Supporting Information

Solutions and Condensed Phases of PEG_{2000} from All-atom Molecular Dynamics

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S1 Parameter File for Solvated PEG_{2000}

GROMOS 54A7 and GAFF force field parameters for ethanol, ethyl acetate, and PEG_{2000} molecules are provided in S5. Appendix to this Supporting Information. Both, GROMACS .top and .itp files are included.

S2 Preparation and Equilibration of PEG_{2000} Solutions

S2.1 Single PEG_{2000} in Vacuo and in Solutions

A single PEG_{2000} molecule constructed with ideal bond lengths and angles forming an extended helical structure is shown in Fig.S1 with properties as in table S1. Additionally, the figure illustrates the RESP atomic charges of the ether oxygen atoms in the GAFF.

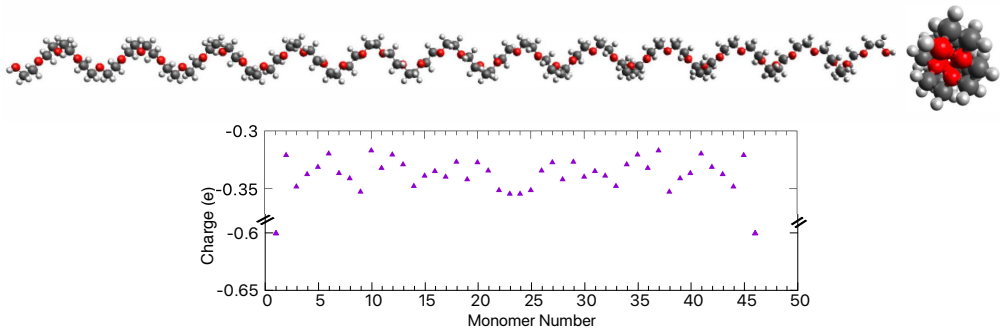

Figure S1: Initial geometry of the PEG_{2000} macromolecule with ideal bond lengths and angles forming a helical structure with view along the macromolecule length (top left) and along the helix from one of its ends (top right). Bottom panel displays the custom generated RESP atomic charges of the ether oxygen atoms along the macromolecule monomer number.

Table S1: PEG_{2000} molecular formula, mass, original elongated radius of gyration R_g and end-to-end distance R_{ee}.

Molecular Formula	$HOCH_2(CH_2OCH_2)_{44}CH_2OH$
Molecular Weight	2000.34 u
D_{ee}	11.1 nm
R_g	3.3 nm

The elongated helical PEG_{2000} is solvated in various solvents. The computational boxes of the solvated macromolecule are prepared with details provided in Table S2.

Table S2: Summary of the systems initiated with one helical PEG_{2000} macromolecule solvated inside an initial cubic box with edge of 10 nm at 300 K and 101.325 kPa.

Solvent	No. of waters	No. ethanol or ethyl acetate	Equilibrated system density (kg/m^3)	Experimental solvent density (kg/m^3)
Water	32,959		998±1	999.8
4% Ethanol	31,131	506	992±0.7	991
Ethyl Acetate		6,106	904±1.3	902

Figure S2 shows the time evolution of the solutions densities and enthalpies along NPT MD simulations at 300 K. Along these simulations, Fig. S3 depicts the R_g and D_{ee} of the solvated PEG_{2000} while the systems relaxed toward equilibrium.

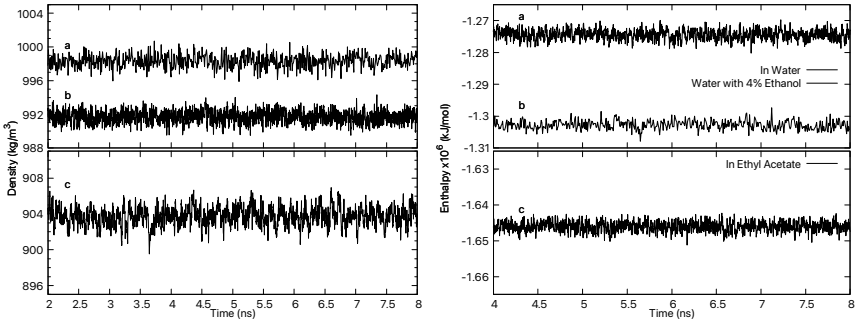

Figure S2: Time evolution of the solutions density and enthalpy along the NPT MD equilibration of PEG_{2000} solvated in the three studied solvents: (a) pure water, (b) water with 4% ethanol, (c) ethyl acetate.

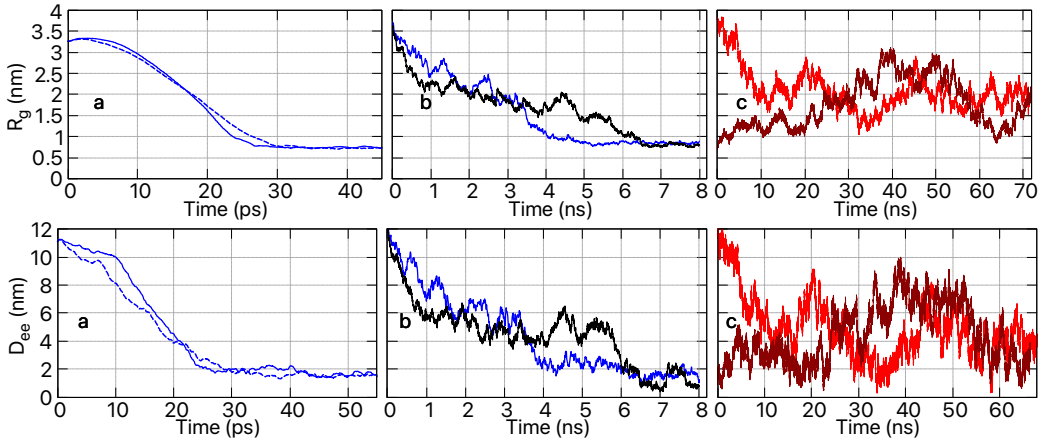

Figure S3: Fate of the PEG_{2000} radius of gyration R_g (top) and the end-to-end distance D_{ee} while relaxing toward equilibrium. (a) In-vacuo, full line is at 300 K and dotted-line at 400K of NVT simulations. NPT simulations at 300 K are: (b) In water (blue), in water with 4% ethanol (black). (c) In ethyl acetate (red) with PEG_{2000} initiated from the helical structure and initiated from the collapsed structure (maroon).

S3 Time Evolution of Solvated PEG_{2000} Properties

Potential energy of the PEG_{2000} macromolecule and its interaction energy with the solvent along with other basic properties are plotted in Fig. S4a,b,c as a function of time during the production lapse of the NVE simulation at 300 K and the equilibrated density of each system of Table S2.

