Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supplementary Information

Sequence-Selective Recognition of Cationic Amphipathic Tripeptides with Similar Structures in Aqueous Solution by Cucurbit[7]uril

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Section S1 Details information on Independent Gradient Method (IGM) analysis

To evaluate the noncovalent interactions between host CB[7] and guest molecules, the Independent Gradient Method (IGM)[1] is performed by Multiwfn program.[2] $\delta g^{inter} = |\nabla \rho^{IGM,\ inter}| - |\nabla \rho|$ is the key descriptor in IGM, which depends on the magnitude of the norm of the electron density gradient calculated by IGM model $\nabla \rho^{IGM,\ inter}$ and the electron density gradient $\nabla \rho$. Spatial representations of the noncovalent interactions are obtained by plotting isosurface volumes for the δg^{inter}, colored by the value of $sign(\lambda_2)\rho$, that is the product of electron density ρ and the sign of the second eigenvalue λ_2 of electron density Hessian matrix. The strong attractive/repulsive interaction and vdW interaction are shown in blue/red and green, respectively. The volume cutoff is set to δg_{inter}= 0.008, and color-coding is $-0.20 \leq sign(\lambda_2)\rho \leq 0.20$ in all systems.

Reference

1. C. Lefebvre, G. Rubez, H. Khartabil, J. C. Boisson, J. Contreras-Garcia and E. Henon, *Phys. Chem. Chem. Phys.*, 2017,
19, 17928-17936.
2. T. Lu and F. Chen, *J. Comput. Chem.*, 2012, **33**, 580-592.

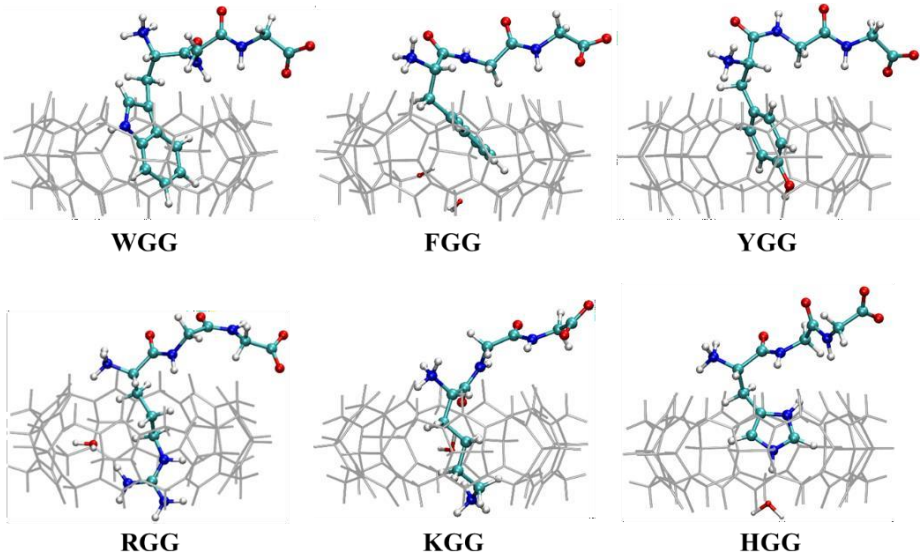

Fig. S1 The initial conformations of CB[7]/X_1GG (X_1= W, F, Y) and CB[7]/X_2GG (X_2= R, K, H). Color code: cyan C, white H, blue N, red O. All the color scheme is the same in this work.

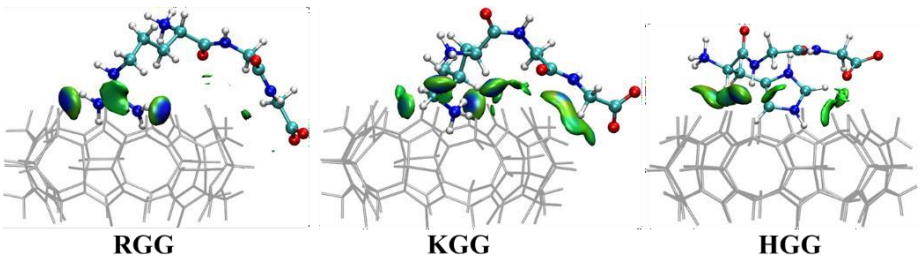

Fig. S2 IGM isosurface analysis of CB[7]/X_2GG (X_2= R, K, H). The strong attractive/repulsive interaction and vdW interaction are shown in blue/red and green, respectively. The color scheme is the same in this work.

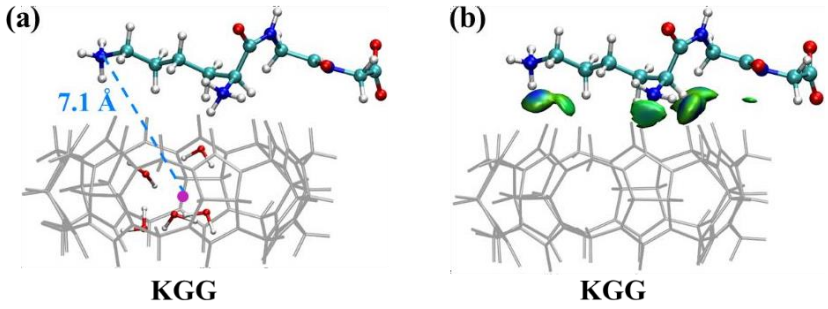

Fig. S3 (a) The conformation of CB[7]/KGG complex. (b) IGM isosurface analysis of CB[7]/KGG complex.

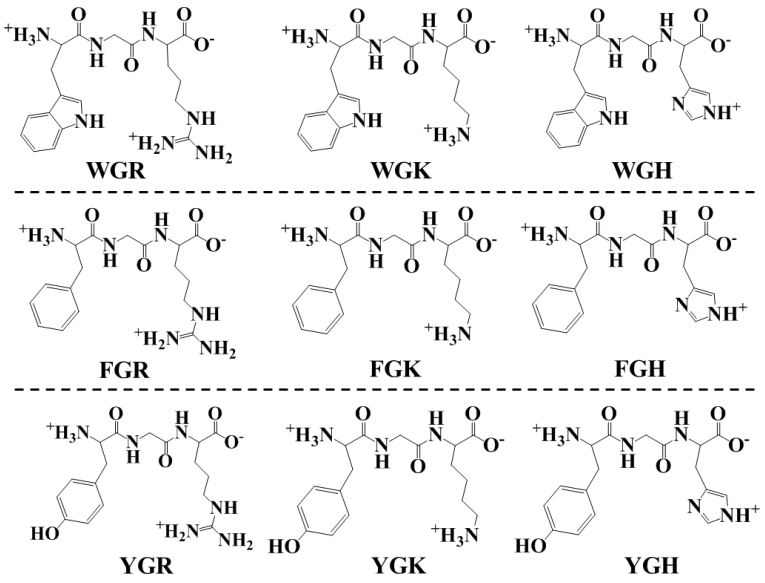

Fig. S4 The structural formulas of cationic amphipathic tripeptides X_1GX_2 (X_1= W, F, Y, and X_2= R, K, H).

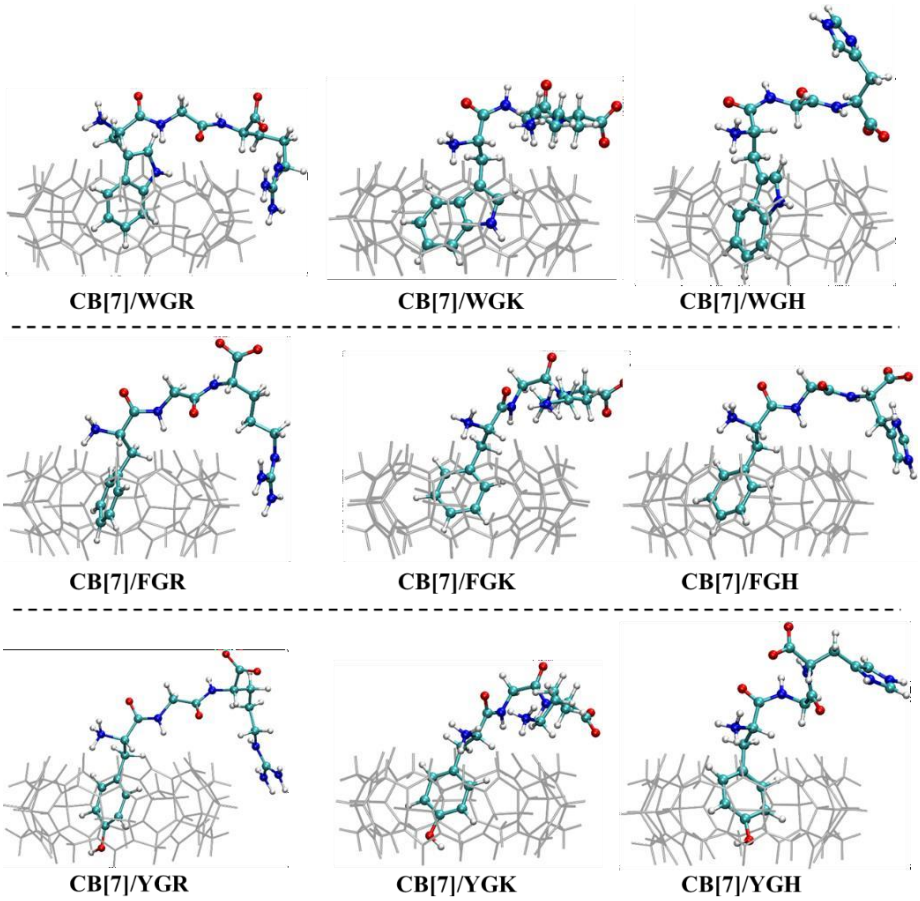

Fig. S5 The conformations of CB[7]/X_1GX_2 (X_1= W, F, Y and X_2= R, K, H).

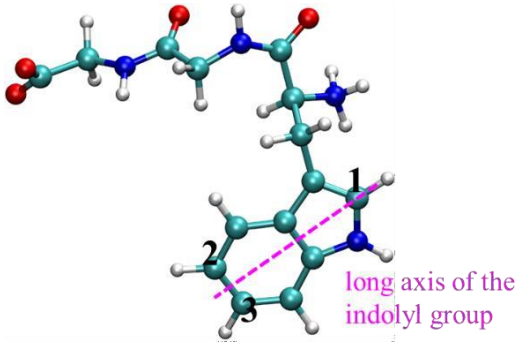

Fig. S6 The purple dashed line between the carbon atom 1 and the center of mass of carbon atom 2 and carbon atom3 refers to the long axis of the indolyl group.

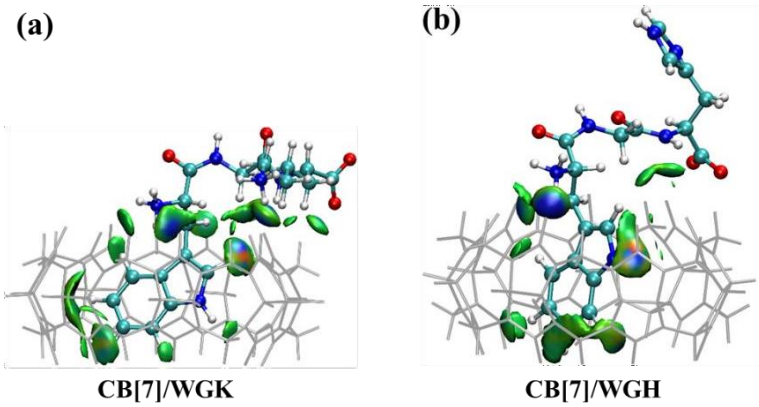

Fig. S7 (a-b) IGM isosurface analysis of CB[7]/WGK and CB[7]/WGH.

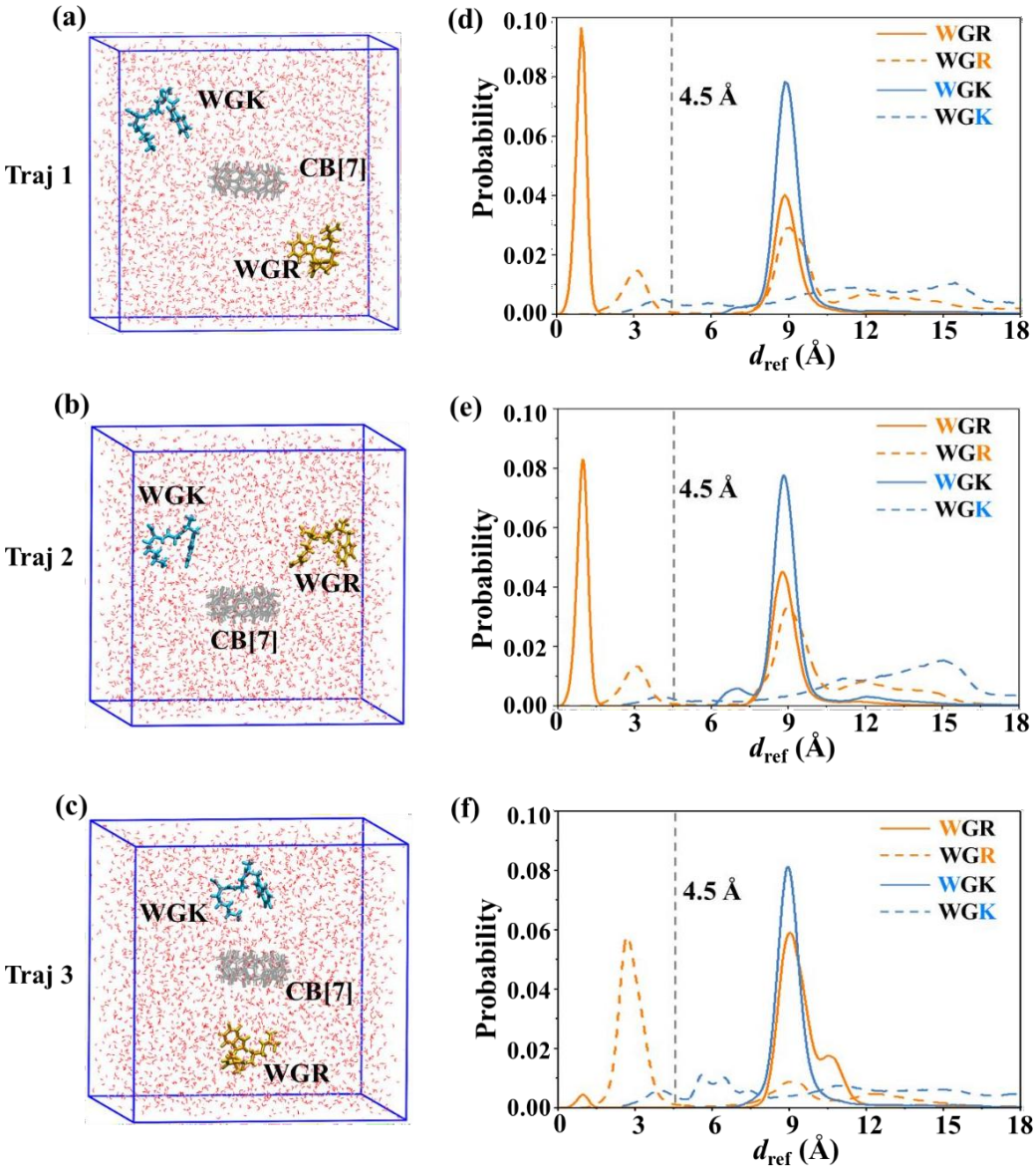

Fig. S8 (a-c) The initial models of the mixed solution containing CB[7], WGK, and WGR. The red points refer to oxygen atoms of water solvent. (d-f) The probability distributions of d_{ref} between CB[7] and the N-terminal W residue of WGR (orange solid line) and WGK (blue solid line), and between CB[7] and the C-terminal R residue of WGR (orange dotted line) and K residue of WGK (blue dotted line).

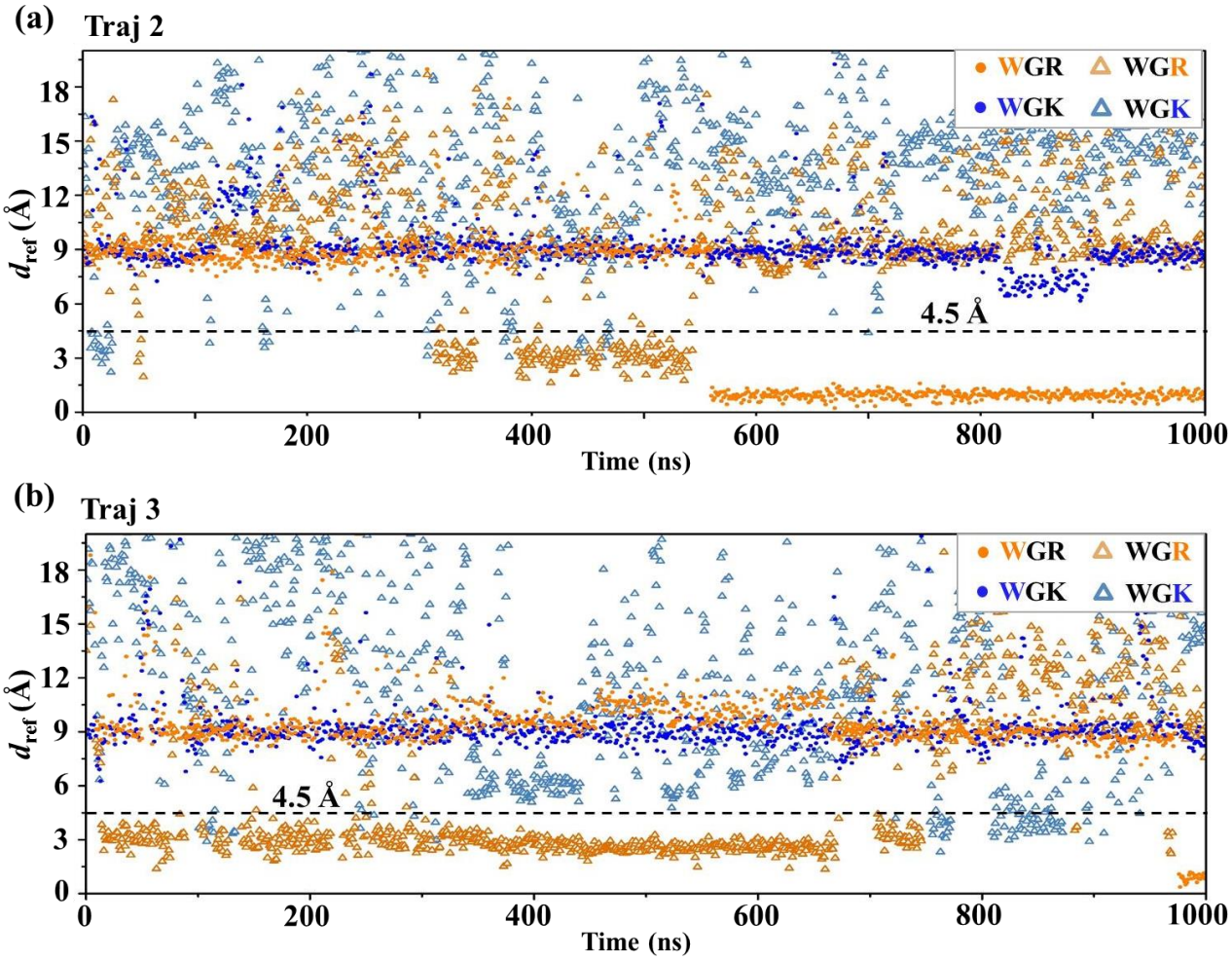

Fig. S9 (a-b) The plot of d_{ref} as a function of simulation time. Here d_{ref} refers to the distances between the reference center of CB[7] and the reference center of the N-terminal W residue of WGR (orange dots) and WGK (blue dots) and between the reference center of CB[7] and the reference center of the C-terminal R residue of WGR (orange triangles) and K residue of WGK (blue triangles).

