522954      17.96
 C      -1.505976     2.802887     2.259667     -30.44
 C      -2.697471     2.441289     1.269743      99.50
 H      -3.251678     3.344870     1.233603      27.60
 O      -3.575414     1.434580     1.935213     223.96
 H      -4.234570     1.097704     1.247860      25.70
 C      -2.350721     2.084361    -0.280920      83.52
 H      -1.747356     3.082530    -0.674895      24.11
 C      -3.716276     1.989432    -1.097875     113.46
 O      -4.713634     1.034928    -0.690125     276.89
 H      -4.353726     0.041948    -0.751085      24.50
 H      -3.443856     2.095877    -2.166988      28.13
 H      -4.324620     2.761153    -1.104546      28.66
 C       2.022968     1.377942    -0.960824     110.02
 H       2.781096     1.960584    -0.332690      21.79
 C       1.168838    -0.743479    -2.018247      93.35
 H       1.571003    -1.756254    -2.289314      20.06
 C      -0.118589    -0.546543    -1.572800      20.82
 O      -1.082595    -1.519748    -1.738786     228.39
 C      -0.668528    -2.889895    -2.059175     107.70
 H       0.245489    -3.102517    -1.288826      25.30
 H      -1.682566    -3.567621    -1.861654      23.93
 H      -0.238933    -3.004304    -2.840986      31.36
 C      -0.497357     0.677546    -0.934248      17.89
 O      -1.804315     0.839776    -0.548841     233.12
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 C       0.503055     1.691010    -0.723043      73.80
 H       0.273043     2.572611    -0.014122      19.14
 C       2.292526     0.255782    -1.689890      51.82
 C       3.767371    -0.117507    -1.713109     107.37
 H       3.749593    -0.835473    -2.423438      29.15
 O       4.694385     0.837223    -2.345597     191.47
 H       4.401229     1.668076    -2.044560      36.95
 C       4.335473    -1.038061    -0.512226      84.09
 H       3.646693    -2.063015    -0.557404      25.06
 O       5.714748    -1.095922    -0.678680     216.28
 H       6.086111    -2.026052    -0.666163      25.21
 C       3.955045    -0.433860     0.832772     105.47
 O       4.618501     0.798153     1.057922     166.05
 H       4.036026     1.538850     1.404334      27.09
 H       4.666471    -1.204513     1.474904      24.89
 H       3.002054    -0.256905     1.096673      23.84
55
name = lig-Water-frame_929
 C      -1.144404     4.116807     2.504954      83.67
 H      -1.752984     4.770946     1.980522      23.32
 C      -0.740225     1.757297     2.988079      55.94
 H      -1.091943     0.762510     2.872692      24.11
 C       0.133448     2.179592     3.966309      -2.08
 O       0.922684     1.250325     4.703802     177.89
 C       0.544584    -0.060400     4.568775     119.11
 H       1.221580    -0.773573     5.132784      26.57
 H       0.753115    -0.519659     3.438495      25.92
 H      -0.502853    -0.234638     4.858480      27.52
 C       0.550583     3.579897     4.089702      18.16
 O       1.353667     3.808236     5.126296     175.49
 H       1.221024     4.793064     5.368763      22.06
 C      -0.267445     4.548508     3.406461      89.87
 H      -0.188668     5.808839     3.802232      17.36
 C      -1.524072     2.810258     2.293321       6.43
 C      -2.747184     2.367119     1.254788      76.93
 H      -3.281667     3.418251     1.126790      27.01
 O      -3.528397     1.404761     1.969632     224.02
 H      -4.170130     1.119433     1.349877      29.79
 C      -2.329205     2.097298    -0.268863     112.63
 H      -1.657951     2.847775    -0.385489      30.14
 C      -3.743819     1.979316    -1.108488      76.17
 O      -4.663983     0.936466    -0.647904     240.32
 H      -4.438073     0.037034    -1.143062      25.41
 H      -3.323590     2.098963    -2.133550      27.12
 H      -4.356711     3.161596    -0.961747      26.44
 C       1.954585     1.375550    -0.899748     134.50
 H       2.721958     2.071564    -0.374875      23.01
 C       1.258987    -0.696202    -2.002093     100.30
 H       1.334347    -1.694010    -2.410611      20.86
 C      -0.115702    -0.559043    -1.608953      19.46
 O      -1.048579    -1.549297    -1.738802     232.74
 C      -0.687710    -2.839888    -1.986141      98.37
 H       0.212110    -2.982900    -1.501532      26.71
 H      -1.417557    -3.602826    -1.916702      26.25
 H      -0.125962    -2.936977    -3.326372      22.46
 C      -0.392703     0.670561    -0.917802      38.59
 O      -1.814743     0.862229    -0.568369     229.40
 C       0.501410     1.643796    -0.672086      75.81
 H       0.410932     2.567221    -0.169060      22.40
 C       2.238531     0.243704    -1.713874      29.96
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 C       3.800387    -0.182502    -1.690706      86.92
 H       3.837569    -1.065388    -2.589586      25.55
 O       4.680328     0.811108    -2.258682     166.35
 H       4.564030     1.802680    -2.069115      30.34
 C       4.286086    -1.021057    -0.489470     103.64
 H       3.988547    -2.058081    -0.428791      28.91
 O       5.737627    -1.067759    -0.673438     198.63
 H       5.920273    -2.049770    -0.569383      26.84
 C       4.033052    -0.442601     0.794526     128.41
 O       4.599231     0.785904     1.076918     207.16
 H       3.940271     1.476849     1.299964      26.97
 H       4.411436    -1.104988     1.528027      29.22
 H       2.805031    -0.356385     0.907329      24.74
55
name = lig-Water-frame_930
 C      -1.137392     4.127704     2.422905      57.83
 H      -1.965149     4.895274     1.991866      17.95
 C      -0.785566     1.790819     2.901083      68.16
 H      -0.927430     0.671295     2.783755      23.59
 C       0.095962     2.120559     3.982603     -23.46
 O       0.946318     1.322800     4.707273     148.18
 C       0.615899    -0.136047     4.547669     114.77
 H       1.049751    -0.912298     5.165816      27.23
 H       0.648279    -0.471303     3.566135      28.93
 H      -0.486156    -0.106775     5.043714      25.42
 C       0.535995     3.622212     4.068293       5.53
 O       1.365457     3.798953     5.133926     184.78
 H       1.243564     4.747667     5.501908      20.54
 C      -0.216511     4.591315     3.471538      63.60
 H      -0.271553     5.489595     3.747612      27.08
 C      -1.537769     2.725539     2.297950      14.99
 C      -2.740861     2.351754     1.280634      90.01
 H      -3.344239     3.249537     1.088707      27.52
 O      -3.481912     1.373846     2.002872     184.92
 H      -4.226000     1.002789     1.346574      24.41
 C      -2.392200     2.100252    -0.212004      90.75
 H      -1.561411     2.954030    -0.466734      24.41
 C      -3.758326     2.069994    -1.101704      83.96
 O      -4.607339     0.859428    -0.636746     244.89
 H      -4.336255     0.085044    -1.068282      28.35
 H      -3.488176     1.749055    -2.174466      27.52
 H      -4.157288     2.940935    -0.825509      29.43
 C       1.826245     1.366371    -0.875589     116.27
 H       2.544389     2.039755    -0.645702      28.93
 C       1.293327    -0.686496    -1.987380      91.08
 H       1.480994    -1.573373    -2.729158      23.21
 C      -0.061490    -0.540579    -1.629594      23.26
 O      -1.065865    -1.539405    -1.727237     232.27
 C      -0.614132    -2.809699    -2.024546     110.76
 H       0.379738    -3.233403    -1.406920      24.47
 H      -1.417336    -3.642291    -1.870192      25.83
 H      -0.457517    -2.870618    -2.986503      28.15
 C      -0.401035     0.655544    -0.905050      33.82
 O      -1.770758     0.825452    -0.597514     199.49
 C       0.607059     1.609338    -0.609767      47.05
 H       0.249379     2.706687    -0.223678      17.54
 C       2.265220     0.240136    -1.674000      41.62
 C       3.769836    -0.282701    -1.768722      94.02
 H       3.945227    -0.980460    -2.518309      29.40
 O       4.679008     0.783308    -2.183620     141.94
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 H       4.596406     1.794920    -1.756676      28.59
 C       4.283497    -0.974758    -0.510703      94.40
 H       3.968405    -2.112242    -0.502219      26.60
 O       5.782471    -1.051165    -0.668812     170.91
 H       5.841482    -2.058623    -0.498986      26.77
 C       4.026665    -0.454980     0.835673     127.29
 O       4.606995     0.809016     1.095913     275.81
 H       3.788207     1.426010     1.205263      24.94
 H       4.074850    -1.239753     1.759336      25.65
 H       3.007303    -0.562240     0.758428      28.03
55
name = lig-Water-frame_931
 C      -1.196485     4.138065     2.363327      33.96
 H      -1.800766     4.883700     2.069885      14.45
 C      -0.792509     1.748049     2.887473      71.02
 H      -0.893493     0.744909     2.614103      26.62
 C       0.107199     2.155056     3.940786     -11.05
 O       0.981571     1.361426     4.708028      94.59
 C       0.623098    -0.194798     4.574427      98.17
 H       1.270350    -0.765084     5.341044      25.78
 H       0.527714    -0.459167     3.406220      26.01
 H      -0.355507    -0.213318     4.887132      28.69
 C       0.481306     3.553421     4.093274       9.53
 O       1.394313     3.812966     5.152589     167.46
 H       1.343719     4.747193     5.603563      22.96
 C      -0.202703     4.581084     3.458733      44.93
 H      -0.221185     5.836390     3.801070      19.78
 C      -1.569661     2.727535     2.223987      34.41
 C      -2.696402     2.353901     1.332490      93.78
 H      -3.433559     3.261040     1.252991      25.80
 O      -3.461900     1.325174     2.027475     177.77
 H      -4.092566     0.909139     1.412754      26.28
 C      -2.431455     2.093349    -0.186914      88.96
 H      -1.968460     2.908900    -0.617473      27.35
 C      -3.720082     2.062228    -1.076330      71.18
 O      -4.562208     0.853588    -0.624489     230.45
 H      -3.993052    -0.112740    -0.810177      19.74
 H      -3.678789     1.794143    -2.098310      27.85
 H      -4.440383     3.145467    -0.806307      24.22
 C       1.858253     1.317660    -0.915396      94.29
 H       2.622337     2.291651    -0.862155      21.16
 C       1.299762    -0.726704    -2.023585      66.95
 H       1.705414    -1.329012    -2.756685      25.56
 C      -0.022342    -0.504304    -1.612524      13.01
 O      -1.086759    -1.489798    -1.700790     174.48
 C      -0.516502    -2.860397    -2.023349      79.74
 H       0.238395    -3.234443    -1.505600      29.18
 H      -1.441149    -3.411815    -1.664969      26.23
 H      -0.549971    -2.918888    -3.402224      22.67
 C      -0.451080     0.642740    -0.897380      13.06
 O      -1.717787     0.769718    -0.620227     145.25
 C       0.552946     1.624759    -0.519762      33.79
 H       0.246648     2.501864    -0.231377      24.07
 C       2.322916     0.214071    -1.603111      38.19
 C       3.714860    -0.295994    -1.835051      55.38
 H       3.919693    -1.119268    -2.742680      27.86
 O       4.688323     0.777694    -2.118546     148.18
 H       4.497003     1.337700    -1.424155      38.36
 C       4.351228    -0.977736    -0.539271      90.82
 H       3.753004    -1.934395    -0.662776      29.32
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 O       5.821681    -1.053908    -0.663505     166.90
 H       6.047612    -2.013635    -0.526199      28.03
 C       3.974059    -0.496570     0.922188     108.18
 O       4.596190     0.835608     1.118938     242.24
 H       3.889266     1.513802     1.224782      27.27
 H       4.117195    -1.201024     1.661479      29.33
 H       2.753033    -0.389679     0.795384      25.25
55
name = lig-Water-frame_932
 C      -1.229288     4.130371     2.391131      84.73
 H      -1.831378     5.061686     1.893738      25.03
 C      -0.773984     1.718967     2.913118     -14.68
 H      -0.962469     0.673136     2.513194      23.09
 C       0.155738     2.197253     3.863404      32.55
 O       0.999662     1.345627     4.692010     144.25
 C       0.638428    -0.201439     4.603222      99.78
 H       1.468833    -0.480809     5.173219      27.30
 H       0.728509    -0.507248     3.543518      29.37
 H      -0.549891    -0.434056     4.883622      26.58
 C       0.421988     3.503476     4.176839       4.30
 O       1.421624     3.825311     5.161767     -18.54
 H       1.269261     4.797145     5.415296      22.34
 C      -0.256686     4.572586     3.375087      62.79
 H       0.009712     5.518555     3.618954      18.55
 C      -1.550233     2.797308     2.149419     -36.96
 C      -2.696741     2.357747     1.361542      87.02
 H      -3.359026     3.251850     1.441608      28.22
 O      -3.440750     1.265808     2.057299     130.68
 H      -3.997130     0.876460     1.355382      26.93
 C      -2.470058     2.064174    -0.211242      83.26
 H      -2.020747     3.046951    -0.734517      26.63
 C      -3.731021     2.014915    -0.990386     105.40
 O      -4.509847     0.853935    -0.612551     280.02
 H      -3.990656     0.108853    -0.423857      29.45
 H      -3.561162     2.145014    -2.180686      26.49
 H      -4.443958     2.759696    -0.996677      28.16
 C       1.972613     1.351838    -0.958292      71.05
 H       2.504785     2.158680    -0.911401      25.40
 C       1.320680    -0.727104    -2.042207      58.84
 H       1.728811    -1.498272    -2.853421      24.97
 C      -0.023108    -0.510052    -1.590766      11.65
 O      -1.058698    -1.443780    -1.681887     148.95
 C      -0.528498    -2.886769    -2.080288      91.05
 H       0.555322    -3.178886    -1.478266      26.01
 H      -1.368550    -3.403639    -1.614530      26.88
 H      -0.352306    -3.017590    -2.960758      31.24
 C      -0.419744     0.672013    -0.880079      24.60
 O      -1.741314     0.728344    -0.616038     172.09
 C       0.461454     1.578822    -0.474866      79.66
 H       0.221836     2.713180     0.007481      25.42
 C       2.332343     0.132056    -1.556988      26.72
 C       3.733108    -0.270121    -1.881790      61.77
 H       3.660510    -0.976398    -2.700758      26.88
 O       4.685250     0.779577    -2.074420      84.36
 H       4.554394     1.109929    -1.041630      29.21
 C       4.397322    -1.013226    -0.553832      81.62
 H       3.840261    -2.020950    -0.659485      28.61
 O       5.848054    -1.066696    -0.655449     139.20
 H       6.129503    -2.043977    -0.595095      24.49
 C       3.867538    -0.486197     0.934326      98.18
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 O       4.578555     0.837252     1.148060     147.39
 H       3.973617     1.617814     1.353918      30.53
 H       4.396144    -1.270853     1.710673      26.10
 H       2.900841    -0.191545     1.052488      26.38
55
name = lig-Water-frame_933
 C      -1.267517     4.184373     2.431947      80.96
 H      -1.714824     4.836048     1.789879      29.38
 C      -0.778897     1.764928     2.895293      50.07
 H      -0.953217     0.714623     2.692026      23.29
 C       0.231324     2.153378     3.811740       4.23
 O       0.979503     1.295923     4.649517     148.62
 C       0.646237    -0.151178     4.629065     114.34
 H       1.600441    -0.526326     5.172327      24.44
 H       0.966381    -0.596464     3.570756      26.23
 H      -0.196230    -0.500023     5.028320      29.10
 C       0.354335     3.555978     4.235123      23.85
 O       1.418378     3.840741     5.139586      63.25
 H       1.211181     4.844959     5.304191      23.07
 C      -0.285991     4.464384     3.307016      60.95
 H       0.181387     5.622211     3.433251      18.20
 C      -1.457601     2.805550     2.146128     -10.01
 C      -2.729204     2.351601     1.358219      68.56
 H      -3.406074     3.266577     1.369747      27.64
 O      -3.407404     1.211009     2.082330     130.19
 H      -4.029509     0.878906     1.295337      23.99
 C      -2.474038     2.066428    -0.246347      87.26
 H      -1.846572     2.860217    -0.555898      28.27
 C      -3.758369     1.923972    -0.966569      99.52
 O      -4.487310     0.866043    -0.594365     280.13
 H      -3.882765     0.063272    -0.341693      25.58
 H      -3.327955     2.139939    -1.916770      27.93
 H      -4.620250     2.900463    -0.800379      24.18
 C       1.971906     1.377661    -0.966750      62.37
 H       2.750453     2.295271    -0.812714      24.21
 C       1.318743    -0.735872    -2.050403      71.79
 H       1.382513    -1.599028    -2.599831      26.25
 C      -0.011512    -0.545120    -1.584369      14.81
 O      -0.996345    -1.437621    -1.690303     176.22
 C      -0.538858    -2.865126    -2.021072      70.58
 H       0.350631    -2.915420    -1.621336      30.00
 H      -1.322531    -3.723943    -1.654570      24.31
 H      -0.122171    -3.152325    -3.324234      23.42
 C      -0.397348     0.679518    -0.866542      10.50
 O      -1.827207     0.717625    -0.586407     185.97
 C       0.523703     1.599286    -0.461636      55.74
 H       0.279947     2.396485     0.083209      28.57
 C       2.321766     0.087676    -1.534649      27.62
 C       3.787591    -0.242563    -1.856393      85.20
 H       3.660677    -0.935183    -2.840504      26.25
 O       4.664361     0.806843    -2.020874     149.08
 H       5.016386     1.163548    -1.138632      29.31
 C       4.368104    -1.072665    -0.565492      81.85
 H       4.215150    -2.221230    -0.516998      24.93
 O       5.864096    -1.086045    -0.636550     149.41
 H       5.964222    -2.088590    -0.636476      26.74
 C       3.857158    -0.451661     0.918148     102.72
 O       4.569434     0.826416     1.173669     173.41
 H       3.926330     1.545752     1.493623      29.95
 H       4.307138    -1.089301     1.555450      29.02
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 H       2.709210    -0.274668     1.257407      24.79
55
name = lig-Water-frame_934
 C      -1.307025     4.178256     2.429115      52.60
 H      -1.746107     4.919374     1.641336      23.94
 C      -0.760512     1.840614     2.871431      68.46
 H      -0.979186     0.777496     2.847067      23.69
 C       0.286870     2.120563     3.813400      12.86
 O       0.939161     1.243626     4.595361     171.38
 C       0.762639    -0.106595     4.632617     125.12
 H       1.433728    -0.606868     5.305454      25.58
 H       0.885859    -0.649421     3.632991      27.91
 H      -0.208095    -0.512792     5.259224      24.00
 C       0.305511     3.560235     4.224195      34.27
 O       1.379561     3.881422     5.088653     140.74
 H       1.324422     4.814257     5.497701      22.85
 C      -0.226634     4.433135     3.326932      66.42
 H       0.080117     5.460415     3.167126      22.25
 C      -1.413002     2.764696     2.168541      11.00
 C      -2.733158     2.338262     1.346664      72.16
 H      -3.504010     3.186014     1.225960      27.02
 O      -3.371534     1.175014     2.077839     201.93
 H      -4.089547     0.886677     1.540801      27.26
 C      -2.447625     2.044845    -0.200292      87.38
 H      -1.641277     2.818271    -0.526763      25.80
 C      -3.800179     1.956336    -0.973216      96.07
 O      -4.499071     0.818360    -0.555967     296.10
 H      -3.891830    -0.034747    -0.672074      23.61
 H      -3.396566     1.814629    -2.097630      26.27
 H      -4.263055     2.793167    -0.580714      28.21
 C       1.917159     1.391021    -0.948755      57.26
 H       2.762050     2.003757    -0.672619      27.29
 C       1.271929    -0.749080    -2.018502      59.50
 H       1.329916    -1.827382    -2.454957      22.64
 C       0.013456    -0.529724    -1.563552      21.36
 O      -0.960198    -1.497386    -1.727212     227.74
 C      -0.554130    -2.844823    -2.022211     118.02
 H       0.527525    -2.893515    -1.358651      25.42
 H      -1.157580    -3.629240    -1.767253      28.75
 H      -0.368170    -2.968992    -2.913998      32.72
 C      -0.424976     0.644542    -0.858876      -0.33
 O      -1.893217     0.729516    -0.543825     169.71
 C       0.684352     1.602477    -0.502455      49.62
 H       0.320891     2.468286     0.295430      23.40
 C       2.322014     0.129153    -1.536687      15.48
 C       3.816796    -0.272529    -1.776786      93.36
 H       4.012622    -0.713229    -2.805135      27.20
 O       4.669389     0.869593    -1.991642     156.74
 H       5.226834     1.172721    -1.339627      31.78
 C       4.319641    -1.125519    -0.563536      88.68
 H       4.091591    -2.159458    -0.479205      27.60
 O       5.859764    -1.110453    -0.605913     170.36
 H       5.986827    -2.100176    -0.617450      26.97
 C       3.868906    -0.395073     0.877161     113.51
 O       4.555912     0.813485     1.196188     205.09
 H       3.869292     1.435017     1.467383      32.61
 H       4.278371    -1.225858     1.685738      25.91
 H       2.842069    -0.590369     1.083889      27.66
55
name = lig-Water-frame_935
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 C      -1.302980     4.117965     2.392178      53.57
 H      -1.700948     4.965278     1.822121      25.63
 C      -0.678687     1.844416     2.896162      53.67
 H      -1.092962     0.787703     2.831748      25.42
 C       0.269901     2.153760     3.832173      47.54
 O       0.931005     1.232070     4.559007     208.70
 C       0.831899    -0.165070     4.667639     119.62
 H       1.576430    -0.518637     5.444801      23.54
 H       0.751598    -0.664239     3.625569      27.63
 H      -0.145946    -0.240652     5.022211      27.27
 C       0.334764     3.489324     4.193194      40.50
 O       1.344642     3.926146     5.043542     113.80
 H       1.194547     4.781312     5.574793      22.81
 C      -0.209191     4.474863     3.310326      46.29
 H       0.157164     5.580638     3.254478      18.40
 C      -1.499087     2.774099     2.154774      14.01
 C      -2.710711     2.293926     1.333726      94.88
 H      -3.450072     3.110418     1.304940      28.25
 O      -3.324825     1.164248     2.069201     194.97
 H      -4.214062     0.850229     1.693028      25.11
 C      -2.400096     2.008673    -0.138073     101.18
 H      -1.758086     2.795623    -0.573253      28.81
 C      -3.761905     1.987082    -1.009440      73.22
 O      -4.531078     0.736763    -0.515876     232.52
 H      -4.105187    -0.011725    -0.922433      28.81
 H      -3.825206     1.785317    -2.051415      28.18
 H      -4.348024     3.060510    -0.618011      25.85
 C       1.952489     1.340445    -0.943976      50.99
 H       2.778094     1.909725    -0.523771      28.54
 C       1.286766    -0.767593    -1.962478      56.16
 H       1.643429    -1.701922    -2.330325      25.17
 C      -0.034557    -0.498307    -1.524770      17.62
 O      -0.970555    -1.562416    -1.765303     211.68
 C      -0.490619    -2.801199    -1.949385      93.08
 H       0.255197    -3.197820    -1.369650      28.51
 H      -1.420046    -3.599506    -1.620056      24.88
 H      -0.348881    -2.877132    -3.319999      22.89
 C      -0.448674     0.635356    -0.835636      11.37
 O      -1.886395     0.734151    -0.498010     180.72
 C       0.685581     1.601205    -0.519733      59.71
 H       0.604903     2.410915     0.207341      27.79
 C       2.309775     0.170064    -1.589894      -4.55
 C       3.842089    -0.286208    -1.687457      74.28
 H       4.110643    -0.828797    -2.691562      28.16
 O       4.672824     0.950158    -1.992799      86.67
 H       5.437373     1.121093    -1.225988      25.17
 C       4.306547    -1.108929    -0.523922      84.91
 H       3.587735    -2.128854    -0.540044      26.58
 O       5.825011    -1.145569    -0.571984     169.67
 H       6.170515    -2.116429    -0.537401      22.77
 C       3.942603    -0.454398     0.843675     121.83
 O       4.527201     0.804228     1.216826     156.80
 H       3.818082     1.536179     1.336217      31.57
 H       4.221283    -1.133009     1.548939      30.12
 H       2.764957    -0.531709     0.817025      27.81
55
name = lig-Water-frame_936
 C      -1.231503     4.096723     2.372326      84.83
 H      -1.798198     4.940743     1.938071      28.87
 C      -0.667467     1.806414     2.876438      59.94
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 H      -0.966597     0.824071     2.771484      31.72
 C       0.219818     2.158921     3.861328      42.11
 O       0.984892     1.266168     4.549638     152.33
 C       0.848237    -0.247655     4.697093     101.72
 H       1.705554    -0.410393     5.332401      24.70
 H       0.848048    -0.761713     3.635493      28.23
 H      -0.284824    -0.298949     4.989539      25.16
 C       0.409919     3.501165     4.131236       2.85
 O       1.332860     3.954792     5.027999     -32.05
 H       0.898403     4.832179     5.357057      21.43
 C      -0.236052     4.515088     3.262712      43.33
 H       0.185848     5.554642     3.631616      12.34
 C      -1.595063     2.760005     2.162784      -6.09
 C      -2.692848     2.231434     1.338207     104.41
 H      -3.409117     3.165336     1.423420      28.02
 O      -3.276452     1.155304     2.066623     178.97
 H      -4.212035     0.891937     1.688966      26.14
 C      -2.394122     1.978734    -0.147921      98.99
 H      -1.834920     2.869004    -0.556743      29.85
 C      -3.746421     2.008309    -0.977801      88.30
 O      -4.575034     0.693978    -0.474477     147.73
 H      -4.245749    -0.117683    -1.102128      26.77
 H      -3.953932     2.012030    -2.143511      26.76
 H      -4.432257     2.833801    -0.935556      29.12
 C       2.028835     1.283035    -0.937010      13.24
 H       2.815385     2.006504    -0.403411      27.14
 C       1.341511    -0.747161    -1.876492      52.65
 H       1.795553    -1.672285    -2.312900      26.37
 C      -0.095905    -0.530128    -1.512519       9.85
 O      -1.006061    -1.552483    -1.768959     194.78
 C      -0.480408    -2.856337    -1.965016     125.51
 H       0.383620    -3.408717    -1.287407      27.96
 H      -1.356610    -3.294306    -1.723560      30.09
 H      -0.176476    -2.999087    -2.855260      32.26
 C      -0.462736     0.679213    -0.791177      16.92
 O      -1.805297     0.715790    -0.452172     189.50
 C       0.590129     1.569194    -0.535870      37.22
 H       0.607664     2.502376     0.176887      29.41
 C       2.324065     0.159060    -1.672745      41.93
 C       3.864985    -0.238776    -1.665381      72.03
 H       3.939315    -1.127747    -2.433590      29.09
 O       4.681639     1.019787    -1.981765     124.24
 H       5.351603     0.976785    -1.263939      26.77
 C       4.306477    -1.072223    -0.459321     118.56
 H       3.657038    -1.875168    -0.582572      32.86
 O       5.774424    -1.193341    -0.542827     223.39
 H       6.040067    -2.154144    -0.442611      22.88
 C       3.970023    -0.547553     0.809939     123.22
 O       4.495811     0.807857     1.238624     108.45
 H       3.837456     1.530342     1.118436      35.69
 H       4.288464    -1.289237     1.688510      27.69
 H       2.938551    -0.204703     0.685711      30.65
55
name = lig-Water-frame_937
 C      -1.181199     4.123433     2.336966      67.28
 H      -2.001551     4.841388     1.952248      18.56
 C      -0.744102     1.782179     2.813801      41.99
 H      -0.747772     0.609405     2.658305      29.60
 C       0.174069     2.131352     3.882953     -37.75
 O       1.075508     1.295065     4.561563      76.48
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 C       0.811688    -0.277909     4.687965     101.60
 H       1.685806    -0.540323     5.302430      27.79
 H       1.065916    -0.834341     3.732268      30.01
 H      -0.104740    -0.649557     5.200615      27.54
 C       0.474615     3.579725     4.014850       9.66