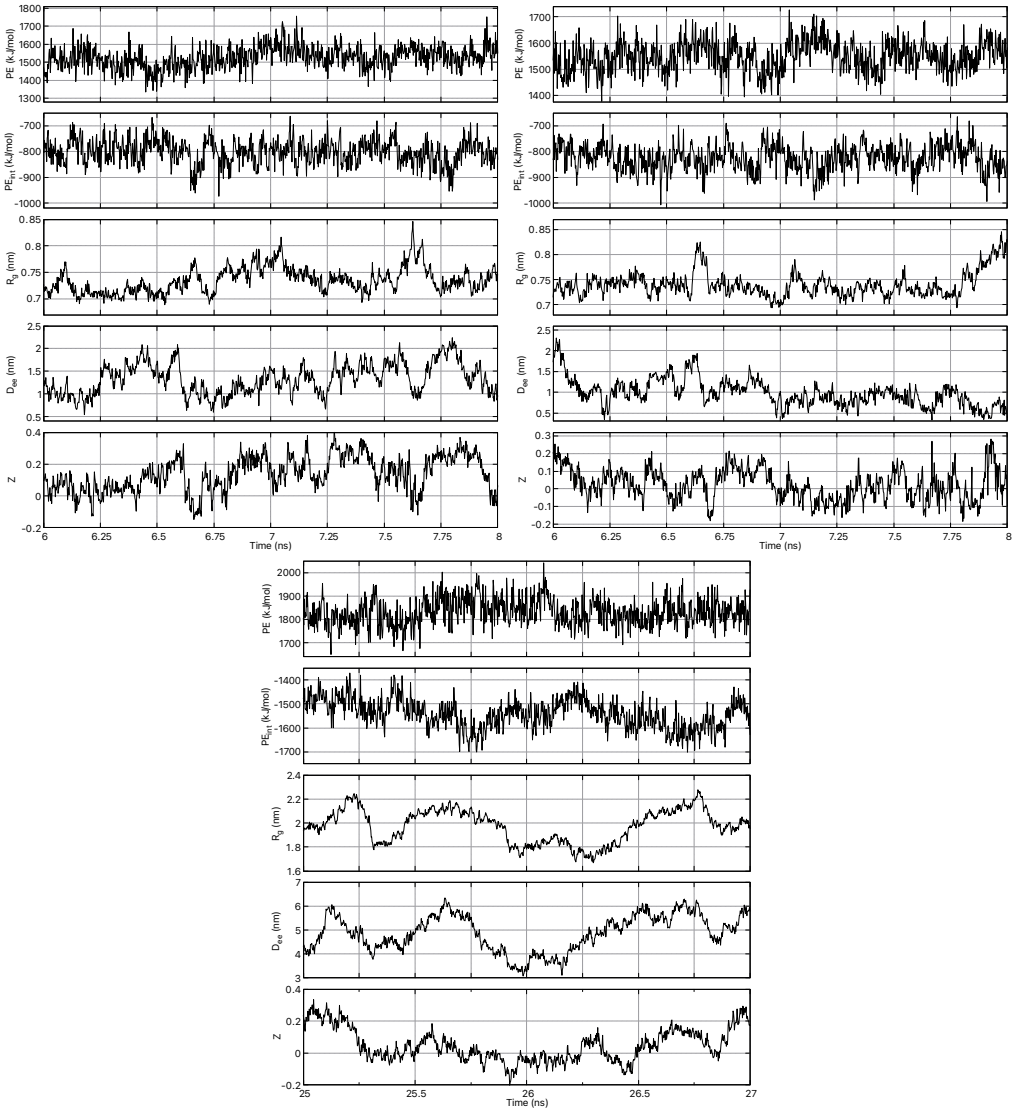

Figure S4: Energetics and basic properties of one PEG_{2000} macromolecule solvated in water (left), in water with 4% ethanol (center), and in ethyl acetate (right) during NVE MD production time at the equilibrium density of each system reported in Table S2.

S4 Condensed System of 216 PEG_{2000} Macromolecules

Figure S5 depicts the simulated equilibrium density of the condensed system of 216 PEG_{2000} macromolecules as a function of temperature across the solid-glass-rubber condensed regions of this polymer at a constant pressure of 101.325 kPa.

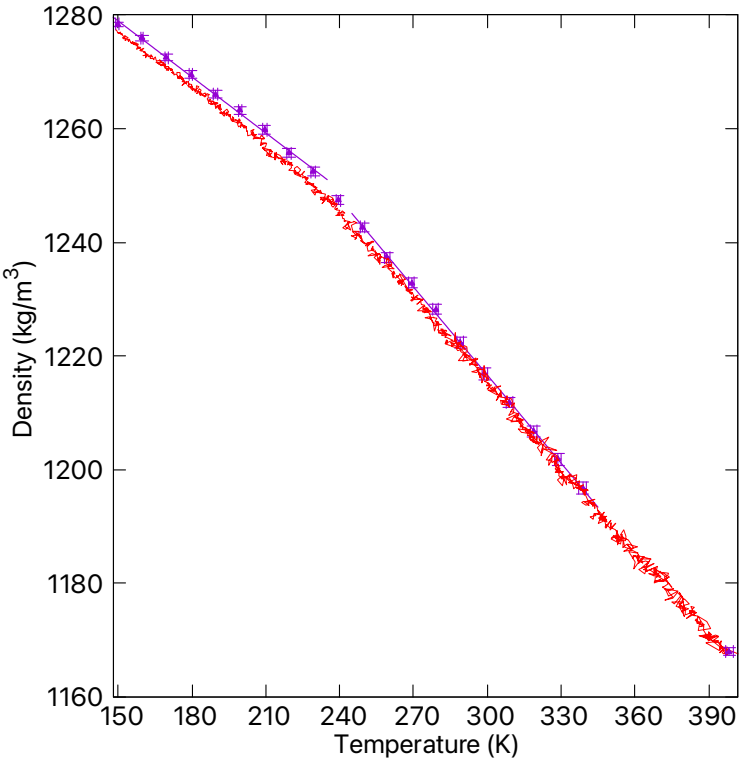

Figure S5: Density of the PEG_{2000} polymer condensed system as a function of temperature equilibrated with NPT MD. Magenta dots and standard deviation correspond to averages over the NPT MD production simulation (last 8 ns of the 16 ns NPT run). Red marks resulted from a fast NPT cooling scan from 400 K to 150 K over 1 million time steps of 1 fs each.

Several properties of the condensed system of PEG_{2000} are provided in Figs. S6, S7, S8 as a function of temperature. Results correspond to fluctuations in the NPT simulations for Fig. S6, and from NVT averages at the previously obtained equilibrium density for the different temperatures for Figs. S7 and S8.

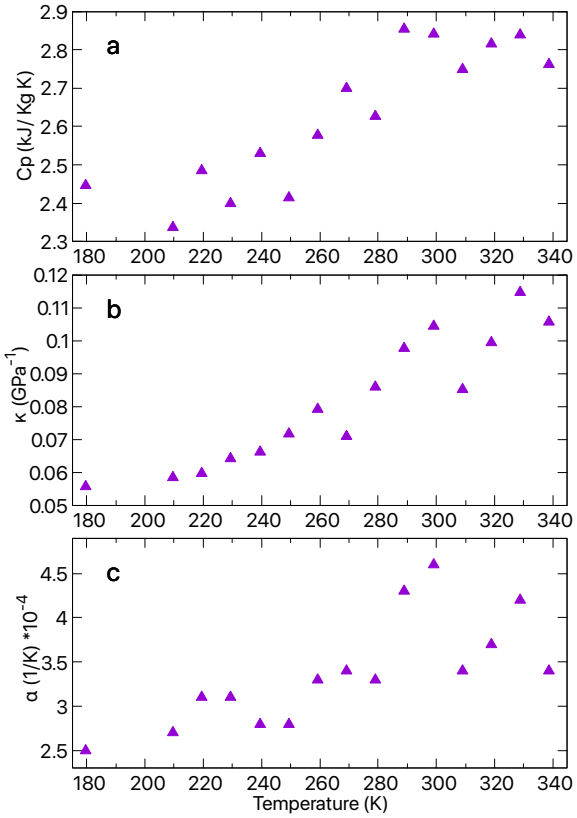

Figure S6: Properties of the PEG_{2000} condensed system as a function of temperature: Heat capacity Cp, thermal compressibility κ, and thermal expansion coefficient α calculated from fluctuations at 101.325 kPa.

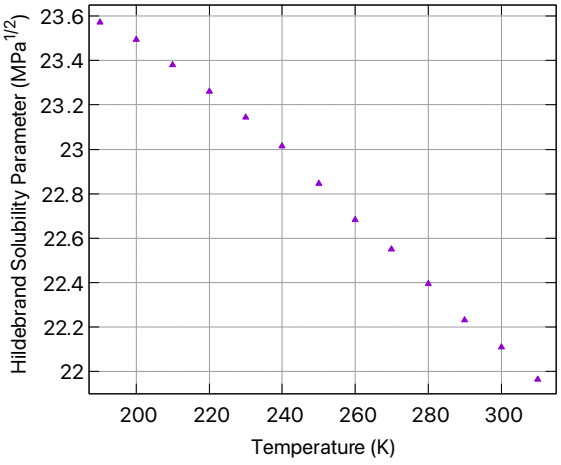

Figure S7: Hildebrand solubility parameter of the PEG_{2000} condensed system as a function of temperature computed from the cohesive energy density. Each point corresponds to an NVT simulation at the appropriate equilibrated density of the system at 101.325 kPa.

The radial distribution function g(r) between monomers of different macromolecules was obtained from:

$$g(r) = \frac{\sum_{k=1}^{m} N_k(r, \Delta r)}{m\rho_o(\frac{1}{2}N)V(r, \Delta r)} \quad (1)$$

where m is the number of time steps used for the averages, r is the distance between the monomers center of mass, N_k(r,Δr) is the number of pair distances within a spherical shell between r and r+Δ r, $N = 46 \times 216$ is the number of monomers in the system, ρ_o=N/V is the system number density (V= system volume) at the calculated temperature, and V_k(r,Δ r) is the volume of the spherical shell between r and r+Δr. Note that at different temperatures the system volume V is different. If a fixed volume is considered for the g(r) calculation at two temperatures, e.g. T_1=180 K and T_2=300 K, then g(r) is not properly scaled. Figure S8 shows the lack of scaling when a volume corresponding to T=150 K is used for plotting g(r) at T=180 and 300 K.