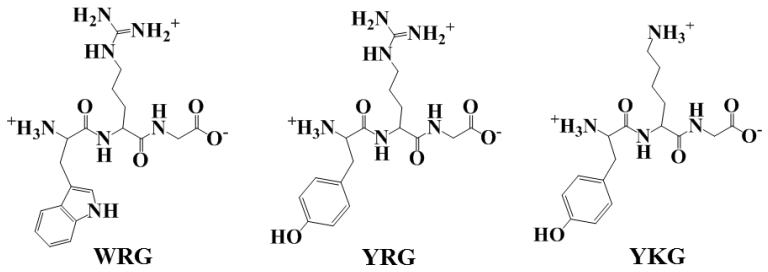

Fig. S10 The structural formulas of tripeptide WRG, YRG and YKG.

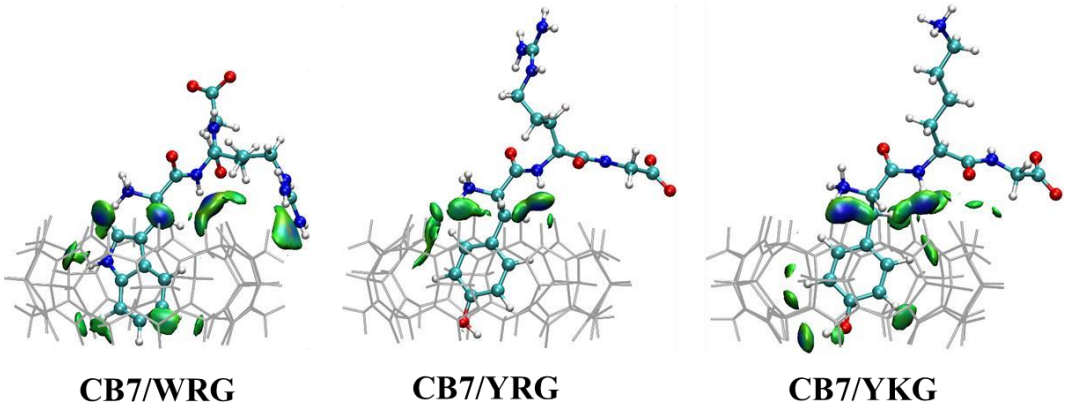

Fig. S11 IGM isosurface analysis of CB[7]/WRG, CB[7]/YRG and CB[7]/YKG.

Table S1 The entropy change of host CB[7] ($-T\Delta S_{CB[7]}$) and guest peptide ($-T\Delta S_{peptide}$) of CB[7]/X_1GG (X_1= W, F, Y) and CB[7]/X_2GG (X_2= R, K, H), in kcal/mol. The average number of embedded water molecules inside CB[7] cavity (N_{water}) of CB[7]/X_1GG and CB[7]/X_2GG, and the average number of intermolecular H-bond ($N_{H\text{-}bond}$), the average distance ($d_{H\text{-}bond}$) in Å between acceptor (A) and donor (D) as well as the average degree of ∠D-H···A between CB[7] and X_1GG, X_2GG.

	$-T\Delta S_{CB[7]}$	$-T\Delta S_{peptide}$	$N_{H\text{-}bond}$	$d_{H\text{-}bond}$	∠ D-H···A (°)	N_{water}
CB[7]/WGG	-3.8	7.1	1.6	2.9	162.2	0.2
CB[7]/FGG	-0.2	6.9	1.3	2.9	161.6	0.6
CB[7]/YGG	-0.6	7.2	1.5	2.9	161.5	0.5
CB[7]/RGG	-0.2	2.2	1.3	3.0	161.4	3.8
CB[7]/KGG	-0.1	1.4	0.6	2.9	160.8	5.6
CB[7]/HGG	-0.3	2.1	0.9	3.0	161.7	4.2

Table S2 The entropy change of host ($-T\Delta S_{CB[7]}$) and guest ($-T\Delta S_{peptide}$) of CB[7]/X_1GX_2 (X_1= W, F, Y, and X_2= R, K, H), in kcal/mol. The average number of embedded water molecules inside CB[7] cavity (N_{water}) of CB[7]/X_1GX_2, and the average number of intermolecular H-bond ($N_{H\text{-}bond}$), the average distance ($d_{H\text{-}bond}$) in Å between acceptor (A) and donor (D) as well as the average degree of ∠D-H···A between CB[7] and X_1GX_2.

	$-T\Delta S_{CB[7]}$	$-T\Delta S_{peptide}$	$N_{H\text{-}bond}$	$d_{H\text{-}bond}$	∠ D-H···A (°)	N_{water}
CB[7]/WGR	-3.7	6.8	2.0	3.0	160.0	0.2
CB[7]/WGK	-2.2	11.0	1.7	2.9	162.5	0.3
CB[7]/WGH	-2.4	7.9	1.6	2.9	162.0	0.2
CB[7]/FGR	0.02	6.7	1.6	2.9	161.8	0.4
CB[7]/FGK	0.06	6.2	1.7	2.9	161.9	0.4
CB[7]/FGH	0.01	7.0	1.6	2.9	159.7	0.4
CB[7]/YGR	-0.3	2.5	2.0	3.0	161.7	0.3
CB[7]/YGK	-0.3	1.6	1.8	3.0	160.0	0.3
CB[7]/YGH	-0.5	2.7	1.5	3.0	161.3	0.4

The Force-field parameters of CB[7] host molecule

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[ moleculetype ]
;name            nrexcl
  CB7              3

[ atoms ]
;     nr    type    resi    res    atom    cgnr        charge        mass       ; qtot     bond_type
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        2       n       1     CB7      N2       2     -0.102391     14.01000 ; qtot -0.202
        3       n       1     CB7      N3       3     -0.131152     14.01000 ; qtot -0.333
        4       n       1     CB7      N4       4     -0.126062     14.01000 ; qtot -0.459
        5       n       1     CB7      N5       5     -0.121824     14.01000 ; qtot -0.581
        6       n       1     CB7      N6       6     -0.116792     14.01000 ; qtot -0.698
        7       n       1     CB7      N7       7     -0.093708     14.01000 ; qtot -0.792
        8       n       1     CB7      N8       8     -0.082855     14.01000 ; qtot -0.875
        9       n       1     CB7      N9       9     -0.081634     14.01000 ; qtot -0.956
       10       n       1     CB7     N10      10     -0.084074     14.01000 ; qtot -1.040
       11       n       1     CB7     N11      11     -0.124779     14.01000 ; qtot -1.165
       12       n       1     CB7     N12      12     -0.123250     14.01000 ; qtot -1.288
       13       n       1     CB7     N13      13     -0.119579     14.01000 ; qtot -1.408
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       15       n       1     CB7     N15      15     -0.113856     14.01000 ; qtot -1.646
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       17       n       1     CB7     N17      17     -0.082530     14.01000 ; qtot -1.837
       18       n       1     CB7     N18      18     -0.072313     14.01000 ; qtot -1.910
       19       n       1     CB7     N19      19     -0.108146     14.01000 ; qtot -2.018
       20       n       1     CB7     N20      20     -0.108911     14.01000 ; qtot -2.127
       21       n       1     CB7     N21      21     -0.131924     14.01000 ; qtot -2.259
       22       n       1     CB7     N22      22     -0.116790     14.01000 ; qtot -2.375
       23       n       1     CB7     N23      23     -0.105346     14.01000 ; qtot -2.481
       24       n       1     CB7     N24      24     -0.124417     14.01000 ; qtot -2.605
       25       n       1     CB7     N25      25     -0.120463     14.01000 ; qtot -2.726
       26       n       1     CB7     N26      26     -0.121403     14.01000 ; qtot -2.847
       27       n       1     CB7     N27      27     -0.064076     14.01000 ; qtot -2.911
       28       n       1     CB7     N28      28     -0.073821     14.01000 ; qtot -2.985
       29       c       1     CB7      C1      29      0.550322     12.01000 ; qtot -2.435
       30       c       1     CB7      C2      30      0.577912     12.01000 ; qtot -1.857
       31      c3       1     CB7      C3      31     -0.155701     12.01000 ; qtot -2.012
       32      h2       1     CB7      H1      32      0.155418      1.00800 ; qtot -1.857
       33      c3       1     CB7      C4      33     -0.096135     12.01000 ; qtot -1.953
       34      h2       1     CB7      H2      34      0.145203      1.00800 ; qtot -1.808
       35      c3       1     CB7      C5      35     -0.085462     12.01000 ; qtot -1.893
       36      h2       1     CB7      H3      36      0.117036      1.00800 ; qtot -1.776
       37      h2       1     CB7      H4      37      0.100836      1.00800 ; qtot -1.675
       38      c3       1     CB7      C6      38     -0.182447     12.01000 ; qtot -1.858
       39      h2       1     CB7      H5      39      0.142906      1.00800 ; qtot -1.715
       40      h2       1     CB7      H6      40      0.129779      1.00800 ; qtot -1.585
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       43      c3       1     CB7      C9      43     -0.099655     12.01000 ; qtot -0.579
       44      h2       1     CB7      H7      44      0.144364      1.00800 ; qtot -0.435
       45      c3       1     CB7     C10      45     -0.157889     12.01000 ; qtot -0.593
       46      h2       1     CB7      H8      46      0.153452      1.00800 ; qtot -0.439
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       50      c3       1     CB7     C12      50     -0.184741     12.01000 ; qtot -0.540
       51      h2       1     CB7     H11      51      0.129598      1.00800 ; qtot -0.410
       52      h2       1     CB7     H12      52      0.138655      1.00800 ; qtot -0.271
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       54       c       1     CB7     C14      54      0.534485     12.01000 ; qtot 0.836
       55      c3       1     CB7     C15      55     -0.180716     12.01000 ; qtot 0.655
       56      h2       1     CB7     H13      56      0.157710      1.00800 ; qtot 0.813
       57      c3       1     CB7     C16      57     -0.074738     12.01000 ; qtot 0.738
       58      h2       1     CB7     H14      58      0.138662      1.00800 ; qtot 0.877
       59      c3       1     CB7     C17      59     -0.182464     12.01000 ; qtot 0.694
       60      h2       1     CB7     H15      60      0.130390      1.00800 ; qtot 0.824
       61      h2       1     CB7     H16      61      0.142557      1.00800 ; qtot 0.967
       62      c3       1     CB7     C18      62     -0.095294     12.01000 ; qtot 0.872
       63      h2       1     CB7     H17      63      0.119226      1.00800 ; qtot 0.991
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    64     h2     1    CB7     H18     64       0.103968     1.00800 ; qtot 1.095
    65      c     1    CB7     C19     65       0.577042    12.01000 ; qtot 1.672
    66      c     1    CB7     C20     66       0.554184    12.01000 ; qtot 2.226
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    69     c3     1    CB7     C22     69      -0.135558    12.01000 ; qtot 2.121
    70     h2     1    CB7     H20     70       0.152242     1.00800 ; qtot 2.273
    71     c3     1    CB7     C23     71      -0.143303    12.01000 ; qtot 2.130
    72     h2     1    CB7     H21     72       0.128501     1.00800 ; qtot 2.258
    73     h2     1    CB7     H22     73       0.118213     1.00800 ; qtot 2.376
    74     c3     1    CB7     C24     74      -0.191086    12.01000 ; qtot 2.185
    75     h2     1    CB7     H23     75       0.131732     1.00800 ; qtot 2.317
    76     h2     1    CB7     H24     76       0.141432     1.00800 ; qtot 2.459
    77      c     1    CB7     C25     77       0.516522    12.01000 ; qtot 2.975
    78      c     1    CB7     C26     78       0.555148    12.01000 ; qtot 3.530
    79     c3     1    CB7     C27     79      -0.172316    12.01000 ; qtot 3.358
    80     h2     1    CB7     H25     80       0.152647     1.00800 ; qtot 3.511
    81     c3     1    CB7     C28     81      -0.075919    12.01000 ; qtot 3.435
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    83     c3     1    CB7     C29     83      -0.104092    12.01000 ; qtot 3.465
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    88     h2     1    CB7     H30     88       0.140899     1.00800 ; qtot 3.780
    89      c     1    CB7     C31     89       0.565677    12.01000 ; qtot 4.346
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    92     h2     1    CB7     H31     92       0.150351     1.00800 ; qtot 4.943
    93     c3     1    CB7     C34     93      -0.147871    12.01000 ; qtot 4.795
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    97     h2     1    CB7     H34     97       0.129286     1.00800 ; qtot 5.040
    98     c3     1    CB7     C36     98      -0.090451    12.01000 ; qtot 4.949
    99     h2     1    CB7     H35     99       0.116936     1.00800 ; qtot 5.066
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   102      c     1    CB7     C38    102       0.522124    12.01000 ; qtot 6.252
   103     c3     1    CB7     C39    103      -0.053144    12.01000 ; qtot 6.199
   104     h2     1    CB7     H37    104       0.132058     1.00800 ; qtot 6.331
   105     c3     1    CB7     C40    105      -0.204281    12.01000 ; qtot 6.126
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   108     h2     1    CB7     H39    108       0.141939     1.00800 ; qtot 6.232
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   110     c3     1    CB7     C42    110      -0.162699    12.01000 ; qtot 6.203
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   113      o     1    CB7      O1    113      -0.467900    16.00000 ; qtot 5.993
   114      o     1    CB7      O2    114      -0.457721    16.00000 ; qtot 5.535
   115      o     1    CB7      O3    115      -0.455316    16.00000 ; qtot 5.080
   116      o     1    CB7      O4    116      -0.468202    16.00000 ; qtot 4.611
   117      o     1    CB7      O5    117      -0.452162    16.00000 ; qtot 4.159
   118      o     1    CB7      O6    118      -0.469551    16.00000 ; qtot 3.690
   119      o     1    CB7      O7    119      -0.454809    16.00000 ; qtot 3.235
   120      o     1    CB7      O8    120      -0.466770    16.00000 ; qtot 2.768
   121      o     1    CB7      O9    121      -0.458347    16.00000 ; qtot 2.310
   122      o     1    CB7     O10    122      -0.451000    16.00000 ; qtot 1.859
   123      o     1    CB7     O11    123      -0.468049    16.00000 ; qtot 1.391
   124      o     1    CB7     O12    124      -0.461524    16.00000 ; qtot 0.929
   125      o     1    CB7     O13    125      -0.460279    16.00000 ; qtot 0.469
   126      o     1    CB7     O14    126      -0.468909    16.00000 ; qtot -0.000