 O       1.322402     3.981676     5.032750     144.48
 H       1.032768     4.922345     5.236837      20.67
 C      -0.225212     4.506540     3.281482      72.61
 H      -0.057322     5.521232     3.618616      24.37
 C      -1.577556     2.709417     2.228733      25.19
 C      -2.710719     2.213526     1.356354      97.69
 H      -3.393917     3.055504     1.313274      30.88
 O      -3.247700     1.127553     2.071199     230.52
 H      -4.001969     0.905506     1.585328      31.44
 C      -2.436469     1.977047    -0.210317      82.63
 H      -1.792322     2.889036    -0.470106      28.11
 C      -3.782082     1.951706    -0.963482      87.77
 O      -4.611425     0.688367    -0.461706     194.57
 H      -4.289492    -0.087213    -0.930417      30.11
 H      -3.498620     2.014954    -2.003663      28.91
 H      -4.583773     2.861243    -0.736881      25.90
 C       2.015978     1.285616    -0.890327       5.94
 H       2.710601     1.943363    -0.610218      27.03
 C       1.330670    -0.760550    -1.805341      31.10
 H       1.570811    -1.727637    -2.327575      24.68
 C      -0.075105    -0.573188    -1.515359       7.43
 O      -1.033389    -1.499866    -1.749455     147.12
 C      -0.466477    -2.956338    -1.937093      70.24
 H       0.294773    -3.120539    -1.186984      29.03
 H      -1.579023    -3.552753    -1.915334      24.08
 H       0.137121    -3.236360    -3.128515      22.23
 C      -0.456050     0.686218    -0.778913      15.65
 O      -1.711243     0.699754    -0.400383     177.62
 C       0.575116     1.544526    -0.547978      64.40
 H       0.308013     2.545540     0.041833      30.47
 C       2.411937     0.172003    -1.705923      56.90
 C       3.864728    -0.168656    -1.699165      86.25
 H       3.941271    -1.091397    -2.457813      26.94
 O       4.671555     1.035834    -1.969346     146.76
 H       5.355146     1.015360    -1.314454      28.56
 C       4.352572    -1.001387    -0.437789     102.40
 H       3.827423    -2.123153    -0.625188      27.89
 O       5.726154    -1.243334    -0.521286     231.93
 H       5.771799    -2.290791    -0.413216      21.48
 C       3.956637    -0.571439     0.878928     152.78
 O       4.496388     0.797846     1.259373     126.16
 H       3.818300     1.404960     0.954972      38.58
 H       4.127890    -1.283212     1.662058      32.42
 H       2.891745    -0.302501     0.844129      32.53
55
name = lig-Water-frame_938
 C      -1.206670     4.113560     2.300530      54.34
 H      -1.926336     4.771083     1.943701      19.72
 C      -0.772035     1.697987     2.821920      52.19
 H      -0.710248     0.726629     2.499706      29.65
 C       0.154134     2.138635     3.860591     -35.98
 O       1.139425     1.287112     4.577011      52.94
 C       0.810758    -0.279056     4.686303      96.55
 H       1.607278    -0.634566     5.406214      27.32
 H       1.158802    -0.821638     3.666327      28.18
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 H      -0.007265    -0.739627     5.231815      27.31
 C       0.537803     3.586540     3.932721      12.25
 O       1.318354     4.005098     5.031965     116.12
 H       1.390028     5.006358     5.347278      25.32
 C      -0.216946     4.512128     3.287546      54.03
 H      -0.387103     5.715715     3.422435      20.98
 C      -1.517303     2.708712     2.262151      28.40
 C      -2.712894     2.233007     1.367999      75.29
 H      -3.574115     3.045948     1.210420      27.10
 O      -3.235684     1.082729     2.078103     188.49
 H      -3.955626     0.692071     1.417744      26.35
 C      -2.475710     1.986367    -0.212949      78.19
 H      -1.841004     2.793891    -0.543399      28.78
 C      -3.843323     1.860961    -0.948018      98.82
 O      -4.634960     0.721563    -0.470451     216.73
 H      -4.175987    -0.145550    -0.745583      28.83
 H      -3.263008     1.814004    -1.934133      26.50
 H      -4.365637     2.720226    -0.451454      26.73
 C       1.930528     1.293991    -0.868129      33.51
 H       2.781583     2.189500    -0.785750      22.96
 C       1.302825    -0.810256    -1.782851      49.38
 H       1.353081    -1.732404    -2.304417      24.21
 C       0.002999    -0.567709    -1.494952      21.67
 O      -1.044181    -1.488329    -1.738451     157.78
 C      -0.502360    -3.048142    -1.969098      95.28
 H       0.162739    -2.995189    -0.965424      27.11
 H      -1.215095    -3.726488    -2.029612      29.58
 H       0.040313    -3.148563    -2.763147      29.26
 C      -0.393134     0.610981    -0.828014      15.91
 O      -1.674208     0.703579    -0.341954     155.73
 C       0.625027     1.559958    -0.552500      73.63
 H       0.206959     2.471242    -0.095522      30.11
 C       2.438188     0.215190    -1.650529      35.29
 C       3.874143    -0.129382    -1.748499      96.68
 H       4.171898    -0.728581    -2.690601      28.81
 O       4.647884     1.022932    -1.967472     158.28
 H       5.514976     1.164361    -1.318083      23.45
 C       4.361296    -0.986497    -0.470235     113.37
 H       3.979608    -1.928738    -0.558056      30.83
 O       5.714465    -1.291392    -0.504677     228.46
 H       5.821271    -2.290348    -0.482052      25.41
 C       3.892100    -0.515647     0.992734     126.73
 O       4.515728     0.763431     1.283204     163.43
 H       3.798237     1.381186     0.903349      33.32
 H       4.114079    -1.342708     1.781997      29.32
 H       2.732064    -0.689753     1.095247      30.50
55
name = lig-Water-frame_939
 C      -1.232304     4.053518     2.316967      88.03
 H      -1.891595     4.896405     1.790773      20.98
 C      -0.725046     1.642848     2.906731      34.78
 H      -0.857102     0.603507     2.392994      28.43
 C       0.202343     2.144896     3.813718     -40.18
 O       1.143340     1.252104     4.584359      69.15
 C       0.880418    -0.266003     4.688684     109.12
 H       1.601127    -0.529861     5.428068      28.67
 H       0.989125    -0.680857     3.703852      30.34
 H      -0.273535    -0.491224     4.995686      26.55
 C       0.586925     3.569094     3.935756      -9.74
 O       1.343570     4.004036     5.027661      52.72
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 H       1.386385     4.967371     5.289413      27.15
 C      -0.276666     4.575804     3.213001      36.78
 H      -0.271110     5.560231     3.393362      22.30
 C      -1.502773     2.735671     2.211770      22.75
 C      -2.718621     2.273590     1.368587      92.15
 H      -3.499002     2.993015     1.418133      30.43
 O      -3.244382     1.029745     2.064596     184.32
 H      -3.807519     0.488731     1.436568      29.51
 C      -2.479241     1.961756    -0.136590      85.65
 H      -1.973022     2.826273    -0.787710      27.58
 C      -3.829712     1.753369    -0.913603      99.72
 O      -4.653945     0.742703    -0.496545     224.83
 H      -4.050275    -0.126405    -0.518945      28.20
 H      -3.746708     1.653925    -2.035972      28.59
 H      -4.352819     2.767429    -0.599120      27.27
 C       1.937188     1.360792    -0.891090      69.27
 H       2.503740     2.170448    -0.853322      26.91
 C       1.364338    -0.836724    -1.800031      59.47
 H       1.489154    -1.834062    -2.378471      20.95
 C       0.026682    -0.585449    -1.464389      18.76
 O      -1.040661    -1.521416    -1.744175     158.28
 C      -0.529658    -3.044206    -1.929201      67.29
 H      -0.082278    -3.225864    -0.870571      26.76
 H      -1.329085    -4.002557    -2.021415      23.86
 H       0.305462    -3.021828    -2.942475      21.10
 C      -0.319015     0.567458    -0.860475       9.30
 O      -1.668428     0.708052    -0.290864     153.73
 C       0.630783     1.558055    -0.558660      50.64
 H       0.240165     2.660368    -0.101909      29.07
 C       2.342928     0.204917    -1.550432       4.33
 C       3.917828    -0.116554    -1.781629      95.18
 H       4.163115    -0.649251    -2.812345      26.42
 O       4.650641     1.049574    -1.968831     214.33
 H       5.410149     1.144495    -1.404397      29.96
 C       4.319427    -0.984089    -0.485707      88.38
 H       3.612009    -2.022879    -0.596260      28.89
 O       5.754053    -1.301301    -0.495455     182.40
 H       5.985403    -2.341601    -0.541365      21.06
 C       3.820250    -0.501257     1.087446     114.32
 O       4.510941     0.725561     1.312773     165.51
 H       3.954797     1.496705     1.059438      34.40
 H       4.419769    -1.217610     1.717814      30.49
 H       2.781680    -0.641834     1.236330      31.88
55
name = lig-Water-frame_940
 C      -1.272839     4.062210     2.334170      97.23
 H      -1.758574     4.706397     1.716978      33.96
 C      -0.696258     1.661551     2.946225      35.68
 H      -0.976343     0.644106     2.696947      30.73
 C       0.331346     2.116989     3.790519       1.70
 O       1.113521     1.226120     4.580908     135.66
 C       0.900541    -0.198594     4.689799     117.62
 H       1.653074    -0.556905     5.471863      25.97
 H       0.910755    -0.711600     3.562216      27.13
 H      -0.130749    -0.170091     4.798983      28.52
 C       0.554750     3.598788     3.952791       5.01
 O       1.392476     3.972640     5.013227      23.19
 H       1.089052     4.957918     5.159399      17.15
 C      -0.290446     4.556172     3.153586      39.80
 H       0.044210     5.717603     3.469812       9.24
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 C      -1.500083     2.666950     2.150979     -37.08
 C      -2.715053     2.272256     1.375029      84.92
 H      -3.509006     3.123072     1.679907      24.73
 O      -3.242989     0.983721     2.046512     215.13
 H      -3.749870     0.494765     1.451062      32.39
 C      -2.458561     1.927819    -0.109239     105.58
 H      -2.138048     2.731183    -0.677577      30.33
 C      -3.794589     1.715363    -0.892081     113.93
 O      -4.683995     0.705246    -0.491961     300.51
 H      -4.159264    -0.038188    -0.482626      33.90
 H      -4.021702     1.637592    -2.006685      26.45
 H      -4.390670     2.696566    -1.053849      27.34
 C       1.960755     1.434222    -0.940882      56.69
 H       2.661289     2.408776    -0.821800      27.33
 C       1.446616    -0.856171    -1.835476      69.78
 H       1.869539    -1.678540    -2.311245      26.27
 C       0.021039    -0.688814    -1.465081       9.66
 O      -1.019271    -1.587636    -1.754056     193.22
 C      -0.552212    -3.025486    -1.902449     122.52
 H      -0.078881    -3.452161    -0.884918      29.22
 H      -1.367823    -3.570405    -2.104005      27.96
 H       0.189456    -3.025888    -2.609665      31.31
 C      -0.319595     0.607084    -0.821408      21.16
 O      -1.657635     0.698450    -0.248661     185.36
 C       0.589845     1.589706    -0.557880      60.39
 H       0.382634     2.496562    -0.174999      32.62
 C       2.275294     0.138554    -1.469493       8.98
 C       3.929601    -0.122600    -1.777423      86.44
 H       3.856337    -0.857505    -2.683445      29.74
 O       4.661020     1.112072    -1.981767     181.59
 H       5.383971     1.072996    -1.348563      29.81
 C       4.227838    -1.040962    -0.489781      77.01
 H       3.620606    -1.809995    -0.664152      32.10
 O       5.796041    -1.289954    -0.487147     185.02
 H       5.912375    -2.288332    -0.550246      24.96
 C       3.836440    -0.516448     1.100668     106.39
 O       4.500117     0.715960     1.361692     141.09
 H       4.042893     1.566376     1.262582      35.60
 H       4.531091    -1.183046     1.628878      29.96
 H       2.677895    -0.377629     1.399833      27.87
55
name = lig-Water-frame_941
 C      -1.308052     4.053363     2.328004      43.46
 H      -1.871847     4.723328     1.527007      28.89
 C      -0.699361     1.740490     2.939292      34.02
 H      -0.975699     0.663069     3.084505      26.73
 C       0.456084     2.101239     3.773771       9.49
 O       1.109282     1.252295     4.575136     148.73
 C       0.892147    -0.131153     4.636635     130.70
 H       1.485682    -0.621360     5.358395      28.68
 H       1.094874    -0.675491     3.754179      28.20
 H      -0.287314    -0.235677     5.012195      24.11
 C       0.479140     3.586725     3.956836      20.42
 O       1.432037     3.961975     4.976898     126.51
 H       1.009297     4.839091     5.307343      20.58
 C      -0.206474     4.522249     3.179197      82.42
 H       0.053564     5.475580     3.245541      22.07
 C      -1.457459     2.576948     2.150868     -21.53
 C      -2.736360     2.222079     1.412719      93.40
 H      -3.400049     2.993019     1.535807      28.67
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 O      -3.221981     0.960481     2.035359     212.22
 H      -3.904237     0.580472     1.314812      24.46
 C      -2.466684     1.882104    -0.130554      83.86
 H      -1.929125     2.894337    -0.569568      25.76
 C      -3.799478     1.724310    -0.936367      89.28
 O      -4.733807     0.647047    -0.447659     245.91
 H      -4.233516    -0.285345    -0.597543      26.34
 H      -3.473023     1.512239    -2.022066      27.80
 H      -4.407321     2.689620    -0.947265      26.70
 C       1.959212     1.498723    -0.992634      46.48
 H       2.764833     2.176881    -0.820314      25.90
 C       1.441195    -0.882698    -1.848117      61.40
 H       2.143127    -1.700762    -2.299103      20.31
 C       0.031451    -0.770221    -1.470606       1.99
 O      -0.973303    -1.660826    -1.748612     224.88
 C      -0.582110    -2.968465    -1.836243     102.61
 H      -0.117240    -3.624686    -0.964490      26.22
 H      -1.662001    -3.334521    -2.322843      23.86
 H       0.351752    -3.128130    -2.723330      23.99
 C      -0.380844     0.603351    -0.771579       9.05
 O      -1.641621     0.678781    -0.211533     193.01
 C       0.608418     1.622025    -0.587793      43.95
 H       0.256054     2.736923     0.012558      26.35
 C       2.336465     0.155797    -1.411041      28.20
 C       3.853105    -0.139316    -1.716125      73.92
 H       3.839832    -0.905828    -2.571019      28.64
 O       4.664472     1.153577    -1.999453     128.74
 H       5.454678     1.002571    -1.248087      26.44
 C       4.185445    -1.034807    -0.476759      72.29
 H       3.614986    -2.144571    -0.756868      23.78
 O       5.794309    -1.270223    -0.474727     163.45
 H       5.867507    -2.261064    -0.535340      27.39
 C       3.874900    -0.513953     1.048751     110.60
 O       4.519358     0.733593     1.420950     159.54
 H       3.827581     1.514303     1.399383      29.88
 H       4.348106    -1.398126     1.678740      27.78
 H       2.930598    -0.410843     1.391995      29.50
55
name = lig-Water-frame_942
 C      -1.293960     4.009340     2.297744      54.21
 H      -1.842361     4.676505     1.699118      30.60
 C      -0.658548     1.767471     2.958693      37.87
 H      -0.999440     0.748792     3.325258      28.98
 C       0.470639     2.156925     3.713074      24.64
 O       1.150024     1.312205     4.587936     117.15
 C       0.796755    -0.101578     4.608727     126.81
 H       1.468138    -0.544287     5.441049      27.22
 H       1.279703    -0.700985     3.630742      27.87
 H      -0.060979    -0.453165     4.997143      29.69
 C       0.469128     3.502486     3.993248      36.27
 O       1.447034     3.970472     4.933006     117.09
 H       1.266371     4.777420     5.466507      22.26
 C      -0.171205     4.445541     3.172681      60.01
 H       0.090822     5.629890     3.103935      18.40
 C      -1.438527     2.586239     2.177902      11.27
 C      -2.724737     2.094906     1.439120      76.99
 H      -3.534851     3.021245     1.323352      26.97
 O      -3.214612     0.941403     2.009214     235.94
 H      -4.005171     0.761471     1.450850      26.99
 C      -2.469344     1.888372    -0.146398      81.18
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 H      -1.857479     2.641176    -0.430188      30.70
 C      -3.788065     1.705704    -1.008917      77.88
 O      -4.751894     0.583244    -0.400772     230.60
 H      -4.453413    -0.299492    -0.808723      27.81
 H      -3.104591     1.429597    -1.855493      26.72
 H      -4.404967     2.665352    -0.699831      25.55
 C       1.945946     1.482406    -1.037209      57.46
 H       2.834249     2.151538    -0.806719      27.94
 C       1.423543    -0.887481    -1.819277      56.89
 H       1.827838    -1.770598    -2.253369      25.26
 C       0.072539    -0.754153    -1.451359      10.09
 O      -0.918758    -1.682281    -1.711881     242.39
 C      -0.615851    -2.997271    -1.869711     142.52
 H      -0.331281    -3.544566    -0.867219      28.63
 H      -1.449447    -3.415040    -2.346758      29.40
 H       0.104805    -3.215576    -2.595035      30.07
 C      -0.394924     0.554213    -0.752277      -5.81
 O      -1.640632     0.650181    -0.180729     162.11
 C       0.603447     1.689781    -0.603738      49.95
 H       0.272780     2.445574    -0.137552      31.64
 C       2.407531     0.230093    -1.405460      34.63
 C       3.746218    -0.138807    -1.628842      90.22
 H       4.086785    -0.745337    -2.602300      26.72
 O       4.660989     1.137443    -1.989543     144.59
 H       5.417919     1.105991    -1.448613      29.77
 C       4.198242    -1.036240    -0.450158     105.76
 H       3.904992    -1.963266    -0.551807      31.40
 O       5.748481    -1.247280    -0.460745     155.83
 H       5.923469    -2.282468    -0.536028      26.22
 C       3.950737    -0.542644     0.981690     126.09
 O       4.543030     0.763917     1.472101     175.79
 H       3.736548     1.284560     1.464447      33.88
 H       4.154762    -1.364897     1.635996      30.97
 H       2.747931    -0.570979     1.244624      29.20
55
name = lig-Water-frame_943
 C      -1.200592     3.951783     2.293892      99.24
 H      -1.862777     4.749646     1.811851      29.09
 C      -0.616087     1.729672     2.996070      49.88
 H      -1.021820     0.792561     3.184607      32.20
 C       0.429794     2.196706     3.679576      22.29
 O       1.185364     1.370908     4.602765     108.71
 C       0.792850    -0.121371     4.587821     113.97
 H       1.470459    -0.296127     5.382704      26.88
 H       1.072896    -0.500173     3.713925      33.13
 H      -0.360648    -0.568378     4.831065      25.60
 C       0.529470     3.506963     4.047619      41.32
 O       1.468437     3.961626     4.895509      26.22
 H       1.357206     4.924697     5.344355      21.83
 C      -0.200148     4.395561     3.117025      60.17
 H       0.091597     5.413895     3.205340      22.63
 C      -1.483001     2.632493     2.200661      14.23
 C      -2.698566     2.030082     1.412727     103.80
 H      -3.414784     2.757511     1.412539      33.21
 O      -3.229795     0.906263     1.999994     217.92
 H      -4.095110     0.706020     1.630156      28.57
 C      -2.465062     1.855628    -0.096037      76.85
 H      -1.749143     2.732635    -0.567747      28.00
 C      -3.754348     1.657089    -0.998636      85.65
 O      -4.733132     0.545357    -0.384226     204.95
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 H      -4.544808    -0.256667    -0.836934      30.61
 H      -3.329126     1.384506    -2.075517      28.47
 H      -4.322758     2.539147    -0.963529      29.90
 C       1.943457     1.466381    -1.046269      77.62
 H       2.671737     2.322210    -0.815004      29.94
 C       1.423204    -0.833648    -1.743434      73.84
 H       1.510143    -1.861816    -2.245111      24.72
 C       0.103503    -0.667878    -1.401668      21.16
 O      -0.881121    -1.643399    -1.663512     196.65
 C      -0.635123    -3.097581    -1.907181      98.45
 H      -0.632248    -3.401580    -0.739156      25.82
 H      -1.562559    -3.724931    -2.359579      26.90
 H       0.316890    -3.328725    -2.703383      25.70
 C      -0.332646     0.528939    -0.754675       1.39
 O      -1.649749     0.600203    -0.166811     140.46
 C       0.567882     1.641263    -0.662221       4.84
 H       0.158520     2.742408    -0.030693      31.35
 C       2.357481     0.250875    -1.472829      47.82
 C       3.770983    -0.125579    -1.580618     110.87
 H       3.973517    -0.638048    -2.493988      30.41
 O       4.629336     1.095063    -1.971748     170.16
 H       5.510433     1.167743    -1.499533      25.93
 C       4.305901    -0.993093    -0.400720     102.76
 H       3.804051    -2.173621    -0.393110      28.94
 O       5.698953    -1.230891    -0.455576     188.53
 H       5.898994    -2.138146    -0.543315      30.03
 C       3.961537    -0.569959     0.949161     131.44
 O       4.553963     0.756848     1.498986     122.98
 H       3.752110     1.385989     1.483514      34.80
 H       4.292566    -1.389342     1.753293      29.34
 H       2.941974    -0.540729     0.860058      33.57
55
name = lig-Water-frame_944
 C      -1.140118     3.943464     2.260956      94.15
 H      -1.806476     4.733652     1.871736      26.49
 C      -0.665741     1.699650     2.961632      45.40
 H      -0.971023     0.550647     2.898238      29.26
 C       0.425404     2.181014     3.759165      -6.21
 O       1.181957     1.410579     4.596271     133.98
 C       0.786350    -0.120679     4.607727      96.24
 H       1.510887    -0.451202     5.403586      25.55
 H       1.017386    -0.503221     3.427101      30.10
 H      -0.199391    -0.184374     4.665205      29.44
 C       0.565610     3.609036     4.013827      47.56
 O       1.516819     3.973771     4.893900      65.23
 H       1.262643     4.918162     4.968568      25.72
 C      -0.175213     4.352207     3.134397      77.75
 H       0.037097     5.473262     3.288040      25.08
 C      -1.524611     2.580112     2.239266      17.40
 C      -2.661377     2.033033     1.371647      86.96
 H      -3.533122     2.865719     1.589438      29.21
 O      -3.245118     0.835073     2.027030     117.96
 H      -4.228600     0.572361     1.709788      23.04
 C      -2.410399     1.802704    -0.079006     101.36
 H      -2.049471     2.623644    -0.553327      32.17
 C      -3.717996     1.563058    -0.954902      94.28
 O      -4.686418     0.555546    -0.385783     201.79
 H      -4.441483    -0.406724    -0.824253      25.66
 H      -3.716476     1.322350    -2.062711      28.69
 H      -4.344954     2.557639    -1.360932      26.42
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 C       1.898683     1.504513    -1.020164      28.99
 H       2.501820     2.347184    -0.891691      27.62
 C       1.422989    -0.779702    -1.669540      81.96
 H       1.584910    -1.734282    -2.195441      27.70
 C       0.095018    -0.600225    -1.345594      32.82
 O      -0.868126    -1.600832    -1.633977     129.50
 C      -0.645032    -3.194728    -1.931591     113.77
 H      -0.577486    -3.540097    -0.897648      29.80
 H      -1.571981    -3.602684    -2.336241      29.62
 H       0.334639    -3.399270    -2.366988      28.32
 C      -0.304411     0.558241    -0.736171      21.64
 O      -1.641568     0.535193    -0.177151     150.19
 C       0.521498     1.611923    -0.697161      67.53
 H       0.302870     2.433797    -0.334056      37.76
 C       2.296008     0.215977    -1.564758      18.78
 C       3.880762    -0.097059    -1.566955      99.16
 H       3.720903    -0.916004    -2.527272      27.47
 O       4.585867     1.050026    -1.945263     168.07
 H       5.565791     1.132425    -1.478079      24.10
 C       4.400219    -1.007561    -0.366087     126.68
 H       3.756803    -1.769727    -0.426083      34.91
 O       5.701992    -1.208513    -0.465104     213.02
 H       5.849431    -2.211551    -0.593466      26.81
 C       3.973899    -0.568719     0.995809     131.13
 O       4.543370     0.724772     1.500014     136.90
 H       3.994239     1.569394     1.436181      33.93
 H       4.334381    -1.243466     1.670735      33.71
 H       2.806485    -0.387011     0.782679      34.21
55
name = lig-Water-frame_945
 C      -1.143457     3.924201     2.216783       2.56
 H      -1.748421     4.703205     1.759682      17.61
 C      -0.721873     1.642479     2.921471      61.77
 H      -0.739859     0.659296     2.684513      30.01
 C       0.379829     2.168676     3.864446     -21.21
 O       1.172831     1.407041     4.591557      58.54
 C       0.843334    -0.074068     4.575324     103.74
 H       1.336949    -0.761150     5.289751      29.24
 H       1.024672    -0.474391     3.697837      34.16
 H      -0.358024     0.108476     4.792712      24.36
 C       0.597009     3.594077     3.932550      35.44
 O       1.570196     4.020649     4.898537     196.01
 H       1.395500     5.042906     4.983592      22.18
 C      -0.114997     4.412388     3.179387      62.04
 H      -0.169957     5.547172     3.240301      22.29
 C      -1.529466     2.511807     2.264815      33.17
 C      -2.699368     2.072108     1.391726      87.77
 H      -3.382123     2.820881     1.424731      33.64
 O      -3.256998     0.756966     2.070109      98.67
 H      -4.102002     0.606860     1.670736      27.72
 C      -2.391051     1.706395    -0.113766      86.27
 H      -1.996872     2.737289    -0.626726      28.33
 C      -3.736258     1.481021    -0.935467     104.98
 O      -4.629276     0.567884    -0.396304     272.01
 H      -4.278471    -0.298172    -0.587034      30.49
 H      -3.589427     1.001697    -2.009869      28.32
 H      -4.199614     2.395456    -1.083726      30.68
 C       1.832497     1.498279    -1.021783      38.02
 H       2.555017     2.456904    -0.994773      24.86
 C       1.395446    -0.782035    -1.633561      64.26
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 H       1.868260    -1.651899    -2.127199      28.02
 C       0.061149    -0.619286    -1.310572      35.29
 O      -0.875933    -1.586965    -1.618218     123.02
 C      -0.643054    -3.205588    -1.901864      78.50
 H      -0.430453    -3.874957    -0.842899      26.44
 H      -1.602402    -3.411804    -2.509109      26.59
 H       0.430360    -3.477654    -2.372971      25.47
 C      -0.385434     0.573725    -0.693570      36.39
 O      -1.613376     0.485089    -0.202445     167.79
 C       0.541592     1.608737    -0.732524      71.30
 H       0.117829     2.795275    -0.321493      29.99
 C       2.349103     0.263109    -1.590748      22.32
 C       3.917646    -0.124461    -1.608971     106.65
 H       3.937985    -0.939486    -2.356894      29.23
 O       4.571646     1.025300    -1.918412     234.27
 H       5.378458     1.014542    -1.523376      32.85
 C       4.391390    -0.954300    -0.350236      98.20
 H       3.626686    -1.903049    -0.619927      30.47
 O       5.799716    -1.228177    -0.485515     183.89
 H       5.880691    -2.224449    -0.650435      26.87
 C       3.944253    -0.484416     1.044205     146.62
 O       4.551714     0.693337     1.495616     177.52
 H       4.116392     1.519425     1.262058      35.02
 H       4.244665    -1.350734     1.849203      30.49
 H       2.896110    -0.424835     1.138245      33.36
55
name = lig-Water-frame_946
 C      -1.145595     3.890274     2.233237      33.38
 H      -1.736093     4.629866     1.555160      21.30
 C      -0.687881     1.601127     2.952543      28.55
 H      -0.601883     0.490826     2.578302      25.69
 C       0.262384     2.160447     3.896501      -5.04
 O       1.199993     1.363154     4.609056     152.78
 C       0.834856     0.007561     4.577536     111.11