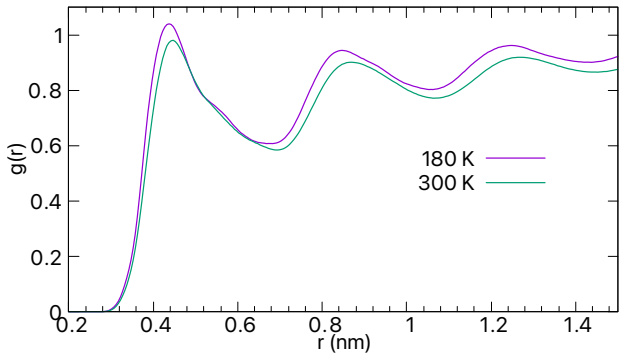

Figure S8: Radial distribution function of the PEG_{2000} condensed system computed between the monomers centers of mass at T=180 K (magenta) and T=300 K (green) at 101.325 kPa. Both curves were calculated from Eq. 1 with a fixed ρ_o corresponding to the system at T=150 K.

S5 Appendix: Force Field Files for Systems

S5.1 Top level topology .top file for PEG2000 in water

```
; Top level topology file for PEG2000 in water
; GAFF parameters
;


; atomtypes for peg2000.itp
[ atomtypes ]
; name at.num mass charge ptype sigma epsilon
ho 1 1.008000 0.00000000 A 0 0
oh 8 16.000000 0.00000000 A 0.30664734 0.8803136
c3 6 12.010000 0.00000000 A 0.33996695 0.4577296
h1 1 1.008000 0.00000000 A 0.2471353 0.0656888
os 8 16.000000 0.00000000 A 0.30000123 0.71128

#include "peg2000.itp"

; Include Position restraint file
#ifdef POSRES
#include "posre.itp"
#endif

[ system ]
; Name
Polyethylene Glycol 2000 in Water

[ molecules ]
; Compound #mols
PEG2000 1
SOL 33327
```

S5.2 Top level topology .top file for PEG2000 in water:ethanol

```
; Top level topology for PolyEthylene Glycol system in water:ethanol
; GAFF parameters
; Include all relevant .itp files here then list and number the molecules.

; Include forcefield parameters

[ atomtypes ]
; name at.num mass charge ptype sigma epsilon
ho 1 1.008000 0.00000000 A 0 0
oh 8 16.000000 0.00000000 A 0.30664734 0.8803136
c3 6 12.010000 0.00000000 A 0.33996695 0.4577296
h1 1 1.008000 0.00000000 A 0.2471353 0.0656888
os 8 16.000000 0.00000000 A 0.30000123 0.71128
hc 1 1.008000 0.00000000 A 0.26495328 0.0656888

#include "peg2000.itp"
#include "Ethanol.itp"
```

```
; Include Position restraint file
#ifdef POSRES
#include "posre.itp"
#endif

[ system ]
; Name
Polyethylene Glycol 2000 in Water with Ethanol in water

[ molecules ]
; Compound #mols
PEG2000 1
_U1K 516
SOL 31715
```

S5.3 Top level topology file .top for PEG2000 in Ethyl Acetate

```
; Top level topology for PolyEthylene system in Ethyl Acetate.
; GAFF force field parameters.
; All atom types must be defined before any listed parameters
; Include all relevant .itp files here then list and number the molecules.

[ defaults ]
; nbfunc comb-rule gen-pairs fudgeLJ fudgeQQ
1 2 yes 0.5 0.83333333

; atomtypes for Peg2000.itp
[ atomtypes ]
; name at.num mass charge ptype sigma epsilon
ho 1 1.008000 0.00000000 A 0 0
oh 8 16.000000 0.00000000 A 0.30664734 0.8803136
c3 6 12.010000 0.00000000 A 0.33996695 0.4577296
h1 1 1.008000 0.00000000 A 0.2471353 0.0656888
os 8 16.000000 0.00000000 A 0.30000123 0.71128

; atomtypes for acetate.itp
[ atomtypes ]
; name at.num mass charge ptype sigma epsilon
c 6 12.010000 0.00000000 A 0.33996695 0.359824
o 8 16.000000 0.00000000 A 0.29599219 0.87864
hc 1 1.008000 0.00000000 A 0.26495328 0.0656888
; os defined above
; os 8 16.000000 0.00000000 A 0.30000123 0.71128
; c3 defined above
; c3 6 12.010000 0.00000000 A 0.33996695 0.4577296
; h1 defined above
; h1 1 1.008000 0.00000000 A 0.2471353 0.0656888

; Include forcefield parameters
#include "peg2000.itp"
#include "acetate.itp"

[ system ]
```

```
; Name
Polyethylene Glycol 2000 in Ethyl Acetate

[ molecules ]
; Compound #mols
PEG2000 1
EthAce 6106
```

S5.4 Topology include .itp file for Ethanol GAFF ff

```
; Topology Include .itp file for Ethanol
; GAFF parameters


[ moleculetype ]
; Name nrexcl
_U1K 3

[ atoms ]
; nr type resnr residue atom cgnr charge mass typeB chargeB massB
; residue 1 TOH rtp TOH q 0.0
1 ho 1 _U1K H9 1 0.37747500 1.008000 ; qtot 0.377475
2 oh 1 _U1K O3 1 -0.62253500 16.000000 ; qtot -0.245060
3 c3 1 _U1K C2 1 0.42688900 12.010000 ; qtot 0.181829
4 h1 1 _U1K H7 1 -0.06513000 1.008000 ; qtot 0.116699
5 h1 1 _U1K H8 1 -0.06513000 1.008000 ; qtot 0.051569
6 c3 1 _U1K C1 2 -0.27216200 12.010000 ; qtot -0.220593
7 hc 1 _U1K H4 2 0.07353100 1.008000 ; qtot -0.147062
8 hc 1 _U1K H5 2 0.07353100 1.008000 ; qtot -0.073531
9 hc 1 _U1K H6 2 0.07353100 1.008000 ; qtot 0.000000

[ bonds ]
; ai aj funct c0 c1 c2 c3
2 3 1 0.14260 262838.880000
3 6 1 0.15350 253634.080000
2 1 1 0.09740 309281.280000
3 4 1 0.10930 281081.120000
3 5 1 0.10930 281081.120000
6 7 1 0.10920 282252.640000
6 8 1 0.10920 282252.640000
6 9 1 0.10920 282252.640000

[ pairs ]
; ai aj funct c0 c1 c2 c3
2 7 1
2 8 1
2 9 1
1 4 1
1 5 1
1 6 1
4 7 1
4 8 1
4 9 1
5 7 1
```

```
5 8 1
5 9 1

[ angles ]
; ai aj ak funct c0 c1 c2 c3
2 3 6 1 109.4300470 566.680960
2 3 4 1 109.8800469 426.516960
2 3 5 1 109.8800469 426.516960
1 2 3 1 108.1600465 394.049120
3 6 7 1 110.0500475 388.024160
3 6 8 1 110.0500475 388.024160
3 6 9 1 110.0500475 388.024160
4 3 5 1 109.5500472 327.858240
4 3 6 1 110.0700471 387.940480
5 3 6 1 110.0700471 387.940480
7 6 8 1 108.3500467 329.950240
7 6 9 1 108.3500467 329.950240
8 6 9 1 108.3500467 329.950240

[ dihedrals ]
; ai aj ak al funct c0 c1 c2 c3 c4
c5 2 3 6 7 1 0.0000000 1.0460000 1
2 3 6 7 1 0.0000000 0.0000000 3
2 3 6 8 1 0.0000000 1.0460000 1
2 3 6 8 1 0.0000000 0.0000000 3
2 3 6 9 1 0.0000000 1.0460000 1
2 3 6 9 1 0.0000000 0.0000000 3
1 2 3 4 1 0.0000000 0.6973333 3
1 2 3 5 1 0.0000000 0.6973333 3
1 2 3 6 1 0.0000000 1.0460000 1
1 2 3 6 1 0.0000000 0.6694400 3
4 3 6 7 1 0.0000000 0.6508444 3
4 3 6 8 1 0.0000000 0.6508444 3
4 3 6 9 1 0.0000000 0.6508444 3
5 3 6 7 1 0.0000000 0.6508444 3
5 3 6 8 1 0.0000000 0.6508444 3
5 3 6 9 1 0.0000000 0.6508444 3
```