[ bonds ]
;    ai     aj funct      r             k
     1     29     1      1.3789e-01     3.5782e+05 ;     N1 - C1
     1     31     1      1.4619e-01     2.7506e+05 ;     N1 - C3
     1    107     1      1.4619e-01     2.7506e+05 ;     N1 - C41
     2     30     1      1.3789e-01     3.5782e+05 ;     N2 - C2
     2     31     1      1.4619e-01     2.7506e+05 ;     N2 - C3
```

2 110 1 1.4619e-01 2.7506e+05 ; N2 - C42
3 29 1 1.3789e-01 3.5782e+05 ; N3 - C1
3 33 1 1.4619e-01 2.7506e+05 ; N3 - C4
3 35 1 1.4619e-01 2.7506e+05 ; N3 - C5
4 30 1 1.3789e-01 3.5782e+05 ; N4 - C2
4 33 1 1.4619e-01 2.7506e+05 ; N4 - C4
4 38 1 1.4619e-01 2.7506e+05 ; N4 - C6
5 35 1 1.4619e-01 2.7506e+05 ; N5 - C5
5 41 1 1.3789e-01 3.5782e+05 ; N5 - C7
5 43 1 1.4619e-01 2.7506e+05 ; N5 - C9
6 38 1 1.4619e-01 2.7506e+05 ; N6 - C6
6 42 1 1.3789e-01 3.5782e+05 ; N6 - C8
6 43 1 1.4619e-01 2.7506e+05 ; N6 - C9
7 41 1 1.3789e-01 3.5782e+05 ; N7 - C7
7 45 1 1.4619e-01 2.7506e+05 ; N7 - C10
7 47 1 1.4619e-01 2.7506e+05 ; N7 - C11
8 42 1 1.3789e-01 3.5782e+05 ; N8 - C8
8 45 1 1.4619e-01 2.7506e+05 ; N8 - C10
8 50 1 1.4619e-01 2.7506e+05 ; N8 - C12
9 47 1 1.4619e-01 2.7506e+05 ; N9 - C11
9 53 1 1.3789e-01 3.5782e+05 ; N9 - C13
9 55 1 1.4619e-01 2.7506e+05 ; N9 - C15
10 50 1 1.4619e-01 2.7506e+05 ; N10 - C12
10 54 1 1.3789e-01 3.5782e+05 ; N10 - C14
10 55 1 1.4619e-01 2.7506e+05 ; N10 - C15
11 53 1 1.3789e-01 3.5782e+05 ; N11 - C13
11 57 1 1.4619e-01 2.7506e+05 ; N11 - C16
11 59 1 1.4619e-01 2.7506e+05 ; N11 - C17
12 54 1 1.3789e-01 3.5782e+05 ; N12 - C14
12 57 1 1.4619e-01 2.7506e+05 ; N12 - C16
12 62 1 1.4619e-01 2.7506e+05 ; N12 - C18
13 59 1 1.4619e-01 2.7506e+05 ; N13 - C17
13 65 1 1.3789e-01 3.5782e+05 ; N13 - C19
13 67 1 1.4619e-01 2.7506e+05 ; N13 - C21
14 62 1 1.4619e-01 2.7506e+05 ; N14 - C18
14 66 1 1.3789e-01 3.5782e+05 ; N14 - C20
14 67 1 1.4619e-01 2.7506e+05 ; N14 - C21
15 65 1 1.3789e-01 3.5782e+05 ; N15 - C19
15 69 1 1.4619e-01 2.7506e+05 ; N15 - C22
15 71 1 1.4619e-01 2.7506e+05 ; N15 - C23
16 66 1 1.3789e-01 3.5782e+05 ; N16 - C20
16 69 1 1.4619e-01 2.7506e+05 ; N16 - C22
16 74 1 1.4619e-01 2.7506e+05 ; N16 - C24
17 71 1 1.4619e-01 2.7506e+05 ; N17 - C23
17 77 1 1.3789e-01 3.5782e+05 ; N17 - C25
17 79 1 1.4619e-01 2.7506e+05 ; N17 - C27
18 74 1 1.4619e-01 2.7506e+05 ; N18 - C24
18 78 1 1.3789e-01 3.5782e+05 ; N18 - C26
18 79 1 1.4619e-01 2.7506e+05 ; N18 - C27
19 77 1 1.3789e-01 3.5782e+05 ; N19 - C25
19 81 1 1.4619e-01 2.7506e+05 ; N19 - C28
19 83 1 1.4619e-01 2.7506e+05 ; N19 - C29
20 78 1 1.3789e-01 3.5782e+05 ; N20 - C26
20 81 1 1.4619e-01 2.7506e+05 ; N20 - C28
20 86 1 1.4619e-01 2.7506e+05 ; N20 - C30
21 83 1 1.4619e-01 2.7506e+05 ; N21 - C29
21 89 1 1.3789e-01 3.5782e+05 ; N21 - C31
21 91 1 1.4619e-01 2.7506e+05 ; N21 - C33
22 86 1 1.4619e-01 2.7506e+05 ; N22 - C30
22 90 1 1.3789e-01 3.5782e+05 ; N22 - C32
22 91 1 1.4619e-01 2.7506e+05 ; N22 - C33
23 89 1 1.3789e-01 3.5782e+05 ; N23 - C31
23 93 1 1.4619e-01 2.7506e+05 ; N23 - C34
23 95 1 1.4619e-01 2.7506e+05 ; N23 - C35
24 90 1 1.3789e-01 3.5782e+05 ; N24 - C32
24 93 1 1.4619e-01 2.7506e+05 ; N24 - C34
24 98 1 1.4619e-01 2.7506e+05 ; N24 - C36
25 95 1 1.4619e-01 2.7506e+05 ; N25 - C35
25 101 1 1.3789e-01 3.5782e+05 ; N25 - C37
25 103 1 1.4619e-01 2.7506e+05 ; N25 - C39
26 98 1 1.4619e-01 2.7506e+05 ; N26 - C36

26	102	1	1.3789e-01	3.5782e+05 ;	N26 - C38
26	103	1	1.4619e-01	2.7506e+05 ;	N26 - C39
27	101	1	1.3789e-01	3.5782e+05 ;	N27 - C37
27	105	1	1.4619e-01	2.7506e+05 ;	N27 - C40
27	107	1	1.4619e-01	2.7506e+05 ;	N27 - C41
28	102	1	1.3789e-01	3.5782e+05 ;	N28 - C38
28	105	1	1.4619e-01	2.7506e+05 ;	N28 - C40
28	110	1	1.4619e-01	2.7506e+05 ;	N28 - C42
29	114	1	1.2183e-01	5.3363e+05 ;	C1 - O2
30	113	1	1.2183e-01	5.3363e+05 ;	C2 - O1
31	32	1	1.0961e-01	2.7757e+05 ;	C3 - H1
31	33	1	1.5375e-01	2.5179e+05 ;	C3 - C4
33	34	1	1.0961e-01	2.7757e+05 ;	C4 - H2
35	36	1	1.0961e-01	2.7757e+05 ;	C5 - H3
35	37	1	1.0961e-01	2.7757e+05 ;	C5 - H4
38	39	1	1.0961e-01	2.7757e+05 ;	C6 - H5
38	40	1	1.0961e-01	2.7757e+05 ;	C6 - H6
41	115	1	1.2183e-01	5.3363e+05 ;	C7 - O3
42	116	1	1.2183e-01	5.3363e+05 ;	C8 - O4
43	44	1	1.0961e-01	2.7757e+05 ;	C9 - H7
43	45	1	1.5375e-01	2.5179e+05 ;	C9 - C10
45	46	1	1.0961e-01	2.7757e+05 ;	C10 - H8
47	48	1	1.0961e-01	2.7757e+05 ;	C11 - H9
47	49	1	1.0961e-01	2.7757e+05 ;	C11 - H10
50	51	1	1.0961e-01	2.7757e+05 ;	C12 - H11
50	52	1	1.0961e-01	2.7757e+05 ;	C12 - H12
53	118	1	1.2183e-01	5.3363e+05 ;	C13 - O6
54	119	1	1.2183e-01	5.3363e+05 ;	C14 - O7
55	56	1	1.0961e-01	2.7757e+05 ;	C15 - H13
55	57	1	1.5375e-01	2.5179e+05 ;	C15 - C16
57	58	1	1.0961e-01	2.7757e+05 ;	C16 - H14
59	60	1	1.0961e-01	2.7757e+05 ;	C17 - H15
59	61	1	1.0961e-01	2.7757e+05 ;	C17 - H16
62	63	1	1.0961e-01	2.7757e+05 ;	C18 - H17
62	64	1	1.0961e-01	2.7757e+05 ;	C18 - H18
65	120	1	1.2183e-01	5.3363e+05 ;	C19 - O8
66	121	1	1.2183e-01	5.3363e+05 ;	C20 - O9
67	68	1	1.0961e-01	2.7757e+05 ;	C21 - H19
67	69	1	1.5375e-01	2.5179e+05 ;	C21 - C22
69	70	1	1.0961e-01	2.7757e+05 ;	C22 - H20
71	72	1	1.0961e-01	2.7757e+05 ;	C23 - H21
71	73	1	1.0961e-01	2.7757e+05 ;	C23 - H22
74	75	1	1.0961e-01	2.7757e+05 ;	C24 - H23
74	76	1	1.0961e-01	2.7757e+05 ;	C24 - H24
77	122	1	1.2183e-01	5.3363e+05 ;	C25 - O10
78	123	1	1.2183e-01	5.3363e+05 ;	C26 - O11
79	80	1	1.0961e-01	2.7757e+05 ;	C27 - H25
79	81	1	1.5375e-01	2.5179e+05 ;	C27 - C28
81	82	1	1.0961e-01	2.7757e+05 ;	C28 - H26
83	84	1	1.0961e-01	2.7757e+05 ;	C29 - H27
83	85	1	1.0961e-01	2.7757e+05 ;	C29 - H28
86	87	1	1.0961e-01	2.7757e+05 ;	C30 - H29
86	88	1	1.0961e-01	2.7757e+05 ;	C30 - H30
89	124	1	1.2183e-01	5.3363e+05 ;	C31 - O12
90	125	1	1.2183e-01	5.3363e+05 ;	C32 - O13
91	92	1	1.0961e-01	2.7757e+05 ;	C33 - H31
91	93	1	1.5375e-01	2.5179e+05 ;	C33 - C34
93	94	1	1.0961e-01	2.7757e+05 ;	C34 - H32
95	96	1	1.0961e-01	2.7757e+05 ;	C35 - H33
95	97	1	1.0961e-01	2.7757e+05 ;	C35 - H34
98	99	1	1.0961e-01	2.7757e+05 ;	C36 - H35
98	100	1	1.0961e-01	2.7757e+05 ;	C36 - H36
101	126	1	1.2183e-01	5.3363e+05 ;	C37 - O14
102	117	1	1.2183e-01	5.3363e+05 ;	C38 - O5
103	104	1	1.0961e-01	2.7757e+05 ;	C39 - H37
103	105	1	1.5375e-01	2.5179e+05 ;	C39 - C40
105	106	1	1.0961e-01	2.7757e+05 ;	C40 - H38
107	108	1	1.0961e-01	2.7757e+05 ;	C41 - H39
107	109	1	1.0961e-01	2.7757e+05 ;	C41 - H40
110	111	1	1.0961e-01	2.7757e+05 ;	C42 - H41
110	112	1	1.0961e-01	2.7757e+05 ;	C42 - H42