 H       1.253631    -0.697304     5.298293      28.24
 H       1.054899    -0.559100     3.473924      28.68
 H      -0.159510    -0.071539     4.886202      28.76
 C       0.672230     3.514404     3.919197      -6.98
 O       1.616260     4.079734     4.878286      74.38
 H       1.527951     4.996179     5.299310      28.08
 C      -0.149445     4.520352     3.129541      36.86
 H      -0.135679     5.576473     3.248433      21.39
 C      -1.527747     2.521931     2.240276      42.55
 C      -2.729213     2.039545     1.421750      69.99
 H      -3.540745     2.955394     1.234635      27.24
 O      -3.250626     0.720516     2.107312      77.61
 H      -4.106172     0.586688     1.586039      25.31
 C      -2.412380     1.646161    -0.161371      84.05
 H      -1.818729     2.395683    -0.556508      30.63
 C      -3.711540     1.395096    -0.951511      96.40
 O      -4.600919     0.559699    -0.372142     266.67
 H      -4.176616    -0.350552    -0.391267      28.75
 H      -3.207897     0.969133    -1.908756      27.68
 H      -4.203319     2.517273    -0.735024      24.92
 C       1.872440     1.492724    -1.077846      73.06
 H       2.440490     2.314923    -1.062461      29.57
 C       1.414206    -0.787972    -1.635090      46.06
 H       1.940076    -1.740718    -2.002690      25.27
 C       0.039178    -0.687691    -1.290225      20.32
 O      -0.904278    -1.627842    -1.605998     191.53
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 C      -0.604867    -3.180040    -1.834493     107.68
 H      -0.571581    -3.737850    -1.027538      31.06
 H      -1.430162    -3.257288    -2.630004      26.27
 H       0.256958    -3.334605    -2.595132      26.41
 C      -0.425627     0.550034    -0.685281       6.34
 O      -1.625139     0.462404    -0.214173     163.72
 C       0.485924     1.708048    -0.706677      85.78
 H       0.122060     2.578013    -0.490756      34.19
 C       2.415700     0.316020    -1.550481      30.40
 C       3.862637    -0.174615    -1.642576      92.77
 H       4.377054    -0.949976    -2.469048      25.44
 O       4.580760     1.039583    -1.910048     197.80
 H       5.534725     0.979853    -1.488086      24.79
 C       4.292975    -0.918784    -0.358198      81.57
 H       3.993324    -1.875125    -0.513650      30.64
 O       5.910773    -1.266975    -0.503485     140.45
 H       5.969909    -2.196354    -0.657621      30.72
 C       3.926190    -0.450094     1.113003     136.58
 O       4.595732     0.686561     1.502016     209.25
 H       4.068310     1.424045     1.057930      32.99
 H       4.116891    -1.201050     1.762017      33.20
 H       2.755976    -0.456606     1.364678      30.38
55
name = lig-Water-frame_947
 C      -1.153364     3.902565     2.271143      83.75
 H      -1.686213     4.441512     1.560730      25.91
 C      -0.638153     1.581301     2.984666      48.29
 H      -0.654832     0.547831     2.782766      27.55
 C       0.200224     2.136919     3.906391     -14.25
 O       1.221855     1.329652     4.625358     166.36
 C       0.825450     0.008042     4.560950     114.42
 H       1.526065    -0.375989     5.378398      25.97
 H       0.940427    -0.367705     3.632710      33.12
 H      -0.317137    -0.285977     4.843098      25.10
 C       0.684763     3.559230     3.923571     -29.46
 O       1.673796     4.096845     4.839344      57.10
 H       1.211656     4.910565     5.363675      20.51
 C      -0.193792     4.518684     3.066432      36.71
 H       0.079968     5.674162     3.242762      17.24
 C      -1.505772     2.535484     2.208880      33.06
 C      -2.754432     1.980141     1.415155      86.81
 H      -3.505603     2.671716     1.354618      33.36
 O      -3.240740     0.736429     2.123171      93.83
 H      -4.134451     0.458397     1.634539      23.35
 C      -2.444282     1.595197    -0.133053      92.67
 H      -1.717687     2.359348    -0.637932      29.06
 C      -3.640021     1.399903    -0.961152     106.46
 O      -4.600113     0.506437    -0.325584     264.18
 H      -4.244260    -0.484508    -0.264096      26.79
 H      -3.144813     1.220205    -1.994740      28.47
 H      -4.126614     2.263237    -0.992456      31.33
 C       1.898286     1.521442    -1.137034      16.67
 H       2.587553     2.506043    -1.101654      23.46
 C       1.468860    -0.789410    -1.643177      65.94
 H       1.723506    -1.786390    -1.886204      28.29
 C       0.075944    -0.746810    -1.281219       6.86
 O      -0.939350    -1.709475    -1.584242     189.08
 C      -0.576909    -3.059125    -1.865068     107.88
 H      -0.746094    -3.772463    -0.748031      24.64
 H      -1.406568    -3.377438    -2.478452      27.23
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 H       0.303692    -3.155626    -2.546175      27.43
 C      -0.352459     0.524719    -0.724457      -5.51
 O      -1.689723     0.428308    -0.202428     138.08
 C       0.436252     1.707668    -0.695425      -2.03
 H       0.019977     2.923762    -0.460465      27.99
 C       2.409673     0.261618    -1.502953      46.16
 C       3.849741    -0.198412    -1.678669     111.59
 H       4.144131    -0.800175    -2.459459      29.58
 O       4.617208     1.076452    -1.894380     178.26
 H       5.623905     0.974336    -1.577075      23.91
 C       4.227906    -0.914250    -0.351813      62.13
 H       4.064500    -2.103511    -0.327957      26.19
 O       5.991520    -1.281339    -0.511594      49.05
 H       5.976555    -2.313760    -0.647992      26.47
 C       3.879686    -0.467723     1.146896     114.85
 O       4.650697     0.716371     1.509229     195.98
 H       4.139462     1.439828     1.058699      33.40
 H       4.312494    -1.357006     1.853648      27.37
 H       2.815866    -0.311562     1.249167      31.18
55
name = lig-Water-frame_948
 C      -1.194103     3.913768     2.287502      69.26
 H      -1.807751     4.569992     1.519163      26.30
 C      -0.652108     1.619714     2.979972      41.45
 H      -0.824188     0.502601     3.009269      26.78
 C       0.284381     2.165036     3.942263     -53.62
 O       1.189089     1.351418     4.620668     119.28
 C       0.825985    -0.055855     4.616689     103.88
 H       1.636473    -0.352173     5.216420      28.51
 H       1.009403    -0.469731     3.444158      30.38
 H      -0.221528    -0.290223     4.845262      27.22
 C       0.600408     3.650444     3.908111       8.24
 O       1.700267     4.092345     4.784236     138.18
 H       1.130967     4.786253     5.140839      21.87
 C      -0.147819     4.463912     3.078644      67.87
 H       0.102017     5.437788     3.000664      21.97
 C      -1.456132     2.495732     2.207882     -15.15
 C      -2.732255     1.886757     1.396519      89.17
 H      -3.675563     2.659342     1.535850      25.41
 O      -3.229574     0.767991     2.129083     125.51
 H      -4.047072     0.472230     1.810914      26.85
 C      -2.430626     1.595997    -0.058802     104.99
 H      -2.017069     2.472908    -0.566694      29.40
 C      -3.586060     1.410295    -0.979706      86.31
 O      -4.599276     0.440047    -0.285197     258.86
 H      -4.340615    -0.443794    -0.393389      30.17
 H      -3.373097     1.196675    -2.106891      26.67
 H      -4.303941     2.383077    -1.383941      24.55
 C       1.879590     1.596255    -1.170641      40.37
 H       2.570152     2.368137    -1.174184      26.87
 C       1.471104    -0.830577    -1.638853      73.91
 H       1.744171    -1.938972    -1.915511      24.57
 C       0.135479    -0.764278    -1.281643      15.12
 O      -0.956160    -1.748501    -1.544191     209.73
 C      -0.588009    -2.971537    -1.884526     130.56
 H      -0.483799    -3.430659    -1.053091      33.51
 H      -1.440308    -3.651833    -2.336482      25.75
 H       0.564109    -3.082299    -2.258577      26.19
 C      -0.313418     0.492340    -0.755092       5.91
 O      -1.715936     0.358856    -0.194981     114.65
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 C       0.457426     1.693076    -0.716651      49.36
 H       0.128261     2.647524    -0.470204      30.84
 C       2.364849     0.189212    -1.465646      15.99
 C       3.875099    -0.151591    -1.658127      85.77
 H       3.683512    -0.916352    -2.707455      25.79
 O       4.661165     1.103470    -1.875425     197.62
 H       5.525757     0.947708    -1.666945      29.83
 C       4.229328    -0.989503    -0.328120      59.60
 H       3.824983    -1.972507    -0.323946      28.67
 O       6.029457    -1.290766    -0.511016      83.76
 H       5.962547    -2.272722    -0.623062      28.34
 C       3.899060    -0.505265     1.147781     109.74
 O       4.698582     0.743457     1.513646     169.48
 H       4.283252     1.564945     1.237113      33.64
 H       4.296356    -1.235572     1.750394      30.48
 H       2.782310    -0.235827     1.170061      29.69
55
name = lig-Water-frame_949
 C      -1.261072     3.902263     2.263873      50.72
 H      -1.775467     4.639423     1.764440      30.29
 C      -0.662631     1.673666     3.006854      47.08
 H      -1.026449     0.627689     3.179225      32.72
 C       0.397397     2.236645     3.929955      12.04
 O       1.127681     1.394618     4.615445     110.51
 C       0.872810    -0.129291     4.621755     107.29
 H       1.665837    -0.744471     5.227781      27.72
 H       1.038249    -0.518043     3.680159      33.77
 H      -0.156111    -0.293319     5.057606      28.53
 C       0.538376     3.636084     3.929222      47.77
 O       1.681831     4.068558     4.695382     222.72
 H       1.480890     5.066605     5.176822      13.40
 C      -0.116692     4.404827     3.075051      57.53
 H       0.147327     5.521437     2.741639      20.53
 C      -1.430741     2.463318     2.208579      -9.62
 C      -2.718250     1.851467     1.417682     101.83
 H      -3.407589     2.646111     1.466803      29.43
 O      -3.195665     0.773135     2.156712     147.65
 H      -4.186553     0.531731     1.820902      19.86
 C      -2.426434     1.617336    -0.024335      85.90
 H      -1.997832     2.626672    -0.372837      28.06
 C      -3.648308     1.428605    -1.024564      88.83
 O      -4.591338     0.413593    -0.267005     167.20
 H      -4.295467    -0.513271    -0.719692      25.34
 H      -3.434885     0.770488    -1.969005      27.04
 H      -4.187605     2.243186    -1.197950      30.64
 C       1.822874     1.571245    -1.190875      74.57
 H       2.606485     2.422536    -1.233617      24.19
 C       1.454421    -0.950794    -1.633505      78.95
 H       1.953093    -1.779620    -1.982334      27.04
 C       0.128868    -0.754701    -1.284893      23.55
 O      -0.960036    -1.674368    -1.491536     192.24
 C      -0.555809    -2.996228    -1.913294     117.58
 H      -0.071909    -3.566511    -0.766000      25.71
 H      -1.253052    -3.564534    -2.404108      28.82
 H       0.422234    -3.048663    -2.316914      28.82
 C      -0.341172     0.455370    -0.757260      22.22
 O      -1.675330     0.297905    -0.203030      95.37
 C       0.544489     1.617759    -0.775230      54.71
 H       0.027761     2.699481    -0.370972      30.43
 C       2.336097     0.216572    -1.430227       6.03
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 C       3.867009    -0.107557    -1.633878     104.05
 H       3.767402    -0.696710    -2.423510      31.90
 O       4.669292     1.101263    -1.862276     195.28
 H       5.707746     0.841343    -1.643097      24.06
 C       4.297472    -1.053269    -0.324212      64.62
 H       3.610046    -2.012619    -0.492814      27.47
 O       6.003125    -1.300380    -0.496071     138.54
 H       6.018701    -2.252982    -0.636012      30.51
 C       3.962701    -0.471560     1.086576     109.68
 O       4.748780     0.741087     1.521244     151.64
 H       4.219322     1.618462     1.441029      30.26
 H       4.215282    -1.299381     1.901353      28.32
 H       2.834051    -0.332002     1.216639      30.28
55
name = lig-Water-frame_950
 C      -1.267134     3.867892     2.267749      75.42
 H      -1.913152     4.729823     1.803875      26.18
 C      -0.637877     1.730484     3.092905      74.12
 H      -0.994376     0.768499     3.244793      33.25
 C       0.404968     2.255293     3.831255      26.92
 O       1.112191     1.396476     4.652048     150.60
 C       0.930002    -0.185092     4.647315     100.65
 H       1.578864    -0.729137     5.266204      28.35
 H       0.941845    -0.623786     3.533580      28.88
 H      -0.075472    -0.321914     5.271508      25.04
 C       0.570784     3.586321     4.006044      37.40
 O       1.655546     4.077059     4.622190     115.12
 H       1.770552     4.934047     4.936882      24.31
 C      -0.179346     4.407326     2.974660      43.31
 H       0.199779     5.371891     2.839652      24.31
 C      -1.464554     2.478877     2.189476      20.26
 C      -2.661641     1.861797     1.469544      86.99
 H      -3.381326     2.869461     1.364933      26.63
 O      -3.185588     0.737629     2.196633     171.32
 H      -4.106019     0.624705     1.856641      24.27
 C      -2.436359     1.623276    -0.065809      69.91
 H      -1.723643     2.480465    -0.208188      27.26
 C      -3.717846     1.361239    -1.007458      92.24
 O      -4.574651     0.398444    -0.276095     173.26
 H      -4.334580    -0.377509    -0.863157      27.65
 H      -3.314589     0.735304    -1.815003      27.94
 H      -4.303728     2.480310    -1.067722      25.41
 C       1.841110     1.478311    -1.218724     145.27
 H       2.424310     2.423726    -1.257785      29.75
 C       1.477719    -0.998635    -1.605111      94.50
 H       2.109025    -1.843487    -2.120880      24.11
 C       0.075457    -0.770642    -1.302739      19.72
 O      -0.951161    -1.599146    -1.451930     164.10
 C      -0.452872    -3.058689    -1.832115      92.04
 H      -0.172928    -3.553835    -1.101160      31.97
 H      -1.336870    -3.501436    -2.525012      26.50
 H       0.340897    -2.893590    -2.851482      24.60
 C      -0.369879     0.442591    -0.739837      25.42
 O      -1.602860     0.294147    -0.218931     117.95
 C       0.522333     1.560130    -0.802999      63.07
 H       0.074981     2.494900    -0.382141      34.01
 C       2.321716     0.250153    -1.419651      13.21
 C       3.840148    -0.047094    -1.544518      87.23
 H       4.184539    -0.822774    -2.590186      25.65
 O       4.679640     1.077249    -1.847134     212.68
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 H       5.622300     0.849566    -1.610332      26.50
 C       4.395097    -1.077515    -0.354090     112.65
 H       3.785972    -1.962205    -0.576322      30.57
 O       5.910122    -1.314123    -0.470279     156.89
 H       6.104964    -2.323261    -0.673393      26.34
 C       4.058708    -0.451439     1.047227     138.61
 O       4.791111     0.727943     1.526015     173.03
 H       4.050725     1.391820     1.578615      32.81
 H       4.115389    -1.169255     1.842945      32.26
 H       2.960805    -0.333463     1.142086      32.54
55
name = lig-Water-frame_951
 C      -1.271915     3.879187     2.251215      76.21
 H      -1.978944     4.463099     1.730011      27.77
 C      -0.670561     1.782378     3.122233      71.71
 H      -0.829694     0.621743     3.307927      31.38
 C       0.396411     2.194081     3.774407       9.43
 O       1.137623     1.352392     4.708535     125.45
 C       0.943595    -0.196821     4.665826     115.97
 H       1.840414    -0.522935     5.306132      25.96
 H       0.740081    -0.603635     3.652937      29.08
 H       0.027222    -0.391548     5.146769      28.50
 C       0.575057     3.622520     3.976185      16.17
 O       1.679677     4.058377     4.570003      70.69
 H       1.552636     5.155680     4.764227      20.81
 C      -0.212144     4.379525     2.940675      54.53
 H       0.148239     5.472113     2.952696      23.25
 C      -1.493902     2.493289     2.211421      40.33
 C      -2.626307     1.915795     1.499038      87.83
 H      -3.371135     2.659511     1.420629      30.80
 O      -3.176325     0.707870     2.233016     167.07
 H      -4.081670     0.544668     1.942021      25.01
 C      -2.418700     1.588509    -0.092961      79.99
 H      -1.687038     2.306332    -0.441899      28.28
 C      -3.765156     1.331439    -0.917819     118.46
 O      -4.569326     0.403307    -0.302676     234.81
 H      -4.384066    -0.523495    -0.698308      25.36
 H      -3.208423     1.101628    -1.976852      27.96
 H      -4.224768     2.207865    -1.163414      31.30
 C       1.848398     1.429770    -1.229589      99.66
 H       2.376447     2.356178    -1.268365      31.92
 C       1.512881    -0.964751    -1.565217      83.37
 H       1.856500    -1.826133    -2.046666      26.97
 C       0.099713    -0.791996    -1.331981      10.44
 O      -0.945049    -1.624271    -1.433903     160.31
 C      -0.397954    -3.039522    -1.893005      95.40
 H      -0.041051    -3.862798    -0.872961      24.88
 H      -1.330036    -3.392248    -2.184111      29.20
 H       0.132762    -2.865429    -2.698064      31.20
 C      -0.342339     0.446791    -0.733493      27.23
 O      -1.569160     0.341997    -0.220667     156.60
 C       0.433515     1.501902    -0.809497      45.05
 H       0.103892     2.587929    -0.389660      31.32
 C       2.366633     0.164203    -1.455002      31.19
 C       3.870783    -0.065792    -1.512226     126.19
 H       4.106750    -0.668725    -2.272286      31.59
 O       4.680374     1.072848    -1.823896     258.10
 H       5.551541     0.898767    -1.519192      29.43
 C       4.495120    -1.032784    -0.384209     132.65
 H       4.007753    -2.046697    -0.499449      30.02
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 O       5.800313    -1.338029    -0.448930     210.76
 H       6.010946    -2.244598    -0.658356      29.06
 C       4.146407    -0.472714     1.028049     131.66
 O       4.814543     0.714639     1.527473     167.91
 H       4.030298     1.305484     1.612351      35.25
 H       4.267440    -1.287643     1.834391      30.41
 H       3.023617    -0.142182     0.856138      30.80
55
name = lig-Water-frame_952
 C      -1.300137     3.880432     2.205265      54.22
 H      -2.021850     4.429056     1.527395      24.24
 C      -0.758937     1.723600     3.098973      60.29
 H      -0.794937     0.725531     3.161236      33.11
 C       0.439210     2.167603     3.830501     -13.44
 O       1.160612     1.296746     4.739530     112.57
 C       0.959244    -0.153453     4.701799     113.19
 H       1.950872    -0.421917     5.050938      26.32
 H       0.853906    -0.594622     3.651837      27.68
 H      -0.069939    -0.557918     5.255770      24.74
 C       0.543267     3.617827     3.823298      23.63
 O       1.715974     4.089482     4.545601     181.95
 H       1.324613     4.913582     4.802674      26.17
 C      -0.170677     4.392422     2.995730      64.24
 H      -0.160137     5.513721     2.982530      23.19
 C      -1.496167     2.508904     2.279919      31.28
 C      -2.637308     1.916079     1.481884      75.41
 H      -3.603111     2.644010     1.534847      25.74
 O      -3.143291     0.696784     2.260670     120.98
 H      -4.162016     0.441531     2.008672      20.03
 C      -2.376983     1.536332    -0.077352      88.99
 H      -1.995840     2.372966    -0.855874      26.35
 C      -3.700753     1.328088    -0.858478      99.66
 O      -4.603673     0.394565    -0.329127     247.41
 H      -4.243978    -0.601332    -0.392568      23.51
 H      -3.440398     1.225908    -1.925944      28.05
 H      -4.406750     2.331346    -1.152736      24.97
 C       1.797558     1.389680    -1.218383       2.29
 H       2.529035     2.334351    -1.265764      27.68
 C       1.497738    -0.926302    -1.533917      81.08
 H       1.726490    -1.970025    -1.924231      25.26
 C       0.171013    -0.771969    -1.333967      23.20
 O      -0.912306    -1.732285    -1.432834     200.09
 C      -0.425775    -3.021912    -1.878066     103.40
 H       0.100288    -3.453295    -1.189887      31.49
 H      -1.457371    -3.550521    -1.986493      26.19
 H       0.420731    -2.896701    -2.887977      25.68
 C      -0.323289     0.396057    -0.746746      20.12
 O      -1.591824     0.397147    -0.201668     176.14
 C       0.432384     1.538333    -0.819556      49.87
 H       0.161149     2.645839    -0.482984      26.64
 C       2.446775     0.079202    -1.488584       8.21
 C       3.936800    -0.124846    -1.494120     107.71
 H       3.907090    -0.955633    -2.562083      24.79
 O       4.668775     1.096009    -1.801902     160.75
 H       5.670277     1.014541    -1.315847      22.54
 C       4.491485    -0.968040    -0.372433     117.84
 H       3.911235    -1.970729    -0.327875      28.42
 O       5.787624    -1.356284    -0.445571     225.71
 H       5.829693    -2.287435    -0.688054      29.16
 C       4.186414    -0.514630     1.015301     145.52
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 O       4.836307     0.705493     1.530289     138.51
 H       4.140012     1.468777     1.562073      33.04
 H       4.368771    -1.381896     1.696483      30.12
 H       3.212734    -0.214861     0.836672      30.73
55
name = lig-Water-frame_953
 C      -1.297669     3.891236     2.177538      56.80
 H      -1.830483     4.556726     1.464533      20.54
 C      -0.746631     1.631088     3.124727      20.97
 H      -1.026186     0.474968     2.937347      28.68
 C       0.405666     2.144481     3.888674       0.91
 O       1.167809     1.280882     4.742388     143.22
 C       0.954789    -0.121946     4.721314     125.79
 H       1.921669    -0.620819     5.024801      29.91
 H       1.051943    -0.485626     3.625050      29.18
 H       0.252086    -0.494951     5.321715      33.03
 C       0.611644     3.528694     3.704320      25.90
 O       1.702121     4.118368     4.519581     136.09
 H       1.386220     4.989687     5.182057      20.11
 C      -0.219642     4.458760     2.998487      45.26
 H      -0.202971     5.509792     3.065300      20.09
 C      -1.536088     2.527639     2.316026      13.83
 C      -2.703008     1.891099     1.453093      87.79
 H      -3.551667     2.578054     1.526152      27.63
 O      -3.106043     0.690067     2.270920     166.62
 H      -4.010955     0.521536     2.073729      22.98
 C      -2.372641     1.553672    -0.078712     103.84
 H      -2.190198     2.398249    -0.701140      26.76
 C      -3.657443     1.374633    -0.835143      96.11
 O      -4.660970     0.378337    -0.328015     287.58
 H      -4.134348    -0.398327    -0.383863      28.67
 H      -3.601134     0.994788    -1.974216      25.70
 H      -4.244345     2.229879    -0.632197      27.86
 C       1.806243     1.343813    -1.213005      74.38
 H       2.442764     2.116130    -1.224541      27.04
 C       1.511716    -0.967301    -1.548102      93.27
 H       1.811045    -2.018797    -1.691520      24.00
 C       0.153643    -0.761337    -1.297815      19.01
 O      -0.839928    -1.830325    -1.437888     221.48
 C      -0.474492    -2.993275    -1.927553     111.60
 H       0.544716    -3.382016    -1.008706      23.53
 H      -1.217508    -3.797763    -2.004470      26.61
 H       0.084844    -3.068686    -2.717804      32.11
 C      -0.345497     0.384926    -0.752362      16.39
 O      -1.611869     0.409994    -0.180763     193.89
 C       0.502327     1.603429    -0.842312      69.15
 H       0.097085     2.625692    -0.555604      26.52
 C       2.477247     0.090107    -1.482418      30.92
 C       3.994866    -0.218304    -1.578285     110.51
 H       4.032584    -0.841473    -2.398643      30.61
 O       4.672904     1.111574    -1.770114     224.62
 H       5.471866     1.178801    -1.306249      28.47
 C       4.417357    -0.940316    -0.332274     110.52
 H       3.657026    -1.743410    -0.321163      29.79
 O       5.863078    -1.388822    -0.463828     204.18
 H       5.716869    -2.367297    -0.778216      28.29
 C       4.203133    -0.521076     1.024324     124.73
 O       4.863554     0.701607     1.542362     140.49
 H       4.298314     1.467636     1.361977      33.23
 H       4.409124    -1.377947     1.661438      29.99
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 H       2.955298    -0.417268     1.166395      27.23
55
name = lig-Water-frame_954
 C      -1.253959     3.926650     2.181717      68.03
 H      -1.722442     4.627925     1.507141      24.81
 C      -0.711759     1.543713     3.141428      56.36
 H      -1.092868     0.610995     2.962587      25.40
 C       0.307817     2.074576     3.907399       5.67
 O       1.174722     1.319801     4.738683      77.03
 C       1.017485    -0.122440     4.687723     114.15
 H       1.842001    -0.682076     5.209011      25.57
 H       0.889234    -0.423011     3.665444      29.70
 H       0.120093    -0.496154     5.505760      24.16
 C       0.720504     3.493018     3.659693     -22.11
 O       1.649838     4.149127     4.511762     169.96
 H       1.458741     4.799442     5.168891      25.81
 C      -0.304951     4.471995     2.968155      18.41
 H       0.019323     5.601437     3.194964      18.27
 C      -1.583912     2.508004     2.317983      18.04
 C      -2.737759     1.852248     1.458668      84.01
 H      -3.614225     2.653693     1.407752      26.89
 O      -3.061465     0.694462     2.261127     154.86
 H      -4.078276     0.507494     2.064142      19.70
 C      -2.422332     1.597627    -0.061573      82.79
 H      -1.835784     2.641242    -0.365775      23.53
 C      -3.698040     1.377684    -0.823189      90.67
 O      -4.704618     0.394390    -0.303761     268.57
 H      -4.188861    -0.536766    -0.537959      22.99
 H      -3.508900     1.111064    -1.817239      28.66
 H      -4.144100     2.451484    -0.407092      25.69
 C       1.878063     1.309160    -1.218774      74.15
 H       2.599273     2.293319    -1.219977      21.27
 C       1.558326    -1.023757    -1.567435      69.85
 H       1.946705    -2.034342    -1.611069      19.36
 C       0.101883    -0.818038    -1.265364       9.03
 O      -0.795076    -1.838851    -1.425658     220.64
 C      -0.411914    -3.085107    -1.902302     109.12
 H       0.299584    -3.380363    -1.402541      34.13
 H      -1.150782    -3.903281    -1.889339      26.93
 H      -0.016932    -3.105382    -3.195691      26.50
 C      -0.371302     0.476223    -0.747745      23.85
 O      -1.604231     0.385103    -0.170038     187.26
 C       0.543332     1.586870    -0.858326      66.17
 H      -0.000938     2.693208    -0.656380      23.25
 C       2.435587     0.094138    -1.467261      39.62
 C       4.018140    -0.212568    -1.633788      66.43
 H       4.481028    -0.981133    -2.633653      24.45
 O       4.653003     1.113757    -1.761368     191.04
 H       5.544464     1.189134    -1.170780      23.91
 C       4.374979    -0.960704    -0.327342      88.02
 H       3.566040    -1.811325    -0.418520      24.10
 O       5.914407    -1.442264    -0.492198     158.96
 H       5.830881    -2.342715    -0.820916      30.42
 C       4.142341    -0.481694     1.107509     113.40
 O       4.893134     0.686258     1.557803     183.22
 H       4.344410     1.424888     1.136540      30.08
 H       4.629129    -1.344791     1.743433      25.77
 H       3.182000    -0.542625     1.450714      29.05
55
name = lig-Water-frame_955
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 C      -1.250558     3.921797     2.177301      53.33
 H      -1.884219     4.623519     1.512539      22.96
 C      -0.749266     1.547152     3.094983      63.95