S5.5 Topology include .itp file for Ethyl Acetate GAFF

```
; Topology Include .itp file for Ethyl Acetate
; GAFF parameters
;

;[ defaults ]
; nbfunc comb-rule gen-pairs fudgeLJ fudgeQQ
;1 2 yes 0.5 0.83333333

[ moleculetype ]
; Name nrexcl
EthAce 3

[ atoms ]
; nr type resnr residue atom cgnr charge mass typeB chargeB massB
```

```
; residue 1 MOL rtp MOL q 0.0
1 hc 1 MOL H3 1 0.15873200 1.008000 ; qtot 0.158732
2 c3 1 MOL C1 2 -0.57420600 12.010000 ; qtot -0.098010
3 hc 1 MOL H1 3 0.15873200 1.008000 ; qtot 0.317464
4 hc 1 MOL H2 4 0.15873200 1.008000 ; qtot 0.476196
5 c 1 MOL C2 5 0.80676700 12.010000 ; qtot 0.160295
6 o 1 MOL OA 6 -0.54846200 16.000000 ; qtot -0.646472
7 os 1 MOL OB 7 -0.45876300 16.000000 ; qtot -0.298468
8 c3 1 MOL C3 8 0.42584100 12.010000 ; qtot 0.127373
9 h1 1 MOL H4 9 -0.02252900 1.008000 ; qtot 0.104844
10 h1 1 MOL H5 10 -0.02252900 1.008000 ; qtot 0.082315
11 c3 1 MOL C4 11 -0.39565300 12.010000 ; qtot -0.104444
12 hc 1 MOL H6 12 0.10444700 1.008000 ; qtot 0.186762
13 hc 1 MOL H7 13 0.10444700 1.008000 ; qtot 0.291209
14 hc 1 MOL H8 14 0.10444400 1.008000 ; qtot 0.000000

[ bonds ]
; ai aj funct c0 c1 c2 c3
2 5 1 0.15241 261918.400000
6 5 1 0.12183 533627.360000
5 7 1 0.13584 327021.440000
7 8 1 0.14316 258236.480000
8 11 1 0.15375 251793.120000
1 2 1 0.10969 276646.080000
4 2 1 0.10969 276646.080000
3 2 1 0.10969 276646.080000
8 9 1 0.10969 276646.080000
8 10 1 0.10969 276646.080000
13 11 1 0.10969 276646.080000
12 11 1 0.10969 276646.080000
11 14 1 0.10969 276646.080000

[ pairs ]
; ai aj funct c0 c1 c2 c3
2 8 1
6 8 1
5 11 1
1 6 1
1 7 1
4 6 1
4 7 1
3 6 1
3 7 1
5 9 1
5 10 1
7 13 1
7 12 1
7 14 1
9 13 1
9 12 1
9 14 1
10 13 1
10 12 1
10 14 1

[ angles ]
```

```
; ai aj ak funct c0 c1 c2 c3
2 5 6 1 123.2000528 564.003200
2 5 7 1 110.7200477 576.471520
6 5 7 1 123.2500525 630.277760
5 7 8 1 115.9800495 529.527040
7 8 11 1 107.9700462 569.024000
1 2 4 1 107.5800459 329.699200
1 2 3 1 107.5800459 329.699200
1 2 5 1 108.7700466 392.710240
4 2 3 1 107.5800459 329.699200
4 2 5 1 108.7700466 392.710240
3 2 5 1 108.7700466 392.710240
7 8 9 1 109.7800468 425.094400
7 8 10 1 109.7800468 425.094400
8 11 13 1 109.8000471 387.773120
8 11 12 1 109.8000471 387.773120
8 11 14 1 109.8000471 387.773120
9 8 10 1 108.4600466 328.360320
9 8 11 1 109.5600471 388.191520
10 8 11 1 109.5600471 388.191520
13 11 12 1 107.5800459 329.699200
13 11 14 1 107.5800459 329.699200
12 11 14 1 107.5800459 329.699200

[ dihedrals ]
; ai aj ak al funct c0 c1 c2 c3 c4
c5 2 5 7 8 1 0.0000000 0.0000000 1
2 5 7 8 1 180.0000771 11.2968000 2
2 5 7 8 1 0.0000000 4.8116000 3
6 5 7 8 1 180.0000771 5.8576000 1
6 5 7 8 1 180.0000771 11.2968000 2
5 7 8 13 1 180.0000771 3.3472000 1
5 7 8 13 1 0.0000000 1.6024720 3
2 6 5 7 4 180.0000771 43.9320000 2
1 2 5 6 1 0.0000000 3.3472000 1
1 2 5 6 1 0.0000000 0.0000000 2
1 2 5 6 1 180.0000771 0.3347200 3
1 2 5 7 1 180.0000771 0.0000000 2
4 2 5 6 1 0.0000000 3.3472000 1
4 2 5 6 1 0.0000000 0.0000000 2
4 2 5 6 1 180.0000771 0.3347200 3
4 2 5 7 1 180.0000771 0.0000000 2
3 2 5 6 1 0.0000000 3.3472000 1
3 2 5 6 1 0.0000000 0.0000000 2
3 2 5 6 1 180.0000771 0.3347200 3
3 2 5 7 1 180.0000771 0.0000000 2
5 7 8 9 1 0.0000000 1.6038667 3
5 7 8 10 1 0.0000000 1.6038667 3
7 8 11 13 1 0.0000000 1.0460000 1
7 8 11 13 1 0.0000000 0.0000000 3
7 8 11 12 1 0.0000000 1.0460000 1
7 8 11 12 1 0.0000000 0.0000000 3
7 8 11 14 1 0.0000000 1.0460000 1
7 8 11 14 1 0.0000000 0.0000000 3
9 8 11 13 1 0.0000000 0.6508444 3
9 8 11 12 1 0.0000000 0.6508444 3
```

```
9 8 11 14 1 0.0000000 0.6508444 3
10 8 11 13 1 0.0000000 0.6508444 3
10 8 11 12 1 0.0000000 0.6508444 3
10 8 11 14 1 0.0000000 0.6508444 3
```