```
[ pairs ]
;     ai      aj      funct
        1       4       1 ;       N1 - N4
        1       30       1 ;       N1 - C2
        1       34       1 ;       N1 - H2
        1       35       1 ;       N1 - C5
        1       101       1 ;       N1 - C37
        1       105       1 ;       N1 - C40
        1       110       1 ;       N1 - C42
        2       3       1 ;       N2 - N3
        2       34       1 ;       N2 - H2
        2       38       1 ;       N2 - C6
        2       102       1 ;       N2 - C38
        2       105       1 ;       N2 - C40
        3       30       1 ;       N3 - C2
        3       32       1 ;       N3 - H1
        3       38       1 ;       N3 - C6
        3       41       1 ;       N3 - C7
        3       43       1 ;       N3 - C9
        4       29       1 ;       N4 - C1
        4       32       1 ;       N4 - H1
        4       35       1 ;       N4 - C5
        4       42       1 ;       N4 - C8
        4       43       1 ;       N4 - C9
        4       110       1 ;       N4 - C42
        5       8       1 ;       N5 - N8
        5       29       1 ;       N5 - C1
        5       33       1 ;       N5 - C4
        5       38       1 ;       N5 - C6
        5       42       1 ;       N5 - C8
        5       46       1 ;       N5 - H8
        5       47       1 ;       N5 - C11
        6       7       1 ;       N6 - N7
        6       30       1 ;       N6 - C2
        6       33       1 ;       N6 - C4
        6       35       1 ;       N6 - C5
        6       41       1 ;       N6 - C7
        6       46       1 ;       N6 - H8
        6       50       1 ;       N6 - C12
        7       35       1 ;       N7 - C5
        7       42       1 ;       N7 - C8
        7       44       1 ;       N7 - H7
        7       50       1 ;       N7 - C12
        7       53       1 ;       N7 - C13
        7       55       1 ;       N7 - C15
        8       38       1 ;       N8 - C6
        8       41       1 ;       N8 - C7
        8       44       1 ;       N8 - H7
        8       47       1 ;       N8 - C11
        8       54       1 ;       N8 - C14
        8       55       1 ;       N8 - C15
        9       12       1 ;       N9 - N12
        9       41       1 ;       N9 - C7
        9       45       1 ;       N9 - C10
        9       50       1 ;       N9 - C12
        9       54       1 ;       N9 - C14
        9       58       1 ;       N9 - H14
        9       59       1 ;       N9 - C17
       10       11       1 ;       N10 - N11
       10       42       1 ;       N10 - C8
       10       45       1 ;       N10 - C10
       10       47       1 ;       N10 - C11
       10       53       1 ;       N10 - C13
       10       58       1 ;       N10 - H14
       10       62       1 ;       N10 - C18
       11       47       1 ;       N11 - C11
       11       54       1 ;       N11 - C14
       11       56       1 ;       N11 - H13
       11       62       1 ;       N11 - C18
       11       65       1 ;       N11 - C19
```

11	67	1 ;	N11 - C21
12	50	1 ;	N12 - C12
12	53	1 ;	N12 - C13
12	56	1 ;	N12 - H13
12	59	1 ;	N12 - C17
12	66	1 ;	N12 - C20
12	67	1 ;	N12 - C21
13	16	1 ;	N13 - N16
13	53	1 ;	N13 - C13
13	57	1 ;	N13 - C16
13	62	1 ;	N13 - C18
13	66	1 ;	N13 - C20
13	70	1 ;	N13 - H20
13	71	1 ;	N13 - C23
14	15	1 ;	N14 - N15
14	54	1 ;	N14 - C14
14	57	1 ;	N14 - C16
14	59	1 ;	N14 - C17
14	65	1 ;	N14 - C19
14	70	1 ;	N14 - H20
14	74	1 ;	N14 - C24
15	59	1 ;	N15 - C17
15	66	1 ;	N15 - C20
15	68	1 ;	N15 - H19
15	74	1 ;	N15 - C24
15	77	1 ;	N15 - C25
15	79	1 ;	N15 - C27
16	62	1 ;	N16 - C18
16	65	1 ;	N16 - C19
16	68	1 ;	N16 - H19
16	71	1 ;	N16 - C23
16	78	1 ;	N16 - C26
16	79	1 ;	N16 - C27
17	20	1 ;	N17 - N20
17	65	1 ;	N17 - C19
17	69	1 ;	N17 - C22
17	74	1 ;	N17 - C24
17	78	1 ;	N17 - C26
17	82	1 ;	N17 - H26
17	83	1 ;	N17 - C29
18	19	1 ;	N18 - N19
18	66	1 ;	N18 - C20
18	69	1 ;	N18 - C22
18	71	1 ;	N18 - C23
18	77	1 ;	N18 - C25
18	82	1 ;	N18 - H26
18	86	1 ;	N18 - C30
19	71	1 ;	N19 - C23
19	78	1 ;	N19 - C26
19	80	1 ;	N19 - H25
19	86	1 ;	N19 - C30
19	89	1 ;	N19 - C31
19	91	1 ;	N19 - C33
20	74	1 ;	N20 - C24
20	77	1 ;	N20 - C25
20	80	1 ;	N20 - H25
20	83	1 ;	N20 - C29
20	90	1 ;	N20 - C32
20	91	1 ;	N20 - C33
21	24	1 ;	N21 - N24
21	77	1 ;	N21 - C25
21	81	1 ;	N21 - C28
21	86	1 ;	N21 - C30
21	90	1 ;	N21 - C32
21	94	1 ;	N21 - H32
21	95	1 ;	N21 - C35
22	23	1 ;	N22 - N23
22	78	1 ;	N22 - C26
22	81	1 ;	N22 - C28
22	83	1 ;	N22 - C29
22	89	1 ;	N22 - C31

22 94 1 ; N22 - H32
22 98 1 ; N22 - C36
23 83 1 ; N23 - C29
23 90 1 ; N23 - C32
23 92 1 ; N23 - H31
23 98 1 ; N23 - C36
23 101 1 ; N23 - C37
23 103 1 ; N23 - C39
24 86 1 ; N24 - C30
24 89 1 ; N24 - C31
24 92 1 ; N24 - H31
24 95 1 ; N24 - C35
24 102 1 ; N24 - C38
24 103 1 ; N24 - C39
25 28 1 ; N25 - N28
25 89 1 ; N25 - C31
25 93 1 ; N25 - C34
25 98 1 ; N25 - C36
25 102 1 ; N25 - C38
25 106 1 ; N25 - H38
25 107 1 ; N25 - C41
26 27 1 ; N26 - N27
26 90 1 ; N26 - C32
26 93 1 ; N26 - C34
26 95 1 ; N26 - C35
26 101 1 ; N26 - C37
26 106 1 ; N26 - H38
26 110 1 ; N26 - C42
27 95 1 ; N27 - C35
27 102 1 ; N27 - C38
27 104 1 ; N27 - H37
27 110 1 ; N27 - C42
28 30 1 ; N28 - C2
28 31 1 ; N28 - C3
28 98 1 ; N28 - C36
28 101 1 ; N28 - C37
28 104 1 ; N28 - H37
28 107 1 ; N28 - C41
29 2 1 ; C1 - N2
29 27 1 ; C1 - N27
29 32 1 ; C1 - H1
29 34 1 ; C1 - H2
29 36 1 ; C1 - H3
29 37 1 ; C1 - H4
29 108 1 ; C1 - H39
29 109 1 ; C1 - H40
30 32 1 ; C2 - H1
30 34 1 ; C2 - H2
30 39 1 ; C2 - H5
30 40 1 ; C2 - H6
30 111 1 ; C2 - H41
30 112 1 ; C2 - H42
31 27 1 ; C3 - N27
31 35 1 ; C3 - C5
31 38 1 ; C3 - C6
31 108 1 ; C3 - H39
31 109 1 ; C3 - H40
31 111 1 ; C3 - H41
31 112 1 ; C3 - H42
31 113 1 ; C3 - O1
31 114 1 ; C3 - O2
32 34 1 ; H1 - H2
32 110 1 ; H1 - C42
33 36 1 ; C4 - H3
33 37 1 ; C4 - H4
33 39 1 ; C4 - H5
33 40 1 ; C4 - H6
33 110 1 ; C4 - C42
33 113 1 ; C4 - O1
33 114 1 ; C4 - O2
34 35 1 ; H2 - C5

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34      38      1 ;     H2 - C6
35      44      1 ;     C5 - H7
35      45      1 ;     C5 - C10
35      114     1 ;     C5 - O2
35      115     1 ;     C5 - O3
36      41      1 ;     H3 - C7
36      43      1 ;     H3 - C9
37      41      1 ;     H4 - C7
37      43      1 ;     H4 - C9
38      44      1 ;     C6 - H7
38      45      1 ;     C6 - C10
38      113     1 ;     C6 - O1
38      116     1 ;     C6 - O4
39      42      1 ;     H5 - C8
39      43      1 ;     H5 - C9
40      42      1 ;     H6 - C8
40      43      1 ;     H6 - C9
41      44      1 ;     C7 - H7
41      46      1 ;     C7 - H8
41      48      1 ;     C7 - H9
41      49      1 ;     C7 - H10
42      44      1 ;     C8 - H7
42      46      1 ;     C8 - H8
42      51      1 ;     C8 - H11
42      52      1 ;     C8 - H12
43      47      1 ;     C9 - C11
43      50      1 ;     C9 - C12
43      115     1 ;     C9 - O3
43      116     1 ;     C9 - O4
44      46      1 ;     H7 - H8
45      48      1 ;     C10 - H9
45      49      1 ;     C10 - H10
45      51      1 ;     C10 - H11
45      52      1 ;     C10 - H12
45      115     1 ;     C10 - O3
45      116     1 ;     C10 - O4
46      47      1 ;     H8 - C11
46      50      1 ;     H8 - C12
47      56      1 ;     C11 - H13
47      57      1 ;     C11 - C16
47      115     1 ;     C11 - O3
47      118     1 ;     C11 - O6
48      53      1 ;     H9 - C13
48      55      1 ;     H9 - C15
49      53      1 ;     H10 - C13
49      55      1 ;     H10 - C15
50      56      1 ;     C12 - H13
50      57      1 ;     C12 - C16
50      116     1 ;     C12 - O4
50      119     1 ;     C12 - O7
51      54      1 ;     H11 - C14
51      55      1 ;     H11 - C15
52      54      1 ;     H12 - C14
52      55      1 ;     H12 - C15
53      56      1 ;     C13 - H13
53      58      1 ;     C13 - H14
53      60      1 ;     C13 - H15
53      61      1 ;     C13 - H16
54      56      1 ;     C14 - H13
54      58      1 ;     C14 - H14
54      63      1 ;     C14 - H17
54      64      1 ;     C14 - H18
55      59      1 ;     C15 - C17
55      62      1 ;     C15 - C18
55      118     1 ;     C15 - O6
55      119     1 ;     C15 - O7
56      58      1 ;     H13 - H14
57      60      1 ;     C16 - H15
57      61      1 ;     C16 - H16
57      63      1 ;     C16 - H17
57      64      1 ;     C16 - H18
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57 118 1 ; C16 - O6
57 119 1 ; C16 - O7
58 59 1 ; H14 - C17
58 62 1 ; H14 - C18
59 68 1 ; C17 - H19
59 69 1 ; C17 - C22
59 118 1 ; C17 - O6
59 120 1 ; C17 - O8
60 65 1 ; H15 - C19
60 67 1 ; H15 - C21
61 65 1 ; H16 - C19
61 67 1 ; H16 - C21
62 68 1 ; C18 - H19
62 69 1 ; C18 - C22
62 119 1 ; C18 - O7
62 121 1 ; C18 - O9
63 66 1 ; H17 - C20
63 67 1 ; H17 - C21
64 66 1 ; H18 - C20
64 67 1 ; H18 - C21
65 68 1 ; C19 - H19
65 70 1 ; C19 - H20
65 72 1 ; C19 - H21
65 73 1 ; C19 - H22
66 68 1 ; C20 - H19
66 70 1 ; C20 - H20
66 75 1 ; C20 - H23
66 76 1 ; C20 - H24
67 71 1 ; C21 - C23
67 74 1 ; C21 - C24
67 120 1 ; C21 - O8
67 121 1 ; C21 - O9
68 70 1 ; H19 - H20
69 72 1 ; C22 - H21
69 73 1 ; C22 - H22
69 75 1 ; C22 - H23
69 76 1 ; C22 - H24
69 120 1 ; C22 - O8
69 121 1 ; C22 - O9
70 71 1 ; H20 - C23
70 74 1 ; H20 - C24
71 80 1 ; C23 - H25
71 81 1 ; C23 - C28
71 120 1 ; C23 - O8
71 122 1 ; C23 - O10
72 77 1 ; H21 - C25
72 79 1 ; H21 - C27
73 77 1 ; H22 - C25
73 79 1 ; H22 - C27
74 80 1 ; C24 - H25
74 81 1 ; C24 - C28
74 121 1 ; C24 - O9
74 123 1 ; C24 - O11
75 78 1 ; H23 - C26
75 79 1 ; H23 - C27
76 78 1 ; H24 - C26
76 79 1 ; H24 - C27
77 80 1 ; C25 - H25
77 82 1 ; C25 - H26
77 84 1 ; C25 - H27
77 85 1 ; C25 - H28
78 80 1 ; C26 - H25
78 82 1 ; C26 - H26
78 87 1 ; C26 - H29
78 88 1 ; C26 - H30
79 83 1 ; C27 - C29
79 86 1 ; C27 - C30
79 122 1 ; C27 - O10
79 123 1 ; C27 - O11
80 82 1 ; H25 - H26
81 84 1 ; C28 - H27

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 81    85    1 ;     C28 - H28
 81    87    1 ;     C28 - H29
 81    88    1 ;     C28 - H30
 81   122     1 ;     C28 - O10
 81   123     1 ;     C28 - O11
 82    83    1 ;     H26 - C29
 82    86    1 ;     H26 - C30
 83    92    1 ;     C29 - H31
 83    93    1 ;     C29 - C34
 83   122     1 ;     C29 - O10
 83   124     1 ;     C29 - O12
 84    89    1 ;     H27 - C31
 84    91    1 ;     H27 - C33
 85    89    1 ;     H28 - C31
 85    91    1 ;     H28 - C33
 86    92    1 ;     C30 - H31
 86    93    1 ;     C30 - C34
 86   123     1 ;     C30 - O11
 86   125     1 ;     C30 - O13
 87    90    1 ;     H29 - C32
 87    91    1 ;     H29 - C33
 88    90    1 ;     H30 - C32
 88    91    1 ;     H30 - C33
 89    92    1 ;     C31 - H31
 89    94    1 ;     C31 - H32
 89    96    1 ;     C31 - H33
 89    97    1 ;     C31 - H34
 90    92    1 ;     C32 - H31
 90    94    1 ;     C32 - H32
 90    99    1 ;     C32 - H35
 90   100     1 ;     C32 - H36
 91    95    1 ;     C33 - C35
 91    98    1 ;     C33 - C36
 91   124     1 ;     C33 - O12
 91   125     1 ;     C33 - O13
 92    94    1 ;     H31 - H32
 93    96    1 ;     C34 - H33
 93    97    1 ;     C34 - H34
 93    99    1 ;     C34 - H35
 93   100     1 ;     C34 - H36
 93   124     1 ;     C34 - O12
 93   125     1 ;     C34 - O13
 94    95    1 ;     H32 - C35
 94    98    1 ;     H32 - C36
 95   104     1 ;     C35 - H37
 95   105     1 ;     C35 - C40
 95   124     1 ;     C35 - O12
 95   126     1 ;     C35 - O14
 96   101     1 ;     H33 - C37
 96   103     1 ;     H33 - C39
 97   101     1 ;     H34 - C37
 97   103     1 ;     H34 - C39
 98   104     1 ;     C36 - H37
 98   105     1 ;     C36 - C40
 98   117     1 ;     C36 - O5
 98   125     1 ;     C36 - O13
 99   102     1 ;     H35 - C38
 99   103     1 ;     H35 - C39
100   102     1 ;     H36 - C38
100   103     1 ;     H36 - C39
101   104     1 ;     C37 - H37
101   106     1 ;     C37 - H38
101   108     1 ;     C37 - H39
101   109     1 ;     C37 - H40
102   104     1 ;     C38 - H37
102   106     1 ;     C38 - H38
102   111     1 ;     C38 - H41
102   112     1 ;     C38 - H42
103   107     1 ;     C39 - C41
103   110     1 ;     C39 - C42
103   117     1 ;     C39 - O5
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   103     126     1 ;     C39 - O14
   104     106     1 ;     H37 - H38
   105     108     1 ;     C40 - H39
   105     109     1 ;     C40 - H40
   105     111     1 ;     C40 - H41
   105     112     1 ;     C40 - H42
   105     117     1 ;     C40 - O5
   105     126     1 ;     C40 - O14
   106     107     1 ;     H38 - C41
   106     110     1 ;     H38 - C42
   107     2     1 ;     C41 - N2
   107     3     1 ;     C41 - N3
   107     32     1 ;     C41 - H1
   107     33     1 ;     C41 - C4
   107     114     1 ;     C41 - O2
   107     126     1 ;     C41 - O14
   110     113     1 ;     C42 - O1
   110     117     1 ;     C42 - O5

[ angles ]
;    ai     aj     ak     funct     theta          cth
     1     29     3     1     1.1356e+02     6.1003e+02 ;     N1 - C1     - N3
     1     29     114     1     1.2305e+02     6.2107e+02 ;     N1 - C1     - O2
     1     31     2     1     1.1265e+02     5.7773e+02 ;     N1 - C3     - N2
     1     31     32     1     1.0728e+02     4.2016e+02 ;     N1 - C3     - H1
     1     31     33     1     1.1161e+02     5.5153e+02 ;     N1 - C3     - C4
     1     107     27     1     1.1265e+02     5.7773e+02 ;     N1 - C41     - N27
     1     107     108     1     1.0728e+02     4.2016e+02 ;     N1 - C41     - H39
     1     107     109     1     1.0728e+02     4.2016e+02 ;     N1 - C41     - H40
     2     30     4     1     1.1356e+02     6.1003e+02 ;     N2 - C2     - N4
     2     30     113     1     1.2305e+02     6.2107e+02 ;     N2 - C2     - O1
     2     31     32     1     1.0728e+02     4.2016e+02 ;     N2 - C3     - H1
     2     31     33     1     1.1161e+02     5.5153e+02 ;     N2 - C3     - C4
     2     110     28     1     1.1265e+02     5.7773e+02 ;     N2 - C42     - N28
     2     110     111     1     1.0728e+02     4.2016e+02 ;     N2 - C42     - H41
     2     110     112     1     1.0728e+02     4.2016e+02 ;     N2 - C42     - H42
     3     29     114     1     1.2305e+02     6.2107e+02 ;     N3 - C1     - O2
     3     33     4     1     1.1265e+02     5.7773e+02 ;     N3 - C4     - N4
     3     33     31     1     1.1161e+02     5.5153e+02 ;     N3 - C4     - C3
     3     33     34     1     1.0728e+02     4.2016e+02 ;     N3 - C4     - H2
     3     35     5     1     1.1265e+02     5.7773e+02 ;     N3 - C5     - N5
     3     35     36     1     1.0728e+02     4.2016e+02 ;     N3 - C5     - H3
     3     35     37     1     1.0728e+02     4.2016e+02 ;     N3 - C5     - H4
     4     30     113     1     1.2305e+02     6.2107e+02 ;     N4 - C2     - O1
     4     33     31     1     1.1161e+02     5.5153e+02 ;     N4 - C4     - C3
     4     33     34     1     1.0728e+02     4.2016e+02 ;     N4 - C4     - H2
     4     38     6     1     1.1265e+02     5.7773e+02 ;     N4 - C6     - N6
     4     38     39     1     1.0728e+02     4.2016e+02 ;     N4 - C6     - H5
     4     38     40     1     1.0728e+02     4.2016e+02 ;     N4 - C6     - H6
     5     35     36     1     1.0728e+02     4.2016e+02 ;     N5 - C5     - H3
     5     35     37     1     1.0728e+02     4.2016e+02 ;     N5 - C5     - H4
     5     41     7     1     1.1356e+02     6.1003e+02 ;     N5 - C7     - N7
     5     41     115     1     1.2305e+02     6.2107e+02 ;     N5 - C7     - O3
     5     43     6     1     1.1265e+02     5.7773e+02 ;     N5 - C9     - N6
     5     43     44     1     1.0728e+02     4.2016e+02 ;     N5 - C9     - H7
     5     43     45     1     1.1161e+02     5.5153e+02 ;     N5 - C9     - C10
     6     38     39     1     1.0728e+02     4.2016e+02 ;     N6 - C6     - H5
     6     38     40     1     1.0728e+02     4.2016e+02 ;     N6 - C6     - H6
     6     42     8     1     1.1356e+02     6.1003e+02 ;     N6 - C8     - N8
     6     42     116     1     1.2305e+02     6.2107e+02 ;     N6 - C8     - O4
     6     43     44     1     1.0728e+02     4.2016e+02 ;     N6 - C9     - H7
     6     43     45     1     1.1161e+02     5.5153e+02 ;     N6 - C9     - C10
     7     41     115     1     1.2305e+02     6.2107e+02 ;     N7 - C7     - O3
     7     45     8     1     1.1265e+02     5.7773e+02 ;     N7 - C10     - N8
     7     45     43     1     1.1161e+02     5.5153e+02 ;     N7 - C10     - C9
     7     45     46     1     1.0728e+02     4.2016e+02 ;     N7 - C10     - H8
     7     47     9     1     1.1265e+02     5.7773e+02 ;     N7 - C11     - N9
     7     47     48     1     1.0728e+02     4.2016e+02 ;     N7 - C11     - H9
     7     47     49     1     1.0728e+02     4.2016e+02 ;     N7 - C11     - H10
     8     42     116     1     1.2305e+02     6.2107e+02 ;     N8 - C8     - O4
     8     45     43     1     1.1161e+02     5.5153e+02 ;     N8 - C10     - C9
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8	45	46	1	1.0728e+02	4.2016e+02 ;	N8 - C10 - H8
8	50	10	1	1.1265e+02	5.7773e+02 ;	N8 - C12 - N10
8	50	51	1	1.0728e+02	4.2016e+02 ;	N8 - C12 - H11
8	50	52	1	1.0728e+02	4.2016e+02 ;	N8 - C12 - H12
9	47	48	1	1.0728e+02	4.2016e+02 ;	N9 - C11 - H9
9	47	49	1	1.0728e+02	4.2016e+02 ;	N9 - C11 - H10
9	53	11	1	1.1356e+02	6.1003e+02 ;	N9 - C13 - N11
9	53	118	1	1.2305e+02	6.2107e+02 ;	N9 - C13 - O6
9	55	10	1	1.1265e+02	5.7773e+02 ;	N9 - C15 - N10
9	55	56	1	1.0728e+02	4.2016e+02 ;	N9 - C15 - H13
9	55	57	1	1.1161e+02	5.5153e+02 ;	N9 - C15 - C16
10	50	51	1	1.0728e+02	4.2016e+02 ;	N10 - C12 - H11
10	50	52	1	1.0728e+02	4.2016e+02 ;	N10 - C12 - H12
10	54	12	1	1.1356e+02	6.1003e+02 ;	N10 - C14 - N12
10	54	119	1	1.2305e+02	6.2107e+02 ;	N10 - C14 - O7
10	55	56	1	1.0728e+02	4.2016e+02 ;	N10 - C15 - H13
10	55	57	1	1.1161e+02	5.5153e+02 ;	N10 - C15 - C16
11	53	118	1	1.2305e+02	6.2107e+02 ;	N11 - C13 - O6
11	57	12	1	1.1265e+02	5.7773e+02 ;	N11 - C16 - N12
11	57	55	1	1.1161e+02	5.5153e+02 ;	N11 - C16 - C15
11	57	58	1	1.0728e+02	4.2016e+02 ;	N11 - C16 - H14
11	59	13	1	1.1265e+02	5.7773e+02 ;	N11 - C17 - N13
11	59	60	1	1.0728e+02	4.2016e+02 ;	N11 - C17 - H15
11	59	61	1	1.0728e+02	4.2016e+02 ;	N11 - C17 - H16
12	54	119	1	1.2305e+02	6.2107e+02 ;	N12 - C14 - O7
12	57	55	1	1.1161e+02	5.5153e+02 ;	N12 - C16 - C15
12	57	58	1	1.0728e+02	4.2016e+02 ;	N12 - C16 - H14
12	62	14	1	1.1265e+02	5.7773e+02 ;	N12 - C18 - N14
12	62	63	1	1.0728e+02	4.2016e+02 ;	N12 - C18 - H17
12	62	64	1	1.0728e+02	4.2016e+02 ;	N12 - C18 - H18
13	59	60	1	1.0728e+02	4.2016e+02 ;	N13 - C17 - H15
13	59	61	1	1.0728e+02	4.2016e+02 ;	N13 - C17 - H16
13	65	15	1	1.1356e+02	6.1003e+02 ;	N13 - C19 - N15
13	65	120	1	1.2305e+02	6.2107e+02 ;	N13 - C19 - O8
13	67	14	1	1.1265e+02	5.7773e+02 ;	N13 - C21 - N14
13	67	68	1	1.0728e+02	4.2016e+02 ;	N13 - C21 - H19
13	67	69	1	1.1161e+02	5.5153e+02 ;	N13 - C21 - C22
14	62	63	1	1.0728e+02	4.2016e+02 ;	N14 - C18 - H17
14	62	64	1	1.0728e+02	4.2016e+02 ;	N14 - C18 - H18
14	66	16	1	1.1356e+02	6.1003e+02 ;	N14 - C20 - N16
14	66	121	1	1.2305e+02	6.2107e+02 ;	N14 - C20 - O9
14	67	68	1	1.0728e+02	4.2016e+02 ;	N14 - C21 - H19
14	67	69	1	1.1161e+02	5.5153e+02 ;	N14 - C21 - C22
15	65	120	1	1.2305e+02	6.2107e+02 ;	N15 - C19 - O8
15	69	16	1	1.1265e+02	5.7773e+02 ;	N15 - C22 - N16
15	69	67	1	1.1161e+02	5.5153e+02 ;	N15 - C22 - C21
15	69	70	1	1.0728e+02	4.2016e+02 ;	N15 - C22 - H20
15	71	17	1	1.1265e+02	5.7773e+02 ;	N15 - C23 - N17
15	71	72	1	1.0728e+02	4.2016e+02 ;	N15 - C23 - H21
15	71	73	1	1.0728e+02	4.2016e+02 ;	N15 - C23 - H22
16	66	121	1	1.2305e+02	6.2107e+02 ;	N16 - C20 - O9
16	69	67	1	1.1161e+02	5.5153e+02 ;	N16 - C22 - C21
16	69	70	1	1.0728e+02	4.2016e+02 ;	N16 - C22 - H20
16	74	18	1	1.1265e+02	5.7773e+02 ;	N16 - C24 - N18
16	74	75	1	1.0728e+02	4.2016e+02 ;	N16 - C24 - H23
16	74	76	1	1.0728e+02	4.2016e+02 ;	N16 - C24 - H24
17	71	72	1	1.0728e+02	4.2016e+02 ;	N17 - C23 - H21
17	71	73	1	1.0728e+02	4.2016e+02 ;	N17 - C23 - H22
17	77	19	1	1.1356e+02	6.1003e+02 ;	N17 - C25 - N19
17	77	122	1	1.2305e+02	6.2107e+02 ;	N17 - C25 - O10
17	79	18	1	1.1265e+02	5.7773e+02 ;	N17 - C27 - N18
17	79	80	1	1.0728e+02	4.2016e+02 ;	N17 - C27 - H25
17	79	81	1	1.1161e+02	5.5153e+02 ;	N17 - C27 - C28
18	74	75	1	1.0728e+02	4.2016e+02 ;	N18 - C24 - H23
18	74	76	1	1.0728e+02	4.2016e+02 ;	N18 - C24 - H24
18	78	20	1	1.1356e+02	6.1003e+02 ;	N18 - C26 - N20
18	78	123	1	1.2305e+02	6.2107e+02 ;	N18 - C26 - O11
18	79	80	1	1.0728e+02	4.2016e+02 ;	N18 - C27 - H25
18	79	81	1	1.1161e+02	5.5153e+02 ;	N18 - C27 - C28
19	77	122	1	1.2305e+02	6.2107e+02 ;	N19 - C25 - O10
19	81	20	1	1.1265e+02	5.7773e+02 ;	N19 - C28 - N20

19	81	79	1	1.1161e+02	5.5153e+02 ;	N19	- C28	- C27
19	81	82	1	1.0728e+02	4.2016e+02 ;	N19	- C28	- H26
19	83	21	1	1.1265e+02	5.7773e+02 ;	N19	- C29	- N21
19	83	84	1	1.0728e+02	4.2016e+02 ;	N19	- C29	- H27
19	83	85	1	1.0728e+02	4.2016e+02 ;	N19	- C29	- H28
20	78	123	1	1.2305e+02	6.2107e+02 ;	N20	- C26	- O11
20	81	79	1	1.1161e+02	5.5153e+02 ;	N20	- C28	- C27
20	81	82	1	1.0728e+02	4.2016e+02 ;	N20	- C28	- H26
20	86	22	1	1.1265e+02	5.7773e+02 ;	N20	- C30	- N22
20	86	87	1	1.0728e+02	4.2016e+02 ;	N20	- C30	- H29
20	86	88	1	1.0728e+02	4.2016e+02 ;	N20	- C30	- H30
21	83	84	1	1.0728e+02	4.2016e+02 ;	N21	- C29	- H27
21	83	85	1	1.0728e+02	4.2016e+02 ;	N21	- C29	- H28
21	89	23	1	1.1356e+02	6.1003e+02 ;	N21	- C31	- N23
21	89	124	1	1.2305e+02	6.2107e+02 ;	N21	- C31	- O12
21	91	22	1	1.1265e+02	5.7773e+02 ;	N21	- C33	- N22
21	91	92	1	1.0728e+02	4.2016e+02 ;	N21	- C33	- H31
21	91	93	1	1.1161e+02	5.5153e+02 ;	N21	- C33	- C34
22	86	87	1	1.0728e+02	4.2016e+02 ;	N22	- C30	- H29
22	86	88	1	1.0728e+02	4.2016e+02 ;	N22	- C30	- H30
22	90	24	1	1.1356e+02	6.1003e+02 ;	N22	- C32	- N24
22	90	125	1	1.2305e+02	6.2107e+02 ;	N22	- C32	- O13
22	91	92	1	1.0728e+02	4.2016e+02 ;	N22	- C33	- H31
22	91	93	1	1.1161e+02	5.5153e+02 ;	N22	- C33	- C34
23	89	124	1	1.2305e+02	6.2107e+02 ;	N23	- C31	- O12
23	93	24	1	1.1265e+02	5.7773e+02 ;	N23	- C34	- N24
23	93	91	1	1.1161e+02	5.5153e+02 ;	N23	- C34	- C33
23	93	94	1	1.0728e+02	4.2016e+02 ;	N23	- C34	- H32
23	95	25	1	1.1265e+02	5.7773e+02 ;	N23	- C35	- N25
23	95	96	1	1.0728e+02	4.2016e+02 ;	N23	- C35	- H33
23	95	97	1	1.0728e+02	4.2016e+02 ;	N23	- C35	- H34
24	90	125	1	1.2305e+02	6.2107e+02 ;	N24	- C32	- O13
24	93	91	1	1.1161e+02	5.5153e+02 ;	N24	- C34	- C33
24	93	94	1	1.0728e+02	4.2016e+02 ;	N24	- C34	- H32
24	98	26	1	1.1265e+02	5.7773e+02 ;	N24	- C36	- N26
24	98	99	1	1.0728e+02	4.2016e+02 ;	N24	- C36	- H35
24	98	100	1	1.0728e+02	4.2016e+02 ;	N24	- C36	- H36
25	95	96	1	1.0728e+02	4.2016e+02 ;	N25	- C35	- H33
25	95	97	1	1.0728e+02	4.2016e+02 ;	N25	- C35	- H34
25	101	27	1	1.1356e+02	6.1003e+02 ;	N25	- C37	- N27
25	101	126	1	1.2305e+02	6.2107e+02 ;	N25	- C37	- O14
25	103	26	1	1.1265e+02	5.7773e+02 ;	N25	- C39	- N26
25	103	104	1	1.0728e+02	4.2016e+02 ;	N25	- C39	- H37
25	103	105	1	1.1161e+02	5.5153e+02 ;	N25	- C39	- C40
26	98	99	1	1.0728e+02	4.2016e+02 ;	N26	- C36	- H35
26	98	100	1	1.0728e+02	4.2016e+02 ;	N26	- C36	- H36
26	102	28	1	1.1356e+02	6.1003e+02 ;	N26	- C38	- N28
26	102	117	1	1.2305e+02	6.2107e+02 ;	N26	- C38	- O5
26	103	104	1	1.0728e+02	4.2016e+02 ;	N26	- C39	- H37
26	103	105	1	1.1161e+02	5.5153e+02 ;	N26	- C39	- C40
27	101	126	1	1.2305e+02	6.2107e+02 ;	N27	- C37	- O14
27	105	28	1	1.1265e+02	5.7773e+02 ;	N27	- C40	- N28
27	105	103	1	1.1161e+02	5.5153e+02 ;	N27	- C40	- C39
27	105	106	1	1.0728e+02	4.2016e+02 ;	N27	- C40	- H38
27	107	108	1	1.0728e+02	4.2016e+02 ;	N27	- C41	- H39
27	107	109	1	1.0728e+02	4.2016e+02 ;	N27	- C41	- H40
28	102	117	1	1.2305e+02	6.2107e+02 ;	N28	- C38	- O5
28	105	103	1	1.1161e+02	5.5153e+02 ;	N28	- C40	- C39
28	105	106	1	1.0728e+02	4.2016e+02 ;	N28	- C40	- H38
28	110	111	1	1.0728e+02	4.2016e+02 ;	N28	- C42	- H41
28	110	112	1	1.0728e+02	4.2016e+02 ;	N28	- C42	- H42
29	1	31	1	1.2069e+02	5.3045e+02 ;	C1	- N1	- C3
29	1	107	1	1.2069e+02	5.3045e+02 ;	C1	- N1	- C41
29	3	33	1	1.2069e+02	5.3045e+02 ;	C1	- N3	- C4
29	3	35	1	1.2069e+02	5.3045e+02 ;	C1	- N3	- C5
30	2	31	1	1.2069e+02	5.3045e+02 ;	C2	- N2	- C3
30	2	110	1	1.2069e+02	5.3045e+02 ;	C2	- N2	- C42
30	4	33	1	1.2069e+02	5.3045e+02 ;	C2	- N4	- C4
30	4	38	1	1.2069e+02	5.3045e+02 ;	C2	- N4	- C6
31	1	107	1	1.1564e+02	5.2744e+02 ;	C3	- N1	- C41
31	2	110	1	1.1564e+02	5.2744e+02 ;	C3	- N2	- C42

31	33	34	1	1.1022e+02	3.8702e+02 ;	C3 - C4	- H2
32	31	33	1	1.1022e+02	3.8702e+02 ;	H1 - C3	- C4
33	3	35	1	1.1564e+02	5.2744e+02 ;	C4 - N3	- C5
33	4	38	1	1.1564e+02	5.2744e+02 ;	C4 - N4	- C6
35	5	41	1	1.2069e+02	5.3045e+02 ;	C5 - N5	- C7
35	5	43	1	1.1564e+02	5.2744e+02 ;	C5 - N5	- C9
36	35	37	1	1.1020e+02	3.2602e+02 ;	H3 - C5	- H4
38	6	42	1	1.2069e+02	5.3045e+02 ;	C6 - N6	- C8
38	6	43	1	1.1564e+02	5.2744e+02 ;	C6 - N6	- C9
39	38	40	1	1.1020e+02	3.2602e+02 ;	H5 - C6	- H6
41	5	43	1	1.2069e+02	5.3045e+02 ;	C7 - N5	- C9
41	7	45	1	1.2069e+02	5.3045e+02 ;	C7 - N7	- C10
41	7	47	1	1.2069e+02	5.3045e+02 ;	C7 - N7	- C11
42	6	43	1	1.2069e+02	5.3045e+02 ;	C8 - N6	- C9
42	8	45	1	1.2069e+02	5.3045e+02 ;	C8 - N8	- C10
42	8	50	1	1.2069e+02	5.3045e+02 ;	C8 - N8	- C12
43	45	46	1	1.1022e+02	3.8702e+02 ;	C9 - C10	- H8
44	43	45	1	1.1022e+02	3.8702e+02 ;	H7 - C9	- C10
45	7	47	1	1.1564e+02	5.2744e+02 ;	C10 - N7	- C11
45	8	50	1	1.1564e+02	5.2744e+02 ;	C10 - N8	- C12
47	9	53	1	1.2069e+02	5.3045e+02 ;	C11 - N9	- C13
47	9	55	1	1.1564e+02	5.2744e+02 ;	C11 - N9	- C15
48	47	49	1	1.1020e+02	3.2602e+02 ;	H9 - C11	- H10
50	10	54	1	1.2069e+02	5.3045e+02 ;	C12 - N10	- C14
50	10	55	1	1.1564e+02	5.2744e+02 ;	C12 - N10	- C15
51	50	52	1	1.1020e+02	3.2602e+02 ;	H11 - C12	- H12
53	9	55	1	1.2069e+02	5.3045e+02 ;	C13 - N9	- C15
53	11	57	1	1.2069e+02	5.3045e+02 ;	C13 - N11	- C16
53	11	59	1	1.2069e+02	5.3045e+02 ;	C13 - N11	- C17
54	10	55	1	1.2069e+02	5.3045e+02 ;	C14 - N10	- C15
54	12	57	1	1.2069e+02	5.3045e+02 ;	C14 - N12	- C16
54	12	62	1	1.2069e+02	5.3045e+02 ;	C14 - N12	- C18
55	57	58	1	1.1022e+02	3.8702e+02 ;	C15 - C16	- H14
56	55	57	1	1.1022e+02	3.8702e+02 ;	H13 - C15	- C16
57	11	59	1	1.1564e+02	5.2744e+02 ;	C16 - N11	- C17
57	12	62	1	1.1564e+02	5.2744e+02 ;	C16 - N12	- C18
59	13	65	1	1.2069e+02	5.3045e+02 ;	C17 - N13	- C19
59	13	67	1	1.1564e+02	5.2744e+02 ;	C17 - N13	- C21
60	59	61	1	1.1020e+02	3.2602e+02 ;	H15 - C17	- H16
62	14	66	1	1.2069e+02	5.3045e+02 ;	C18 - N14	- C20
62	14	67	1	1.1564e+02	5.2744e+02 ;	C18 - N14	- C21
63	62	64	1	1.1020e+02	3.2602e+02 ;	H17 - C18	- H18
65	13	67	1	1.2069e+02	5.3045e+02 ;	C19 - N13	- C21
65	15	69	1	1.2069e+02	5.3045e+02 ;	C19 - N15	- C22
65	15	71	1	1.2069e+02	5.3045e+02 ;	C19 - N15	- C23
66	14	67	1	1.2069e+02	5.3045e+02 ;	C20 - N14	- C21
66	16	69	1	1.2069e+02	5.3045e+02 ;	C20 - N16	- C22
66	16	74	1	1.2069e+02	5.3045e+02 ;	C20 - N16	- C24
67	69	70	1	1.1022e+02	3.8702e+02 ;	C21 - C22	- H20
68	67	69	1	1.1022e+02	3.8702e+02 ;	H19 - C21	- C22
69	15	71	1	1.1564e+02	5.2744e+02 ;	C22 - N15	- C23
69	16	74	1	1.1564e+02	5.2744e+02 ;	C22 - N16	- C24
71	17	77	1	1.2069e+02	5.3045e+02 ;	C23 - N17	- C25
71	17	79	1	1.1564e+02	5.2744e+02 ;	C23 - N17	- C27
72	71	73	1	1.1020e+02	3.2602e+02 ;	H21 - C23	- H22
74	18	78	1	1.2069e+02	5.3045e+02 ;	C24 - N18	- C26
74	18	79	1	1.1564e+02	5.2744e+02 ;	C24 - N18	- C27
75	74	76	1	1.1020e+02	3.2602e+02 ;	H23 - C24	- H24
77	17	79	1	1.2069e+02	5.3045e+02 ;	C25 - N17	- C27
77	19	81	1	1.2069e+02	5.3045e+02 ;	C25 - N19	- C28
77	19	83	1	1.2069e+02	5.3045e+02 ;	C25 - N19	- C29
78	18	79	1	1.2069e+02	5.3045e+02 ;	C26 - N18	- C27
78	20	81	1	1.2069e+02	5.3045e+02 ;	C26 - N20	- C28
78	20	86	1	1.2069e+02	5.3045e+02 ;	C26 - N20	- C30
79	81	82	1	1.1022e+02	3.8702e+02 ;	C27 - C28	- H26
80	79	81	1	1.1022e+02	3.8702e+02 ;	H25 - C27	- C28
81	19	83	1	1.1564e+02	5.2744e+02 ;	C28 - N19	- C29
81	20	86	1	1.1564e+02	5.2744e+02 ;	C28 - N20	- C30
83	21	89	1	1.2069e+02	5.3045e+02 ;	C29 - N21	- C31
83	21	91	1	1.1564e+02	5.2744e+02 ;	C29 - N21	- C33
84	83	85	1	1.1020e+02	3.2602e+02 ;	H27 - C29	- H28

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    86    22    90     1    1.2069e+02    5.3045e+02 ;    C30 - N22    - C32
    86    22    91     1    1.1564e+02    5.2744e+02 ;    C30 - N22    - C33
    87    86    88     1    1.1020e+02    3.2602e+02 ;    H29 - C30    - H30
    89    21    91     1    1.2069e+02    5.3045e+02 ;    C31 - N21    - C33
    89    23    93     1    1.2069e+02    5.3045e+02 ;    C31 - N23    - C34
    89    23    95     1    1.2069e+02    5.3045e+02 ;    C31 - N23    - C35
    90    22    91     1    1.2069e+02    5.3045e+02 ;    C32 - N22    - C33
    90    24    93     1    1.2069e+02    5.3045e+02 ;    C32 - N24    - C34
    90    24    98     1    1.2069e+02    5.3045e+02 ;    C32 - N24    - C36
    91    93    94     1    1.1022e+02    3.8702e+02 ;    C33 - C34    - H32
    92    91    93     1    1.1022e+02    3.8702e+02 ;    H31 - C33    - C34
    93    23    95     1    1.1564e+02    5.2744e+02 ;    C34 - N23    - C35
    93    24    98     1    1.1564e+02    5.2744e+02 ;    C34 - N24    - C36
    95    25   101     1    1.2069e+02    5.3045e+02 ;    C35 - N25    - C37
    95    25   103     1    1.1564e+02    5.2744e+02 ;    C35 - N25    - C39
    96    95    97     1    1.1020e+02    3.2602e+02 ;    H33 - C35    - H34
    98    26   102     1    1.2069e+02    5.3045e+02 ;    C36 - N26    - C38
    98    26   103     1    1.1564e+02    5.2744e+02 ;    C36 - N26    - C39
    99    98   100     1    1.1020e+02    3.2602e+02 ;    H35 - C36    - H36
   101    25   103     1    1.2069e+02    5.3045e+02 ;    C37 - N25    - C39
   101    27   105     1    1.2069e+02    5.3045e+02 ;    C37 - N27    - C40
   101    27   107     1    1.2069e+02    5.3045e+02 ;    C37 - N27    - C41
   102    26   103     1    1.2069e+02    5.3045e+02 ;    C38 - N26    - C39
   102    28   105     1    1.2069e+02    5.3045e+02 ;    C38 - N28    - C40
   102    28   110     1    1.2069e+02    5.3045e+02 ;    C38 - N28    - C42
   103   105   106     1    1.1022e+02    3.8702e+02 ;    C39 - C40    - H38
   104   103   105     1    1.1022e+02    3.8702e+02 ;    H37 - C39    - C40
   105    27   107     1    1.1564e+02    5.2744e+02 ;    C40 - N27    - C41
   105    28   110     1    1.1564e+02    5.2744e+02 ;    C40 - N28    - C42
   108   107   109     1    1.1020e+02    3.2602e+02 ;    H39 - C41    - H40
   111   110   112     1    1.1020e+02    3.2602e+02 ;    H41 - C42    - H42

[ dihedrals ] ; propers
; treated as RBs in GROMACS to use combine multiple AMBER torsions per quartet
;    i    j    k    l  func       C0         C1         C2         C3         C4         C5
1    29   3    33   3   20.92000    0.00000  -20.92000    0.00000    0.00000    0.00000 ;   N1-   C1-   N3-   C4
1    29   3    35   3   20.92000    0.00000  -20.92000    0.00000    0.00000    0.00000 ;   N1-   C1-   N3-   C5
1    31   2    30   3    0.00000    0.00000    0.00000    0.00000    0.00000    0.00000 ;   N1-   C3-   N2-   C2
1    31   2    110  3    0.00000    0.00000    0.00000    0.00000    0.00000    0.00000 ;   N1-   C3-   N2-   C42
1    31   33   3    3    0.65084    1.95253    0.00000   -2.60338    0.00000    0.00000 ;   N1-   C3-   C4-   N3
1    31   33   4    3    0.65084    1.95253    0.00000   -2.60338    0.00000    0.00000 ;   N1-   C3-   C4-   N4
1    31   33   34   3    0.65084    1.95253    0.00000   -2.60338    0.00000    0.00000 ;   N1-   C3-   C4-   H2
1    107  27   101  3    0.00000    0.00000    0.00000    0.00000    0.00000    0.00000 ;   N1-   C41-  N27-  C37
1    107  27   105  3    0.00000    0.00000    0.00000    0.00000    0.00000    0.00000 ;   N1-   C41-  N27-  C40
2    30   4    33   3   20.92000    0.00000   -20.92000    0.00000    0.00000    0.00000 ;   N2-   C2-   N4-   C4
2    30   4    38   3   20.92000    0.00000   -20.92000    0.00000    0.00000    0.00000 ;   N2-   C2-   N4-   C6
2    31   33   3    3    0.65084    1.95253    0.00000   -2.60338    0.00000    0.00000 ;   N2-   C3-   C4-   N3
2    31   33   4    3    0.65084    1.95253    0.00000   -2.60338    0.00000    0.00000 ;   N2-   C3-   C4-   N4
2    31   33   34   3    0.65084    1.95253    0.00000   -2.60338    0.00000    0.00000 ;   N2-   C3-   C4-   H2
2    110  28   102  3    0.00000    0.00000    0.00000    0.00000    0.00000    0.00000 ;   N2-   C42-  N28-  C38
2    110  28   105  3    0.00000    0.00000    0.00000    0.00000    0.00000    0.00000 ;   N2-   C42-  N28-  C40
3    33   4    30   3    0.00000    0.00000    0.00000    0.00000    0.00000    0.00000 ;   N3-   C4-   N4-   C2
3    33   4    38   3    0.00000    0.00000    0.00000    0.00000    0.00000    0.00000 ;   N3-   C4-   N4-   C6
3    33   31   32   3    0.65084    1.95253    0.00000   -2.60338    0.00000    0.00000 ;   N3-   C4-   C3-   H1
3    35   5    41   3    0.00000    0.00000    0.00000    0.00000    0.00000    0.00000 ;   N3-   C5-   N5-   C7
3    35   5    43   3    0.00000    0.00000    0.00000    0.00000    0.00000    0.00000 ;   N3-   C5-   N5-   C9
4    30   2    31   3   20.92000    0.00000   -20.92000    0.00000    0.00000    0.00000 ;   N4-   C2-   N2-   C3
4    30   2    110  3   20.92000    0.00000   -20.92000    0.00000    0.00000    0.00000 ;   N4-   C2-   N2-   C42
4    33   3    29   3    0.00000    0.00000    0.00000    0.00000    0.00000    0.00000 ;   N4-   C4-   N3-   C1
4    33   3    35   3    0.00000    0.00000    0.00000    0.00000    0.00000    0.00000 ;   N4-   C4-   N3-   C5
4    33   31   32   3    0.65084    1.95253    0.00000   -2.60338    0.00000    0.00000 ;   N4-   C4-   C3-   H1
4    38   6    42   3    0.00000    0.00000    0.00000    0.00000    0.00000    0.00000 ;   N4-   C6-   N6-   C8
4    38   6    43   3    0.00000    0.00000    0.00000    0.00000    0.00000    0.00000 ;   N4-   C6-   N6-   C9
5    35   3    29   3    0.00000    0.00000    0.00000    0.00000    0.00000    0.00000 ;   N5-   C5-   N3-   C1
5    35   3    33   3    0.00000    0.00000    0.00000    0.00000    0.00000    0.00000 ;   N5-   C5-   N3-   C4
5    41   7    45   3   20.92000    0.00000   -20.92000    0.00000    0.00000    0.00000 ;   N5-   C7-   N7-   C10
5    41   7    47   3   20.92000    0.00000   -20.92000    0.00000    0.00000    0.00000 ;   N5-   C7-   N7-   C11
5    43   6    38   3    0.00000    0.00000    0.00000    0.00000    0.00000    0.00000 ;   N5-   C9-   N6-   C6
5    43   6    42   3    0.00000    0.00000    0.00000    0.00000    0.00000    0.00000 ;   N5-   C9-   N6-   C8
5    43   45   7    3    0.65084    1.95253    0.00000   -2.60338    0.00000    0.00000 ;   N5-   C9-   C10-  N7
5    43   45   8    3    0.65084    1.95253    0.00000   -2.60338    0.00000    0.00000 ;   N5-   C9-   C10-  N8
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5 43 45 46 3 0.65084 1.95253 0.00000 -2.60338 0.00000 0.00000 ; N5- C9- C10- H8
6 38 4 30 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; N6- C6- N4- C2
6 38 4 33 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; N6- C6- N4- C4
6 42 8 45 3 20.92000 0.00000 -20.92000 0.00000 0.00000 0.00000 ; N6- C8- N8- C10
6 42 8 50 3 20.92000 0.00000 -20.92000 0.00000 0.00000 0.00000 ; N6- C8- N8- C12
6 43 5 35 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; N6- C9- N5- C5
6 43 5 41 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; N6- C9- N5- C7
6 43 45 7 3 0.65084 1.95253 0.00000 -2.60338 0.00000 0.00000 ; N6- C9- C10- N7
6 43 45 8 3 0.65084 1.95253 0.00000 -2.60338 0.00000 0.00000 ; N6- C9- C10- N8
6 43 45 46 3 0.65084 1.95253 0.00000 -2.60338 0.00000 0.00000 ; N6- C9- C10- H8
7 41 5 35 3 20.92000 0.00000 -20.92000 0.00000 0.00000 0.00000 ; N7- C7- N5- C5
7 41 5 43 3 20.92000 0.00000 -20.92000 0.00000 0.00000 0.00000 ; N7- C7- N5- C9
7 45 8 42 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; N7- C10- N8- C8
7 45 8 50 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; N7- C10- N8- C12
7 45 43 44 3 0.65084 1.95253 0.00000 -2.60338 0.00000 0.00000 ; N7- C10- C9- H7
7 47 9 53 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; N7- C11- N9- C13
7 47 9 55 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; N7- C11- N9- C15
8 42 6 38 3 20.92000 0.00000 -20.92000 0.00000 0.00000 0.00000 ; N8- C8- N6- C6
8 42 6 43 3 20.92000 0.00000 -20.92000 0.00000 0.00000 0.00000 ; N8- C8- N6- C9
8 45 7 41 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; N8- C10- N7- C7
8 45 7 47 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; N8- C10- N7- C11
8 45 43 44 3 0.65084 1.95253 0.00000 -2.60338 0.00000 0.00000 ; N8- C10- C9- H7
8 50 10 54 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; N8- C12- N10- C14
8 50 10 55 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; N8- C12- N10- C15
9 47 7 41 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; N9- C11- N7- C7
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9 53 11 59 3 20.92000 0.00000 -20.92000 0.00000 0.00000 0.00000 ; N9- C13- N11- C17
9 55 10 50 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; N9- C15- N10- C12
9 55 10 54 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; N9- C15- N10- C14
9 55 57 11 3 0.65084 1.95253 0.00000 -2.60338 0.00000 0.00000 ; N9- C15- C16- N11
9 55 57 12 3 0.65084 1.95253 0.00000 -2.60338 0.00000 0.00000 ; N9- C15- C16- N12
9 55 57 58 3 0.65084 1.95253 0.00000 -2.60338 0.00000 0.00000 ; N9- C15- C16- H14
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10 50 8 45 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; N10- C12- N8- C10
10 54 12 57 3 20.92000 0.00000 -20.92000 0.00000 0.00000 0.00000 ; N10- C14- N12- C16
10 54 12 62 3 20.92000 0.00000 -20.92000 0.00000 0.00000 0.00000 ; N10- C14- N12- C18
10 55 9 47 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; N10- C15- N9- C11
10 55 9 53 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; N10- C15- N9- C13
10 55 57 11 3 0.65084 1.95253 0.00000 -2.60338 0.00000 0.00000 ; N10- C15- C16- N11
10 55 57 12 3 0.65084 1.95253 0.00000 -2.60338 0.00000 0.00000 ; N10- C15- C16- N12
10 55 57 58 3 0.65084 1.95253 0.00000 -2.60338 0.00000 0.00000 ; N10- C15- C16- H14
11 53 9 47 3 20.92000 0.00000 -20.92000 0.00000 0.00000 0.00000 ; N11- C13- N9- C11
11 53 9 55 3 20.92000 0.00000 -20.92000 0.00000 0.00000 0.00000 ; N11- C13- N9- C15
11 57 12 54 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; N11- C16- N12- C14
11 57 12 62 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; N11- C16- N12- C18
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11 59 13 65 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; N11- C17- N13- C19
11 59 13 67 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; N11- C17- N13- C21
12 54 10 50 3 20.92000 0.00000 -20.92000 0.00000 0.00000 0.00000 ; N12- C14- N10- C12
12 54 10 55 3 20.92000 0.00000 -20.92000 0.00000 0.00000 0.00000 ; N12- C14- N10- C15
12 57 11 53 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; N12- C16- N11- C13
12 57 11 59 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; N12- C16- N11- C17
12 57 55 56 3 0.65084 1.95253 0.00000 -2.60338 0.00000 0.00000 ; N12- C16- C15- H13
12 62 14 66 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; N12- C18- N14- C20
12 62 14 67 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; N12- C18- N14- C21
13 59 11 53 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; N13- C17- N11- C13
13 59 11 57 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; N13- C17- N11- C16
13 65 15 69 3 20.92000 0.00000 -20.92000 0.00000 0.00000 0.00000 ; N13- C19- N15- C22
13 65 15 71 3 20.92000 0.00000 -20.92000 0.00000 0.00000 0.00000 ; N13- C19- N15- C23
13 67 14 62 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; N13- C21- N14- C18
13 67 14 66 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; N13- C21- N14- C20
13 67 69 15 3 0.65084 1.95253 0.00000 -2.60338 0.00000 0.00000 ; N13- C21- C22- N15
13 67 69 16 3 0.65084 1.95253 0.00000 -2.60338 0.00000 0.00000 ; N13- C21- C22- N16
13 67 69 70 3 0.65084 1.95253 0.00000 -2.60338 0.00000 0.00000 ; N13- C21- C22- H20
14 62 12 54 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; N14- C18- N12- C14
14 62 12 57 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; N14- C18- N12- C16
14 66 16 69 3 20.92000 0.00000 -20.92000 0.00000 0.00000 0.00000 ; N14- C20- N16- C22
14 66 16 74 3 20.92000 0.00000 -20.92000 0.00000 0.00000 0.00000 ; N14- C20- N16- C24
14 67 13 59 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; N14- C21- N13- C17
14 67 13 65 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; N14- C21- N13- C19

14	67	69	15	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000 ;	N14-	C21-	C22-	N15
14	67	69	16	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000 ;	N14-	C21-	C22-	N16
14	67	69	70	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000 ;	N14-	C21-	C22-	H20
15	65	13	59	3	20.92000	0.00000	-20.92000	0.00000	0.00000	0.00000 ;	N15-	C19-	N13-	C17
15	65	13	67	3	20.92000	0.00000	-20.92000	0.00000	0.00000	0.00000 ;	N15-	C19-	N13-	C21
15	69	16	66	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 ;	N15-	C22-	N16-	C20
15	69	16	74	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 ;	N15-	C22-	N16-	C24
15	69	67	68	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000 ;	N15-	C22-	C21-	H19
15	71	17	77	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 ;	N15-	C23-	N17-	C25
15	71	17	79	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 ;	N15-	C23-	N17-	C27
16	66	14	62	3	20.92000	0.00000	-20.92000	0.00000	0.00000	0.00000 ;	N16-	C20-	N14-	C18
16	66	14	67	3	20.92000	0.00000	-20.92000	0.00000	0.00000	0.00000 ;	N16-	C20-	N14-	C21
16	69	15	65	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 ;	N16-	C22-	N15-	C19
16	69	15	71	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 ;	N16-	C22-	N15-	C23
16	69	67	68	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000 ;	N16-	C22-	C21-	H19
16	74	18	78	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 ;	N16-	C24-	N18-	C26
16	74	18	79	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 ;	N16-	C24-	N18-	C27
17	71	15	65	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 ;	N17-	C23-	N15-	C19
17	71	15	69	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 ;	N17-	C23-	N15-	C22
17	77	19	81	3	20.92000	0.00000	-20.92000	0.00000	0.00000	0.00000 ;	N17-	C25-	N19-	C28
17	77	19	83	3	20.92000	0.00000	-20.92000	0.00000	0.00000	0.00000 ;	N17-	C25-	N19-	C29
17	79	18	74	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 ;	N17-	C27-	N18-	C24
17	79	18	78	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 ;	N17-	C27-	N18-	C26
17	79	81	19	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000 ;	N17-	C27-	C28-	N19
17	79	81	20	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000 ;	N17-	C27-	C28-	N20
17	79	81	82	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000 ;	N17-	C27-	C28-	H26
18	74	16	66	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 ;	N18-	C24-	N16-	C20
18	74	16	69	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 ;	N18-	C24-	N16-	C22
18	78	20	81	3	20.92000	0.00000	-20.92000	0.00000	0.00000	0.00000 ;	N18-	C26-	N20-	C28
18	78	20	86	3	20.92000	0.00000	-20.92000	0.00000	0.00000	0.00000 ;	N18-	C26-	N20-	C30
18	79	17	71	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 ;	N18-	C27-	N17-	C23
18	79	17	77	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 ;	N18-	C27-	N17-	C25
18	79	81	19	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000 ;	N18-	C27-	C28-	N19
18	79	81	20	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000 ;	N18-	C27-	C28-	N20
18	79	81	82	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000 ;	N18-	C27-	C28-	H26
19	77	17	71	3	20.92000	0.00000	-20.92000	0.00000	0.00000	0.00000 ;	N19-	C25-	N17-	C23
19	77	17	79	3	20.92000	0.00000	-20.92000	0.00000	0.00000	0.00000 ;	N19-	C25-	N17-	C27
19	81	20	78	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 ;	N19-	C28-	N20-	C26
19	81	20	86	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 ;	N19-	C28-	N20-	C30
19	81	79	80	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000 ;	N19-	C28-	C27-	H25
19	83	21	89	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 ;	N19-	C29-	N21-	C31
19	83	21	91	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 ;	N19-	C29-	N21-	C33
20	78	18	74	3	20.92000	0.00000	-20.92000	0.00000	0.00000	0.00000 ;	N20-	C26-	N18-	C24
20	78	18	79	3	20.92000	0.00000	-20.92000	0.00000	0.00000	0.00000 ;	N20-	C26-	N18-	C27
20	81	19	77	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 ;	N20-	C28-	N19-	C25
20	81	19	83	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 ;	N20-	C28-	N19-	C29
20	81	79	80	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000 ;	N20-	C28-	C27-	H25
20	86	22	90	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 ;	N20-	C30-	N22-	C32
20	86	22	91	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 ;	N20-	C30-	N22-	C33
21	83	19	77	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 ;	N21-	C29-	N19-	C25
21	83	19	81	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 ;	N21-	C29-	N19-	C28
21	89	23	93	3	20.92000	0.00000	-20.92000	0.00000	0.00000	0.00000 ;	N21-	C31-	N23-	C34
21	89	23	95	3	20.92000	0.00000	-20.92000	0.00000	0.00000	0.00000 ;	N21-	C31-	N23-	C35
21	91	22	86	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 ;	N21-	C33-	N22-	C30
21	91	22	90	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 ;	N21-	C33-	N22-	C32
21	91	93	23	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000 ;	N21-	C33-	C34-	N23
21	91	93	24	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000 ;	N21-	C33-	C34-	N24
21	91	93	94	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000 ;	N21-	C33-	C34-	H32
22	86	20	78	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 ;	N22-	C30-	N20-	C26
22	86	20	81	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 ;	N22-	C30-	N20-	C28
22	90	24	93	3	20.92000	0.00000	-20.92000	0.00000	0.00000	0.00000 ;	N22-	C32-	N24-	C34
22	90	24	98	3	20.92000	0.00000	-20.92000	0.00000	0.00000	0.00000 ;	N22-	C32-	N24-	C36
22	91	21	83	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 ;	N22-	C33-	N21-	C29
22	91	21	89	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 ;	N22-	C33-	N21-	C31
22	91	93	23	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000 ;	N22-	C33-	C34-	N23
22	91	93	24	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000 ;	N22-	C33-	C34-	N24
22	91	93	94	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000 ;	N22-	C33-	C34-	H32
23	89	21	83	3	20.92000	0.00000	-20.92000	0.00000	0.00000	0.00000 ;	N23-	C31-	N21-	C29
23	89	21	91	3	20.92000	0.00000	-20.92000	0.00000	0.00000	0.00000 ;	N23-	C31-	N21-	C33
23	93	24	90	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 ;	N23-	C34-	N24-	C32
23	93	24	98	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 ;	N23-	C34-	N24-	C36

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23   93   91   92    3    0.65084    1.95253    0.00000   -2.60338    0.00000    0.00000 ;   N23-   C34-   C33-   H31
23   95   25   101   3    0.00000    0.00000    0.00000    0.00000    0.00000    0.00000 ;   N23-   C35-   N25-   C37
23   95   25   103   3    0.00000    0.00000    0.00000    0.00000    0.00000    0.00000 ;   N23-   C35-   N25-   C39
24   90   22   86    3   20.92000    0.00000  -20.92000    0.00000    0.00000    0.00000 ;   N24-   C32-   N22-   C30
24   90   22   91    3   20.92000    0.00000  -20.92000    0.00000    0.00000    0.00000 ;   N24-   C32-   N22-   C33
24   93   23   89    3    0.00000    0.00000    0.00000    0.00000    0.00000    0.00000 ;   N24-   C34-   N23-   C31
24   93   23   95    3    0.00000    0.00000    0.00000    0.00000    0.00000    0.00000 ;   N24-   C34-   N23-   C35
24   93   91   92    3    0.65084    1.95253    0.00000   -2.60338    0.00000    0.00000 ;   N24-   C34-   C33-   H31
24   98   26   102   3    0.00000    0.00000    0.00000    0.00000    0.00000    0.00000 ;   N24-   C36-   N26-   C38
24   98   26   103   3    0.00000    0.00000    0.00000    0.00000    0.00000    0.00000 ;   N24-   C36-   N26-   C39
25   95   23   89    3    0.00000    0.00000    0.00000    0.00000    0.00000    0.00000 ;   N25-   C35-   N23-   C31
25   95   23   93    3    0.00000    0.00000    0.00000    0.00000    0.00000    0.00000 ;   N25-   C35-   N23-   C34
25   101  27   105   3   20.92000    0.00000  -20.92000    0.00000    0.00000    0.00000 ;   N25-   C37-   N27-   C40
25   101  27   107   3   20.92000    0.00000  -20.92000    0.00000    0.00000    0.00000 ;   N25-   C37-   N27-   C41
25   103  26   98    3    0.00000    0.00000    0.00000    0.00000    0.00000    0.00000 ;   N25-   C39-   N26-   C36
25   103  26   102   3    0.00000    0.00000    0.00000    0.00000    0.00000    0.00000 ;   N25-   C39-   N26-   C38
25   103  105  27    3    0.65084    1.95253    0.00000   -2.60338    0.00000    0.00000 ;   N25-   C39-   C40-   N27
25   103  105  28    3    0.65084    1.95253    0.00000   -2.60338    0.00000    0.00000 ;   N25-   C39-   C40-   N28
25   103  105  106   3    0.65084    1.95253    0.00000   -2.60338    0.00000    0.00000 ;   N25-   C39-   C40-   H38
26   98   24   90    3    0.00000    0.00000    0.00000    0.00000    0.00000    0.00000 ;   N26-   C36-   N24-   C32
26   98   24   93    3    0.00000    0.00000    0.00000    0.00000    0.00000    0.00000 ;   N26-   C36-   N24-   C34
26   102  28   105   3   20.92000    0.00000  -20.92000    0.00000    0.00000    0.00000 ;   N26-   C38-   N28-   C40
26   102  28   110   3   20.92000    0.00000  -20.92000    0.00000    0.00000    0.00000 ;   N26-   C38-   N28-   C42
26   103  25   95    3    0.00000    0.00000    0.00000    0.00000    0.00000    0.00000 ;   N26-   C39-   N25-   C35
26   103  25   101   3    0.00000    0.00000    0.00000    0.00000    0.00000    0.00000 ;   N26-   C39-   N25-   C37
26   103  105  27    3    0.65084    1.95253    0.00000   -2.60338    0.00000    0.00000 ;   N26-   C39-   C40-   N27
26   103  105  28    3    0.65084    1.95253    0.00000   -2.60338    0.00000    0.00000 ;   N26-   C39-   C40-   N28
26   103  105  106   3    0.65084    1.95253    0.00000   -2.60338    0.00000    0.00000 ;   N26-   C39-   C40-   H38
27   101  25   95    3   20.92000    0.00000  -20.92000    0.00000    0.00000    0.00000 ;   N27-   C37-   N25-   C35
27   101  25   103   3   20.92000    0.00000  -20.92000    0.00000    0.00000    0.00000 ;   N27-   C37-   N25-   C39
27   105  28   102   3    0.00000    0.00000    0.00000    0.00000    0.00000    0.00000 ;   N27-   C40-   N28-   C38
27   105  28   110   3    0.00000    0.00000    0.00000    0.00000    0.00000    0.00000 ;   N27-   C40-   N28-   C42
27   105  103  104   3    0.65084    1.95253    0.00000   -2.60338    0.00000    0.00000 ;   N27-   C40-   C39-   H37
28   102  26   98    3   20.92000    0.00000  -20.92000    0.00000    0.00000    0.00000 ;   N28-   C38-   N26-   C36
28   102  26   103   3   20.92000    0.00000  -20.92000    0.00000    0.00000    0.00000 ;   N28-   C38-   N26-   C39
28   105  27   101   3    0.00000    0.00000    0.00000    0.00000    0.00000    0.00000 ;   N28-   C40-   N27-   C37
28   105  27   107   3    0.00000    0.00000    0.00000    0.00000    0.00000    0.00000 ;   N28-   C40-   N27-   C41
28   105  103  104   3    0.65084    1.95253    0.00000   -2.60338    0.00000    0.00000 ;   N28-   C40-   C39-   H37
28   110  2    30    3    0.00000    0.00000    0.00000    0.00000    0.00000    0.00000 ;   N28-   C42-   N2-    C2
28   110  2    31    3    0.00000    0.00000    0.00000    0.00000    0.00000    0.00000 ;   N28-   C42-   N2-    C3
29   1    31   2     3    0.00000    0.00000    0.00000    0.00000    0.00000    0.00000 ;   C1-    N1-    C3-    N2
29   1    31   32    3    0.00000    0.00000    0.00000    0.00000    0.00000    0.00000 ;   C1-    N1-    C3-    H1
29   1    31   33    3    2.84512   -4.10032   16.73600    2.51040  -16.73600    0.00000 ;   C1-    N1-    C3-    C4
29   1    107  27    3    0.00000    0.00000    0.00000    0.00000    0.00000    0.00000 ;   C1-    N1-    C41-   N27
29   1    107  108   3    0.00000    0.00000    0.00000    0.00000    0.00000    0.00000 ;   C1-    N1-    C41-   H39
29   1    107  109   3    0.00000    0.00000    0.00000    0.00000    0.00000    0.00000 ;   C1-    N1-    C41-   H40
29   3    33   31    3    2.84512   -4.10032   16.73600    2.51040  -16.73600    0.00000 ;   C1-    N3-    C4-    C3
29   3    33   34    3    0.00000    0.00000    0.00000    0.00000    0.00000    0.00000 ;   C1-    N3-    C4-    H2
29   3    35   36    3    0.00000    0.00000    0.00000    0.00000    0.00000    0.00000 ;   C1-    N3-    C5-    H3
29   3    35   37    3    0.00000    0.00000    0.00000    0.00000    0.00000    0.00000 ;   C1-    N3-    C5-    H4
30   2    31   32    3    0.00000    0.00000    0.00000    0.00000    0.00000    0.00000 ;   C2-    N2-    C3-    H1
30   2    31   33    3    2.84512   -4.10032   16.73600    2.51040  -16.73600    0.00000 ;   C2-    N2-    C3-    C4
30   2    110  111   3    0.00000    0.00000    0.00000    0.00000    0.00000    0.00000 ;   C2-    N2-    C42-   H41
30   2    110  112   3    0.00000    0.00000    0.00000    0.00000    0.00000    0.00000 ;   C2-    N2-    C42-   H42
30   4    33   31    3    2.84512   -4.10032   16.73600    2.51040  -16.73600    0.00000 ;   C2-    N4-    C4-    C3
30   4    33   34    3    0.00000    0.00000    0.00000    0.00000    0.00000    0.00000 ;   C2-    N4-    C4-    H2
30   4    38   39    3    0.00000    0.00000    0.00000    0.00000    0.00000    0.00000 ;   C2-    N4-    C6-    H5
30   4    38   40    3    0.00000    0.00000    0.00000    0.00000    0.00000    0.00000 ;   C2-    N4-    C6-    H6
31   1    29   3     3   20.92000    0.00000  -20.92000    0.00000    0.00000    0.00000 ;   C3-    N1-    C1-    N3
31   1    29   114   3   20.92000    0.00000  -20.92000    0.00000    0.00000    0.00000 ;   C3-    N1-    C1-    O2
31   1    107  27    3    0.00000    0.00000    0.00000    0.00000    0.00000    0.00000 ;   C3-    N1-    C41-   N27
31   1    107  108   3    0.00000    0.00000    0.00000    0.00000    0.00000    0.00000 ;   C3-    N1-    C41-   H39
31   1    107  109   3    0.00000    0.00000    0.00000    0.00000    0.00000    0.00000 ;   C3-    N1-    C41-   H40
31   2    30   113   3   20.92000    0.00000  -20.92000    0.00000    0.00000    0.00000 ;   C3-    N2-    C2-    O1
31   2    110  111   3    0.00000    0.00000    0.00000    0.00000    0.00000    0.00000 ;   C3-    N2-    C42-   H41
31   2    110  112   3    0.00000    0.00000    0.00000    0.00000    0.00000    0.00000 ;   C3-    N2-    C42-   H42
31   33   3    35    3    0.00000    0.00000    0.00000    0.00000    0.00000    0.00000 ;   C3-    C4-    N3-    C5
31   33   4    38    3    0.00000    0.00000    0.00000    0.00000    0.00000    0.00000 ;   C3-    C4-    N4-    C6
32   31   2    110   3    0.00000    0.00000    0.00000    0.00000    0.00000    0.00000 ;   H1-    C3-    N2-    C42
32   31   33   34    3    0.65084    1.95253    0.00000   -2.60338    0.00000    0.00000 ;   H1-    C3-    C4-    H2
33   3    29   114   3   20.92000    0.00000  -20.92000    0.00000    0.00000    0.00000 ;   C4-    N3-    C1-    O2
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33   3   35   36   3   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000 ;   C4-   N3-   C5-   H3
33   3   35   37   3   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000 ;   C4-   N3-   C5-   H4
33   4   30   113   3   20.92000   0.00000   -20.92000   0.00000   0.00000   0.00000 ;   C4-   N4-   C2-   O1
33   4   38   39   3   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000 ;   C4-   N4-   C6-   H5
33   4   38   40   3   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000 ;   C4-   N4-   C6-   H6
33   31   2   110   3   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000 ;   C4-   C3-   N2-   C42
34   33   3   35   3   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000 ;   H2-   C4-   N3-   C5
34   33   4   38   3   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000 ;   H2-   C4-   N4-   C6
35   3   29   114   3   20.92000   0.00000   -20.92000   0.00000   0.00000   0.00000 ;   C5-   N3-   C1-   O2
35   5   41   115   3   20.92000   0.00000   -20.92000   0.00000   0.00000   0.00000 ;   C5-   N5-   C7-   O3
35   5   43   44   3   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000 ;   C5-   N5-   C9-   H7
35   5   43   45   3   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000 ;   C5-   N5-   C9-   C10
36   35   5   41   3   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000 ;   H3-   C5-   N5-   C7
36   35   5   43   3   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000 ;   H3-   C5-   N5-   C9
37   35   5   41   3   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000 ;   H4-   C5-   N5-   C7
37   35   5   43   3   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000 ;   H4-   C5-   N5-   C9
38   4   30   113   3   20.92000   0.00000   -20.92000   0.00000   0.00000   0.00000 ;   C6-   N4-   C2-   O1
38   6   42   116   3   20.92000   0.00000   -20.92000   0.00000   0.00000   0.00000 ;   C6-   N6-   C8-   O4
38   6   43   44   3   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000 ;   C6-   N6-   C9-   H7
38   6   43   45   3   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000 ;   C6-   N6-   C9-   C10
39   38   6   42   3   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000 ;   H5-   C6-   N6-   C8
39   38   6   43   3   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000 ;   H5-   C6-   N6-   C9
40   38   6   42   3   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000 ;   H6-   C6-   N6-   C8
40   38   6   43   3   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000 ;   H6-   C6-   N6-   C9
41   5   43   44   3   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000 ;   C7-   N5-   C9-   H7
41   5   43   45   3   2.84512   -4.10032   16.73600   2.51040   -16.73600   0.00000 ;   C7-   N5-   C9-   C10
41   7   45   43   3   2.84512   -4.10032   16.73600   2.51040   -16.73600   0.00000 ;   C7-   N7-   C10-   C9
41   7   45   46   3   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000 ;   C7-   N7-   C10-   H8
41   7   47   48   3   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000 ;   C7-   N7-   C11-   H9
41   7   47   49   3   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000 ;   C7-   N7-   C11-   H10
42   6   43   44   3   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000 ;   C8-   N6-   C9-   H7
42   6   43   45   3   2.84512   -4.10032   16.73600   2.51040   -16.73600   0.00000 ;   C8-   N6-   C9-   C10
42   8   45   43   3   2.84512   -4.10032   16.73600   2.51040   -16.73600   0.00000 ;   C8-   N8-   C10-   C9
42   8   45   46   3   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000 ;   C8-   N8-   C10-   H8
42   8   50   51   3   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000 ;   C8-   N8-   C12-   H11
42   8   50   52   3   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000 ;   C8-   N8-   C12-   H12
43   5   41   115   3   20.92000   0.00000   -20.92000   0.00000   0.00000   0.00000 ;   C9-   N5-   C7-   O3
43   6   42   116   3   20.92000   0.00000   -20.92000   0.00000   0.00000   0.00000 ;   C9-   N6-   C8-   O4
43   45   7   47   3   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000 ;   C9-   C10-   N7-   C11
43   45   8   50   3   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000 ;   C9-   C10-   N8-   C12
44   43   45   46   3   0.65084   1.95253   0.00000   -2.60338   0.00000   0.00000 ;   H7-   C9-   C10-   H8
45   7   41   115   3   20.92000   0.00000   -20.92000   0.00000   0.00000   0.00000 ;   C10-   N7-   C7-   O3
45   7   47   48   3   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000 ;   C10-   N7-   C11-   H9
45   7   47   49   3   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000 ;   C10-   N7-   C11-   H10
45   8   42   116   3   20.92000   0.00000   -20.92000   0.00000   0.00000   0.00000 ;   C10-   N8-   C8-   O4
45   8   50   51   3   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000 ;   C10-   N8-   C12-   H11
45   8   50   52   3   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000 ;   C10-   N8-   C12-   H12
46   45   7   47   3   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000 ;   H8-   C10-   N7-   C11
46   45   8   50   3   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000 ;   H8-   C10-   N8-   C12
47   7   41   115   3   20.92000   0.00000   -20.92000   0.00000   0.00000   0.00000 ;   C11-   N7-   C7-   O3
47   9   53   118   3   20.92000   0.00000   -20.92000   0.00000   0.00000   0.00000 ;   C11-   N9-   C13-   O6
47   9   55   56   3   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000 ;   C11-   N9-   C15-   H13
47   9   55   57   3   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000 ;   C11-   N9-   C15-   C16
48   47   9   53   3   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000 ;   H9-   C11-   N9-   C13
48   47   9   55   3   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000 ;   H9-   C11-   N9-   C15
49   47   9   53   3   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000 ;   H10-   C11-   N9-   C13
49   47   9   55   3   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000 ;   H10-   C11-   N9-   C15
50   8   42   116   3   20.92000   0.00000   -20.92000   0.00000   0.00000   0.00000 ;   C12-   N8-   C8-   O4
50   10   54   119   3   20.92000   0.00000   -20.92000   0.00000   0.00000   0.00000 ;   C12-   N10-   C14-   O7
50   10   55   56   3   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000 ;   C12-   N10-   C15-   H13
50   10   55   57   3   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000 ;   C12-   N10-   C15-   C16
51   50   10   54   3   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000 ;   H11-   C12-   N10-   C14
51   50   10   55   3   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000 ;   H11-   C12-   N10-   C15
52   50   10   54   3   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000 ;   H12-   C12-   N10-   C14
52   50   10   55   3   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000 ;   H12-   C12-   N10-   C15
53   9   55   56   3   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000 ;   C13-   N9-   C15-   H13
53   9   55   57   3   2.84512   -4.10032   16.73600   2.51040   -16.73600   0.00000 ;   C13-   N9-   C15-   C16
53   11   57   55   3   2.84512   -4.10032   16.73600   2.51040   -16.73600   0.00000 ;   C13-   N11-   C16-   C15
53   11   57   58   3   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000 ;   C13-   N11-   C16-   H14
53   11   59   60   3   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000 ;   C13-   N11-   C17-   H15
53   11   59   61   3   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000 ;   C13-   N11-   C17-   H16
```