 H      -1.042550     0.430653     3.177627      26.05
 C       0.268724     2.042562     3.913759     -17.82
 O       1.180440     1.371546     4.730672      64.24
 C       1.047753    -0.153405     4.708157     113.45
 H       1.913429    -0.508347     5.206266      26.81
 H       0.636251    -0.516075     3.646602      27.63
 H       0.170796    -0.294346     5.148962      29.03
 C       0.724024     3.518329     3.651134     -27.75
 O       1.616581     4.126673     4.494201      58.85
 H       1.107479     4.969338     5.085071      16.13
 C      -0.252424     4.437090     3.012209      35.23
 H       0.044111     5.398024     3.068417      21.29
 C      -1.582059     2.475555     2.308594      29.88
 C      -2.741216     1.847674     1.498832      99.73
 H      -3.587827     2.581613     1.390339      30.68
 O      -3.057252     0.693664     2.236251     187.21
 H      -4.017426     0.379000     2.076623      22.08
 C      -2.437029     1.639184    -0.002069      90.15
 H      -1.775370     2.397473    -0.134113      30.10
 C      -3.792070     1.416342    -0.770753     106.39
 O      -4.697538     0.410332    -0.282252     304.86
 H      -4.589744    -0.463244    -0.689007      27.92
 H      -3.410839     1.448024    -1.933302      27.34
 H      -4.202138     2.432521    -0.816893      29.21
 C       1.971501     1.373166    -1.226513      68.43
 H       2.587701     2.156872    -1.286685      28.96
 C       1.543290    -1.056361    -1.557796      47.51
 H       2.053901    -2.080290    -1.718684      23.37
 C       0.129868    -0.868089    -1.243459       7.20
 O      -0.798892    -1.821136    -1.401382     150.39
 C      -0.340639    -3.211325    -1.987071      80.05
 H       0.786169    -3.751623    -1.392274      24.11
 H      -1.313692    -3.759358    -1.653132      25.31
 H      -0.264613    -3.022663    -2.933471      31.24
 C      -0.356461     0.528865    -0.769400      19.09
 O      -1.599676     0.374592    -0.163198     166.59
 C       0.540648     1.545496    -0.868880      79.44
 H       0.233998     2.557564    -0.764490      28.81
 C       2.414654     0.033507    -1.488012      22.01
 C       4.038379    -0.165726    -1.669210     100.33
 H       4.389010    -0.720158    -2.369074      31.98
 O       4.641029     1.114407    -1.755253     229.45
 H       5.510993     1.019708    -1.187909      24.95
 C       4.359828    -1.023862    -0.354733      78.68
 H       3.867769    -1.937058    -0.421915      28.25
 O       5.919528    -1.489588    -0.512905     166.10
 H       5.941209    -2.402484    -0.843593      31.23
 C       4.153979    -0.482266     1.212587     107.45
 O       4.904131     0.682250     1.565018     167.63
 H       4.446974     1.448303     1.094135      30.55
 H       4.745332    -1.204951     1.684192      28.96
 H       3.004538    -0.493966     1.714539      26.41
55
name = lig-Water-frame_956
 C      -1.285677     3.861425     2.183452      53.55
 H      -1.963951     4.452682     1.660923      22.71
 C      -0.815674     1.571538     3.044583      46.00
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 H      -0.947753     0.531678     3.352992      24.50
 C       0.298682     2.102672     3.883576     -38.50
 O       1.177470     1.402261     4.707002       7.12
 C       1.038384    -0.148687     4.697708      95.45
 H       2.065403    -0.467176     5.136212      26.15
 H       0.944192    -0.563017     3.745414      31.48
 H      -0.046163    -0.285215     5.267838      23.17
 C       0.618055     3.516890     3.672494      24.82
 O       1.580292     4.112328     4.514135     131.89
 H       1.154700     4.923106     4.712629      23.76
 C      -0.149120     4.343437     3.046809      57.62
 H       0.050094     5.520152     2.889799      19.80
 C      -1.546348     2.466883     2.285093      37.98
 C      -2.722597     1.863443     1.549718     103.03
 H      -3.642072     2.595669     1.576382      30.86
 O      -3.081384     0.663032     2.223631     170.59
 H      -3.973042     0.366098     2.015372      24.70
 C      -2.453882     1.601859     0.087289      81.18
 H      -1.751076     2.533607    -0.364461      27.48
 C      -3.834084     1.488614    -0.781576     100.49
 O      -4.681605     0.449064    -0.266194     271.96
 H      -4.654163    -0.365005    -0.837897      28.25
 H      -3.568816     1.412683    -1.764946      30.78
 H      -4.566447     2.482507    -0.986538      26.95
 C       1.994754     1.372548    -1.251848      32.50
 H       2.763444     2.291100    -1.373746      25.00
 C       1.501130    -1.089294    -1.533443      72.72
 H       1.888268    -1.986388    -1.874650      27.69
 C       0.206606    -0.860942    -1.223468      20.47
 O      -0.805574    -1.842642    -1.375677     116.47
 C      -0.277123    -3.331110    -1.970712      91.68
 H       0.549663    -3.652387    -1.729505      32.58
 H      -1.158087    -3.709650    -1.618442      26.80
 H      -0.387348    -2.960638    -3.223391      24.72
 C      -0.329460     0.453886    -0.808000      20.57
 O      -1.603802     0.392058    -0.162781     148.66
 C       0.591135     1.521573    -0.892244      53.29
 H       0.393096     2.778716    -0.757715      26.59
 C       2.446820     0.015471    -1.528125      20.99
 C       3.982391    -0.111589    -1.602375      78.47
 H       4.282818    -0.896092    -2.708089      24.96
 O       4.645213     1.119732    -1.744209     184.77
 H       5.502225     1.057485    -1.298092      27.59
 C       4.395004    -1.069156    -0.373427      62.58
 H       3.997309    -2.162092    -0.422152      26.28
 O       5.898179    -1.516442    -0.522622     114.62
 H       5.910858    -2.510605    -0.824404      29.75
 C       4.173346    -0.516172     1.286604     103.42
 O       4.907806     0.698822     1.567290     169.18
 H       4.512657     1.489598     1.197813      33.74
 H       4.826954    -1.379382     1.794083      27.29
 H       3.227381    -0.432437     1.579937      29.93
55
name = lig-Water-frame_957
 C      -1.273403     3.780740     2.248479      60.25
 H      -2.055117     4.475418     1.729095      28.10
 C      -0.783203     1.615358     3.085188      63.22
 H      -1.098406     0.599361     3.226359      40.07
 C       0.316366     2.165889     3.795576      19.11
 O       1.165053     1.409102     4.664906     191.36
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 C       1.001621    -0.099416     4.712132     116.79
 H       1.852833    -0.460809     5.194832      28.30
 H       1.296367    -0.566466     3.638480      28.66
 H       0.285687    -0.458935     5.343814      26.91
 C       0.556213     3.455461     3.783737      38.96
 O       1.557944     4.066079     4.528399    -110.97
 H       1.359917     5.103910     4.748095      27.99
 C      -0.173327     4.325770     2.935088      61.08
 H       0.087571     5.340856     2.904751      27.81
 C      -1.530859     2.462068     2.246597       5.15
 C      -2.722081     1.883421     1.597484      89.60
 H      -3.577715     2.614394     1.781985      27.23
 O      -3.098877     0.614012     2.232596     158.14
 H      -4.102128     0.424388     1.886270      18.01
 C      -2.453259     1.604751     0.093153      95.59
 H      -2.145803     2.405441    -0.426996      30.38
 C      -3.860014     1.585455    -0.794131      82.68
 O      -4.672578     0.491388    -0.252545     211.09
 H      -4.433653    -0.286953    -0.874926      26.95
 H      -3.585370     1.083724    -1.895535      26.13
 H      -4.613647     2.352675    -0.715159      26.55
 C       1.987334     1.317790    -1.310040      84.11
 H       2.639044     2.157398    -1.375813      29.58
 C       1.533235    -1.075075    -1.519457      92.30
 H       1.702067    -2.099111    -2.075655      23.94
 C       0.195460    -0.854239    -1.201948      26.66
 O      -0.774516    -1.893633    -1.349130     143.71
 C      -0.318604    -3.317334    -2.014985      80.30
 H       0.935445    -3.663396    -1.718409      23.36
 H      -1.140641    -4.123289    -1.578040      25.56
 H      -0.340853    -3.295963    -2.981355      31.12
 C      -0.291368     0.372115    -0.827616      -5.17
 O      -1.609082     0.415742    -0.170144     135.81
 C       0.664802     1.557794    -0.920517      67.85
 H       0.344582     2.486293    -0.714712      34.24
 C       2.478647     0.055183    -1.552520      33.95
 C       3.920892    -0.158171    -1.563795     105.14
 H       4.027279    -0.682848    -2.430655      28.85
 O       4.643100     1.129165    -1.736324     156.24
 H       5.665149     1.174161    -1.311003      22.52
 C       4.473848    -1.105996    -0.360812      91.98
 H       3.755608    -1.891454    -0.456117      31.20
 O       5.867062    -1.532615    -0.528784     212.80
 H       5.774239    -2.459612    -0.741942      31.58
 C       4.275307    -0.582252     1.281045     107.88
 O       4.926508     0.708617     1.582696     124.09
 H       4.326164     1.479270     1.249737      29.73
 H       4.600666    -1.340786     1.899255      31.56
 H       3.032392    -0.450288     1.461036      28.32
55
name = lig-Water-frame_958
 C      -1.283004     3.782771     2.282790      73.13
 H      -1.909695     4.443313     1.802458      25.97
 C      -0.731101     1.651982     3.130101      83.19
 H      -1.170945     0.602539     3.040891      29.88
 C       0.335886     2.106924     3.741899      33.74
 O       1.141538     1.394688     4.618436     192.00
 C       1.027341    -0.035192     4.691052     128.27
 H       1.874215    -0.340750     5.460717      26.14
 H       1.168610    -0.449161     3.763610      31.79
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 H       0.149612    -0.629033     5.288785      26.24
 C       0.518485     3.521651     3.874830      31.92
 O       1.557053     4.013901     4.552423     121.87
 H       1.490308     4.938168     5.002162      20.46
 C      -0.215229     4.300608     2.825706      51.05
 H       0.099491     5.399561     2.899201      24.36
 C      -1.515329     2.398122     2.249875      32.75
 C      -2.737033     1.869620     1.626285      90.41
 H      -3.555440     2.657804     1.758895      27.32
 O      -3.110770     0.574848     2.238784     184.70
 H      -4.017147     0.413077     2.011435      23.45
 C      -2.488527     1.627430     0.033942      74.45
 H      -2.091080     2.703239    -0.481575      24.92
 C      -3.848869     1.580050    -0.797432      92.59
 O      -4.671505     0.515516    -0.246097     228.60
 H      -4.271472    -0.289189    -0.595154      30.12
 H      -3.615908     1.324510    -1.745186      30.40
 H      -4.445947     2.631298    -0.573050      25.35
 C       1.950458     1.286949    -1.375591     102.49
 H       2.655408     2.156993    -1.393010      26.74
 C       1.598911    -1.041655    -1.543097      85.66
 H       1.731157    -1.927829    -2.034744      27.20
 C       0.154252    -0.910919    -1.207069       6.60
 O      -0.728143    -1.983721    -1.336462     197.24
 C      -0.352891    -3.298134    -1.970121     102.54
 H       0.588692    -3.347574    -1.624201      30.92
 H      -0.782847    -4.148489    -1.649911      29.46
 H      -0.361499    -3.456500    -3.272969      25.48
 C      -0.258928     0.407691    -0.800931      -2.12
 O      -1.608022     0.438582    -0.188280     135.08
 C       0.678376     1.506843    -0.951207      58.79
 H       0.072314     2.575658    -0.566061      27.13
 C       2.462322     0.049827    -1.544052      52.82
 C       3.932847    -0.195374    -1.491349      78.28
 H       4.098771    -0.891774    -2.635665      25.96
 O       4.649363     1.137778    -1.733397     148.07
 H       5.447045     1.114420    -1.271613      26.06
 C       4.525736    -1.094816    -0.304525      99.20
 H       3.582843    -1.793324    -0.406240      28.77
 O       5.824704    -1.549869    -0.538300     228.98
 H       5.743546    -2.507485    -0.711864      29.14
 C       4.327046    -0.616426     1.196628     145.45
 O       4.941928     0.706126     1.599704     148.61
 H       4.142789     1.246901     1.332600      33.65
 H       4.525258    -1.389866     2.092750      29.32
 H       3.342736    -0.561621     1.256091      31.06
55
name = lig-Water-frame_959
 C      -1.355927     3.778278     2.242841      58.00
 H      -1.986229     4.531143     1.621169      22.58
 C      -0.757050     1.598806     3.096021      78.97
 H      -0.874155     0.558067     3.120238      26.78
 C       0.406929     2.085436     3.777190      13.08
 O       1.123901     1.373377     4.584149     179.31
 C       1.062808    -0.013488     4.735185     118.72
 H       1.831834    -0.161209     5.420282      25.40
 H       1.089038    -0.537304     3.644733      26.79
 H       0.028535    -0.304216     4.847662      26.88
 C       0.455280     3.606534     3.860450      27.82
 O       1.596267     3.964518     4.609284     201.90
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 H       1.272157     4.792298     5.175530      18.80
 C      -0.145890     4.310518     2.851501      56.48
 H      -0.072507     5.463630     2.754221      25.96
 C      -1.507003     2.365522     2.292067      34.74
 C      -2.757686     1.814422     1.610394      81.68
 H      -3.592391     2.635938     1.632161      25.76
 O      -3.084920     0.561176     2.244302     204.89
 H      -4.127868     0.318271     2.248633      20.87
 C      -2.512895     1.710479    -0.053697      73.51
 H      -1.940950     2.526378    -0.226020      26.66
 C      -3.828631     1.564111    -0.735673     106.94
 O      -4.678102     0.536555    -0.239846     224.42
 H      -4.197729    -0.351315    -0.289864      26.25
 H      -3.635878     1.681072    -1.983165      25.28
 H      -4.033379     2.647910    -0.624243      26.13
 C       1.928203     1.332165    -1.432397      58.87
 H       2.708155     2.201751    -1.434145      24.59
 C       1.570100    -1.022904    -1.568117      59.31
 H       2.087912    -1.992898    -2.017880      23.33
 C       0.171324    -0.970776    -1.239794       0.46
 O      -0.716369    -2.078201    -1.328643     217.31
 C      -0.365689    -3.243506    -1.969137      95.69
 H       0.873996    -3.330311    -1.530353      22.63
 H      -0.854774    -4.219776    -1.425358      25.51
 H      -0.402936    -3.248236    -2.972491      29.93
 C      -0.268689     0.441822    -0.754848      14.84
 O      -1.595942     0.473859    -0.220932     146.83
 C       0.567011     1.465961    -0.945376      80.29
 H       0.287255     2.345613    -0.700586      28.43
 C       2.461885     0.005531    -1.515028      20.25
 C       4.010422    -0.218666    -1.489328      98.36
 H       4.294870    -0.895830    -2.278346      29.69
 O       4.628836     1.120027    -1.739820     162.54
 H       5.499201     1.082344    -1.106108      21.83
 C       4.506835    -1.063676    -0.237097     105.24
 H       3.817817    -1.944611    -0.237558      28.01
 O       5.794554    -1.584775    -0.556993     235.19
 H       5.836671    -2.603905    -0.726223      26.63
 C       4.395563    -0.644956     1.120321     127.78
 O       4.935919     0.677532     1.600324     157.90
 H       4.159001     1.291173     1.460282      31.01
 H       4.628960    -1.342311     1.848462      30.46
 H       3.134669    -0.508877     1.150233      25.85
55
name = lig-Water-frame_960
 C      -1.387636     3.779535     2.186437      56.12
 H      -1.996101     4.353749     1.512839      22.12
 C      -0.713820     1.496184     3.082911      52.08
 H      -0.657655     0.370814     3.166916      22.31
 C       0.378085     2.153404     3.793137       7.32
 O       1.159027     1.377833     4.578803     166.21
 C       1.050547    -0.027171     4.707831     106.67
 H       1.812978    -0.352540     5.517421      24.30
 H       1.374664    -0.556188     3.841571      30.22
 H      -0.095922    -0.093428     4.873125      24.64
 C       0.469694     3.576623     3.827130      30.03
 O       1.626231     3.951232     4.684891     212.77
 H       1.134177     4.667543     5.272572      17.61
 C      -0.145265     4.374530     2.880463      54.29
 H      -0.052189     5.392074     2.720850      26.81
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 C      -1.576472     2.397544     2.301959      10.45
 C      -2.773174     1.757258     1.554014      96.28
 H      -3.621910     2.457067     1.646755      26.32
 O      -3.063164     0.546020     2.245268     229.99
 H      -4.028562     0.433080     2.538098      22.96
 C      -2.484677     1.728602    -0.065075      64.10
 H      -1.727905     2.656762    -0.205606      22.25
 C      -3.761907     1.575926    -0.748866     112.10
 O      -4.686403     0.564753    -0.232603     221.67
 H      -4.122266    -0.269526    -0.123716      26.42
 H      -3.820482     1.678529    -1.735604      29.99
 H      -4.235140     2.679774    -0.492978      25.18
 C       1.917220     1.357586    -1.459812      61.58
 H       2.530499     2.202240    -1.499906      27.59
 C       1.510355    -1.093370    -1.610409      69.59
 H       2.158535    -1.898305    -1.779379      23.89
 C       0.203183    -0.988546    -1.269838      11.28
 O      -0.739066    -2.099698    -1.295946     204.79
 C      -0.281532    -3.250620    -1.884104     120.48
 H       0.698752    -3.611707    -1.888421      28.26
 H      -0.959097    -3.893490    -1.433541      28.00
 H      -0.459274    -3.056951    -3.167374      25.01
 C      -0.350280     0.356507    -0.724283      21.75
 O      -1.583132     0.507313    -0.262181     158.29
 C       0.514795     1.449216    -0.964035      42.38
 H       0.303570     2.695930    -0.735845      24.78
 C       2.489781     0.035481    -1.484759      11.58
 C       4.051846    -0.207476    -1.484942      90.85
 H       4.624951    -1.100858    -2.247335      23.79
 O       4.622719     1.074456    -1.727153     198.73
 H       5.516138     1.222646    -1.259510      23.61
 C       4.488814    -1.076543    -0.243923     100.76
 H       3.917730    -1.992465    -0.141440      28.56
 O       5.803735    -1.625494    -0.581226     211.21
 H       5.817064    -2.569717    -0.698417      28.81
 C       4.371401    -0.595943     1.111250     140.27
 O       4.926794     0.636761     1.582793     171.96
 H       4.288015     1.435271     1.536728      29.13
 H       4.838281    -1.509036     1.725221      27.83
 H       3.389835    -0.523294     1.252378      27.64
55
name = lig-Water-frame_961
 C      -1.331785     3.778796     2.167644      55.39
 H      -2.008631     4.294760     1.436447      27.43
 C      -0.637065     1.454818     3.068629      46.80
 H      -0.702041     0.380885     3.007594      24.82
 C       0.266177     2.173437     3.784508      16.82
 O       1.248331     1.420146     4.589285     149.22
 C       1.016335    -0.051331     4.689370     115.58
 H       1.460345    -0.497450     5.595338      28.47
 H       1.563381    -0.637192     3.838015      28.57
 H       0.006000    -0.302435     5.086622      26.42
 C       0.569694     3.522114     3.805324      23.12
 O       1.611136     3.956682     4.749313     105.51
 H       1.324457     4.718653     5.301035      29.07
 C      -0.247619     4.409074     2.884364      69.21
 H       0.195089     5.576835     2.768009      15.53
 C      -1.650153     2.393662     2.310017     -13.51
 C      -2.763806     1.729329     1.501376     100.38
 H      -3.782900     2.333594     1.683994      25.05
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 O      -3.033382     0.519221     2.243983     240.67
 H      -3.983797     0.545705     2.490275      23.77
 C      -2.369443     1.717186    -0.007114      91.28
 H      -1.983927     2.615870    -0.362029      27.29
 C      -3.752747     1.656793    -0.754906      84.81
 O      -4.673707     0.591614    -0.223582     179.15
 H      -4.140187    -0.178227    -0.095696      30.40
 H      -3.851096     1.476569    -1.997791      25.40
 H      -4.486687     2.336489    -0.338849      26.14
 C       1.875211     1.318860    -1.443575      74.52
 H       2.406489     2.410334    -1.613467      23.51
 C       1.540377    -1.122151    -1.629533      51.97
 H       1.969226    -2.191353    -1.673162      23.03
 C       0.155723    -0.979773    -1.262491      17.07
 O      -0.741473    -2.037609    -1.228502     198.70
 C      -0.235013    -3.287132    -1.896282     121.84
 H       0.812650    -3.689906    -1.878515      26.37
 H      -1.110487    -4.012745    -1.569311      26.13
 H      -0.505928    -3.122410    -2.871422      29.72
 C      -0.375386     0.271085    -0.754359      17.76
 O      -1.616876     0.510454    -0.292766     183.45
 C       0.518522     1.491216    -0.997868      43.91
 H       0.154519     2.394112    -0.834508      29.29
 C       2.490098     0.073272    -1.488173      16.12
 C       4.065793    -0.242353    -1.495098     107.66
 H       4.436400    -0.886306    -2.335330      28.09
 O       4.631404     1.043768    -1.715790     245.12
 H       5.530569     1.181056    -1.395269      26.26
 C       4.499833    -1.109120    -0.316954      86.90
 H       3.655502    -1.966116    -0.206609      27.59
 O       5.838000    -1.647233    -0.598817     220.79
 H       5.734504    -2.625716    -0.645989      27.37
 C       4.352057    -0.554520     1.176657     117.87
 O       4.948071     0.616618     1.565974     187.43
 H       4.317239     1.354770     1.436382      30.74
 H       4.887444    -1.354479     1.636440      30.98
 H       3.148283    -0.624969     1.553827      26.39
55
name = lig-Water-frame_962
 C      -1.267760     3.766988     2.164330      59.04
 H      -1.911016     4.394593     1.483095      25.28
 C      -0.660745     1.500572     2.985535      64.38
 H      -0.768481     0.432449     2.885336      26.59
 C       0.240781     2.124325     3.828015      -4.57
 O       1.324448     1.446766     4.598619      70.69
 C       0.993700    -0.080352     4.704601     111.52
 H       1.448455    -0.377074     5.682254      27.49
 H       1.398850    -0.638423     3.828328      29.16
 H      -0.045003    -0.492594     4.862345      26.56
 C       0.638405     3.553798     3.765404      -9.76
 O       1.574040     3.952991     4.778920     102.42
 H       1.356731     4.946611     5.192663      21.42
 C      -0.296598     4.420585     2.928447      51.10
 H       0.070751     5.307640     2.815812      22.10
 C      -1.640270     2.356677     2.340934      25.69
 C      -2.748239     1.742156     1.509139     102.02
 H      -3.646805     2.296011     1.516731      28.58
 O      -2.995753     0.487621     2.220137     233.31
 H      -4.070704     0.414567     2.256169      22.67
 C      -2.306906     1.673651     0.029797      92.26
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 H      -1.987176     2.705963    -0.444502      24.75
 C      -3.801531     1.694046    -0.783511      77.97
 O      -4.648913     0.602774    -0.216318     154.22
 H      -4.138881    -0.272121    -0.151740      27.09
 H      -3.581656     1.486750    -1.766512      29.03
 H      -4.457793     2.579666    -0.460935      26.93
 C       1.824978     1.331096    -1.406692     118.01
 H       2.304806     2.157566    -1.650622      32.23
 C       1.606284    -1.100076    -1.604521      61.93
 H       1.683043    -2.174029    -1.659014      18.90
 C       0.105624    -0.954130    -1.237258       5.27
 O      -0.723380    -1.988335    -1.157774     197.61
 C      -0.275017    -3.333712    -1.901807      72.50
 H       0.870865    -3.468041    -1.435001      22.64
 H      -0.885605    -4.204812    -1.687701      26.65
 H      -0.482701    -3.160557    -3.113133      25.01
 C      -0.310348     0.299531    -0.833219      28.18
 O      -1.682490     0.474455    -0.315833     189.97
 C       0.510405     1.425693    -1.038767      61.38
 H      -0.124517     2.478731    -0.877120      24.85
 C       2.468387     0.016663    -1.523701       3.54
 C       4.035388    -0.271144    -1.520628      99.87
 H       3.986240    -0.723197    -2.699553      23.58
 O       4.642138     1.041552    -1.708475     201.27
 H       5.709756     0.957584    -1.385368      21.47
 C       4.477545    -1.139391    -0.365561      96.68
 H       3.700970    -1.817772    -0.430359      28.99
 O       5.860668    -1.663846    -0.605005     234.24
 H       5.752164    -2.702166    -0.580682      27.84
 C       4.292543    -0.575080     1.225294     103.21
 O       4.989905     0.635867     1.557459     200.23
 H       4.273834     1.317084     1.287693      29.71
 H       4.909489    -1.335758     1.839666      27.37
 H       3.379403    -0.715641     1.649460      29.85
55
name = lig-Water-frame_963
 C      -1.243465     3.738518     2.175415      67.89
 H      -1.781764     4.449058     1.592117      25.98
 C      -0.721580     1.566587     2.908062      54.15
 H      -0.817968     0.456019     2.847565      29.09
 C       0.337426     2.113855     3.886305     -28.85
 O       1.333081     1.423167     4.593048      45.13
 C       0.981727    -0.098222     4.750070     116.84
 H       1.633722    -0.248182     5.661630      26.30
 H       1.362970    -0.606147     3.830615      27.50
 H      -0.113917    -0.300448     4.483883      23.89
 C       0.619290     3.578240     3.736080      14.12
 O       1.528767     3.974501     4.778981     176.71
 H       1.170856     4.847149     5.009157      22.07
 C      -0.268917     4.350177     3.017962      59.11
 H      -0.089175     5.593492     2.746190      19.31
 C      -1.576535     2.369115     2.348624      55.28
 C      -2.688099     1.751821     1.558573      87.82
 H      -3.637610     2.517421     1.409582      26.22
 O      -2.990692     0.463319     2.165124     260.11
 H      -3.873040     0.149437     2.051418      28.00
 C      -2.342847     1.657169     0.010290      87.32
 H      -1.731408     2.522693    -0.239968      27.93
 C      -3.834020     1.693144    -0.743691      89.57
 O      -4.629162     0.608576    -0.217857     193.80
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 H      -4.080620    -0.226624    -0.372502      27.10
 H      -3.400979     1.562482    -1.885110      26.57
 H      -4.108354     2.812783    -0.877141      26.59
 C       1.807932     1.303539    -1.369120     -11.14
 H       2.529219     2.240130    -1.726956      28.19
 C       1.568643    -1.063004    -1.540168      70.63
 H       1.914290    -2.083425    -1.757282      24.48
 C       0.153001    -0.916665    -1.230765      12.60
 O      -0.732462    -2.007774    -1.105352     184.03
 C      -0.309851    -3.326519    -1.894752      99.75
 H       0.564249    -3.459332    -1.401419      29.43
 H      -0.830294    -4.283892    -1.560477      26.31
 H      -0.069954    -3.189268    -2.974757      28.59
 C      -0.301766     0.364765    -0.896396      29.29
 O      -1.717478     0.408876    -0.353687     154.82
 C       0.454119     1.393746    -1.069329      90.28
 H      -0.016347     2.347205    -1.026074      24.81
 C       2.438993    -0.048935    -1.546745     -26.43
 C       3.948207    -0.242495    -1.617770     119.86
 H       3.944407    -0.803003    -2.596226      24.68
 O       4.676714     1.033807    -1.690538     225.15
 H       5.514198     0.876052    -1.378422      28.14
 C       4.461850    -1.152170    -0.377647      85.82
 H       3.735358    -2.125178    -0.579884      22.39
 O       5.853300    -1.684739    -0.599745     212.74
 H       5.897988    -2.633511    -0.553400      31.57
 C       4.316577    -0.656531     1.233623      86.78
 O       5.006895     0.673374     1.546330     148.95
 H       4.367730     1.403770     1.263362      30.52
 H       4.845551    -1.375736     1.889790      27.85
 H       3.150352    -0.670442     1.690820      26.74
55
name = lig-Water-frame_964