S5.6 Topology include .itp file for Polyethylene Glycol 2000 GAFF

```
; Topology include .itp file for Polyethylene Glycol 2000 GAFF
; GAFF force field
;

[ moleculetype ]
; Name nrexcl
PEG2000 3

[ atoms ]
; nr type resnr residue atom cgnr charge mass typeB chargeB massB
; residue 1 MOL rtp MOL q -0.0
1 ho 1 LIB H21 1 0.37755200 1.008000 ; qtot 0.377552
2 oh 1 LIB OO2 1 -0.60057900 16.000000 ; qtot -0.223027
3 c3 1 LIB C1 1 0.28304200 12.010000 ; qtot 0.060015
4 h1 1 LIB H11 1 0.00482800 1.008000 ; qtot 0.064843
5 h1 1 LIB H12 1 0.00482800 1.008000 ; qtot 0.069671
6 c3 2 LIG C3 2 -0.04312400 12.010000 ; qtot 0.026547
7 h1 2 LIG H31 2 0.05936600 1.008000 ; qtot 0.085913
8 h1 2 LIG H32 2 0.05936600 1.008000 ; qtot 0.145279
9 os 2 LIG OO2 2 -0.32101400 16.000000 ; qtot -0.175735
10 c3 2 LIG C1 2 0.04898800 12.010000 ; qtot -0.126747
11 h1 2 LIG H11 2 0.05347500 1.008000 ; qtot -0.073272
12 h1 2 LIG H12 2 0.05347500 1.008000 ; qtot -0.019797
13 c3 3 LIG C3 3 0.13212200 12.010000 ; qtot 0.112325
14 h1 3 LIG H31 3 0.02596800 1.008000 ; qtot 0.138293
15 h1 3 LIG H32 3 0.02596800 1.008000 ; qtot 0.164261
16 os 3 LIG OO2 3 -0.34827500 16.000000 ; qtot -0.184014
17 c3 3 LIG C1 3 0.13420900 12.010000 ; qtot -0.049805
18 h1 3 LIG H11 3 0.02790400 1.008000 ; qtot -0.021901
19 h1 3 LIG H12 3 0.02790400 1.008000 ; qtot 0.006003
20 c3 4 LIG C3 4 0.08279600 12.010000 ; qtot 0.088799
21 h1 4 LIG H31 4 0.03567400 1.008000 ; qtot 0.124473
22 h1 4 LIG H32 4 0.03567400 1.008000 ; qtot 0.160147
23 os 4 LIG OO2 4 -0.33740600 16.000000 ; qtot -0.177259
24 c3 4 LIG C1 4 0.14568000 12.010000 ; qtot -0.031579
25 h1 4 LIG H11 4 0.02432700 1.008000 ; qtot -0.007252
26 h1 4 LIG H12 4 0.02432700 1.008000 ; qtot 0.017075
27 c3 5 LIG C3 5 0.06001900 12.010000 ; qtot 0.077094
28 h1 5 LIG H31 5 0.04163300 1.008000 ; qtot 0.118727
29 h1 5 LIG H32 5 0.04163300 1.008000 ; qtot 0.160360
30 os 5 LIG OO2 5 -0.33132000 16.000000 ; qtot -0.170960
31 c3 5 LIG C1 5 0.12646500 12.010000 ; qtot -0.044495
32 h1 5 LIG H11 5 0.02762200 1.008000 ; qtot -0.016873
33 h1 5 LIG H12 5 0.02762200 1.008000 ; qtot 0.010749
34 c3 6 LIG C3 6 0.05496400 12.010000 ; qtot 0.065713
35 h1 6 LIG H31 6 0.04449200 1.008000 ; qtot 0.110205
36 h1 6 LIG H32 6 0.04449200 1.008000 ; qtot 0.154697
```

```
37 os 6 LIG OO2 6 -0.31973900 16.000000 ; qtot -0.165042
38 c3 6 LIG C1 6 0.08563500 12.010000 ; qtot -0.079407
39 h1 6 LIG H11 6 0.04132000 1.008000 ; qtot -0.038087
40 h1 6 LIG H12 6 0.04132000 1.008000 ; qtot 0.003233
41 c3 7 LIG C3 7 0.07366700 12.010000 ; qtot 0.076900
42 h1 7 LIG H31 7 0.04424200 1.008000 ; qtot 0.121142
43 h1 7 LIG H32 7 0.04424200 1.008000 ; qtot 0.165384
44 os 7 LIG OO2 7 -0.33652600 16.000000 ; qtot -0.171142
45 c3 7 LIG C1 7 0.14011900 12.010000 ; qtot -0.031023
46 h1 7 LIG H11 7 0.02078600 1.008000 ; qtot -0.010237
47 h1 7 LIG H12 7 0.02078600 1.008000 ; qtot 0.010549
48 c3 8 LIG C3 8 0.04250500 12.010000 ; qtot 0.053054
49 h1 8 LIG H31 8 0.05446100 1.008000 ; qtot 0.107515
50 h1 8 LIG H32 8 0.05446100 1.008000 ; qtot 0.161976
51 os 8 LIG OO2 8 -0.34100800 16.000000 ; qtot -0.179032
52 c3 8 LIG C1 8 0.10024900 12.010000 ; qtot -0.078783
53 h1 8 LIG H11 8 0.03274700 1.008000 ; qtot -0.046036
54 h1 8 LIG H12 8 0.03274700 1.008000 ; qtot -0.013289
55 c3 9 LIG C3 9 0.06028000 12.010000 ; qtot 0.046991
56 h1 9 LIG H31 9 0.06074700 1.008000 ; qtot 0.107738
57 h1 9 LIG H32 9 0.06074700 1.008000 ; qtot 0.168485
58 os 9 LIG OO2 9 -0.35270300 16.000000 ; qtot -0.184218
59 c3 9 LIG C1 9 0.08709800 12.010000 ; qtot -0.097120
60 h1 9 LIG H11 9 0.05772300 1.008000 ; qtot -0.039397
61 h1 9 LIG H12 9 0.05772300 1.008000 ; qtot 0.018326
62 c3 10 LIG C3 10 0.04504900 12.010000 ; qtot 0.063375
63 h1 10 LIG H31 10 0.04614600 1.008000 ; qtot 0.109521
64 h1 10 LIG H32 10 0.04614600 1.008000 ; qtot 0.155667
65 os 10 LIG OO2 10 -0.31679000 16.000000 ; qtot -0.161123
66 c3 10 LIG C1 10 0.10114900 12.010000 ; qtot -0.059974
67 h1 10 LIG H11 10 0.03112000 1.008000 ; qtot -0.028854
68 h1 10 LIG H12 10 0.03112000 1.008000 ; qtot 0.002266
69 c3 11 LIG C3 11 0.09576100 12.010000 ; qtot 0.098027
70 h1 11 LIG H31 11 0.03498700 1.008000 ; qtot 0.133014
71 h1 11 LIG H32 11 0.03498700 1.008000 ; qtot 0.168001
72 os 11 LIG OO2 11 -0.33223100 16.000000 ; qtot -0.164230
73 c3 11 LIG C1 11 0.07742100 12.010000 ; qtot -0.086809
74 h1 11 LIG H11 11 0.03708000 1.008000 ; qtot -0.049729
75 h1 11 LIG H12 11 0.03708000 1.008000 ; qtot -0.012649
76 c3 12 LIG C3 12 0.10849200 12.010000 ; qtot 0.095843
77 h1 12 LIG H31 12 0.03117900 1.008000 ; qtot 0.127022
78 h1 12 LIG H32 12 0.03117900 1.008000 ; qtot 0.158201
79 os 12 LIG OO2 12 -0.32029400 16.000000 ; qtot -0.162093
80 c3 12 LIG C1 12 0.05746900 12.010000 ; qtot -0.104624
81 h1 12 LIG H11 12 0.04460300 1.008000 ; qtot -0.060021
82 h1 12 LIG H12 12 0.04460300 1.008000 ; qtot -0.015418
83 c3 13 LIG C3 13 0.12762300 12.010000 ; qtot 0.112205
84 h1 13 LIG H31 13 0.02863500 1.008000 ; qtot 0.140840
85 h1 13 LIG H32 13 0.02863500 1.008000 ; qtot 0.169475
86 os 13 LIG OO2 13 -0.32898200 16.000000 ; qtot -0.159507
87 c3 13 LIG C1 13 0.05201500 12.010000 ; qtot -0.107492
88 h1 13 LIG H11 13 0.04276800 1.008000 ; qtot -0.064724
89 h1 13 LIG H12 13 0.04276800 1.008000 ; qtot -0.021956
90 c3 14 LIG C3 14 0.15284200 12.010000 ; qtot 0.130886
91 h1 14 LIG H31 14 0.02278800 1.008000 ; qtot 0.153674
92 h1 14 LIG H32 14 0.02278800 1.008000 ; qtot 0.176462
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93 os 14 LIG OO2 14 -0.34783800 16.000000 ; qtot -0.171376
94 c3 14 LIG C1 14 0.11460900 12.010000 ; qtot -0.056767
95 h1 14 LIG H11 14 0.02687100 1.008000 ; qtot -0.029896
96 h1 14 LIG H12 14 0.02687100 1.008000 ; qtot -0.003025
97 c3 15 LIG C3 15 0.11918000 12.010000 ; qtot 0.116155
98 h1 15 LIG H31 15 0.02661600 1.008000 ; qtot 0.142771
99 h1 15 LIG H32 15 0.02661600 1.008000 ; qtot 0.169387
100 os 15 LIG OO2 15 -0.33895500 16.000000 ; qtot -0.169568
101 c3 15 LIG C1 15 0.11960800 12.010000 ; qtot -0.049960
102 h1 15 LIG H11 15 0.02601300 1.008000 ; qtot -0.023947
103 h1 15 LIG H12 15 0.02601300 1.008000 ; qtot 0.002066
104 c3 16 LIG C3 16 0.09861000 12.010000 ; qtot 0.100676
105 h1 16 LIG H31 16 0.02995200 1.008000 ; qtot 0.130628
106 h1 16 LIG H32 16 0.02995200 1.008000 ; qtot 0.160580
107 os 16 LIG OO2 16 -0.33498100 16.000000 ; qtot -0.174401