54 10 55 56 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; C14- N10- C15- H13
54 10 55 57 3 2.84512 -4.10032 16.73600 2.51040 -16.73600 0.00000 ; C14- N10- C15- C16
54 12 57 55 3 2.84512 -4.10032 16.73600 2.51040 -16.73600 0.00000 ; C14- N12- C16- C15
54 12 57 58 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; C14- N12- C16- H14
54 12 62 63 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; C14- N12- C18- H17
54 12 62 64 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; C14- N12- C18- H18
55 9 53 118 3 20.92000 0.00000 -20.92000 0.00000 0.00000 0.00000 ; C15- N9- C13- O6
55 10 54 119 3 20.92000 0.00000 -20.92000 0.00000 0.00000 0.00000 ; C15- N10- C14- O7
55 57 11 59 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; C15- C16- N11- C17
55 57 12 62 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; C15- C16- N12- C18
56 55 57 58 3 0.65084 1.95253 0.00000 -2.60338 0.00000 0.00000 ; H13- C15- C16- H14
57 11 53 118 3 20.92000 0.00000 -20.92000 0.00000 0.00000 0.00000 ; C16- N11- C13- O6
57 11 59 60 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; C16- N11- C17- H15
57 11 59 61 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; C16- N11- C17- H16
57 12 54 119 3 20.92000 0.00000 -20.92000 0.00000 0.00000 0.00000 ; C16- N12- C14- O7
57 12 62 63 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; C16- N12- C18- H17
57 12 62 64 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; C16- N12- C18- H18
58 57 11 59 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; H14- C16- N11- C17
58 57 12 62 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; H14- C16- N12- C18
59 11 53 118 3 20.92000 0.00000 -20.92000 0.00000 0.00000 0.00000 ; C17- N11- C13- O6
59 13 65 120 3 20.92000 0.00000 -20.92000 0.00000 0.00000 0.00000 ; C17- N13- C19- O8
59 13 67 68 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; C17- N13- C21- H19
59 13 67 69 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; C17- N13- C21- C22
60 59 13 65 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; H15- C17- N13- C19
60 59 13 67 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; H15- C17- N13- C21
61 59 13 65 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; H16- C17- N13- C19
61 59 13 67 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; H16- C17- N13- C21
62 12 54 119 3 20.92000 0.00000 -20.92000 0.00000 0.00000 0.00000 ; C18- N12- C14- O7
62 14 66 121 3 20.92000 0.00000 -20.92000 0.00000 0.00000 0.00000 ; C18- N14- C20- O9
62 14 67 68 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; C18- N14- C21- H19
62 14 67 69 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; C18- N14- C21- C22
63 62 14 66 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; H17- C18- N14- C20
63 62 14 67 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; H17- C18- N14- C21
64 62 14 66 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; H18- C18- N14- C20
64 62 14 67 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; H18- C18- N14- C21
65 13 67 68 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; C19- N13- C21- H19
65 13 67 69 3 2.84512 -4.10032 16.73600 2.51040 -16.73600 0.00000 ; C19- N13- C21- C22
65 15 69 67 3 2.84512 -4.10032 16.73600 2.51040 -16.73600 0.00000 ; C19- N15- C22- C21
65 15 69 70 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; C19- N15- C22- H20
65 15 71 72 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; C19- N15- C23- H21
65 15 71 73 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; C19- N15- C23- H22
66 14 67 68 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; C20- N14- C21- H19
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66 16 69 67 3 2.84512 -4.10032 16.73600 2.51040 -16.73600 0.00000 ; C20- N16- C22- C21
66 16 69 70 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; C20- N16- C22- H20
66 16 74 75 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; C20- N16- C24- H23
66 16 74 76 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; C20- N16- C24- H24
67 13 65 120 3 20.92000 0.00000 -20.92000 0.00000 0.00000 0.00000 ; C21- N13- C19- O8
67 14 66 121 3 20.92000 0.00000 -20.92000 0.00000 0.00000 0.00000 ; C21- N14- C20- O9
67 69 15 71 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; C21- C22- N15- C23
67 69 16 74 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; C21- C22- N16- C24
68 67 69 70 3 0.65084 1.95253 0.00000 -2.60338 0.00000 0.00000 ; H19- C21- C22- H20
69 15 65 120 3 20.92000 0.00000 -20.92000 0.00000 0.00000 0.00000 ; C22- N15- C19- O8
69 15 71 72 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; C22- N15- C23- H21
69 15 71 73 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; C22- N15- C23- H22
69 16 66 121 3 20.92000 0.00000 -20.92000 0.00000 0.00000 0.00000 ; C22- N16- C20- O9
69 16 74 75 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; C22- N16- C24- H23
69 16 74 76 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; C22- N16- C24- H24
70 69 15 71 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; H20- C22- N15- C23
70 69 16 74 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; H20- C22- N16- C24
71 15 65 120 3 20.92000 0.00000 -20.92000 0.00000 0.00000 0.00000 ; C23- N15- C19- O8
71 17 77 122 3 20.92000 0.00000 -20.92000 0.00000 0.00000 0.00000 ; C23- N17- C25- O10
71 17 79 80 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; C23- N17- C27- H25
71 17 79 81 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; C23- N17- C27- C28
72 71 17 77 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; H21- C23- N17- C25
72 71 17 79 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; H21- C23- N17- C27
73 71 17 77 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; H22- C23- N17- C25
73 71 17 79 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; H22- C23- N17- C27
74 16 66 121 3 20.92000 0.00000 -20.92000 0.00000 0.00000 0.00000 ; C24- N16- C20- O9
74 18 78 123 3 20.92000 0.00000 -20.92000 0.00000 0.00000 0.00000 ; C24- N18- C26- O11
74 18 79 80 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; C24- N18- C27- H25