 C      -1.225833     3.740649     2.225732      78.17
 H      -1.848239     4.494990     1.590965      22.80
 C      -0.647006     1.572011     2.971783      30.87
 H      -0.887876     0.547484     2.841490      26.84
 C       0.430511     2.138216     3.849524     -30.92
 O       1.296450     1.368505     4.579363      56.49
 C       0.990535    -0.073732     4.754053     129.38
 H       1.490313    -0.405235     5.640106      32.34
 H       1.597119    -0.582051     3.896696      29.13
 H      -0.074850    -0.051488     4.675319      26.91
 C       0.590713     3.513534     3.787429      53.93
 O       1.483453     4.002451     4.739821     160.73
 H       1.038011     4.937213     5.164181      16.91
 C      -0.231182     4.334067     3.047561      51.34
 H      -0.274444     5.301519     2.976679      22.98
 C      -1.552850     2.446099     2.282352      31.02
 C      -2.660536     1.765356     1.575525      99.65
 H      -3.420946     2.462671     1.667697      30.27
 O      -2.973257     0.455219     2.101346     234.00
 H      -3.899809     0.066030     1.824936      23.22
 C      -2.422738     1.637762    -0.010588      75.55
 H      -1.594950     2.395196    -0.143880      24.99
 C      -3.748013     1.695334    -0.756395     109.75
 O      -4.617418     0.627007    -0.240568     258.36
 H      -4.069580    -0.063568    -0.618910      28.77
 H      -3.571459     1.443291    -1.779913      29.03
 H      -4.106582     2.689690    -0.890592      28.47
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 C       1.871804     1.259255    -1.365318     102.75
 H       2.420744     2.077285    -1.550117      36.58
 C       1.479681    -1.102099    -1.478730     108.22
 H       2.148144    -1.918618    -1.829156      20.41
 C       0.210971    -0.919953    -1.225028      19.05
 O      -0.750477    -2.053332    -1.082839     191.07
 C      -0.325545    -3.280757    -1.840149      85.97
 H       0.801936    -3.692433    -1.277014      23.01
 H      -1.115834    -4.095610    -1.533864      25.45
 H       0.060893    -3.152600    -2.910331      27.44
 C      -0.430663     0.337368    -0.916887      14.85
 O      -1.716076     0.335857    -0.407343     141.50
 C       0.463139     1.465686    -1.119353      56.76
 H       0.053255     2.552571    -1.110543      25.09
 C       2.404920     0.007830    -1.538265      26.23
 C       3.869293    -0.198521    -1.692612      85.91
 H       4.350384    -1.065037    -2.454507      23.59
 O       4.665748     1.013541    -1.687286     202.15
 H       5.652164     0.851903    -1.230455      21.57
 C       4.431808    -1.210071    -0.378177      88.59
 H       3.940030    -2.048865    -0.418255      28.69
 O       5.835396    -1.676014    -0.591341     204.57
 H       5.931957    -2.701114    -0.538275      28.54
 C       4.331299    -0.720930     1.215991      87.66
 O       5.007453     0.681377     1.536165     134.52
 H       4.389060     1.409102     1.306513      33.98
 H       4.828566    -1.486232     1.815544      27.65
 H       3.322606    -0.521172     1.371219      29.27
55
name = lig-Water-frame_965
 C      -1.237131     3.832311     2.262536      57.94
 H      -1.861436     4.410876     1.694876      23.89
 C      -0.541293     1.593527     3.076131      50.61
 H      -0.819106     0.522410     2.966667      27.07
 C       0.464857     2.094526     3.734469      56.28
 O       1.274140     1.323694     4.582494     219.51
 C       1.025889    -0.029129     4.721583     135.47
 H       1.231084    -0.545288     5.770742      24.34
 H       1.531808    -0.610830     4.004370      26.59
 H      -0.128933    -0.163723     4.990347      24.42
 C       0.578842     3.465186     3.893321      15.98
 O       1.445966     4.053650     4.713464      17.26
 H       1.164364     4.887887     5.203765      28.95
 C      -0.220546     4.291187     3.039393      38.90
 H      -0.212837     5.541305     3.302858      23.37
 C      -1.482472     2.435453     2.235618     -14.73
 C      -2.654266     1.749912     1.541827      93.18
 H      -3.592637     2.461656     1.941235      23.02
 O      -2.951846     0.444500     2.047201     201.06
 H      -3.877763     0.357427     1.651152      21.48
 C      -2.457237     1.621937    -0.009030      76.67
 H      -1.711406     2.425031    -0.322638      24.21
 C      -3.641462     1.692497    -0.801515      91.17
 O      -4.602724     0.655859    -0.276705     227.12
 H      -4.235549    -0.167440    -0.793034      25.91
 H      -3.600728     1.294372    -1.926215      24.37
 H      -4.368881     2.622224    -0.576289      24.21
 C       1.878555     1.254327    -1.360164      67.68
 H       2.552949     2.248378    -1.429466      27.45
 C       1.522518    -1.135154    -1.458504      88.93
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 H       1.939499    -2.083764    -1.794107      23.04
 C       0.129209    -0.974800    -1.183570       4.32
 O      -0.745643    -2.089646    -1.089686     221.93
 C      -0.290437    -3.248978    -1.714876     119.14
 H       0.518565    -3.729044    -1.347856      28.98
 H      -1.253133    -3.789469    -1.739918      25.18
 H      -0.119984    -3.065873    -2.889066      27.57
 C      -0.513825     0.338295    -0.937102       8.13
 O      -1.730473     0.266275    -0.456216     112.71
 C       0.462339     1.531471    -1.164884      49.63
 H       0.210045     2.672680    -1.149658      22.30
 C       2.368501     0.047884    -1.530180      47.29
 C       3.890480    -0.226734    -1.693435      84.31
 H       4.354992    -0.891542    -2.416190      26.27
 O       4.642255     0.986963    -1.687607     230.65
 H       5.516397     0.920919    -1.194959      25.84
 C       4.435674    -1.233622    -0.339513      71.15
 H       3.693349    -2.233395    -0.238458      21.81
 O       5.820061    -1.655501    -0.588166     213.43
 H       5.826617    -2.665477    -0.555888      27.11
 C       4.365745    -0.721478     1.123774      82.62
 O       5.013865     0.642579     1.532677     113.08
 H       4.207835     1.292179     1.339710      28.70
 H       4.786101    -1.571843     1.826866      25.00
 H       3.214370    -0.509682     1.258827      24.41
55
name = lig-Water-frame_966
 C      -1.280362     3.874545     2.274014      46.72
 H      -2.009796     4.603690     1.686312      22.29
 C      -0.576811     1.588763     3.057357      67.04
 H      -0.601046     0.501691     3.207359      25.89
 C       0.555354     2.042942     3.692049      28.83
 O       1.283844     1.315222     4.598568     181.08
 C       1.000532    -0.044864     4.757846     129.44
 H       1.366215    -0.289500     5.705908      26.59
 H       1.328216    -0.814490     3.894174      26.51
 H      -0.003043    -0.365094     4.797407      28.44
 C       0.534950     3.478700     3.944416      10.65
 O       1.466855     4.078436     4.722780      61.39
 H       1.082441     5.074762     5.032726      19.54
 C      -0.194241     4.321372     3.080100      54.57
 H      -0.016199     5.255306     3.463558      25.15
 C      -1.355692     2.377634     2.239788      19.22
 C      -2.658237     1.755135     1.526258      98.92
 H      -3.506881     2.281954     1.713213      28.26
 O      -2.940527     0.435514     1.996344     232.56
 H      -3.838884     0.387765     1.650281      25.02
 C      -2.410115     1.621055    -0.019301      88.32
 H      -1.878252     2.452361    -0.480536      26.02
 C      -3.653341     1.673535    -0.865412     100.34
 O      -4.581971     0.661006    -0.328758     317.75
 H      -4.564933    -0.241139    -0.691391      29.35
 H      -3.427258     1.606264    -1.978398      26.87
 H      -4.168972     2.475968    -0.535479      27.95
 C       1.818495     1.367978    -1.350155      46.02
 H       2.585554     2.127985    -1.353371      31.71
 C       1.554888    -1.140127    -1.456802      68.28
 H       1.695902    -2.222498    -1.655484      20.23
 C       0.045418    -1.011724    -1.136671      -2.12
 O      -0.733963    -2.078152    -1.080147     223.72
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 C      -0.315118    -3.231105    -1.651066      96.94
 H       0.565373    -4.044170    -1.111155      23.30
 H      -1.312176    -3.776134    -1.980442      24.26
 H      -0.153555    -2.979192    -2.736968      26.99
 C      -0.453814     0.372908    -0.983240       8.93
 O      -1.797037     0.231515    -0.477777     115.90
 C       0.435963     1.536756    -1.191247      62.44
 H       0.188248     2.586303    -1.133534      23.39
 C       2.387286    -0.031844    -1.538379       6.33
 C       3.947958    -0.292935    -1.590769      86.41
 H       4.083662    -0.779014    -2.782288      25.65
 O       4.605427     0.977441    -1.687001     198.69
 H       5.440652     0.956198    -1.203927      27.67
 C       4.433637    -1.258931    -0.303619     112.05
 H       3.693300    -1.954276    -0.227137      29.94
 O       5.796582    -1.639892    -0.591697     242.86
 H       5.837899    -2.594601    -0.598038      28.42
 C       4.367959    -0.683409     1.037446     126.03
 O       5.002629     0.573541     1.522010     185.24
 H       4.258220     1.182126     1.420083      32.24
 H       4.672953    -1.397425     1.722139      29.74
 H       3.295987    -0.681668     1.333344      28.48
55
name = lig-Water-frame_967
 C      -1.302467     3.859573     2.285545      53.83
 H      -1.924943     4.540931     1.831703      24.67
 C      -0.602126     1.527500     3.009690      43.47
 H      -0.716598     0.483041     3.170333      25.42
 C       0.634340     2.073469     3.717359      13.28
 O       1.311698     1.322627     4.608491     140.08
 C       0.971201    -0.132767     4.789929      91.67
 H       1.709097    -0.180308     5.706979      22.19
 H       1.341834    -0.644612     3.976346      30.69
 H      -0.176344    -0.375638     4.652466      24.73
 C       0.515243     3.465619     3.929713      23.24
 O       1.515611     4.104173     4.758284      90.82
 H       1.074711     5.028843     4.962826      21.08
 C      -0.205938     4.339850     3.130182      41.01
 H       0.040577     5.513338     3.378750      22.09
 C      -1.321391     2.375843     2.220862      26.33
 C      -2.585472     1.745366     1.498224      78.05
 H      -3.589939     2.487004     1.445397      24.17
 O      -2.936412     0.422733     1.961933     182.79
 H      -3.920403     0.117126     1.722266      23.31
 C      -2.350978     1.598900    -0.077178      84.26
 H      -1.779248     2.528747    -0.527874      23.94
 C      -3.693009     1.624055    -0.896911      79.77
 O      -4.586973     0.661701    -0.381173     350.25
 H      -4.633666    -0.230292    -0.719053      30.54
 H      -3.359137     1.841522    -2.025770      25.15
 H      -4.098958     2.793687    -0.681058      24.79
 C       1.784387     1.387069    -1.353798     -28.67
 H       2.549146     2.222045    -1.394034      28.43
 C       1.476147    -1.149879    -1.448285      47.72
 H       1.834877    -2.212560    -1.495770      25.03
 C       0.096288    -0.946201    -1.123284      17.33
 O      -0.760563    -2.039277    -1.024457     209.82
 C      -0.360107    -3.310095    -1.659625     101.89
 H       0.221391    -3.826315    -1.070302      29.79
 H      -1.208658    -3.917386    -1.835954      27.44
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 H       0.312854    -2.957676    -2.621450      24.72
 C      -0.384464     0.355661    -1.014961      16.26
 O      -1.843756     0.267046    -0.489619     108.03
 C       0.401186     1.501536    -1.200305      65.78
 H      -0.158884     2.588520    -1.038763      21.89
 C       2.413992    -0.079125    -1.518306     -50.93
 C       3.962188    -0.367069    -1.510710     114.53
 H       3.944206    -0.802170    -2.536085      28.21
 O       4.568698     0.975263    -1.675851     140.66
 H       5.543905     1.043960    -1.167249      21.71
 C       4.452799    -1.223491    -0.352666     109.22
 H       3.636762    -2.127064    -0.346388      26.63
 O       5.777759    -1.631830    -0.598039     202.19
 H       5.965511    -2.665320    -0.616502      24.37
 C       4.333378    -0.630536     1.027375     122.51
 O       4.988157     0.494853     1.502829     152.26
 H       4.382125     1.352765     1.411723      28.58
 H       4.807865    -1.498913     1.737072      26.79
 H       3.246749    -0.657006     1.359475      27.53
55
name = lig-Water-frame_968
 C      -1.241845     3.798828     2.340611      55.83
 H      -1.996142     4.498585     1.792735      24.82
 C      -0.519740     1.483909     2.993979      13.14
 H      -1.009127     0.426755     2.889800      28.00
 C       0.587318     2.093259     3.740028      23.59
 O       1.350431     1.326531     4.617071     154.30
 C       0.963023    -0.192477     4.819887     107.52
 H       1.573136    -0.480645     5.636062      29.43
 H       1.586623    -0.601457     3.891641      29.17
 H      -0.060174    -0.259838     4.980833      30.08
 C       0.581358     3.476389     3.912193      18.35
 O       1.565070     4.102691     4.782224       1.77
 H       1.128880     5.012644     5.174965      23.43
 C      -0.275460     4.379015     3.161832      50.73
 H      -0.134682     5.455159     2.955954      21.81
 C      -1.397202     2.403923     2.183399      -9.35
 C      -2.535106     1.747325     1.417112      97.49
 H      -3.227606     2.466688     1.445350      30.05
 O      -2.938469     0.404820     1.956252     202.04
 H      -3.831791     0.141693     1.728328      26.19
 C      -2.322977     1.578097    -0.169971     101.62
 H      -1.697883     2.377927    -0.422551      28.75
 C      -3.709900     1.657030    -0.899393     106.07
 O      -4.621870     0.674560    -0.429825     341.67
 H      -4.440194    -0.165041    -1.014294      27.22
 H      -3.503396     1.636549    -2.038754      27.45
 H      -4.108765     2.574535    -0.832822      29.26
 C       1.809770     1.304675    -1.372876     -21.29
 H       2.330687     2.337707    -1.525275      28.19
 C       1.428814    -1.152467    -1.432110      76.20
 H       1.965067    -2.063594    -1.382582      26.64
 C       0.180172    -0.905009    -1.140485      33.79
 O      -0.807829    -1.998258    -0.963939     123.41
 C      -0.375125    -3.340947    -1.706389      80.74
 H       0.267060    -3.819860    -0.643351      23.78
 H      -1.353763    -4.067404    -1.796103      24.67
 H       0.407970    -3.240126    -2.409901      27.49
 C      -0.402275     0.321903    -1.003272      20.53
 O      -1.815290     0.343241    -0.514152     144.72
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 C       0.353584     1.486793    -1.189618      81.75
 H      -0.181728     2.308437    -1.063890      29.42
 C       2.384748    -0.051285    -1.453212     -53.03
 C       3.917578    -0.371758    -1.465098     111.42
 H       4.169316    -1.191741    -2.429039      27.03
 O       4.559790     0.968398    -1.645826     159.00
 H       5.391125     1.075355    -1.279435      23.95
 C       4.436499    -1.206375    -0.418386     122.07
 H       3.941167    -2.150816    -0.436174      28.96
 O       5.797435    -1.635294    -0.616230     206.86
 H       5.911165    -2.603505    -0.510116      28.04
 C       4.273543    -0.661944     1.090637     124.21
 O       4.988560     0.473471     1.487190     173.99
 H       4.582989     1.345624     1.264375      31.05
 H       4.760050    -1.429423     1.535456      31.60
 H       3.143769    -0.526985     1.302511      29.00
55
name = lig-Water-frame_969
 C      -1.219709     3.736697     2.363345      62.97
 H      -1.906961     4.336615     1.805645      25.05
 C      -0.468975     1.499197     2.931849      76.45
 H      -0.811947     0.537053     2.792894      28.58
 C       0.473740     2.048482     3.777937     -13.43
 O       1.390857     1.317378     4.634050     134.29
 C       1.023629    -0.198193     4.810457     105.49
 H       1.442494    -0.749371     5.769930      27.51
 H       1.320975    -0.732006     3.950816      29.84
 H      -0.075025    -0.271854     5.197107      25.50
 C       0.672744     3.568275     3.891873       1.65
 O       1.606049     4.085994     4.800445      34.85
 H       1.166685     4.921441     5.211157      28.37
 C      -0.326495     4.376201     3.180827      69.51
 H      -0.204493     5.458535     2.900270      19.97
 C      -1.430048     2.371163     2.203476      36.74
 C      -2.489096     1.718785     1.314858      79.69
 H      -3.368098     2.588724     1.539998      26.15
 O      -2.924868     0.411116     1.967377     167.32
 H      -3.852992     0.319880     1.608578      25.77
 C      -2.345875     1.582101    -0.236063     103.47
 H      -1.591001     2.474787    -0.465747      27.25
 C      -3.699158     1.693884    -0.912725      84.07
 O      -4.661844     0.670454    -0.492176     277.81
 H      -4.300663     0.012397    -1.101637      27.70
 H      -3.599214     1.330045    -2.101742      25.32
 H      -4.331683     2.729668    -0.750756      24.97
 C       1.804024     1.227729    -1.400579     102.56
 H       2.269497     2.129869    -1.607050      33.41
 C       1.518389    -1.122570    -1.416389      74.38
 H       1.958653    -2.197411    -1.336928      25.96
 C       0.135006    -0.961724    -1.148115     -16.01
 O      -0.834230    -1.968440    -0.947511     147.73
 C      -0.389708    -3.372387    -1.608462     101.61
 H       0.031316    -3.777912    -0.867837      30.19
 H      -1.222150    -3.839059    -1.908156      29.34
 H       0.455390    -3.513839    -2.531866      25.69
 C      -0.477267     0.343491    -0.957340      45.29
 O      -1.719070     0.386392    -0.564442     199.61
 C       0.363674     1.408807    -1.179608      44.49
 H      -0.131927     2.585098    -1.145859      27.59
 C       2.334220     0.004495    -1.383894      48.93
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 C       3.859811    -0.331819    -1.504201     105.34
 H       4.263066    -1.127172    -2.363705      27.94
 O       4.533846     0.946802    -1.626235     145.36
 H       5.517871     1.011322    -1.222668      21.55
 C       4.431235    -1.212701    -0.393631     107.00
 H       3.884838    -2.227811    -0.451290      28.47
 O       5.842055    -1.618792    -0.643548     184.46
 H       5.824242    -2.601627    -0.398281      27.62
 C       4.189155    -0.711943     1.110704     109.74
 O       5.019618     0.483217     1.479955     164.43
 H       4.545249     1.277080     1.102467      33.23
 H       4.675159    -1.654394     1.736706      27.96
 H       3.143501    -0.547034     1.311110      30.28
55
name = lig-Water-frame_970
 C      -1.260163     3.670070     2.345234      57.47
 H      -1.910701     4.361905     1.752125      23.74
 C      -0.465464     1.542410     2.845504      71.40
 H      -0.382524     0.349948     2.839236      28.84
 C       0.410171     2.047048     3.855094     -47.81
 O       1.411590     1.277916     4.646894      88.66
 C       1.060769    -0.175704     4.841915     125.83
 H       1.585178    -0.632740     5.678348      29.19
 H       1.000897    -0.848530     3.893958      26.70
 H      -0.002355    -0.233189     5.008247      27.26
 C       0.712940     3.626022     3.860971      -6.84
 O       1.640689     4.061443     4.807502     105.16
 H       1.176210     4.978687     5.188873      20.49
 C      -0.298520     4.348486     3.211668      55.91
 H      -0.214540     5.541840     3.172951      20.92
 C      -1.391699     2.292366     2.242796      58.43
 C      -2.501621     1.717439     1.274504      98.15
 H      -3.328588     2.261264     1.389342      32.19
 O      -2.912062     0.447765     1.963983     200.80
 H      -3.869505     0.367973     1.538814      25.57
 C      -2.356696     1.654083    -0.261118      92.98
 H      -1.853507     2.473542    -0.616574      29.70
 C      -3.727407     1.743505    -0.964566     103.60
 O      -4.690602     0.664590    -0.549756     246.50
 H      -4.414426    -0.181584    -1.008013      27.21
 H      -3.569853     1.433166    -2.017272      27.28
 H      -4.139111     2.652198    -0.770414      29.83
 C       1.721685     1.220434    -1.418606      76.28
 H       2.547682     2.094497    -1.709207      27.02
 C       1.568042    -1.137800    -1.366509      75.67
 H       1.869166    -2.112522    -1.417035      25.91
 C       0.061761    -1.021028    -1.146693     -10.28
 O      -0.829833    -1.981215    -0.979467     191.51
 C      -0.394971    -3.358248    -1.524465      86.76
 H       0.047508    -4.164237    -0.551846      23.26
 H      -1.454131    -3.701587    -2.071825      25.23
 H       0.179527    -3.352168    -2.354962      29.72
 C      -0.448069     0.348114    -0.935175      43.22
 O      -1.681867     0.395099    -0.611324     184.15
 C       0.401730     1.393830    -1.178087     101.62
 H       0.255336     2.338521    -1.274295      29.79
 C       2.358654    -0.012334    -1.347267      45.48
 C       3.829176    -0.279285    -1.541813      97.84
 H       4.069286    -0.798268    -2.586283      27.15
 O       4.525008     0.937530    -1.608875     175.08
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 H       5.467326     0.832355    -1.194665      25.35
 C       4.413035    -1.242847    -0.315547     102.97
 H       3.712622    -2.127406    -0.447895      27.19
 O       5.866845    -1.587092    -0.665173     198.84
 H       5.940752    -2.600289    -0.389562      26.51
 C       4.175390    -0.791156     1.119332     110.24
 O       5.039759     0.479958     1.468707     164.09
 H       4.429813     1.229453     1.095880      29.66
 H       4.329895    -1.468332     1.864251      31.03
 H       3.020459    -0.572118     1.363590      29.18
55
name = lig-Water-frame_971
 C      -1.297155     3.658620     2.343129      45.14
 H      -1.963816     4.351003     1.756609      23.17
 C      -0.390481     1.488177     2.853356      54.73
 H      -0.117930     0.493153     2.725810      29.85
 C       0.424214     2.118699     3.921768     -45.21
 O       1.401199     1.232084     4.638204      46.59
 C       1.058956    -0.138677     4.845230     126.43
 H       1.864342    -0.447881     5.586079      27.63
 H       1.063753    -0.696300     3.875472      26.49
 H      -0.075409    -0.127308     5.080429      25.59
 C       0.704354     3.563795     3.864891      18.36
 O       1.656441     4.063589     4.806007     188.60
 H       1.338413     4.912828     5.151934      24.83
 C      -0.263608     4.326027     3.214873      49.09
 H      -0.260857     5.365149     3.396256      22.58
 C      -1.391806     2.250063     2.201771      34.81
 C      -2.504994     1.701366     1.297520      88.04
 H      -3.553627     2.383723     1.339637      25.17
 O      -2.913453     0.492297     1.931024     249.09
 H      -3.756031     0.181932     1.677890      29.93
 C      -2.367047     1.703385    -0.271003      78.79
 H      -1.907370     2.678407    -0.821322      25.82
 C      -3.746963     1.718660    -1.014275      74.54
 O      -4.716826     0.670577    -0.597584     222.61
 H      -4.547260    -0.292764    -0.836416      26.09
 H      -3.478365     1.758917    -2.253466      24.55
 H      -4.163748     2.863363    -0.813695      24.95
 C       1.759314     1.239595    -1.447728      97.34
 H       2.370634     1.962215    -1.642742      34.57
 C       1.488773    -1.178718    -1.286904      87.67
 H       1.975103    -2.231384    -1.546081      24.28
 C       0.092793    -1.004647    -1.141794      26.08
 O      -0.824478    -2.051957    -1.024342     223.64
 C      -0.471927    -3.365628    -1.406505     121.63
 H      -0.194886    -4.004277    -0.781664      31.93
 H      -1.336123    -3.650809    -1.800826      31.05
 H       0.317509    -3.027971    -2.337038      24.70
 C      -0.324518     0.285354    -0.946454      22.19
 O      -1.749215     0.410320    -0.642771     102.23
 C       0.447177     1.409671    -1.184575      63.39
 H       0.159279     2.629592    -1.351561      25.70
 C       2.393069    -0.063409    -1.343756      19.73
 C       3.827760    -0.238888    -1.538292      86.30
 H       3.852351    -0.764971    -2.775727      23.97
 O       4.539486     0.954168    -1.589894     192.82
 H       5.361517     0.818176    -1.204138      29.61
 C       4.387506    -1.280277    -0.286188     113.79
 H       3.746433    -2.154392    -0.409101      28.89
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 O       5.849600    -1.555206    -0.665260     209.20
 H       6.097985    -2.495044    -0.555596      27.93
 C       4.168296    -0.804315     1.135497     118.31
 O       5.022547     0.449758     1.448743     167.08
 H       4.471757     1.234868     1.284114      32.41
 H       4.278849    -1.533653     2.087634      27.87
 H       3.153637    -0.534552     1.189504      30.19
55
name = lig-Water-frame_972
 C      -1.296132     3.685413     2.376250      47.88
 H      -2.031978     4.282349     1.880754      24.53
 C      -0.287723     1.462550     2.926539      10.02
 H      -0.093013     0.375611     2.537578      26.40
 C       0.486055     2.148232     3.927258      11.03
 O       1.380545     1.246298     4.611356      97.62
 C       1.022966    -0.094594     4.835258     146.18
 H       1.922152    -0.413894     5.447813      30.19
 H       1.281624    -0.647845     3.880523      27.59
 H       0.107887    -0.214372     5.451675      30.53
 C       0.677254     3.459210     3.932403      36.00
 O       1.667689     4.054366     4.782872      89.04
 H       1.340231     5.043393     5.183140      20.19
 C      -0.267358     4.259678     3.165951      56.09
 H      -0.363631     5.439749     3.533793      18.74
 C      -1.380651     2.248652     2.136122     -31.51
 C      -2.573491     1.729459     1.328624      94.79
 H      -3.227621     2.499947     1.457272      27.52
 O      -2.903027     0.510323     1.901862     254.29
 H      -3.793164     0.069953     1.727900      26.31
 C      -2.379579     1.726989    -0.308545      92.03
 H      -1.873878     2.558487    -0.647360      27.25
 C      -3.759633     1.694412    -1.082610     107.25
 O      -4.748543     0.703669    -0.638980     279.64
 H      -4.412632    -0.176100    -0.865589      28.73
 H      -3.534885     1.984094    -2.106432      27.00
 H      -4.296716     2.569297    -0.808415      27.71
 C       1.875131     1.202257    -1.461977      45.49
 H       2.470528     2.307854    -1.661938      22.93
 C       1.451371    -1.241849    -1.225390      94.33
 H       1.882819    -2.128075    -1.486927      25.53
 C       0.157756    -1.030886    -1.120000      20.38
 O      -0.833474    -2.077641    -1.034707     222.39
 C      -0.520092    -3.316628    -1.396794      99.22
 H      -0.049975    -4.139932    -0.429752      23.40
 H      -1.558765    -3.926764    -1.779593      24.43
 H       0.254871    -3.329669    -2.029873      29.61
 C      -0.302688     0.276526    -0.947402       0.40
 O      -1.803045     0.427843    -0.684093     115.63
 C       0.467458     1.491061    -1.206710      49.59
 H      -0.127312     2.305403    -1.226175      24.52
 C       2.346064    -0.094011    -1.353252      31.27
 C       3.852249    -0.269116    -1.527299      97.00
 H       3.830998    -0.824037    -2.426997      28.41
 O       4.551471     0.993512    -1.578599     169.04
 H       5.548552     0.905747    -1.102110      22.69
 C       4.396751    -1.319182    -0.326460     104.39
 H       3.869710    -2.389862    -0.400340      26.19
 O       5.803652    -1.503794    -0.652532     219.14
 H       6.060286    -2.530586    -0.700518      26.75
 C       4.184787    -0.771815     1.178382     114.25
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 O       4.991402     0.394268     1.433231     177.11