108 c3 16 LIG C1 16 0.11059300 12.010000 ; qtot -0.063808
109 h1 16 LIG H11 16 0.03223200 1.008000 ; qtot -0.031576
110 h1 16 LIG H12 16 0.03223200 1.008000 ; qtot 0.000656
111 c3 17 LIG C3 17 0.10191300 12.010000 ; qtot 0.102569
112 h1 17 LIG H31 17 0.03255500 1.008000 ; qtot 0.135124
113 h1 17 LIG H32 17 0.03255500 1.008000 ; qtot 0.167679
114 os 17 LIG OO2 17 -0.33972800 16.000000 ; qtot -0.172049
115 c3 17 LIG C1 17 0.10742000 12.010000 ; qtot -0.064629
116 h1 17 LIG H11 17 0.03256200 1.008000 ; qtot -0.032067
117 h1 17 LIG H12 17 0.03256200 1.008000 ; qtot 0.000495
118 c3 18 LIG C3 18 0.07653600 12.010000 ; qtot 0.077031
119 h1 18 LIG H31 18 0.04370400 1.008000 ; qtot 0.120735
120 h1 18 LIG H32 18 0.04370400 1.008000 ; qtot 0.164439
121 os 18 LIG OO2 18 -0.32686500 16.000000 ; qtot -0.162426
122 c3 18 LIG C1 18 0.10447600 12.010000 ; qtot -0.057950
123 h1 18 LIG H11 18 0.03045200 1.008000 ; qtot -0.027498
124 h1 18 LIG H12 18 0.03045200 1.008000 ; qtot 0.002954
125 c3 19 LIG C3 19 0.11549300 12.010000 ; qtot 0.118447
126 h1 19 LIG H31 19 0.02616800 1.008000 ; qtot 0.144615
127 h1 19 LIG H32 19 0.02616800 1.008000 ; qtot 0.170783
128 os 19 LIG OO2 19 -0.34175300 16.000000 ; qtot -0.170970
129 c3 19 LIG C1 19 0.09762100 12.010000 ; qtot -0.073349
130 h1 19 LIG H11 19 0.03734100 1.008000 ; qtot -0.036008
131 h1 19 LIG H12 19 0.03734100 1.008000 ; qtot 0.001333
132 c3 20 LIG C3 20 0.09866200 12.010000 ; qtot 0.099995
133 h1 20 LIG H31 20 0.03218100 1.008000 ; qtot 0.132176
134 h1 20 LIG H32 20 0.03218100 1.008000 ; qtot 0.164357
135 os 20 LIG OO2 20 -0.32712500 16.000000 ; qtot -0.162768
136 c3 20 LIG C1 20 0.08040700 12.010000 ; qtot -0.082361
137 h1 20 LIG H11 20 0.03825100 1.008000 ; qtot -0.044110
138 h1 20 LIG H12 20 0.03825100 1.008000 ; qtot -0.005859
139 c3 21 LIG C3 21 0.10815800 12.010000 ; qtot 0.102299
140 h1 21 LIG H31 21 0.03670600 1.008000 ; qtot 0.139005
141 h1 21 LIG H32 21 0.03670600 1.008000 ; qtot 0.175711
142 os 21 LIG OO2 21 -0.33441500 16.000000 ; qtot -0.158704
143 c3 21 LIG C1 21 0.06041800 12.010000 ; qtot -0.098286
144 h1 21 LIG H11 21 0.04127000 1.008000 ; qtot -0.057016
145 h1 21 LIG H12 21 0.04127000 1.008000 ; qtot -0.015746
146 c3 22 LIG C3 22 0.14158900 12.010000 ; qtot 0.125843
147 h1 22 LIG H31 22 0.02443900 1.008000 ; qtot 0.150282
148 h1 22 LIG H32 22 0.02443900 1.008000 ; qtot 0.174721
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149 os 22 LIG OO2 22 -0.35114400 16.000000 ; qtot -0.176423
150 c3 22 LIG C1 22 0.16706000 12.010000 ; qtot -0.009363
151 h1 22 LIG H11 22 0.01036400 1.008000 ; qtot 0.001001
152 h1 22 LIG H12 22 0.01036400 1.008000 ; qtot 0.011365
153 c3 23 LIG C3 23 0.09016800 12.010000 ; qtot 0.101533
154 h1 23 LIG H31 23 0.03744400 1.008000 ; qtot 0.138977
155 h1 23 LIG H32 23 0.03744400 1.008000 ; qtot 0.176421
156 os 23 LIG OO2 23 -0.35448700 16.000000 ; qtot -0.178066
157 c3 23 LIG C1 23 0.13084700 12.010000 ; qtot -0.047219
158 h1 23 LIG H11 23 0.02360900 1.008000 ; qtot -0.023610
159 h1 23 LIG H12 23 0.02360900 1.008000 ; qtot -0.000001
160 c3 24 LIG C3 24 0.13084700 12.010000 ; qtot 0.130846
161 h1 24 LIG H31 24 0.02360900 1.008000 ; qtot 0.154455
162 h1 24 LIG H32 24 0.02360900 1.008000 ; qtot 0.178064
163 os 24 LIG OO2 24 -0.35448700 16.000000 ; qtot -0.176423
164 c3 24 LIG C1 24 0.09016800 12.010000 ; qtot -0.086255
165 h1 24 LIG H11 24 0.03744400 1.008000 ; qtot -0.048811
166 h1 24 LIG H12 24 0.03744400 1.008000 ; qtot -0.011367
167 c3 25 LIG C3 25 0.16706000 12.010000 ; qtot 0.155693
168 h1 25 LIG H31 25 0.01036400 1.008000 ; qtot 0.166057
169 h1 25 LIG H32 25 0.01036400 1.008000 ; qtot 0.176421
170 os 25 LIG OO2 25 -0.35114400 16.000000 ; qtot -0.174723
171 c3 25 LIG C1 25 0.14158900 12.010000 ; qtot -0.033134
172 h1 25 LIG H11 25 0.02443900 1.008000 ; qtot -0.008695
173 h1 25 LIG H12 25 0.02443900 1.008000 ; qtot 0.015744
174 c3 26 LIG C3 26 0.06041800 12.010000 ; qtot 0.076162
175 h1 26 LIG H31 26 0.04127000 1.008000 ; qtot 0.117432
176 h1 26 LIG H32 26 0.04127000 1.008000 ; qtot 0.158702
177 os 26 LIG OO2 26 -0.33441500 16.000000 ; qtot -0.175713
178 c3 26 LIG C1 26 0.10815800 12.010000 ; qtot -0.067555
179 h1 26 LIG H11 26 0.03670600 1.008000 ; qtot -0.030849
180 h1 26 LIG H12 26 0.03670600 1.008000 ; qtot 0.005857
181 c3 27 LIG C3 27 0.08040700 12.010000 ; qtot 0.086264
182 h1 27 LIG H31 27 0.03825100 1.008000 ; qtot 0.124515
183 h1 27 LIG H32 27 0.03825100 1.008000 ; qtot 0.162766
184 os 27 LIG OO2 27 -0.32712500 16.000000 ; qtot -0.164359
185 c3 27 LIG C1 27 0.09866200 12.010000 ; qtot -0.065697
186 h1 27 LIG H11 27 0.03218100 1.008000 ; qtot -0.033516
187 h1 27 LIG H12 27 0.03218100 1.008000 ; qtot -0.001335
188 c3 28 LIG C3 28 0.09762100 12.010000 ; qtot 0.096286
189 h1 28 LIG H31 28 0.03734100 1.008000 ; qtot 0.133627
190 h1 28 LIG H32 28 0.03734100 1.008000 ; qtot 0.170968
191 os 28 LIG OO2 28 -0.34175300 16.000000 ; qtot -0.170785
192 c3 28 LIG C1 28 0.11549300 12.010000 ; qtot -0.055292
193 h1 28 LIG H11 28 0.02616800 1.008000 ; qtot -0.029124
194 h1 28 LIG H12 28 0.02616800 1.008000 ; qtot -0.002956
195 c3 29 LIG C3 29 0.10447600 12.010000 ; qtot 0.101520
196 h1 29 LIG H31 29 0.03045200 1.008000 ; qtot 0.131972
197 h1 29 LIG H32 29 0.03045200 1.008000 ; qtot 0.162424
198 os 29 LIG OO2 29 -0.32686500 16.000000 ; qtot -0.164441
199 c3 29 LIG C1 29 0.07653600 12.010000 ; qtot -0.087905
200 h1 29 LIG H11 29 0.04370400 1.008000 ; qtot -0.044201
201 h1 29 LIG H12 29 0.04370400 1.008000 ; qtot -0.000497
202 c3 30 LIG C3 30 0.10742000 12.010000 ; qtot 0.106923
203 h1 30 LIG H31 30 0.03256200 1.008000 ; qtot 0.139485
204 h1 30 LIG H32 30 0.03256200 1.008000 ; qtot 0.172047
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205 os 30 LIG OO2 30 -0.33972800 16.000000 ; qtot -0.167681
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207 h1 30 LIG H11 30 0.03255500 1.008000 ; qtot -0.033213
208 h1 30 LIG H12 30 0.03255500 1.008000 ; qtot -0.000658
209 c3 31 LIG C3 31 0.11059300 12.010000 ; qtot 0.109935
210 h1 31 LIG H31 31 0.03223200 1.008000 ; qtot 0.142167
211 h1 31 LIG H32 31 0.03223200 1.008000 ; qtot 0.174399
212 os 31 LIG OO2 31 -0.33498100 16.000000 ; qtot -0.160582
213 c3 31 LIG C1 31 0.09861000 12.010000 ; qtot -0.061972
214 h1 31 LIG H11 31 0.02995200 1.008000 ; qtot -0.032020
215 h1 31 LIG H12 31 0.02995200 1.008000 ; qtot -0.002068