74	18	79	81	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 ;	C24-	N18-	C27-	C28
75	74	18	78	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 ;	H23-	C24-	N18-	C26
75	74	18	79	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 ;	H23-	C24-	N18-	C27
76	74	18	78	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 ;	H24-	C24-	N18-	C26
76	74	18	79	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 ;	H24-	C24-	N18-	C27
77	17	79	80	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 ;	C25-	N17-	C27-	H25
77	17	79	81	3	2.84512	-4.10032	16.73600	2.51040	-16.73600	0.00000 ;	C25-	N17-	C27-	C28
77	19	81	79	3	2.84512	-4.10032	16.73600	2.51040	-16.73600	0.00000 ;	C25-	N19-	C28-	C27
77	19	81	82	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 ;	C25-	N19-	C28-	H26
77	19	83	84	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 ;	C25-	N19-	C29-	H27
77	19	83	85	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 ;	C25-	N19-	C29-	H28
78	18	79	80	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 ;	C26-	N18-	C27-	H25
78	18	79	81	3	2.84512	-4.10032	16.73600	2.51040	-16.73600	0.00000 ;	C26-	N18-	C27-	C28
78	20	81	79	3	2.84512	-4.10032	16.73600	2.51040	-16.73600	0.00000 ;	C26-	N20-	C28-	C27
78	20	81	82	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 ;	C26-	N20-	C28-	H26
78	20	86	87	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 ;	C26-	N20-	C30-	H29
78	20	86	88	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 ;	C26-	N20-	C30-	H30
79	17	77	122	3	20.92000	0.00000	-20.92000	0.00000	0.00000	0.00000 ;	C27-	N17-	C25-	O10
79	18	78	123	3	20.92000	0.00000	-20.92000	0.00000	0.00000	0.00000 ;	C27-	N18-	C26-	O11
79	81	19	83	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 ;	C27-	C28-	N19-	C29
79	81	20	86	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 ;	C27-	C28-	N20-	C30
80	79	81	82	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000 ;	H25-	C27-	C28-	H26
81	19	77	122	3	20.92000	0.00000	-20.92000	0.00000	0.00000	0.00000 ;	C28-	N19-	C25-	O10
81	19	83	84	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 ;	C28-	N19-	C29-	H27
81	19	83	85	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 ;	C28-	N19-	C29-	H28
81	20	78	123	3	20.92000	0.00000	-20.92000	0.00000	0.00000	0.00000 ;	C28-	N20-	C26-	O11
81	20	86	87	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 ;	C28-	N20-	C30-	H29
81	20	86	88	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 ;	C28-	N20-	C30-	H30
82	81	19	83	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 ;	H26-	C28-	N19-	C29
82	81	20	86	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 ;	H26-	C28-	N20-	C30
83	19	77	122	3	20.92000	0.00000	-20.92000	0.00000	0.00000	0.00000 ;	C29-	N19-	C25-	O10
83	21	89	124	3	20.92000	0.00000	-20.92000	0.00000	0.00000	0.00000 ;	C29-	N21-	C31-	O12
83	21	91	92	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 ;	C29-	N21-	C33-	H31
83	21	91	93	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 ;	C29-	N21-	C33-	C34
84	83	21	89	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 ;	H27-	C29-	N21-	C31
84	83	21	91	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 ;	H27-	C29-	N21-	C33
85	83	21	89	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 ;	H28-	C29-	N21-	C31
85	83	21	91	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 ;	H28-	C29-	N21-	C33
86	20	78	123	3	20.92000	0.00000	-20.92000	0.00000	0.00000	0.00000 ;	C30-	N20-	C26-	O11
86	22	90	125	3	20.92000	0.00000	-20.92000	0.00000	0.00000	0.00000 ;	C30-	N22-	C32-	O13
86	22	91	92	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 ;	C30-	N22-	C33-	H31
86	22	91	93	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 ;	C30-	N22-	C33-	C34
87	86	22	90	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 ;	H29-	C30-	N22-	C32
87	86	22	91	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 ;	H29-	C30-	N22-	C33
88	86	22	90	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 ;	H30-	C30-	N22-	C32
88	86	22	91	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 ;	H30-	C30-	N22-	C33
89	21	91	92	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 ;	C31-	N21-	C33-	H31
89	21	91	93	3	2.84512	-4.10032	16.73600	2.51040	-16.73600	0.00000 ;	C31-	N21-	C33-	C34
89	23	93	91	3	2.84512	-4.10032	16.73600	2.51040	-16.73600	0.00000 ;	C31-	N23-	C34-	C33
89	23	93	94	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 ;	C31-	N23-	C34-	H32
89	23	95	96	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 ;	C31-	N23-	C35-	H33
89	23	95	97	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 ;	C31-	N23-	C35-	H34
90	22	91	92	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 ;	C32-	N22-	C33-	H31
90	22	91	93	3	2.84512	-4.10032	16.73600	2.51040	-16.73600	0.00000 ;	C32-	N22-	C33-	C34
90	24	93	91	3	2.84512	-4.10032	16.73600	2.51040	-16.73600	0.00000 ;	C32-	N24-	C34-	C33
90	24	93	94	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 ;	C32-	N24-	C34-	H32
90	24	98	99	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 ;	C32-	N24-	C36-	H35
90	24	98	100	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 ;	C32-	N24-	C36-	H36
91	21	89	124	3	20.92000	0.00000	-20.92000	0.00000	0.00000	0.00000 ;	C33-	N21-	C31-	O12
91	22	90	125	3	20.92000	0.00000	-20.92000	0.00000	0.00000	0.00000 ;	C33-	N22-	C32-	O13
91	93	23	95	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 ;	C33-	C34-	N23-	C35
91	93	24	98	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 ;	C33-	C34-	N24-	C36
92	91	93	94	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000 ;	H31-	C33-	C34-	H32
93	23	89	124	3	20.92000	0.00000	-20.92000	0.00000	0.00000	0.00000 ;	C34-	N23-	C31-	O12
93	23	95	96	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 ;	C34-	N23-	C35-	H33
93	23	95	97	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 ;	C34-	N23-	C35-	H34
93	24	90	125	3	20.92000	0.00000	-20.92000	0.00000	0.00000	0.00000 ;	C34-	N24-	C32-	O13
93	24	98	99	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 ;	C34-	N24-	C36-	H35
93	24	98	100	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 ;	C34-	N24-	C36-	H36
94	93	23	95	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 ;	H32-	C34-	N23-	C35
94	93	24	98	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000 ;	H32-	C34-	N24-	C36