 H       4.479472     1.284252     1.436635      29.41
 H       4.405108    -1.523526     1.867566      30.31
 H       3.056951    -0.384474     1.013938      26.00
55
name = lig-Water-frame_973
 C      -1.281436     3.674933     2.405651      45.48
 H      -2.158481     4.361247     2.050165      23.44
 C      -0.270108     1.483528     2.935327      58.99
 H      -0.193745     0.435250     2.611565      29.03
 C       0.560993     2.032218     3.877433      30.81
 O       1.374408     1.320544     4.597370     228.66
 C       1.029579    -0.077543     4.840123     136.84
 H       1.857604    -0.469461     5.462653      27.94
 H       1.140500    -0.759796     3.905475      26.23
 H       0.240713    -0.371832     5.549560      29.00
 C       0.633408     3.466099     4.011907      13.34
 O       1.665473     4.056160     4.761878      48.17
 H       1.243037     4.835686     5.034615      27.43
 C      -0.274744     4.213237     3.152472      52.84
 H      -0.367778     5.171380     3.336561      26.57
 C      -1.283207     2.262283     2.132886     -36.80
 C      -2.604882     1.774791     1.328440      65.70
 H      -3.298290     2.751319     1.630831      22.53
 O      -2.898546     0.490109     1.890306     223.82
 H      -3.888785     0.259272     1.655773      24.76
 C      -2.429825     1.685221    -0.323830      87.41
 H      -1.702029     2.610488    -0.512729      22.72
 C      -3.779758     1.708086    -1.092515      85.26
 O      -4.762218     0.731445    -0.691216     266.80
 H      -4.285825    -0.087523    -1.010335      26.82
 H      -3.620825     1.791155    -2.326861      23.23
 H      -4.451156     2.607830    -0.664160      23.46
 C       1.942993     1.250721    -1.461050      81.71
 H       2.563307     2.001444    -1.614490      27.68
 C       1.522106    -1.270322    -1.194141      82.06
 H       1.877274    -2.368049    -1.350298      23.30
 C       0.123457    -1.088197    -1.069717       4.24
 O      -0.855980    -2.017790    -1.021356     222.68
 C      -0.561230    -3.408112    -1.362936     120.97
 H      -0.199713    -3.637138    -0.488952      30.49
 H      -1.339325    -3.943749    -1.687404      29.67
 H       0.354622    -3.806167    -2.133604      26.45
 C      -0.361163     0.358267    -0.948045       5.45
 O      -1.804172     0.437773    -0.736286     173.05
 C       0.485415     1.457100    -1.221185      53.70
 H      -0.268986     2.389700    -1.167619      20.95
 C       2.309017    -0.105961    -1.365500      31.61
 C       3.869501    -0.339650    -1.442128      69.81
 H       4.135546    -1.111479    -2.579791      23.83
 O       4.578975     1.022078    -1.562301     160.36
 H       5.438238     1.037268    -1.140955      26.60
 C       4.416907    -1.345005    -0.384650     115.70
 H       3.981587    -2.274868    -0.425501      28.51
 O       5.771221    -1.459524    -0.642040     276.59
 H       5.870916    -2.410800    -0.654920      29.42
 C       4.164372    -0.709514     1.134323     117.75
 O       4.976861     0.354024     1.435590     191.17
 H       4.415931     1.182161     1.415225      31.02
 H       4.465299    -1.627811     1.822175      27.63
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 H       3.163833    -0.488690     1.219718      29.05
55
name = lig-Water-frame_974
 C      -1.293798     3.624873     2.406760      62.79
 H      -2.034747     4.297766     2.187131      28.67
 C      -0.336844     1.507291     2.860488      80.39
 H      -0.301436     0.410938     2.780258      32.37
 C       0.599249     1.984102     3.784041      14.44
 O       1.410412     1.349334     4.638804     161.29
 C       1.083565    -0.103971     4.860168     117.33
 H       1.978057    -0.468915     5.491755      23.49
 H       0.854933    -0.688312     3.978061      24.90
 H       0.058917    -0.267466     5.412827      25.28
 C       0.573500     3.470938     4.035011       3.33
 O       1.648202     4.045397     4.742039      29.88
 H       1.148092     4.989953     5.084916      20.94
 C      -0.246824     4.168962     3.203565      53.58
 H      -0.262123     5.442871     3.181930      23.89
 C      -1.186446     2.290047     2.158721      35.37
 C      -2.580988     1.827075     1.333861      74.02
 H      -3.369107     2.457121     1.574326      28.85
 O      -2.925545     0.472887     1.878517     253.64
 H      -3.823422     0.443796     1.659962      29.98
 C      -2.476408     1.654050    -0.308446      88.85
 H      -1.867715     2.486491    -0.522949      27.84
 C      -3.824280     1.797083    -1.092896      98.36
 O      -4.750560     0.722971    -0.745356     274.74
 H      -4.413388    -0.141338    -1.145514      27.42
 H      -3.760500     1.471264    -2.124933      25.46
 H      -4.214289     2.792746    -0.803099      26.99
 C       1.894930     1.258046    -1.431986      62.85
 H       2.896223     1.996967    -1.620163      25.43
 C       1.561118    -1.300419    -1.182128      66.29
 H       1.925930    -2.319971    -1.103853      26.01
 C       0.086598    -1.064331    -1.011127     -14.79
 O      -0.896200    -1.956025    -1.033522     146.92
 C      -0.530669    -3.510584    -1.336336      67.35
 H      -0.210646    -3.700281    -0.109323      22.79
 H      -1.616246    -4.051180    -1.631782      24.02
 H       0.108153    -3.770966    -2.075675      28.02
 C      -0.419942     0.392716    -0.959771      17.78
 O      -1.774293     0.449604    -0.786834     165.64
 C       0.478910     1.405559    -1.225820      72.18
 H       0.246165     2.486512    -1.258520      25.96
 C       2.363351    -0.110549    -1.387077      25.57
 C       3.879320    -0.436769    -1.432346      99.92
 H       4.331176    -0.776783    -2.209641      31.53
 O       4.578951     1.017356    -1.548774      86.30
 H       5.491014     1.051638    -1.082336      23.57
 C       4.408701    -1.272794    -0.395518     112.40
 H       3.791229    -2.338504    -0.488711      25.80
 O       5.777482    -1.423317    -0.635916     218.10
 H       6.011450    -2.445897    -0.499416      22.94
 C       4.145717    -0.744301     1.053333     126.30
 O       4.983821     0.356117     1.454063     184.89
 H       4.430461     1.137606     1.273703      33.22
 H       4.413828    -1.541193     1.736677      31.00
 H       3.021423    -0.605462     1.506802      28.66
55
name = lig-Water-frame_975
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 C      -1.254452     3.614280     2.436397      54.46
 H      -2.114903     4.305400     2.019416      27.70
 C      -0.354679     1.460562     2.803317      31.53
 H      -0.562631     0.311051     2.848846      30.59
 C       0.598771     2.049424     3.698416       8.47
 O       1.459890     1.322187     4.696459     123.51
 C       1.130600    -0.126458     4.908863     121.61
 H       1.957488    -0.509630     5.399994      27.75
 H       0.795585    -0.579274     3.853040      26.86
 H       0.135502     0.018366     5.346344      26.39
 C       0.561171     3.413399     4.013154      11.58
 O       1.595362     4.060865     4.742209      21.64
 H       1.360155     4.905225     5.105138      26.66
 C      -0.255176     4.229456     3.252260      65.33
 H      -0.061308     5.176532     3.201037      30.06
 C      -1.228193     2.312471     2.118739      27.25
 C      -2.497299     1.784404     1.333993      73.62
 H      -3.497228     2.431955     1.518592      25.82
 O      -2.949202     0.477392     1.867973     198.14
 H      -3.975242     0.402982     1.706217      24.92
 C      -2.506594     1.650464    -0.278980      75.53
 H      -1.934534     2.583133    -0.733091      26.54
 C      -3.841199     1.836435    -1.073508      85.03
 O      -4.757178     0.702642    -0.767846     267.72
 H      -4.495743    -0.073628    -1.273746      29.17
 H      -3.601646     1.651099    -2.222477      25.52
 H      -4.170907     2.983460    -1.021469      25.51
 C       1.864983     1.187436    -1.402359      72.56
 H       2.601978     1.945308    -1.516366      32.63
 C       1.510664    -1.270034    -1.164067      51.24
 H       1.989132    -2.249942    -0.956866      25.90
 C       0.117945    -0.967933    -0.973194       2.69
 O      -0.946380    -1.951029    -1.067682     108.90
 C      -0.561041    -3.579390    -1.222115      85.40
 H      -0.244568    -4.066785    -0.348234      26.91
 H      -1.560153    -3.854634    -1.343390      25.87
 H       0.194690    -3.611497    -2.167235      24.01
 C      -0.433665     0.350290    -0.977366      24.31
 O      -1.767167     0.468826    -0.824760     124.22
 C       0.515390     1.413836    -1.233315      70.55
 H       0.443783     2.532098    -1.319316      29.33
 C       2.437894    -0.139348    -1.404459       6.47
 C       3.873328    -0.408701    -1.457114      90.30
 H       4.471742    -0.802859    -2.607281      24.44
 O       4.570482     0.992906    -1.527835     105.92
 H       5.521678     0.979442    -1.016479      20.91
 C       4.359592    -1.229055    -0.343288     125.38
 H       3.850331    -2.075997    -0.483166      31.44
 O       5.819019    -1.416026    -0.628475     201.27
 H       6.178791    -2.283906    -0.271241      24.44
 C       4.107790    -0.813645     1.023575     131.34
 O       4.986806     0.371256     1.471408      83.61
 H       4.539434     1.259101     1.136723      31.91
 H       4.507377    -1.658651     1.704357      29.80
 H       3.156626    -0.656968     1.335168      30.62
55
name = lig-Water-frame_976
 C      -1.228087     3.704426     2.453260      53.42
 H      -1.927237     4.190560     1.864279      28.16
 C      -0.344646     1.389796     2.783404       8.95
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 H      -0.649754     0.410996     2.756184      30.49
 C       0.605533     2.056954     3.676221      10.64
 O       1.500763     1.300738     4.713748     137.09
 C       1.131034    -0.100265     4.901350     121.56
 H       1.985035    -0.742786     5.442020      26.88
 H       1.083351    -0.556361     3.980185      29.68
 H       0.226225     0.036470     5.655866      25.72
 C       0.597863     3.403586     3.969300      24.16
 O       1.553986     4.041810     4.751054     -64.01
 H       1.223405     4.990015     5.096264      26.76
 C      -0.299305     4.261782     3.281714      60.41
 H       0.070174     5.461567     3.324172      21.19
 C      -1.335747     2.275235     2.058544     -47.91
 C      -2.471372     1.704850     1.313979     102.99
 H      -3.161608     2.524125     1.432543      27.57
 O      -2.969339     0.484797     1.864653     238.45
 H      -3.959452     0.304369     1.783131      25.69
 C      -2.479410     1.708703    -0.274512      78.74
 H      -2.014163     2.563746    -0.748810      26.96
 C      -3.828622     1.809505    -1.079562      92.87
 O      -4.779627     0.710145    -0.770335     280.03
 H      -4.410356     0.032241    -1.431317      27.72
 H      -3.325250     2.042223    -2.080311      26.51
 H      -4.367765     2.820183    -1.056818      26.21
 C       1.867413     1.053071    -1.379462      36.84
 H       2.441860     2.135615    -1.490478      25.41
 C       1.466291    -1.182946    -1.144800      52.30
 H       1.845316    -2.238029    -0.915326      26.73
 C       0.133864    -0.921474    -0.964463      22.11
 O      -0.958352    -1.982708    -1.087261     100.52
 C      -0.594952    -3.559630    -1.139176      88.35
 H      -0.104153    -4.096103    -0.303794      26.13
 H      -1.706336    -3.886093    -1.301049      23.36
 H       0.059754    -3.537398    -2.022212      25.33
 C      -0.392483     0.350213    -0.998151      -5.26
 O      -1.795862     0.486921    -0.852107     105.06
 C       0.542603     1.434431    -1.231117      52.63
 H       0.135797     2.540331    -1.304008      29.88
 C       2.432871    -0.190993    -1.408602      24.18
 C       3.941910    -0.303165    -1.574534     141.67
 H       4.006341    -0.898960    -2.369358      35.18
 O       4.562465     0.957469    -1.495515     197.72
 H       5.382909     0.878315    -1.110571      29.02
 C       4.372190    -1.210593    -0.332780      87.76
 H       3.825113    -2.325784    -0.489488      27.30
 O       5.857534    -1.392348    -0.608055     180.79
 H       6.081700    -2.283142    -0.196226      23.85
 C       4.132029    -0.850358     1.076422     120.51
 O       4.972836     0.377408     1.475992     107.99
 H       4.581085     1.211689     1.192625      33.95
 H       4.565842    -1.719618     1.636078      29.95
 H       2.945828    -0.622801     1.152302      27.93
55
name = lig-Water-frame_977
 C      -1.244348     3.743236     2.398949      47.84
 H      -1.859025     4.467777     1.724776      23.73
 C      -0.360897     1.408227     2.764215      39.63
 H      -0.516005     0.199388     2.668072      26.89
 C       0.619242     1.968830     3.705071     -35.48
 O       1.531874     1.301851     4.684387     153.22
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 C       1.139437    -0.065995     4.940470     117.94
 H       1.868977    -0.583269     5.444168      30.42
 H       1.111227    -0.734870     3.917637      28.56
 H       0.361759    -0.271516     5.642505      28.62
 C       0.642292     3.452519     3.906547      -3.11
 O       1.525031     4.018929     4.782057     -29.58
 H       0.955975     4.864652     4.968280      24.55
 C      -0.304836     4.316824     3.307523      36.61
 H      -0.232219     5.337979     3.449659      21.77
 C      -1.339175     2.231993     2.092772     -29.25
 C      -2.498993     1.654145     1.253039      94.81
 H      -3.153541     2.658190     1.420349      23.92
 O      -2.980628     0.476223     1.877553     262.03
 H      -3.902226     0.355949     1.755918      28.23
 C      -2.433630     1.754320    -0.288164      80.12
 H      -1.866452     2.726032    -0.569010      24.34
 C      -3.804328     1.788810    -1.060777      87.49
 O      -4.775998     0.731785    -0.801309     283.65
 H      -4.400565    -0.009544    -1.365908      27.95
 H      -3.374585     1.916207    -2.113261      25.54
 H      -4.513413     2.659937    -0.746230      24.94
 C       1.884860     1.039342    -1.373611      47.73
 H       2.476349     1.985201    -1.548621      25.74
 C       1.462551    -1.154489    -1.119297      72.90
 H       1.627842    -2.187349    -1.031081      28.07
 C       0.079552    -0.955991    -0.982888     -10.65
 O      -0.928627    -2.019973    -1.078482     176.70
 C      -0.666293    -3.461582    -1.084668      98.91
 H       0.043208    -3.631789    -0.071358      24.69
 H      -1.599447    -4.110622    -1.295425      24.31
 H      -0.038963    -3.694948    -2.022735      25.45
 C      -0.380975     0.423873    -1.011489     -10.56
 O      -1.816884     0.506325    -0.876357     131.17
 C       0.503069     1.420748    -1.213126      96.03
 H       0.025724     2.341104    -1.255045      30.53
 C       2.402255    -0.214787    -1.401642      34.83
 C       3.963756    -0.248160    -1.598322     110.66
 H       3.924848    -1.113197    -2.623256      26.85
 O       4.544371     0.937780    -1.489670     155.58
 H       5.570985     0.813933    -1.093422      21.87
 C       4.423759    -1.246514    -0.407257     102.44
 H       4.034381    -2.150969    -0.480080      31.38
 O       5.878132    -1.354653    -0.567225     216.08
 H       5.964032    -2.417913    -0.429422      21.83
 C       4.156820    -0.820936     1.141482     130.04
 O       4.950370     0.346467     1.485753     180.41
 H       4.396055     1.189930     1.299825      29.56
 H       4.460341    -1.678767     1.777564      30.26
 H       3.110501    -0.710625     1.179519      28.14
55
name = lig-Water-frame_978
 C      -1.272097     3.731240     2.306405      65.05
 H      -1.766472     4.561033     1.852301      22.34
 C      -0.369504     1.414269     2.775701      74.71
 H      -0.261974     0.437999     2.620267      26.37
 C       0.620087     1.927140     3.745004      -7.21
 O       1.529739     1.307536     4.619195     158.78
 C       1.169932    -0.079115     4.951177     108.85
 H       2.157563    -0.353212     5.573589      23.50
 H       0.970588    -0.639196     4.136557      27.05
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 H       0.145425    -0.398398     5.505734      24.89
 C       0.674331     3.445076     3.834363       1.42
 O       1.492253     4.000616     4.821493     127.37
 H       1.095223     4.870028     5.145778      27.79
 C      -0.328539     4.302243     3.286364      64.28
 H      -0.498773     5.495329     3.546879      18.64
 C      -1.284174     2.250875     2.164485      28.41
 C      -2.542266     1.689089     1.213916      85.83
 H      -3.342649     2.395847     1.421403      24.96
 O      -2.987155     0.458789     1.892861     232.15
 H      -4.011980     0.406935     1.648760      24.27
 C      -2.389640     1.762171    -0.317035      87.35
 H      -1.795100     2.705403    -0.329272      23.23
 C      -3.781298     1.809278    -1.027630      80.21
 O      -4.745938     0.732798    -0.843164     267.41
 H      -4.451218    -0.132482    -1.157974      29.29
 H      -3.807805     1.686546    -2.180828      22.29
 H      -4.340584     2.629160    -0.415060      23.93
 C       1.867878     1.134180    -1.383377      47.63
 H       2.735650     1.905845    -1.632805      23.53
 C       1.421724    -1.222963    -1.090057      64.72
 H       1.675558    -2.375386    -1.249100      22.74
 C       0.009690    -0.995891    -1.024868       7.86
 O      -0.907350    -2.022732    -1.063745     215.80
 C      -0.667010    -3.341511    -1.037525     131.34
 H      -0.143515    -3.431624    -0.108154      28.22
 H      -1.571590    -4.073800    -1.025983      25.83
 H      -0.098649    -3.919180    -1.856322      26.96
 C      -0.455199     0.413456    -1.005989      22.95
 O      -1.807746     0.547629    -0.898987     176.09
 C       0.487459     1.385661    -1.193425      70.12
 H       0.090641     2.553039    -1.241889      23.15
 C       2.404141    -0.174272    -1.388116      24.48
 C       3.899987    -0.374041    -1.585027     102.71
 H       4.241275    -0.628179    -2.509794      28.50
 O       4.568443     0.953145    -1.500256     168.60
 H       5.459555     0.946112    -1.123858      25.56
 C       4.501890    -1.235722    -0.468544      94.04
 H       3.984346    -2.360296    -0.625535      24.74
 O       5.899690    -1.341620    -0.524108     226.93
 H       6.089622    -2.292811    -0.675776      27.25
 C       4.200146    -0.790302     1.147425     110.72
 O       4.916613     0.314706     1.505895     217.76
 H       4.301156     1.119353     1.465506      27.47
 H       4.363092    -1.621371     1.956023      26.67
 H       3.039009    -0.654149     1.388767      25.74
55
name = lig-Water-frame_979
 C      -1.243946     3.695757     2.272964      58.26
 H      -1.996121     4.405608     1.816927      21.96
 C      -0.320827     1.439360     2.846905      57.98
 H      -0.198244     0.288572     2.466223      22.81
 C       0.594842     1.994625     3.749971      19.84
 O       1.496775     1.301770     4.539857     159.59
 C       1.210394    -0.111963     4.997449     114.27
 H       2.081501    -0.266759     5.535748      26.93
 H       1.068978    -0.758118     3.984293      23.55
 H       0.260147    -0.053799     5.448627      28.31
 C       0.674693     3.422637     3.809324       8.33
 O       1.472603     3.971896     4.859928     164.11
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 H       1.282312     4.901112     5.303270      31.95
 C      -0.370957     4.249798     3.209907      85.48
 H      -0.541582     5.266161     3.578036      18.55
 C      -1.285325     2.326587     2.170061      21.06
 C      -2.560112     1.729489     1.254008      68.07
 H      -3.530157     2.353708     1.441641      21.89
 O      -3.008307     0.440903     1.886944     241.68
 H      -3.952791     0.323948     1.639068      26.25
 C      -2.370443     1.731578    -0.338316      91.85
 H      -1.770698     2.650466    -0.488062      22.29
 C      -3.779519     1.833506    -1.002439      94.87
 O      -4.727254     0.713775    -0.843178     267.40
 H      -4.299215    -0.193302    -1.034199      27.07
 H      -3.876022     2.004797    -2.078445      25.12
 H      -4.170700     2.751621    -0.506280      25.60
 C       1.865552     1.226543    -1.402201      40.05
 H       2.786350     1.933365    -1.663111      22.13
 C       1.384160    -1.322406    -1.100692      78.51
 H       1.778929    -2.230734    -1.332566      24.56
 C      -0.005203    -1.005815    -1.073092      21.95
 O      -0.940359    -1.956730    -1.070530     190.93
 C      -0.632255    -3.320881    -0.984767     112.79
 H      -0.103094    -3.611444     0.136539      24.88
 H      -1.701450    -3.687636    -0.616738      23.83
 H      -0.039528    -3.795308    -1.748647      27.16
 C      -0.512318     0.319847    -0.996235      33.39
 O      -1.800190     0.599290    -0.919435     192.14
 C       0.488211     1.423479    -1.181739      53.13
 H       0.297618     2.389001    -1.209979      23.72
 C       2.355892    -0.141260    -1.357975      10.95
 C       3.858675    -0.472420    -1.528452      75.57
 H       4.439639    -0.533130    -2.628837      20.96
 O       4.575173     0.987714    -1.520722     100.45
 H       5.473106     1.050119    -0.993175      23.56
 C       4.516993    -1.278417    -0.466315     119.57
 H       4.114738    -2.182596    -0.644060      30.05
 O       5.944496    -1.312805    -0.501707     208.32
 H       6.257084    -2.302375    -0.699041      25.04
 C       4.173315    -0.814282     1.121863     114.48
 O       4.901673     0.316988     1.548166     215.96
 H       4.406028     1.137569     1.471314      29.20
 H       4.482573    -1.611234     1.785946      28.45
 H       3.158280    -0.550329     1.368449      26.82
55
name = lig-Water-frame_980
 C      -1.237432     3.687232     2.253085      44.87
 H      -2.186381     4.042700     1.826747      20.06
 C      -0.297940     1.456877     2.874947      58.54
 H      -0.337387     0.486959     2.570536      25.60
 C       0.573472     2.080203     3.733575      13.38
 O       1.478336     1.288965     4.465688     159.65
 C       1.226351    -0.118917     4.965948     109.66
 H       2.072523    -0.441901     5.687435      26.79
 H       1.320029    -0.837751     4.215922      26.86
 H       0.299279     0.189230     5.653509      25.64
 C       0.629947     3.461757     3.845833      26.43
 O       1.477833     3.926311     4.889247     166.62
 H       1.067859     4.815984     5.125196      29.51
 C      -0.356036     4.170289     3.149142      86.84
 H      -0.442912     5.238662     3.532896      20.79
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 C      -1.320058     2.322030     2.128220       6.31
 C      -2.563112     1.754437     1.345908      65.44
 H      -3.412270     2.503672     1.418331      24.13
 O      -3.015913     0.427254     1.864648     247.28
 H      -3.929351     0.237824     1.654670      27.58
 C      -2.387323     1.720227    -0.332809      89.65
 H      -1.837015     2.612776    -0.829133      21.87
 C      -3.790185     1.861199    -0.991982      83.13
 O      -4.710279     0.697643    -0.808155     281.38
 H      -4.082698    -0.014970    -1.053000      28.13
 H      -3.562071     2.438264    -2.035566      23.42
 H      -4.259172     2.893759    -0.567294      25.10
 C       1.882404     1.233374    -1.416602      40.93
 H       2.555439     2.107154    -1.610860      23.01
 C       1.389726    -1.306098    -1.151470     106.46
 H       1.878188    -2.372195    -1.338096      22.73
 C       0.025584    -1.005997    -1.113130      19.99
 O      -1.008784    -1.890139    -1.083809     182.85
 C      -0.617127    -3.337741    -0.833674     107.18
 H      -0.005903    -3.573916     0.001315      27.92
 H      -1.577634    -3.633579    -0.694232      27.16
 H      -0.047489    -3.670960    -1.846032      24.74
 C      -0.438069     0.301917    -0.998760      30.11
 O      -1.820810     0.605771    -0.946199     203.90
 C       0.486886     1.418573    -1.171715      50.80
 H       0.130328     2.617419    -1.146340      20.02
 C       2.270788    -0.162247    -1.321226      35.75
 C       3.878701    -0.453509    -1.509614      69.73
 H       4.064828    -0.938683    -2.449626      26.53
 O       4.571878     1.021345    -1.529433     111.65
 H       5.350008     1.077301    -0.802555      24.66
 C       4.504782    -1.306060    -0.395375      91.33
 H       4.115970    -2.477602    -0.537072      24.26
 O       6.005189    -1.282084    -0.499563     206.42
 H       6.176361    -2.236892    -0.457577      29.00
 C       4.136411    -0.848752     1.064980      96.36
 O       4.917118     0.328934     1.602144     140.58
 H       4.511822     1.258094     1.277390      25.77
 H       4.658075    -1.781898     1.575294      25.25
 H       3.021747    -0.647831     1.177571      23.94
55
name = lig-Water-frame_981
 C      -1.293740     3.640784     2.214661      56.25
 H      -2.178112     4.189067     1.892687      20.50
 C      -0.365447     1.524152     2.829841      62.12
 H      -0.414872     0.333519     2.790144      24.09
 C       0.571223     2.090127     3.712612       6.74
 O       1.502238     1.276189     4.401843     163.30
 C       1.228546    -0.068941     4.971580     121.44
 H       1.971486    -0.363216     5.731227      27.56
 H       1.233532    -1.011399     4.240516      26.01
 H       0.377600    -0.133888     5.571075      29.49
 C       0.588262     3.491200     3.918758      29.63
 O       1.469965     3.897520     4.894486     120.33
 H       0.946848     4.761448     5.128250      25.03
 C      -0.296637     4.176436     3.140111      78.89
 H      -0.302712     5.363345     3.291141      20.93
 C      -1.328788     2.221410     2.102465      24.81
 C      -2.545676     1.753695     1.406302      67.14
 H      -3.278705     2.620698     1.515447      23.12
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 O      -3.000989     0.431231     1.838974     231.51
 H      -4.024761     0.263281     1.614162      24.11
 C      -2.427176     1.751489    -0.316863      90.75
 H      -1.960685     2.608158    -0.742723      24.93
 C      -3.806235     1.949025    -0.984451      95.89
 O      -4.668767     0.720936    -0.773912     285.56
 H      -4.095666     0.026367    -1.171951      27.82
 H      -3.481630     2.197560    -1.962148      27.09
 H      -4.383918     2.664899    -0.466522      27.35
 C       1.852857     1.167685    -1.406501      51.00
 H       2.356526     2.287814    -1.527826      22.46
 C       1.437779    -1.256134    -1.233134      82.82
 H       1.731256    -2.244177    -1.190082      24.64
 C       0.040310    -1.008896    -1.138138      12.62
 O      -1.064688    -1.865835    -1.079642     164.57
 C      -0.616140    -3.314769    -0.746188      89.45
 H       0.317389    -3.362725     0.107672      24.37
 H      -1.638361    -4.071557    -0.857379      23.42
 H      -0.260630    -3.627740    -1.647122      28.24
 C      -0.334132     0.390856    -1.011265      21.91
 O      -1.833535     0.550276    -0.976368     156.49
 C       0.477595     1.438679    -1.165838      56.43
 H      -0.013851     2.291633    -1.094630      23.46
 C       2.260020    -0.177018    -1.302052      36.33
 C       3.880870    -0.375032    -1.473813      78.81
 H       3.793322    -1.197676    -2.440345      26.08
 O       4.546591     1.009365    -1.516143     141.07
 H       5.233078     1.020512    -0.907222      30.08
 C       4.487254    -1.319149    -0.327528     113.15
 H       4.194756    -2.306697    -0.365275      28.86