216 c3 32 LIG C3 32 0.11960800 12.010000 ; qtot 0.117540
217 h1 32 LIG H31 32 0.02601300 1.008000 ; qtot 0.143553
218 h1 32 LIG H32 32 0.02601300 1.008000 ; qtot 0.169566
219 os 32 LIG OO2 32 -0.33895500 16.000000 ; qtot -0.169389
220 c3 32 LIG C1 32 0.11918000 12.010000 ; qtot -0.050209
221 h1 32 LIG H11 32 0.02661600 1.008000 ; qtot -0.023593
222 h1 32 LIG H12 32 0.02661600 1.008000 ; qtot 0.003023
223 c3 33 LIG C3 33 0.11460900 12.010000 ; qtot 0.117632
224 h1 33 LIG H31 33 0.02687100 1.008000 ; qtot 0.144503
225 h1 33 LIG H32 33 0.02687100 1.008000 ; qtot 0.171374
226 os 33 LIG OO2 33 -0.34783800 16.000000 ; qtot -0.176464
227 c3 33 LIG C1 33 0.15284200 12.010000 ; qtot -0.023622
228 h1 33 LIG H11 33 0.02278800 1.008000 ; qtot -0.000834
229 h1 33 LIG H12 33 0.02278800 1.008000 ; qtot 0.021954
230 c3 34 LIG C3 34 0.05201500 12.010000 ; qtot 0.073969
231 h1 34 LIG H31 34 0.04276800 1.008000 ; qtot 0.116737
232 h1 34 LIG H32 34 0.04276800 1.008000 ; qtot 0.159505
233 os 34 LIG OO2 34 -0.32898200 16.000000 ; qtot -0.169477
234 c3 34 LIG C1 34 0.12762300 12.010000 ; qtot -0.041854
235 h1 34 LIG H11 34 0.02863500 1.008000 ; qtot -0.013219
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237 c3 35 LIG C3 35 0.05746900 12.010000 ; qtot 0.072885
238 h1 35 LIG H31 35 0.04460300 1.008000 ; qtot 0.117488
239 h1 35 LIG H32 35 0.04460300 1.008000 ; qtot 0.162091
240 os 35 LIG OO2 35 -0.32029400 16.000000 ; qtot -0.158203
241 c3 35 LIG C1 35 0.10849200 12.010000 ; qtot -0.049711
242 h1 35 LIG H11 35 0.03117900 1.008000 ; qtot -0.018532
243 h1 35 LIG H12 35 0.03117900 1.008000 ; qtot 0.012647
244 c3 36 LIG C3 36 0.07742100 12.010000 ; qtot 0.090068
245 h1 36 LIG H31 36 0.03708000 1.008000 ; qtot 0.127148
246 h1 36 LIG H32 36 0.03708000 1.008000 ; qtot 0.164228
247 os 36 LIG OO2 36 -0.33223100 16.000000 ; qtot -0.168003
248 c3 36 LIG C1 36 0.09576100 12.010000 ; qtot -0.072242
249 h1 36 LIG H11 36 0.03498700 1.008000 ; qtot -0.037255
250 h1 36 LIG H12 36 0.03498700 1.008000 ; qtot -0.002268
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254 os 37 LIG OO2 37 -0.31679000 16.000000 ; qtot -0.155669
255 c3 37 LIG C1 37 0.04504900 12.010000 ; qtot -0.110620
256 h1 37 LIG H11 37 0.04614600 1.008000 ; qtot -0.064474
257 h1 37 LIG H12 37 0.04614600 1.008000 ; qtot -0.018328
258 c3 38 LIG C3 38 0.08709800 12.010000 ; qtot 0.068770
259 h1 38 LIG H31 38 0.05772300 1.008000 ; qtot 0.126493
260 h1 38 LIG H32 38 0.05772300 1.008000 ; qtot 0.184216
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261 os 38 LIG OO2 38 -0.35270300 16.000000 ; qtot -0.168487
262 c3 38 LIG C1 38 0.06028000 12.010000 ; qtot -0.108207
263 h1 38 LIG H11 38 0.06074700 1.008000 ; qtot -0.047460
264 h1 38 LIG H12 38 0.06074700 1.008000 ; qtot 0.013287
265 c3 39 LIG C3 39 0.10024900 12.010000 ; qtot 0.113536
266 h1 39 LIG H31 39 0.03274700 1.008000 ; qtot 0.146283
267 h1 39 LIG H32 39 0.03274700 1.008000 ; qtot 0.179030
268 os 39 LIG OO2 39 -0.34100800 16.000000 ; qtot -0.161978
269 c3 39 LIG C1 39 0.04250500 12.010000 ; qtot -0.119473
270 h1 39 LIG H11 39 0.05446100 1.008000 ; qtot -0.065012
271 h1 39 LIG H12 39 0.05446100 1.008000 ; qtot -0.010551
272 c3 40 LIG C3 40 0.14011900 12.010000 ; qtot 0.129568
273 h1 40 LIG H31 40 0.02078600 1.008000 ; qtot 0.150354
274 h1 40 LIG H32 40 0.02078600 1.008000 ; qtot 0.171140
275 os 40 LIG OO2 40 -0.33652600 16.000000 ; qtot -0.165386
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281 h1 41 LIG H32 41 0.04132000 1.008000 ; qtot 0.165040
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283 c3 41 LIG C1 41 0.05496400 12.010000 ; qtot -0.099735
284 h1 41 LIG H11 41 0.04449200 1.008000 ; qtot -0.055243
285 h1 41 LIG H12 41 0.04449200 1.008000 ; qtot -0.010751
286 c3 42 LIG C3 42 0.12646500 12.010000 ; qtot 0.115714
287 h1 42 LIG H31 42 0.02762200 1.008000 ; qtot 0.143336
288 h1 42 LIG H32 42 0.02762200 1.008000 ; qtot 0.170958
289 os 42 LIG OO2 42 -0.33132000 16.000000 ; qtot -0.160362
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291 h1 42 LIG H11 42 0.04163300 1.008000 ; qtot -0.058710
292 h1 42 LIG H12 42 0.04163300 1.008000 ; qtot -0.017077
293 c3 43 LIG C3 43 0.14568000 12.010000 ; qtot 0.128603
294 h1 43 LIG H31 43 0.02432700 1.008000 ; qtot 0.152930
295 h1 43 LIG H32 43 0.02432700 1.008000 ; qtot 0.177257
296 os 43 LIG OO2 43 -0.33740600 16.000000 ; qtot -0.160149
297 c3 43 LIG C1 43 0.08279600 12.010000 ; qtot -0.077353
298 h1 43 LIG H11 43 0.03567400 1.008000 ; qtot -0.041679
299 h1 43 LIG H12 43 0.03567400 1.008000 ; qtot -0.006005
300 c3 44 LIG C3 44 0.13420900 12.010000 ; qtot 0.128204
301 h1 44 LIG H31 44 0.02790400 1.008000 ; qtot 0.156108
302 h1 44 LIG H32 44 0.02790400 1.008000 ; qtot 0.184012
303 os 44 LIG OO2 44 -0.34827500 16.000000 ; qtot -0.164263
304 c3 44 LIG C1 44 0.13212200 12.010000 ; qtot -0.032141
305 h1 44 LIG H11 44 0.02596800 1.008000 ; qtot -0.006173
306 h1 44 LIG H12 44 0.02596800 1.008000 ; qtot 0.019795
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308 h1 45 LIG H31 45 0.05347500 1.008000 ; qtot 0.122258
309 h1 45 LIG H32 45 0.05347500 1.008000 ; qtot 0.175733
310 os 45 LIG OO2 45 -0.32101400 16.000000 ; qtot -0.145281
311 c3 45 LIG C1 45 -0.04312400 12.010000 ; qtot -0.188405
312 h1 45 LIG H11 45 0.05936600 1.008000 ; qtot -0.129039
313 h1 45 LIG H12 45 0.05936600 1.008000 ; qtot -0.069673
314 c3 46 LIE C3 46 0.28304200 12.010000 ; qtot 0.213369
315 h1 46 LIE H31 46 0.00482800 1.008000 ; qtot 0.218197
316 h1 46 LIE H32 46 0.00482800 1.008000 ; qtot 0.223025
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[ bonds ]
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3 6 1 0.15375 251793.120000
6 9 1 0.14316 258236.480000
9 10 1 0.14316 258236.480000
10 13 1 0.15375 251793.120000
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[ dihedrals ]
; ai aj ak al funct c0 c1 c2 c3 c4
c5 2 3 6 9 1 0.0000000 4.9162000 2
2 3 6 9 1 0.0000000 0.6024960 3
3 6 9 10 1 180.0000771 0.4184000 2
3 6 9 10 1 0.0000000 1.6024720 3
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31 34 37 38 1 0.0000000 1.6024720 3
34 37 38 41 1 180.0000771 0.4184000 2
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90 93 94 96 1 0.0000000 1.6038667 3
91 90 93 94 1 0.0000000 1.6038667 3
92 90 93 94 1 0.0000000 1.6038667 3
93 94 97 98 1 0.0000000 1.0460000 1
93 94 97 98 1 0.0000000 0.0000000 3
```