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95    23    89    124   3    20.92000 0.00000  -20.92000  0.00000   0.00000   0.00000 ;  C35-  N23-  C31-  O12
95    25    101   126   3    20.92000 0.00000  -20.92000  0.00000   0.00000   0.00000 ;  C35-  N25-  C37-  O14
95    25    103   104   3    0.00000  0.00000  0.00000    0.00000   0.00000   0.00000 ;  C35-  N25-  C39-  H37
95    25    103   105   3    0.00000  0.00000  0.00000    0.00000   0.00000   0.00000 ;  C35-  N25-  C39-  C40
96    95    25    101   3    0.00000  0.00000  0.00000    0.00000   0.00000   0.00000 ;  H33-  C35-  N25-  C37
96    95    25    103   3    0.00000  0.00000  0.00000    0.00000   0.00000   0.00000 ;  H33-  C35-  N25-  C39
97    95    25    101   3    0.00000  0.00000  0.00000    0.00000   0.00000   0.00000 ;  H34-  C35-  N25-  C37
97    95    25    103   3    0.00000  0.00000  0.00000    0.00000   0.00000   0.00000 ;  H34-  C35-  N25-  C39
98    24    90    125   3    20.92000 0.00000  -20.92000  0.00000   0.00000   0.00000 ;  C36-  N24-  C32-  O13
98    26    102   117   3    20.92000 0.00000  -20.92000  0.00000   0.00000   0.00000 ;  C36-  N26-  C38-  O5
98    26    103   104   3    0.00000  0.00000  0.00000    0.00000   0.00000   0.00000 ;  C36-  N26-  C39-  H37
98    26    103   105   3    0.00000  0.00000  0.00000    0.00000   0.00000   0.00000 ;  C36-  N26-  C39-  C40
99    98    26    102   3    0.00000  0.00000  0.00000    0.00000   0.00000   0.00000 ;  H35-  C36-  N26-  C38
99    98    26    103   3    0.00000  0.00000  0.00000    0.00000   0.00000   0.00000 ;  H35-  C36-  N26-  C39
100   98    26    102   3    0.00000  0.00000  0.00000    0.00000   0.00000   0.00000 ;  H36-  C36-  N26-  C38
100   98    26    103   3    0.00000  0.00000  0.00000    0.00000   0.00000   0.00000 ;  H36-  C36-  N26-  C39
101   25    103   104   3    0.00000  0.00000  0.00000    0.00000   0.00000   0.00000 ;  C37-  N25-  C39-  H37
101   25    103   105   3    2.84512  -4.10032 16.73600   2.51040   -16.73600 0.00000 ;  C37-  N25-  C39-  C40
101   27    105   103   3    2.84512  -4.10032 16.73600   2.51040   -16.73600 0.00000 ;  C37-  N27-  C40-  C39
101   27    105   106   3    0.00000  0.00000  0.00000    0.00000   0.00000   0.00000 ;  C37-  N27-  C40-  H38
101   27    107   108   3    0.00000  0.00000  0.00000    0.00000   0.00000   0.00000 ;  C37-  N27-  C41-  H39
101   27    107   109   3    0.00000  0.00000  0.00000    0.00000   0.00000   0.00000 ;  C37-  N27-  C41-  H40
102   26    103   104   3    0.00000  0.00000  0.00000    0.00000   0.00000   0.00000 ;  C38-  N26-  C39-  H37
102   26    103   105   3    2.84512  -4.10032 16.73600   2.51040   -16.73600 0.00000 ;  C38-  N26-  C39-  C40
102   28    105   103   3    2.84512  -4.10032 16.73600   2.51040   -16.73600 0.00000 ;  C38-  N28-  C40-  C39
102   28    105   106   3    0.00000  0.00000  0.00000    0.00000   0.00000   0.00000 ;  C38-  N28-  C40-  H38
102   28    110   111   3    0.00000  0.00000  0.00000    0.00000   0.00000   0.00000 ;  C38-  N28-  C42-  H41
102   28    110   112   3    0.00000  0.00000  0.00000    0.00000   0.00000   0.00000 ;  C38-  N28-  C42-  H42
103   25    101   126   3    20.92000 0.00000  -20.92000  0.00000   0.00000   0.00000 ;  C39-  N25-  C37-  O14
103   26    102   117   3    20.92000 0.00000  -20.92000  0.00000   0.00000   0.00000 ;  C39-  N26-  C38-  O5
103   105   27    107   3    0.00000  0.00000  0.00000    0.00000   0.00000   0.00000 ;  C39-  C40-  N27-  C41
103   105   28    110   3    0.00000  0.00000  0.00000    0.00000   0.00000   0.00000 ;  C39-  C40-  N28-  C42
104   103   105   106   3    0.65084  1.95253  0.00000    -2.60338  0.00000   0.00000 ;  H37-  C39-  C40-  H38
105   27    101   126   3    20.92000 0.00000 -20.92000  0.00000   0.00000   0.00000 ;  C40-  N27-  C37-  O14
105   27    107   108   3    0.00000  0.00000  0.00000    0.00000   0.00000   0.00000 ;  C40-  N27-  C41-  H39
105   27    107   109   3    0.00000  0.00000  0.00000    0.00000   0.00000   0.00000 ;  C40-  N27-  C41-  H40
105   28    102   117   3    20.92000 0.00000  -20.92000  0.00000   0.00000   0.00000 ;  C40-  N28-  C38-  O5
105   28    110   111   3    0.00000  0.00000  0.00000    0.00000   0.00000   0.00000 ;  C40-  N28-  C42-  H41
105   28    110   112   3    0.00000  0.00000  0.00000    0.00000   0.00000   0.00000 ;  C40-  N28-  C42-  H42
106   105   27    107   3    0.00000  0.00000  0.00000    0.00000   0.00000   0.00000 ;  H38-  C40-  N27-  C41
106   105   28    110   3    0.00000  0.00000  0.00000    0.00000   0.00000   0.00000 ;  H38-  C40-  N28-  C42
107   1     29    3     3    20.92000 0.00000  -20.92000  0.00000   0.00000   0.00000 ;  C41-  N1-   C1-   N3
107   1     29    114   3    20.92000 0.00000  -20.92000  0.00000   0.00000   0.00000 ;  C41-  N1-   C1-   O2
107   1     31    2     3    0.00000  0.00000  0.00000    0.00000   0.00000   0.00000 ;  C41-  N1-   C3-   N2
107   1     31    32    3    0.00000  0.00000  0.00000    0.00000   0.00000   0.00000 ;  C41-  N1-   C3-   H1
107   1     31    33    3    0.00000  0.00000  0.00000    0.00000   0.00000   0.00000 ;  C41-  N1-   C3-   C4
107   27    101   126   3    20.92000 0.00000  -20.92000  0.00000   0.00000   0.00000 ;  C41-  N27-  C37-  O14
110   2     30    113   3    20.92000 0.00000  -20.92000  0.00000   0.00000   0.00000 ;  C42-  N2-   C2-   O1
110   28    102   117   3    20.92000 0.00000  -20.92000  0.00000   0.00000   0.00000 ;  C42-  N28-  C38-  O5