 O       6.031867    -1.264761    -0.491872     197.61
 H       6.183033    -2.257985    -0.233534      27.57
 C       4.142114    -0.887479     1.015745     106.62
 O       4.921321     0.331615     1.636512     146.66
 H       4.604334     1.128699     1.198389      30.82
 H       4.473655    -1.669185     1.601432      28.54
 H       3.005557    -0.940029     1.055217      25.28
55
name = lig-Water-frame_982
 C      -1.319613     3.589693     2.226267      52.20
 H      -1.953036     4.480551     1.916593      23.78
 C      -0.427136     1.513804     2.785042      78.73
 H      -0.468782     0.476869     3.063715      29.32
 C       0.558492     2.052481     3.680097      27.52
 O       1.539619     1.257576     4.350865     140.45
 C       1.223626    -0.042681     4.970636     118.85
 H       2.051954    -0.105554     5.663132      24.87
 H       1.099250    -0.820767     4.222496      25.78
 H       0.146867    -0.335532     5.442469      24.45
 C       0.567756     3.437386     3.982637      15.07
 O       1.445053     3.908999     4.896945      43.50
 H       1.205627     4.770715     5.431920      17.35
 C      -0.281530     4.262253     3.094284      45.20
 H      -0.212834     5.331860     3.073616      26.70
 C      -1.339549     2.167912     2.087621      43.30
 C      -2.543471     1.709969     1.384259      83.47
 H      -3.279442     2.558406     1.706619      25.46
 O      -2.992468     0.447520     1.814665     272.04
 H      -3.916912     0.394690     1.590944      28.20
 C      -2.469317     1.778273    -0.280084      75.58
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 H      -1.832897     2.784073    -0.415589      24.99
 C      -3.815617     1.985493    -0.951716      79.41
 O      -4.613588     0.767387    -0.746166     214.69
 H      -4.328844    -0.063163    -1.317826      25.49
 H      -3.735842     1.887273    -2.152374      23.45
 H      -4.593913     2.710158    -0.323246      24.29
 C       1.791570     1.146286    -1.371223      85.01
 H       2.430325     1.936619    -1.483770      29.82
 C       1.423144    -1.228678    -1.305633      73.07
 H       1.778562    -2.302662    -1.102478      24.51
 C       0.029976    -0.971023    -1.150131       7.91
 O      -1.086283    -1.880669    -1.052873     186.95
 C      -0.644844    -3.284093    -0.695801     112.97
 H       0.003993    -3.176818     0.019766      32.56
 H      -1.316351    -4.013488    -0.537610      29.66
 H      -0.091751    -3.705225    -1.721750      26.77
 C      -0.345281     0.411163    -1.030762      17.38
 O      -1.823491     0.500566    -0.988215      97.43
 C       0.493826     1.454276    -1.167577      68.72
 H      -0.100709     2.500522    -1.099343      24.70
 C       2.368246    -0.124418    -1.304807      34.15
 C       3.843640    -0.328471    -1.433075     108.99
 H       3.943164    -0.850980    -2.355587      30.84
 O       4.484753     0.946929    -1.509372     145.29
 H       5.458409     0.928279    -0.977325      22.77
 C       4.524204    -1.251385    -0.322613     112.45
 H       4.082450    -2.384620    -0.419452      27.78
 O       6.010449    -1.275736    -0.467116     180.64
 H       6.338309    -2.201340    -0.217709      26.72
 C       4.163841    -0.904661     1.041802     111.70
 O       4.903040     0.287322     1.641018     141.14
 H       4.524739     1.163461     1.255734      29.28
 H       4.330386    -1.671152     1.958379      26.30
 H       3.066474    -0.918599     1.110401      27.98
55
name = lig-Water-frame_983
 C      -1.264474     3.622026     2.295391      63.77
 H      -1.819543     4.330829     1.696992      28.16
 C      -0.414089     1.431055     2.820915      51.87
 H      -0.612603     0.343071     3.000355      29.22
 C       0.541633     2.021037     3.651899      36.73
 O       1.553673     1.246806     4.301455     128.35
 C       1.176298    -0.036278     4.958544     113.81
 H       2.110058    -0.089701     5.645097      25.08
 H       1.295354    -0.759827     4.052162      26.21
 H       0.225230     0.015569     5.370430      27.90
 C       0.522590     3.403340     3.987419      16.83
 O       1.449175     3.920863     4.919316      52.43
 H       1.220660     4.756954     5.389109      21.04
 C      -0.296283     4.268564     3.045915      39.90
 H      -0.111783     5.495327     2.917743      22.23
 C      -1.385080     2.212783     2.060241      12.08
 C      -2.575964     1.651252     1.309120      99.48
 H      -3.390107     2.368662     1.662970      26.72
 O      -2.982120     0.452180     1.800505     269.27
 H      -3.931295     0.351370     1.576731      26.08
 C      -2.466131     1.825224    -0.228224      62.87
 H      -1.820371     2.613316    -0.241693      28.10
 C      -3.854168     1.956200    -0.940702     118.46
 O      -4.588515     0.791805    -0.704191     283.55
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 H      -4.396347     0.077176    -1.305069      27.88
 H      -3.934971     2.124504    -1.955874      28.99
 H      -4.342544     2.768801    -0.581713      30.89
 C       1.796099     1.155175    -1.326501      56.11
 H       2.841393     1.860261    -1.498817      23.28
 C       1.403311    -1.223069    -1.345244      59.29
 H       1.832782    -2.213170    -1.184367      24.71
 C       0.013980    -0.929985    -1.156947       8.26
 O      -1.082279    -1.909773    -1.020790     179.28
 C      -0.641303    -3.233684    -0.745258     103.66
 H       0.035091    -3.014660     0.369793      25.44
 H      -1.496116    -3.919072    -0.053235      23.80
 H      -0.003871    -3.657679    -1.395811      30.44
 C      -0.476152     0.368657    -1.056958      23.47
 O      -1.804532     0.501632    -0.970587      88.68
 C       0.448783     1.511269    -1.164922      66.79
 H       0.276168     2.575657    -1.214296      27.68
 C       2.414376    -0.096598    -1.314522      25.73
 C       3.841427    -0.300360    -1.373269      88.19
 H       4.237238    -0.729442    -2.603014      24.92
 O       4.456767     0.897331    -1.484925     168.21
 H       5.386486     0.881771    -1.251683      26.56
 C       4.570493    -1.226933    -0.345948     120.69
 H       4.070806    -2.135049    -0.620731      30.97
 O       5.971801    -1.284690    -0.445410     250.94
 H       6.259655    -2.189998    -0.341579      28.61
 C       4.177600    -0.911771     1.182686     120.17
 O       4.871557     0.231113     1.619640     167.96
 H       4.410347     1.134168     1.486750      29.86
 H       4.353223    -1.659975     1.857481      30.41
 H       3.053114    -0.566164     1.178375      28.74
55
name = lig-Water-frame_984
 C      -1.220587     3.667902     2.307849      69.70
 H      -1.815119     4.097145     1.471496      24.65
 C      -0.443427     1.343343     2.849987      25.32
 H      -0.639169     0.224808     2.658052      29.36
 C       0.540669     1.991734     3.656790      10.24
 O       1.551844     1.259590     4.253083     131.96
 C       1.175660    -0.020047     4.898436     117.35
 H       1.841734    -0.309408     5.655485      30.21
 H       1.405149    -0.835739     4.154763      27.17
 H       0.183899     0.291254     5.443920      25.70
 C       0.478526     3.428357     3.943425       7.91
 O       1.464707     3.897623     4.926540      42.11
 H       0.943204     4.893888     5.136333      17.12
 C      -0.259900     4.255811     3.060110      78.27
 H      -0.128961     5.227759     2.977413      26.82
 C      -1.385507     2.263286     2.094656     -47.02
 C      -2.619928     1.642091     1.242699      93.81
 H      -3.547283     2.336144     1.396173      25.23
 O      -2.975037     0.407470     1.797509     252.65
 H      -3.976923     0.083867     1.638791      22.16
 C      -2.457607     1.826259    -0.213190      55.67
 H      -1.653608     2.698606    -0.444456      24.22
 C      -3.855020     1.916705    -0.939162      92.01
 O      -4.613761     0.803811    -0.635089     263.02
 H      -4.220400     0.105464    -1.282763      24.72
 H      -3.776341     2.448374    -2.058282      24.65
 H      -4.236416     3.045369    -0.540049      25.26
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 C       1.894335     1.207415    -1.285043      66.83
 H       2.520831     1.951339    -1.389776      33.14
 C       1.409423    -1.185388    -1.352569      71.99
 H       1.761033    -2.223525    -1.356273      28.16
 C       0.000096    -0.940629    -1.165419     -11.01
 O      -1.059247    -1.916004    -1.013776     209.22
 C      -0.628191    -3.179382    -0.638987     131.69
 H      -0.052848    -3.075529     0.122999      33.82
 H      -1.468516    -3.537301    -0.310182      29.47
 H       0.122187    -3.847048    -1.354144      26.92
 C      -0.563146     0.403270    -1.092307      11.64
 O      -1.839322     0.544956    -0.925185     126.99
 C       0.418297     1.514496    -1.172247      16.19
 H       0.354205     2.660128    -1.278293      26.31
 C       2.320886    -0.141119    -1.328528      36.39
 C       3.919262    -0.342455    -1.398583     115.99
 H       4.140750    -0.808211    -2.220635      33.50
 O       4.461978     0.930906    -1.458764     203.68
 H       5.421258     0.880720    -1.262897      27.53
 C       4.551056    -1.218566    -0.328824      99.92
 H       4.091399    -2.255417    -0.718059      29.73
 O       5.948504    -1.283659    -0.439775     232.37
 H       6.083572    -2.328554    -0.494352      23.55
 C       4.134436    -0.885509     1.269739     122.82
 O       4.875676     0.205414     1.621994     171.88
 H       4.321932     0.993188     1.546131      33.58
 H       4.430296    -1.926485     1.831300      27.76
 H       3.148786    -0.556113     1.291688      31.02
55
name = lig-Water-frame_985
 C      -1.233578     3.650013     2.225895      61.62
 H      -1.789707     4.257848     1.476669      24.93
 C      -0.521681     1.313638     2.833315      26.29
 H      -0.442403     0.313271     2.483164      32.54
 C       0.508096     1.959091     3.662052     -16.10
 O       1.568329     1.275506     4.219637      93.06
 C       1.173520     0.011276     4.841020     121.41
 H       1.740682    -0.333803     5.809524      26.93
 H       1.098666    -0.924546     4.193310      26.10
 H       0.167204     0.139450     5.271079      28.02
 C       0.504252     3.416425     3.905435      21.52
 O       1.428758     3.891916     4.898805     167.45
 H       1.144979     4.777488     5.100501      24.07
 C      -0.206121     4.226851     3.114399      65.45
 H      -0.066846     5.503332     3.149856      20.24
 C      -1.362614     2.255659     2.186432      -6.95
 C      -2.660429     1.688537     1.244180      82.86
 H      -3.519308     2.394874     1.305626      27.15
 O      -2.968525     0.328184     1.793058     246.19
 H      -3.848500    -0.007900     1.750512      24.50
 C      -2.420697     1.802505    -0.293470     106.79
 H      -1.883102     2.599279    -0.628309      29.59
 C      -3.805217     2.004281    -0.947205     106.60
 O      -4.658737     0.807225    -0.589857     271.20
 H      -4.145658     0.032349    -0.998224      27.19
 H      -3.587590     2.140929    -1.938694      30.41
 H      -4.242128     2.684007    -0.377073      31.24
 C       1.891588     1.229848    -1.237018       6.86
 H       2.423169     2.380027    -1.286743      26.77
 C       1.366927    -1.173863    -1.338763      74.24
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 H       1.655019    -2.255266    -1.577350      27.01
 C      -0.031509    -0.935174    -1.177494      -2.10
 O      -1.009781    -1.874313    -1.042916     191.60
 C      -0.581219    -3.167329    -0.548308     102.36
 H       0.202822    -3.073076     0.434569      25.94
 H      -1.740975    -3.697405    -0.535752      23.81
 H      -0.243286    -3.789468    -1.308317      28.76
 C      -0.518145     0.477797    -1.131445       4.41
 O      -1.938111     0.605759    -0.863463     184.50
 C       0.456434     1.476433    -1.196012      47.33
 H       0.048918     2.561454    -1.240369      27.77
 C       2.275115    -0.153909    -1.343878       2.66
 C       3.945810    -0.390121    -1.405641      76.79
 H       4.106852    -1.230658    -2.470305      27.10
 O       4.491910     1.009938    -1.439343     100.68
 H       5.532434     0.978475    -1.064685      21.25
 C       4.446918    -1.247510    -0.268736     102.17
 H       4.196502    -2.296900    -0.463954      29.53
 O       5.946221    -1.303284    -0.444738     226.05
 H       6.124724    -2.252238    -0.550481      27.03
 C       4.091449    -0.929871     1.269303     116.20
 O       4.921909     0.209926     1.657610     168.41
 H       4.319998     1.048796     1.452495      29.52
 H       4.368482    -1.788745     1.783387      31.00
 H       2.899929    -0.829726     1.475190      28.61
55
name = lig-Water-frame_986
 C      -1.211261     3.640705     2.163092      56.50
 H      -1.755672     4.426313     1.685394      22.96
 C      -0.553540     1.353984     2.838762      56.96
 H      -0.259115     0.302993     2.401631      27.97
 C       0.441833     1.937654     3.645430     -12.11
 O       1.589956     1.269327     4.200397     126.33
 C       1.157140     0.007064     4.815525     112.35
 H       1.782630    -0.076836     5.638313      27.22
 H       0.836425    -0.832650     4.100005      23.73
 H       0.029749     0.051216     5.106731      27.01
 C       0.590039     3.343949     3.905393      -1.63
 O       1.391961     3.855204     4.845823      31.87
 H       1.285040     4.917044     5.234534      18.55
 C      -0.220214     4.265103     3.109887      39.82
 H      -0.073303     5.195212     3.317889      20.92
 C      -1.415691     2.222433     2.226891      20.53
 C      -2.651116     1.727499     1.301184      65.63
 H      -3.531317     2.489920     1.567272      26.63
 O      -2.930129     0.276284     1.773761     166.71
 H      -3.978763     0.047960     1.777301      21.57
 C      -2.423502     1.769844    -0.366884     101.62
 H      -1.863140     2.804221    -0.703909      26.16
 C      -3.752605     2.038985    -0.922332      70.20
 O      -4.693575     0.819216    -0.567439     213.86
 H      -4.248357    -0.009212    -0.717999      30.30
 H      -3.635724     1.898136    -2.130549      25.38
 H      -4.479951     2.770259    -0.271755      24.14
 C       1.829325     1.272785    -1.199051      63.08
 H       2.419498     2.059870    -1.185319      31.40
 C       1.282893    -1.201896    -1.336860      69.87
 H       1.593988    -2.147870    -1.639125      26.48
 C      -0.063726    -0.861736    -1.191816      26.44
 O      -0.959438    -1.831704    -1.077243     198.38
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 C      -0.602168    -3.182328    -0.465017     105.71
 H      -0.165302    -2.989269     0.448495      29.52
 H      -1.412506    -3.761102    -0.364482      29.93
 H      -0.209538    -3.756355    -1.437138      25.22
 C      -0.462439     0.491602    -1.151047       7.72
 O      -1.988103     0.635453    -0.828621     167.75
 C       0.486587     1.455963    -1.221215      88.99
 H      -0.055037     2.388239    -1.151620      30.39
 C       2.335825    -0.090797    -1.356783     -21.71
 C       3.896795    -0.440997    -1.452362      90.52
 H       4.122257    -0.913322    -2.237797      33.22
 O       4.543100     1.050128    -1.420436     165.61
 H       5.341684     1.114190    -0.989275      28.05
 C       4.365075    -1.294323    -0.186021      99.45
 H       4.008806    -2.389382    -0.235949      28.38
 O       5.935507    -1.318334    -0.445209     179.90
 H       6.271681    -2.244597    -0.515130      26.50
 C       4.036698    -0.967172     1.220957     110.74
 O       4.939707     0.221760     1.693919     112.34
 H       4.593865     1.101827     1.406566      33.15
 H       4.460784    -1.832672     1.945842      26.62
 H       3.058601    -1.001703     1.512872      29.41
55
name = lig-Water-frame_987
 C      -1.143425     3.660802     2.180657      66.10
 H      -1.924481     4.425260     1.793837      22.60
 C      -0.521256     1.383934     2.847453      66.93
 H      -0.410127     0.422335     2.537859      29.28
 C       0.438309     1.947060     3.646546       6.66
 O       1.572734     1.240720     4.174583     117.07
 C       1.088126    -0.001034     4.776132     109.59
 H       1.920291    -0.145059     5.549416      25.62
 H       1.116769    -0.790865     3.975058      24.86
 H       0.074188     0.226045     5.204212      27.63
 C       0.601424     3.312087     3.857491      13.69
 O       1.404476     3.820932     4.832784      71.81
 H       1.062033     4.715984     4.982330      26.05
 C      -0.255451     4.193339     3.081680      47.78
 H      -0.113963     5.425415     3.400593      21.76
 C      -1.533196     2.230037     2.179062      10.34
 C      -2.614405     1.739297     1.391331      84.62
 H      -3.442720     2.336248     1.739509      27.71
 O      -2.895958     0.266236     1.737184     194.73
 H      -3.884345     0.189865     1.750688      24.76
 C      -2.448148     1.856459    -0.348069      89.59
 H      -1.825001     2.653994    -0.523832      27.10
 C      -3.796579     1.998874    -0.917689     113.53
 O      -4.731075     0.854062    -0.545051     236.91
 H      -4.235671    -0.034470    -0.592135      27.57
 H      -3.890920     2.048902    -1.936156      29.17
 H      -4.281039     2.921948    -0.718093      28.18
 C       1.814681     1.237407    -1.182769      23.84
 H       2.728945     2.054621    -1.115198      25.35
 C       1.281389    -1.145450    -1.354929      74.82
 H       1.566015    -2.258152    -1.604903      24.16
 C      -0.060191    -0.804629    -1.202019      28.60
 O      -0.968992    -1.829324    -1.099847     196.00
 C      -0.633093    -3.173312    -0.478182      88.36
 H      -0.181953    -2.937204     0.644300      25.98
 H      -1.642439    -3.829566    -0.074179      23.87
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 H       0.197568    -3.611759    -1.058305      25.26
 C      -0.486992     0.455568    -1.143480      26.20
 O      -1.937613     0.597993    -0.848635     144.51
 C       0.445395     1.483497    -1.234950      67.04
 H       0.048669     2.607912    -1.006030      25.91
 C       2.361325    -0.047345    -1.363388      22.52
 C       3.804855    -0.401485    -1.398515      58.09
 H       4.346497    -0.825434    -2.580669      24.08
 O       4.560369     1.047304    -1.419387      98.16
 H       5.470963     1.099688    -0.835746      23.66
 C       4.341871    -1.367984    -0.167309      88.46
 H       3.754255    -2.356344    -0.234170      28.06
 O       5.893204    -1.332406    -0.437413     147.96
 H       6.277896    -2.313934    -0.379153      23.89
 C       4.066232    -0.984480     1.225981     105.58
 O       4.928702     0.214203     1.713696      90.08
 H       4.633402     1.141609     1.431310      32.32
 H       4.560606    -1.693135     1.871240      28.03
 H       2.889235    -0.882336     1.505535      27.02
55
name = lig-Water-frame_988
 C      -1.169153     3.667303     2.205275      68.47
 H      -1.915594     4.253873     1.806177      21.50
 C      -0.531008     1.437741     2.815024      24.65
 H      -0.678165     0.249665     2.729268      23.78
 C       0.508602     1.963316     3.651472      -3.43
 O       1.522605     1.210012     4.144542     160.34
 C       1.055277    -0.010890     4.744568     125.83
 H       1.804599    -0.428356     5.445144      28.96
 H       1.348359    -0.812488     3.968885      25.98
 H       0.153328     0.192508     5.323250      28.19
 C       0.557565     3.328895     3.784147      29.93
 O       1.433716     3.777439     4.824435      47.91
 H       0.969145     4.732456     4.949895      19.27
 C      -0.238908     4.145701     3.101080      84.50
 H      -0.293974     5.134880     3.130226      27.84
 C      -1.517351     2.282420     2.163444      -3.84
 C      -2.614448     1.687850     1.430743      87.34
 H      -3.663552     2.225612     1.740488      24.61
 O      -2.847062     0.303065     1.692394     226.10
 H      -3.803925     0.133067     1.697960      25.83
 C      -2.476736     1.918001    -0.256881      41.70
 H      -1.669835     2.745467    -0.431658      22.54
 C      -3.897009     1.936876    -0.935002     102.88
 O      -4.767573     0.906950    -0.510888     269.20
 H      -4.168423     0.120087    -0.628222      27.88
 H      -3.900548     2.090971    -2.141266      24.96
 H      -4.158899     3.055860    -0.811696      24.91
 C       1.864291     1.213964    -1.188797      29.03
 H       2.599808     1.993094    -1.081755      27.98
 C       1.366441    -1.058741    -1.395078      71.55
 H       1.528102    -2.070011    -1.436709      24.71
 C      -0.016257    -0.857954    -1.210604      16.19
 O      -1.023141    -1.863493    -1.117138     215.80
 C      -0.649168    -3.126576    -0.441142     116.48
 H      -0.255884    -2.815646     0.542440      28.48
 H      -1.577775    -3.638316    -0.331466      26.90
 H       0.313255    -3.654059    -0.707506      26.37
 C      -0.581661     0.490777    -1.113239      18.37
 O      -1.844003     0.557225    -0.885188     111.93
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 C       0.384121     1.570727    -1.213150      55.19
 H       0.273657     2.557522    -1.014222      26.47
 C       2.299921    -0.070520    -1.363089      52.57
 C       3.796258    -0.332888    -1.363653      91.33
 H       4.094002    -0.666910    -2.182237      32.89
 O       4.569917     1.019944    -1.405117     184.77
 H       5.423224     0.914443    -0.868649      26.09
 C       4.347208    -1.408736    -0.233064      94.34
 H       3.794271    -2.354310    -0.422496      28.03
 O       5.819768    -1.375383    -0.420114     243.21
 H       6.076129    -2.267405    -0.279126      30.00
 C       4.108808    -0.939568     1.281022     114.16
 O       4.899044     0.195211     1.711857     155.23
 H       4.394984     1.069127     1.484976      30.19
 H       4.556521    -1.812488     1.904451      26.86
 H       3.113083    -0.731174     1.379384      29.34
55
name = lig-Water-frame_989
 C      -1.268374     3.635306     2.220329      64.07
 H      -1.947967     4.395472     1.666671      23.09
 C      -0.556838     1.456655     2.785327      64.00
 H      -0.843347     0.485784     2.937160      26.20
 C       0.538009     1.951816     3.585022      -2.05
 O       1.486237     1.180036     4.138776     200.42
 C       1.082012    -0.065585     4.710816     129.65
 H       1.763067    -0.383151     5.508970      28.05
 H       0.972122    -0.853095     3.966920      27.45
 H       0.035071    -0.095893     5.294904      27.12
 C       0.588268     3.335529     3.793269      30.86
 O       1.442650     3.758034     4.796910     213.46
 H       1.292825     4.709673     5.256631      25.35
 C      -0.259550     4.144196     3.073521      62.72
 H      -0.264429     5.355434     3.062264      21.39
 C      -1.399859     2.318785     2.187168      34.47
 C      -2.692780     1.645672     1.397967     101.86
 H      -3.595984     2.153384     1.585895      27.46
 O      -2.782560     0.337585     1.657282     232.98
 H      -3.764966    -0.091440     1.641031      22.30
 C      -2.501293     1.919404    -0.159346      43.61
 H      -1.859221     2.755148    -0.445862      24.98
 C      -3.959334     1.948021    -1.004723      90.48
 O      -4.798051     0.960365    -0.468628     279.87
 H      -4.295873     0.176630    -0.726570      29.84
 H      -3.670457     1.775107    -2.013366      28.43
 H      -4.313239     2.952580    -0.559000      26.02
 C       1.819697     1.235222    -1.208760      36.23
 H       2.533615     2.132634    -1.093251      27.07
 C       1.379015    -1.044181    -1.430254      60.69
 H       1.781419    -2.136947    -1.340033      22.77
 C       0.006219    -0.894723    -1.223910      12.84
 O      -1.054559    -1.903989    -1.145074     205.51
 C      -0.639119    -3.031988    -0.394549      97.47
 H      -0.403486    -2.619442     0.750065      24.87
 H      -1.637939    -3.734099    -0.599741      24.32
 H       0.142778    -3.800564    -0.774344      25.32
 C      -0.551340     0.537180    -1.093733      13.01
 O      -1.833378     0.557562    -0.896193     108.94
 C       0.395823     1.594297    -1.172281      52.13
 H       0.263113     2.822386    -1.012204      24.01
 C       2.289159    -0.061185    -1.345675      49.78
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 C       3.814331    -0.245987    -1.276790      76.29
 H       4.018015    -0.953663    -2.498576      25.92
 O       4.561283     0.967986    -1.377619     197.81
 H       5.382293     0.828250    -0.910076      27.73
 C       4.357123    -1.356550    -0.300180     106.32
 H       3.979493    -2.425891    -0.631432      25.80
 O       5.735392    -1.433323    -0.410090     225.22
 H       6.006771    -2.417044    -0.243638      26.68
 C       4.176744    -0.924145     1.310456     122.08
 O       4.862119     0.187260     1.695537     189.98
 H       4.285095     0.953883     1.555143      30.08
 H       4.253822    -1.880884     1.931917      27.18
 H       3.023710    -0.658166     1.422352      27.05
55
name = lig-Water-frame_990
 C      -1.357500     3.690459     2.239896      66.36
 H      -1.885500     4.370864     1.636389      27.39
 C      -0.528997     1.458024     2.814531      84.82
 H      -0.870780     0.411109     2.937076      27.68
 C       0.521410     1.945546     3.478813      34.94
 O       1.471798     1.137285     4.160560     137.77
 C       1.077688    -0.165079     4.693087     127.11
 H       1.885067    -0.242553     5.490134      24.99
 H       0.637389    -0.903770     3.922322      23.77
 H       0.087568    -0.137168     5.118032      27.62
 C       0.636810     3.347321     3.829905      10.16
 O       1.481132     3.750890     4.792215     141.85
 H       1.331388     4.592210     5.176927      26.58
 C      -0.316262     4.227225     3.011835      46.69
 H      -0.024767     5.261936     3.206873      22.26
 C      -1.392012     2.281069     2.147130      29.07
 C      -2.717448     1.674185     1.326888      98.40
 H      -3.712061     2.344257     1.631235      25.12
 O      -2.730359     0.301215     1.647425     288.90
 H      -3.568862    -0.121177     1.599882      27.11
 C      -2.556636     1.861450    -0.129265      74.99
 H      -2.017482     2.790274    -0.436856      26.52
 C      -3.941472     1.987356    -0.998055      86.18
 O      -4.833008     0.987299    -0.429726     238.91
 H      -4.607536     0.051066    -0.824911      27.42
 H      -3.577905     1.645749    -2.060135      25.68
 H      -4.526580     2.780177    -0.704751      27.43
 C       1.737686     1.306157    -1.229662      79.31
 H       2.475431     2.218030    -1.178343      27.98
 C       1.344453    -1.156659    -1.442475      51.05
 H       1.924589    -2.033849    -1.396429      22.74
 C      -0.019747    -0.863067    -1.244577       6.86
 O      -1.035288    -1.908371    -1.194339     223.83
 C      -0.673434    -2.980099    -0.333945     129.81
 H      -0.705697    -2.734558     0.745029      28.73
 H      -1.422257    -3.741708    -0.548492      27.59
 H       0.081583    -3.565290    -0.863300      26.29
 C      -0.423105     0.529212    -1.088194       5.43
 O      -1.896492     0.606777    -0.877201      68.20
 C       0.446670     1.623556    -1.118375      81.38
 H       0.084386     2.535634    -1.072862      28.75
 C       2.339106     0.030872    -1.307423       4.01
 C       3.834673    -0.251271    -1.300136     128.35
 H       3.903194    -0.766823    -2.101590      32.05
 O       4.543181     0.916783    -1.344405     222.41
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 H       5.514503     0.869719    -0.835924      22.54
 C       4.341590    -1.279425    -0.310991     127.65
 H       3.921805    -2.204903    -0.600956      30.50
 O       5.712347    -1.503513    -0.420676     243.77
 H       5.981722    -2.472334    -0.302721      26.11
 C       4.115633    -0.971480     1.278797     130.29
 O       4.860897     0.191091     1.689838     172.50
 H       4.292341     1.068623     1.567508      26.74
 H       4.218976    -1.831694     1.978899      28.65
 H       3.102603    -0.762602     1.467663      29.15
55
name = lig-Water-frame_991
 C      -1.391215     3.747149     2.263069      60.04
 H      -2.039554     4.372267     1.600272      27.47
 C      -0.542654     1.419870     2.824793      41.65
 H      -0.611968     0.280618     2.703042      31.33
 C       0.571610     1.976847     3.455865      29.16
 O       1.460802     1.096038     4.176819     101.52
 C       1.036088    -0.252026     4.667127     121.08
 H       1.865069    -0.492304     5.271399      29.68
 H       0.938121    -0.999849     3.887459      26.45
 H       0.072770     0.082808     5.305928      25.59
 C       0.602438     3.361838     3.781454      10.42
 O       1.549917     3.735274     4.796213      38.76
 H       1.111670     4.787836     5.038539      17.05
 C      -0.301051     4.283177     3.021165      53.38
 H      -0.019402     5.362220     3.217789      20.72
 C      -1.493001     2.259065     2.059642      -7.78
 C      -2.704499     1.731424     1.311287     107.33
 H      -3.521925     2.234568     1.680104      29.42
 O      -2.675497     0.247908     1.655678     226.95
 H      -3.669625    -0.113024     1.560408      22.27
 C      -2.615070     1.802188    -0.216600      94.15
 H      -2.054199     2.806019    -0.343277      28.35
 C      -3.880189     1.960142    -0.944814     100.87
 O      -4.877939     0.975365    -0.404578     234.39
 H      -4.840385     0.122669    -0.863169      29.64
 H      -3.729642     1.835881    -2.043239      27.02
 H      -4.618595     2.947290    -1.136748      23.85
 C       1.782832     1.389996    -1.251171     105.20
 H       2.425550     2.233855    -1.280972      30.94
 C       1.367117    -1.181610    -1.425310      34.79
 H       1.811748    -2.229530    -1.522558      22.88
 C      -0.044985    -0.842443    -1.268440      16.86
 O      -1.002565    -1.860589    -1.251485     209.71
 C      -0.728112    -2.977070    -0.314641      89.87
 H      -0.747880    -2.786426     0.873718      28.17
 H      -1.578757    -3.827904    -0.404122      25.42
 H       0.419096    -3.210821    -0.626275      23.82
 C      -0.383608     0.488305    -1.068290      10.80
 O      -1.936904     0.686184    -0.848066      62.07
 C       0.425311     1.607552    -1.067279      60.97
 H      -0.199561     2.652006    -1.089141      28.43
 C       2.306197     0.081257    -1.266367      -2.07
 C       3.819654    -0.271299    -1.308167      82.34
 H       4.033593    -0.914068    -2.520604      26.07
 O       4.573094     0.918076    -1.309998     206.16
 H       5.339290     0.934713    -0.778246      27.88
 C       4.304995    -1.234310    -0.231720     102.98
 H       3.513235    -2.135099    -0.456072      27.99
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 O       5.747044    -1.565690    -0.457335     228.83
 H       5.901279    -2.497278    -0.342012      26.63
 C       4.004555    -1.015799     1.213743     107.43
 O       4.869566     0.195474     1.694895     129.56
 H       4.491814     1.081148     1.498762      31.69
 H       4.512929    -1.813309     1.924030      25.79
 H       2.882951    -0.832075     1.436718      28.49
55
name = lig-Water-frame_992
 C      -1.387866     3.746711     2.267255      40.15
 H      -2.177516     4.398268     1.789079      27.01
 C      -0.587951     1.396308     2.758839       9.49
 H      -0.392702     0.386353     2.512862      38.12
 C       0.611272     1.976628     3.487484       9.31
 O       1.462819     1.071955     4.177773      74.32
 C       0.971043    -0.279211     4.648361     127.07
 H       1.870994    -0.780285     5.185601      28.54
 H       1.121083    -1.061854     3.812167      27.52
 H       0.234276    -0.127241     5.330206      30.17
 C       0.567829     3.381654     3.711222      28.51
 O       1.574546     3.770345     4.775969     131.52
 H       1.333994     4.587009     5.073802      27.67
 C      -0.253935     4.298957     3.072361      83.03
 H      -0.262635     5.469090     3.088029      22.04
 C      -1.552749     2.293027     2.033263      -4.85
 C      -2.650329     1.703603     1.318810      93.05
 H      -3.701819     2.170901     1.798816      25.83
 O      -2.649442     0.208579     1.662667     202.94
 H      -3.643415    -0.001978     1.626803      22.97
 C      -2.611173     1.802300    -0.311029      97.08
 H      -2.052324     2.738504    -0.424517      30.57
 C      -3.926616     1.927871    -0.940642     114.25
 O      -4.922059     0.969446    -0.388075     244.54
 H      -4.834540     0.186386    -0.951529      29.19
 H      -3.757871     1.772318    -2.061954      27.57
 H      -4.175295     2.891329    -1.079847      29.65
 C       1.856201     1.446657    -1.255244      -2.77
 H       2.604978     2.429541    -1.431748      29.95
 C       1.405049    -1.095961    -1.383816      65.76
 H       1.519609    -2.150641    -1.664289      27.25
 C      -0.012476    -0.876940    -1.286788      14.88
 O      -0.990409    -1.808236    -1.294756     190.89
 C      -0.744977    -2.977647    -0.297499      96.88
 H      -0.774965    -2.553379     0.760834      31.13
 H      -1.505000    -3.799686    -0.504495      27.13
 H       0.229837    -3.184753    -0.228120      31.56
 C      -0.467346     0.482369    -1.019948      12.18
 O      -1.933167     0.742661    -0.835886     107.14
 C       0.354490     1.606602    -1.036439      28.44
 H      -0.079445     2.540428    -1.038315      30.69
 C       2.245362     0.038735    -1.253666      -1.70
 C       3.809408    -0.300125    -1.369810     107.55
 H       4.056221    -0.734255    -2.249750      32.64
 O       4.602903     0.954840    -1.294877     151.68
 H       5.374930     0.926342    -0.564245      23.46
 C       4.242196    -1.272565    -0.178270     112.39
 H       3.562706    -2.051112    -0.279350      33.51
 O       5.760753    -1.609353    -0.501490     180.35
 H       5.863119    -2.639957    -0.313413      24.29
 C       3.937813    -0.995988     1.197616     116.35
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 O       4.869514     0.171393     1.706081     119.72
 H       4.553429     1.097752     1.398047      31.70
 H       4.468720    -1.769643     1.643591      31.72
 H       2.857029    -0.972034     1.395409      32.08
55
name = lig-Water-frame_993
 C      -1.360282     3.712663     2.278578      61.21
 H      -2.131509     4.427025     2.062052      26.41
 C      -0.575941     1.455891     2.672945       3.85
 H      -0.399069     0.350875     2.284818      43.14
 C       0.541443     1.923550     3.499681     -53.53
 O       1.469078     1.061704     4.178060      56.98
 C       0.986474    -0.303735     4.599098     132.65
 H       1.820166    -0.575142     5.180314      29.32
 H       0.740943    -0.915844     3.732695      26.52
 H       0.009036    -0.492081     5.343067      27.22
 C       0.619577     3.402013     3.713300      -8.19
 O       1.579146     3.786494     4.711529      24.93
 H       1.460709     4.805439     5.271828      14.83
 C      -0.287136     4.296620     3.072513      98.89
 H      -0.320642     5.327252     3.131044      30.22
 C      -1.510062     2.355930     2.095367      29.53
 C      -2.662308     1.618906     1.324886     103.66
 H      -3.549924     1.973222     1.608020      35.54
 O      -2.637205     0.203131     1.658587     210.03
 H      -3.601571    -0.080849     1.745123      23.12
 C      -2.559992     1.848147    -0.327266      77.61
 H      -2.019023     2.836605    -0.676695      28.68
 C      -4.005984     1.873869    -0.988938      91.12
 O      -4.952385     0.984268    -0.385539     201.99
 H      -4.780623     0.179086    -1.009057      28.10
 H      -3.798054     1.468197    -2.036168      26.81
 H      -4.087530     3.099819    -0.682608      24.37
 C       1.852920     1.462033    -1.239820      94.62
 H       2.511470     2.175236    -1.427305      39.49
 C       1.366050    -0.989541    -1.344685      82.15
 H       1.645350    -1.977164    -1.714235      30.47
 C       0.019392    -0.853693    -1.274429      18.95
 O      -0.983630    -1.804579    -1.321722     205.11
 C      -0.780094    -2.918465    -0.292285      81.53
 H      -1.065827    -2.288712     0.725525      30.73
 H      -1.422898    -3.768274    -0.652574      28.37
 H       0.316243    -3.489682    -0.174820      27.89
 C      -0.588437     0.508666    -0.962492      11.80
 O      -1.888210     0.722743    -0.861565     129.80
 C       0.373912     1.589040    -1.034854      42.18
 H      -0.016378     2.699802    -0.932959      32.75
 C       2.265862     0.023688    -1.278751      19.08
 C       3.791191    -0.284081    -1.344723      85.99
 H       4.177474    -0.857389    -2.508073      26.96
 O       4.631418     0.995280    -1.281853     180.32
 H       5.341289     0.857408    -0.519887      23.80
 C       4.205957    -1.318139    -0.236557      90.24
 H       3.671671    -2.416204    -0.350471      29.08
 O       5.723654    -1.653301    -0.531886     170.76
 H       5.957606    -2.571430    -0.301740      26.89
 C       3.947822    -0.912450     1.230312     121.79
 O       4.842118     0.128857     1.718131     170.66
 H       4.479514     1.022074     1.410645      32.85
 H       4.302645    -1.995869     1.716646      29.12
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 H       2.856968    -0.947830     1.470718      33.27
55
name = lig-Water-frame_994
 C      -1.328179     3.715180     2.313638      82.45
 H      -2.183625     4.477717     2.168178      20.92
 C      -0.479792     1.512305     2.594086     109.58
 H      -0.650573     0.571278     2.248295      32.51
 C       0.433204     1.899749     3.506209     -56.26
 O       1.441749     1.062497     4.173077     114.94
 C       0.978521    -0.319817     4.556296     115.40
 H       1.906565    -0.551356     5.146837      26.37
 H       0.516773    -0.796480     3.629834      28.90
 H       0.112511    -0.422969     5.075164      30.60
 C       0.688247     3.401658     3.754345       0.03
 O       1.586175     3.822388     4.650431      96.79
 H       1.358908     4.696634     4.987156      21.65
 C      -0.333017     4.234108     3.057018      34.65
 H      -0.232963     5.427745     3.341118      21.96
 C      -1.467493     2.359893     2.154531      38.78
 C      -2.640453     1.550032     1.305448      89.49
 H      -3.784556     2.025487     1.518398      26.64
 O      -2.627140     0.207821     1.642237     215.24
 H      -3.582029    -0.239253     1.844738      21.46
 C      -2.515862     1.888242    -0.314225      71.09
 H      -2.073020     2.761468    -0.707078      26.81
 C      -4.026193     1.866607    -1.008153     102.96
 O      -4.970407     0.996270    -0.398917     243.86
 H      -4.907658     0.127766    -0.808000      30.31
 H      -3.960188     1.580390    -2.061220      27.22
 H      -4.462364     2.729798    -0.697027      28.89
 C       1.757941     1.357787    -1.201124      70.17
 H       2.615832     2.280109    -1.407035      27.64
 C       1.321860    -0.943206    -1.333062      50.11
 H       1.931754    -1.850134    -1.611924      25.79
 C      -0.054812    -0.739773    -1.219743      34.22
 O      -0.951893    -1.843440    -1.344632     237.85
 C      -0.804562    -2.840710    -0.285800     115.70
 H      -1.407405    -2.419800     0.559635      30.48
 H      -1.537173    -3.673444    -0.735699      28.43
 H       0.040520    -3.341081    -0.351497      32.31
 C      -0.571016     0.542000    -0.934053      12.94
 O      -1.877507     0.662533    -0.904567     149.14
 C       0.425875     1.599784    -1.042821      75.15
 H       0.129631     2.631253    -0.823181      31.32
 C       2.349320     0.114320    -1.317925      19.51
 C       3.803147    -0.279774    -1.349765     113.69
 H       4.029216    -0.712870    -2.268767      32.11
 O       4.637885     1.007944    -1.259428     213.59
 H       5.369825     0.885460    -0.699863      26.52
 C       4.201822    -1.402931    -0.333431     107.60
 H       3.807745    -2.297708    -0.517009      31.02
 O       5.655613    -1.669206    -0.555617     237.00
 H       5.995942    -2.541202    -0.277089      28.65
 C       3.996550    -0.908351     1.273861     129.04
 O       4.797099     0.086457     1.731665     210.48
 H       4.402221     0.947608     1.553045      32.78
 H       4.097983    -1.725914     1.875649      32.80
 H       2.908330    -0.623012     1.534874      32.43
55
name = lig-Water-frame_995
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 C      -1.374180     3.755128     2.341879      63.05
 H      -2.165269     4.361081     2.056210      22.19
 C      -0.392750     1.538694     2.517495      37.01
 H      -0.752146     0.426101     2.315872      26.42
 C       0.436891     1.946967     3.573334     -21.00
 O       1.373573     1.076424     4.156094     120.90
 C       0.977833    -0.303705     4.479680     104.96
 H       1.847658    -0.889197     4.893618      27.48
 H       0.808385    -0.854349     3.545340      29.36
 H       0.037613    -0.083843     5.247924      25.11
 C       0.657438     3.341132     3.737193      13.17
 O       1.616032     3.850039     4.594070      88.31
 H       1.217555     4.933112     4.860759      16.05
 C      -0.270005     4.203762     3.127214      60.52
 H      -0.240840     5.163594     3.349085      26.19
 C      -1.486379     2.324926     2.148288      -1.33
 C      -2.642378     1.591907     1.282945     102.53
 H      -3.515173     1.976617     1.509306      30.43
 O      -2.616632     0.184314     1.625728     251.22
 H      -3.540189    -0.131087     1.746282      23.68
 C      -2.533063     1.840707    -0.305756      67.46
 H      -1.949106     2.859437    -0.595596      23.53
 C      -4.008357     1.852820    -0.996337      96.00
 O      -4.991950     0.983064    -0.403138     246.11
 H      -4.963694     0.030165    -0.617163      28.79
 H      -4.060365     1.969272    -2.193215      23.96
 H      -4.784009     2.813735    -0.928250      23.28
 C       1.755646     1.316518    -1.176592      71.67
 H       2.236407     2.150492    -1.195954      31.00
 C       1.357327    -0.894724    -1.340673      34.26
 H       1.733974    -1.902280    -1.414810      25.35
 C      -0.121242    -0.675080    -1.160318      10.50
 O      -0.906445    -1.860183    -1.373943     209.20
 C      -0.916690    -2.781834    -0.337303     107.83
 H      -1.406665    -2.540018     0.741616      27.02
 H      -1.621726    -3.534398    -0.681331      26.81
 H       0.274201    -3.211644    -0.252953      24.55
 C      -0.463383     0.595773    -0.939169      20.33
 O      -1.918583     0.623543    -0.942435     129.46
 C       0.422367     1.618047    -1.027952      89.37
 H       0.186389     2.655166    -0.794052      29.57
 C       2.366187     0.153849    -1.342375      39.69
 C       3.835725    -0.243888    -1.329120      86.73
 H       3.990706    -0.707522    -2.578503      25.97
 O       4.614667     0.997079    -1.241940     155.51
 H       5.641214     0.913501    -0.816779      20.04
 C       4.246911    -1.441004    -0.369710      83.74
 H       3.507095    -2.403554    -0.701470      24.61
 O       5.588880    -1.658404    -0.586320     224.39
 H       5.897982    -2.604011    -0.254697      26.81
 C       3.973679    -0.952253     1.266694     100.60
 O       4.794961     0.079566     1.759243     181.67
 H       4.330824     0.998059     1.672859      29.52
 H       4.052787    -1.787420     2.176125      26.14
 H       3.002497    -0.430325     1.340008      29.46
55
name = lig-Water-frame_996
 C      -1.425386     3.746178     2.381627      51.16
 H      -2.218404     4.453009     1.871356      19.98
 C      -0.373708     1.509630     2.472636      15.05
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 H      -0.378283     0.466045     2.496952      23.98
 C       0.499565     1.967651     3.615859       3.25
 O       1.326865     1.098664     4.143836     146.06
 C       0.951827    -0.269268     4.406165     124.72
 H       1.746476    -0.890480     4.748658      28.09
 H       0.841545    -0.897483     3.484137      27.25
 H       0.278897    -0.160332     5.157907      28.66
 C       0.609065     3.285948     3.728238      38.61
 O       1.641596     3.906388     4.548157     206.19
 H       1.369334     4.797149     4.853763      25.48
 C      -0.235389     4.167832     3.180094      58.10
 H      -0.176820     5.370446     3.397934      19.56
 C      -1.516438     2.316585     2.084648      -6.18
 C      -2.594241     1.658642     1.259864      80.51
 H      -3.675623     2.156040     1.701097      23.13
 O      -2.595678     0.168104     1.603401     209.02
 H      -3.639260    -0.070647     1.605650      21.10
 C      -2.586943     1.772063    -0.323039      91.49
 H      -2.020931     2.623339    -0.409963      25.10
 C      -4.027713     1.897747    -0.997850     103.62
 O      -5.014224     0.955173    -0.401351     267.28
 H      -4.739754    -0.034408    -0.583281      25.16
 H      -3.880923     1.900601    -2.061659      26.96
 H      -4.432288     2.882796    -0.938430      27.01
 C       1.777069     1.380689    -1.150768      -4.51
 H       2.356885     2.493546    -0.999572      26.04
 C       1.370546    -0.867237    -1.343770      62.95
 H       1.402293    -1.997902    -1.286941      21.71
 C      -0.034585    -0.720259    -1.135946       8.61
 O      -0.873500    -1.813435    -1.410884     252.69
 C      -0.995418    -2.769880    -0.353731     114.93
 H      -1.089482    -2.437627     0.718449      25.89
 H      -1.682046    -3.705831    -0.710178      23.67
 H      -0.064255    -3.029521    -0.050986      28.29
 C      -0.491864     0.639141    -0.959745      10.15
 O      -1.947216     0.633390    -0.965194     144.47
 C       0.407377     1.663487    -0.994306      64.29
 H       0.129022     2.794587    -0.821705      24.82
 C       2.345776     0.072281    -1.346018      14.36
 C       3.875448    -0.211870    -1.363499      95.38
 H       4.044418    -0.600535    -2.410047      29.10
 O       4.609167     0.984055    -1.217831     268.69
 H       5.506560     0.876331    -0.931695      25.60
 C       4.232100    -1.453205    -0.358765     102.85
 H       3.539570    -2.115694    -0.610923      31.15
 O       5.563156    -1.665580    -0.622351     288.79
 H       5.741841    -2.552832    -0.362164      31.28
 C       3.911522    -1.022886     1.256788      88.64
 O       4.830001     0.098844     1.794355     226.84
 H       4.362479     0.944021     1.664757      31.21
 H       3.944434    -1.771545     1.906120      27.99
 H       2.868077    -0.575688     1.007213      26.55
55
name = lig-Water-frame_997
 C      -1.451013     3.712864     2.421137      61.49
 H      -2.015436     4.456673     1.961625      25.87
 C      -0.378806     1.505179     2.515126      48.11
 H      -0.136281     0.393908     2.388928      20.09
 C       0.497509     1.919051     3.531816      18.40
 O       1.347949     1.104601     4.160185     207.09
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 C       0.946836    -0.256302     4.312967      96.90
 H       1.954931    -0.625237     4.817903      22.99
 H       0.461432    -0.770407     3.425356      24.04
 H       0.086818    -0.478925     5.171439      24.02
 C       0.632550     3.331335     3.794908       4.27
 O       1.680211     3.913909     4.494320     -24.32
 H       1.300525     5.015910     4.968270      15.72
 C      -0.330698     4.201886     3.159738      62.58
 H      -0.054382     5.174200     3.350606      17.72
 C      -1.482196     2.324704     2.014518      16.06
 C      -2.606728     1.692478     1.264344     100.04
 H      -3.421351     2.122571     1.616818      27.50
 O      -2.587485     0.186775     1.577283     231.19
 H      -3.483263    -0.168208     1.545073      25.04
 C      -2.668600     1.706244    -0.326603      83.47
 H      -2.005342     2.707232    -0.529885      21.66
 C      -4.025183     1.930422    -0.978687      78.25
 O      -5.015126     0.932858    -0.411955     266.51
 H      -4.501265     0.170978    -0.682696      27.89
 H      -3.701818     1.470562    -2.052466      23.63
 H      -4.192265     3.057830    -0.688691      24.77
 C       1.825220     1.512122    -1.116315      45.32
 H       2.538352     2.218683    -1.015144      28.47
 C       1.333949    -0.942492    -1.333781      52.09
 H       1.539518    -2.011525    -1.369091      21.06
 C       0.071086    -0.718471    -1.135796      21.03
 O      -0.857693    -1.743120    -1.445895     207.54
 C      -1.052454    -2.783059    -0.343474      83.89
 H      -1.361994    -2.106407     0.629453      21.75
 H      -1.586419    -3.592059    -0.645956      25.62
 H       0.067364    -3.300360    -0.086908      22.57
 C      -0.603441     0.599714    -0.996801       1.42
 O      -1.948901     0.667545    -0.979576     132.95
 C       0.404726     1.745264    -0.955244      35.48
 H       0.052488     2.707089    -0.881625      23.48
 C       2.342503     0.055182    -1.324893      -0.28
 C       3.870816    -0.209591    -1.375806      74.41
 H       4.273658    -0.722031    -2.479913      25.69
 O       4.598709     0.994082    -1.198340     217.38
 H       5.503794     0.771901    -0.817761      24.89
 C       4.197109    -1.354225    -0.303416      84.21
 H       3.424186    -2.308483    -0.578953      21.56
 O       5.572652    -1.693614    -0.665281     235.87
 H       5.798076    -2.659622    -0.484229      28.53
 C       3.855709    -1.025536     1.166626      61.88
 O       4.848321     0.082482     1.820158     186.15
 H       4.390607     0.945522     1.581538      27.95
 H       3.849357    -2.068251     1.832710      22.83
 H       2.812310    -0.825605     1.070850      25.66
55
name = lig-Water-frame_998
 C      -1.445587     3.663554     2.442088      70.91
 H      -2.095904     4.507301     2.007167      27.32
 C      -0.411944     1.487044     2.570854      66.48
 H      -0.297399     0.556384     1.976523      23.34
 C       0.491238     1.943325     3.432250       9.59
 O       1.386859     1.100167     4.186422     190.70
 C       0.943140    -0.284360     4.284409     121.47
 H       1.862558    -0.617808     4.585434      26.94
 H       0.448116    -0.637489     3.393075      26.94
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 H       0.172061    -0.529359     4.931403      28.77
 C       0.624707     3.403130     3.832854      -7.03
 O       1.707088     3.952036     4.471937      80.17
 H       1.340091     4.711084     4.810439      26.76
 C      -0.409452     4.196791     3.152710      81.74
 H      -0.149968     5.344757     3.234572      20.58
 C      -1.389627     2.329993     1.975009      12.87
 C      -2.612751     1.644003     1.246300      85.54
 H      -3.666351     2.229210     1.635658      23.24
 O      -2.564900     0.234045     1.558482     236.91
 H      -3.504806    -0.241444     1.536760      23.14
 C      -2.679035     1.737263    -0.305617     103.34
 H      -2.277778     2.594041    -0.714827      26.81
 C      -3.999732     1.902489    -0.956332     100.84
 O      -4.991561     0.943200    -0.434955     286.67
 H      -4.514833     0.124973    -0.794550      26.61
 H      -3.908671     1.614611    -1.922278      28.73
 H      -4.217751     3.003244    -0.692358      26.94
 C       1.841986     1.528875    -1.092638      40.48
 H       2.809633     2.262267    -1.115504      24.69
 C       1.412152    -1.035125    -1.327502      24.43
 H       1.845013    -2.023767    -1.561684      20.47
 C       0.009294    -0.657658    -1.148626      16.36
 O      -0.858270    -1.707261    -1.468573     183.76
 C      -1.013734    -2.745949    -0.297554      92.70
 H      -1.736504    -2.124717     0.244109      21.57
 H      -1.855580    -3.565484    -0.742431      24.18
 H      -0.192889    -3.351438    -0.215274      25.75
 C      -0.594946     0.575744    -1.028898      14.64
 O      -1.958512     0.679613    -0.999348     150.27
 C       0.396189     1.761583    -0.929897      -0.78
 H      -0.094660     2.869980    -0.887957      21.86
 C       2.320380     0.132801    -1.292115      -9.72
 C       3.835103    -0.251322    -1.384784      91.74
 H       4.252649    -0.756174    -2.369090      26.03
 O       4.600738     1.019238    -1.179924     174.40
 H       5.466412     0.729913    -0.590182      23.31
 C       4.156563    -1.275556    -0.287629     115.50
 H       3.679795    -2.140598    -0.455891      27.84
 O       5.588792    -1.726294    -0.697943     210.06
 H       5.856520    -2.718842    -0.576217      27.19
 C       3.844147    -1.032114     1.098364      91.58
 O       4.819580     0.027398     1.822707     155.63
 H       4.440500     0.935668     1.543057      29.58
 H       4.041233    -1.883670     1.630917      26.71
 H       2.719679    -0.787670     1.398046      24.87
55
name = lig-Water-frame_999
 C      -1.459385     3.637236     2.408935      44.84
 H      -2.288513     4.258597     2.071258      30.99
 C      -0.479209     1.456408     2.544659      19.56
 H      -0.465917     0.602845     1.901365      30.18
 C       0.567747     2.032336     3.440522      -2.15
 O       1.402586     1.117221     4.193152      92.26
 C       0.953184    -0.309674     4.246885     101.70
 H       1.887024    -1.112975     4.354950      24.74
 H       0.725626    -0.615924     3.146023      25.92
 H       0.117874    -0.397233     5.099997      25.60
 C       0.556432     3.424775     3.781815      23.18
 O       1.736912     3.943848     4.441828     -43.12
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H	1.330582	5.040326	4.943114	16.01
C	-0.392812	4.220130	3.207474	72.81
H	-0.562078	5.310610	3.089314	19.75
C	-1.343526	2.330546	1.958688	-12.98
C	-2.636463	1.614594	1.233650	102.39
H	-3.481132	2.046610	1.560775	30.57
O	-2.550730	0.271283	1.552454	233.81
H	-3.487780	-0.087107	1.549588	24.66
C	-2.633355	1.798852	-0.298316	84.44
H	-2.236367	2.834170	-0.763299	27.35
C	-4.012406	1.848165	-0.909896	101.64
O	-4.956986	0.954137	-0.462702	232.21
H	-4.859559	0.006246	-0.830060	25.70
H	-4.070248	2.034666	-2.182672	24.86
H	-4.475819	2.856327	-0.807402	27.54
C	1.833017	1.486013	-1.076180	72.41
H	2.523555	2.316199	-1.263912	25.72
C	1.503550	-1.008063	-1.313561	31.67
H	1.922051	-1.972273	-1.714543	21.94
C	-0.041827	-0.677087	-1.199818	-15.09
O	-0.875401	-1.710163	-1.480021	208.63
C	-1.059428	-2.700203	-0.350492	100.38
H	-1.531928	-2.146823	0.469949	28.33
H	-1.739375	-3.264859	-0.796459	28.30
H	-0.056378	-3.334839	-0.002914	25.37
C	-0.493632	0.648449	-1.034453	15.11
O	-1.971758	0.668644	-1.024912	77.77
C	0.385161	1.751633	-0.928958	51.90
H	0.026091	2.679606	-0.858540	30.66
C	2.278791	0.184652	-1.263472	8.52
C	3.781544	-0.246447	-1.361408	92.84
H	4.087816	-0.755111	-2.456249	26.46
O	4.618803	1.026314	-1.153045	188.98
H	5.316268	0.876350	-0.600395	31.40
C	4.170614	-1.234300	-0.341397	94.00
H	3.538090	-2.265570	-0.528620	24.31
O	5.605373	-1.739059	-0.716363	207.35
H	5.722679	-2.651385	-0.539727	31.26
C	3.865229	-0.978922	1.128988	108.15
O	4.761337	-0.040702	1.799960	180.35
H	4.446073	0.846362	1.619760	35.49
H	4.325141	-1.963001	1.665187	25.60
H	2.941532	-0.704382	1.461712	31.04