[ dihedrals ] ; impropers
; treated as propers in GROMACS to use correct AMBER analytical function
;    i     j     k     l     func  phase    kd       pn
     1     3     29    114   1     180.00   43.93200 2 ;  N1-   N3-   C1-   O2
     2     4     30    113   1     180.00   43.93200 2 ;  N2-   N4-   C2-   O1
     5     7     41    115   1     180.00   43.93200 2 ;  N5-   N7-   C7-   O3
     6     8     42    116   1     180.00   43.93200 2 ;  N6-   N8-   C8-   O4
     9     11    53    118   1     180.00   43.93200 2 ;  N9-   N11-  C13-  O6
     10    12    54    119   1     180.00   43.93200 2 ;  N10-  N12-  C14-  O7
     13    15    65    120   1     180.00   43.93200 2 ;  N13-  N15-  C19-  O8
     14    16    66    121   1     180.00   43.93200 2 ;  N14-  N16-  C20-  O9
     17    19    77    122   1     180.00   43.93200 2 ;  N17-  N19-  C25-  O10
     18    20    78    123   1     180.00   43.93200 2 ;  N18-  N20-  C26-  O11
     21    23    89    124   1     180.00   43.93200 2 ;  N21-  N23-  C31-  O12
     22    24    90    125   1     180.00   43.93200 2 ;  N22-  N24-  C32-  O13
     25    27    101   126   1     180.00   43.93200 2 ;  N25-  N27-  C37-  O14
     26    28    102   117   1     180.00   43.93200 2 ;  N26-  N28-  C38-  O5
     29    33    3     35    1     180.00   4.60240  2 ;  C1-   C4-   N3-   C5
     30    31    2     110   1     180.00   4.60240  2 ;  C2-   C3-   N2-   C42
     30    33    4     38    1     180.00   4.60240  2 ;  C2-   C4-   N4-   C6
     41    35    5     43    1     180.00   4.60240  2 ;  C7-   C5-   N5-   C9
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  41   45    7   47    1   180.00    4.60240    2 ;    C7-   C10-   N7-   C11
  42   38    6   43    1   180.00    4.60240    2 ;    C8-    C6-   N6-    C9
  42   45    8   50    1   180.00    4.60240    2 ;    C8-   C10-   N8-   C12
  53   47    9   55    1   180.00    4.60240    2 ;   C13-   C11-   N9-   C15
  53   57   11   59    1   180.00    4.60240    2 ;   C13-   C16-  N11-   C17
  54   50   10   55    1   180.00    4.60240    2 ;   C14-   C12-  N10-   C15
  54   57   12   62    1   180.00    4.60240    2 ;   C14-   C16-  N12-   C18
  65   59   13   67    1   180.00    4.60240    2 ;   C19-   C17-  N13-   C21
  65   69   15   71    1   180.00    4.60240    2 ;   C19-   C22-  N15-   C23
  66   62   14   67    1   180.00    4.60240    2 ;   C20-   C18-  N14-   C21
  66   69   16   74    1   180.00    4.60240    2 ;   C20-   C22-  N16-   C24
  77   71   17   79    1   180.00    4.60240    2 ;   C25-   C23-  N17-   C27
  77   81   19   83    1   180.00    4.60240    2 ;   C25-   C28-  N19-   C29
  78   74   18   79    1   180.00    4.60240    2 ;   C26-   C24-  N18-   C27
  78   81   20   86    1   180.00    4.60240    2 ;   C26-   C28-  N20-   C30
  89   83   21   91    1   180.00    4.60240    2 ;   C31-   C29-  N21-   C33
  89   93   23   95    1   180.00    4.60240    2 ;   C31-   C34-  N23-   C35
  90   86   22   91    1   180.00    4.60240    2 ;   C32-   C30-  N22-   C33
  90   93   24   98    1   180.00    4.60240    2 ;   C32-   C34-  N24-   C36
 101   95   25  103    1   180.00    4.60240    2 ;   C37-   C35-  N25-   C39
 101  105   27  107    1   180.00    4.60240    2 ;   C37-   C40-  N27-   C41
 102   98   26  103    1   180.00    4.60240    2 ;   C38-   C36-  N26-   C39
 102  105   28  110    1   180.00    4.60240    2 ;   C38-   C40-  N28-   C42
 107    1   31   29    1   180.00    4.60240    2 ;   C41-    N1-   C3-    C1
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