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93 94 97 99 1 0.0000000 1.0460000 1
93 94 97 99 1 0.0000000 0.0000000 3
95 94 97 98 1 0.0000000 0.6508444 3
95 94 97 99 1 0.0000000 0.6508444 3
95 94 97 100 1 0.0000000 1.0460000 1
95 94 97 100 1 0.0000000 0.0000000 3
96 94 97 98 1 0.0000000 0.6508444 3
96 94 97 99 1 0.0000000 0.6508444 3
96 94 97 100 1 0.0000000 1.0460000 1
96 94 97 100 1 0.0000000 0.0000000 3
97 100 101 102 1 0.0000000 1.6038667 3
97 100 101 103 1 0.0000000 1.6038667 3
98 97 100 101 1 0.0000000 1.6038667 3
99 97 100 101 1 0.0000000 1.6038667 3
100 101 104 105 1 0.0000000 1.0460000 1
100 101 104 105 1 0.0000000 0.0000000 3
100 101 104 106 1 0.0000000 1.0460000 1
100 101 104 106 1 0.0000000 0.0000000 3
102 101 104 105 1 0.0000000 0.6508444 3
102 101 104 106 1 0.0000000 0.6508444 3
102 101 104 107 1 0.0000000 1.0460000 1
102 101 104 107 1 0.0000000 0.0000000 3
103 101 104 105 1 0.0000000 0.6508444 3
103 101 104 106 1 0.0000000 0.6508444 3
103 101 104 107 1 0.0000000 1.0460000 1
103 101 104 107 1 0.0000000 0.0000000 3
104 107 108 109 1 0.0000000 1.6038667 3
104 107 108 110 1 0.0000000 1.6038667 3
105 104 107 108 1 0.0000000 1.6038667 3
106 104 107 108 1 0.0000000 1.6038667 3
107 108 111 112 1 0.0000000 1.0460000 1
107 108 111 112 1 0.0000000 0.0000000 3
107 108 111 113 1 0.0000000 1.0460000 1
107 108 111 113 1 0.0000000 0.0000000 3
109 108 111 112 1 0.0000000 0.6508444 3
109 108 111 113 1 0.0000000 0.6508444 3
109 108 111 114 1 0.0000000 1.0460000 1
109 108 111 114 1 0.0000000 0.0000000 3
110 108 111 112 1 0.0000000 0.6508444 3
110 108 111 113 1 0.0000000 0.6508444 3
110 108 111 114 1 0.0000000 1.0460000 1
110 108 111 114 1 0.0000000 0.0000000 3
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111 114 115 117 1 0.0000000 1.6038667 3
112 111 114 115 1 0.0000000 1.6038667 3
113 111 114 115 1 0.0000000 1.6038667 3
114 115 118 119 1 0.0000000 1.0460000 1
114 115 118 119 1 0.0000000 0.0000000 3
114 115 118 120 1 0.0000000 1.0460000 1
114 115 118 120 1 0.0000000 0.0000000 3
116 115 118 119 1 0.0000000 0.6508444 3
116 115 118 120 1 0.0000000 0.6508444 3
116 115 118 121 1 0.0000000 1.0460000 1
116 115 118 121 1 0.0000000 0.0000000 3
117 115 118 119 1 0.0000000 0.6508444 3
117 115 118 120 1 0.0000000 0.6508444 3
```

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117 115 118 121 1 0.0000000 0.0000000 3
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119 118 121 122 1 0.0000000 1.6038667 3
120 118 121 122 1 0.0000000 1.6038667 3
121 122 125 126 1 0.0000000 1.0460000 1
121 122 125 126 1 0.0000000 0.0000000 3
121 122 125 127 1 0.0000000 1.0460000 1
121 122 125 127 1 0.0000000 0.0000000 3
123 122 125 126 1 0.0000000 0.6508444 3
123 122 125 127 1 0.0000000 0.6508444 3
123 122 125 128 1 0.0000000 1.0460000 1
123 122 125 128 1 0.0000000 0.0000000 3
124 122 125 126 1 0.0000000 0.6508444 3
124 122 125 127 1 0.0000000 0.6508444 3
124 122 125 128 1 0.0000000 1.0460000 1
124 122 125 128 1 0.0000000 0.0000000 3
125 128 129 130 1 0.0000000 1.6038667 3
125 128 129 131 1 0.0000000 1.6038667 3
126 125 128 129 1 0.0000000 1.6038667 3
127 125 128 129 1 0.0000000 1.6038667 3
128 129 132 133 1 0.0000000 1.0460000 1
128 129 132 133 1 0.0000000 0.0000000 3
128 129 132 134 1 0.0000000 1.0460000 1
128 129 132 134 1 0.0000000 0.0000000 3
130 129 132 133 1 0.0000000 0.6508444 3
130 129 132 134 1 0.0000000 0.6508444 3
130 129 132 135 1 0.0000000 1.0460000 1
130 129 132 135 1 0.0000000 0.0000000 3
131 129 132 133 1 0.0000000 0.6508444 3
131 129 132 134 1 0.0000000 0.6508444 3
131 129 132 135 1 0.0000000 1.0460000 1
131 129 132 135 1 0.0000000 0.0000000 3
132 135 136 137 1 0.0000000 1.6038667 3
132 135 136 138 1 0.0000000 1.6038667 3
133 132 135 136 1 0.0000000 1.6038667 3
134 132 135 136 1 0.0000000 1.6038667 3
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135 136 139 140 1 0.0000000 0.0000000 3
135 136 139 141 1 0.0000000 1.0460000 1
135 136 139 141 1 0.0000000 0.0000000 3
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137 136 139 142 1 0.0000000 0.0000000 3
138 136 139 140 1 0.0000000 0.6508444 3
138 136 139 141 1 0.0000000 0.6508444 3
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138 136 139 142 1 0.0000000 0.0000000 3
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139 142 143 145 1 0.0000000 1.6038667 3
140 139 142 143 1 0.0000000 1.6038667 3
141 139 142 143 1 0.0000000 1.6038667 3
142 143 146 147 1 0.0000000 1.0460000 1
142 143 146 147 1 0.0000000 0.0000000 3
```

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144 143 146 149 1 0.0000000 0.0000000 3
145 143 146 147 1 0.0000000 0.6508444 3
145 143 146 148 1 0.0000000 0.6508444 3
145 143 146 149 1 0.0000000 1.0460000 1
145 143 146 149 1 0.0000000 0.0000000 3
146 149 150 151 1 0.0000000 1.6038667 3
146 149 150 152 1 0.0000000 1.6038667 3
147 146 149 150 1 0.0000000 1.6038667 3
148 146 149 150 1 0.0000000 1.6038667 3
149 150 153 154 1 0.0000000 1.0460000 1
149 150 153 154 1 0.0000000 0.0000000 3
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151 150 153 156 1 0.0000000 0.0000000 3
152 150 153 154 1 0.0000000 0.6508444 3
152 150 153 155 1 0.0000000 0.6508444 3
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152 150 153 156 1 0.0000000 0.0000000 3
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153 156 157 159 1 0.0000000 1.6038667 3
154 153 156 157 1 0.0000000 1.6038667 3
155 153 156 157 1 0.0000000 1.6038667 3
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156 157 160 161 1 0.0000000 0.0000000 3
156 157 160 162 1 0.0000000 1.0460000 1
156 157 160 162 1 0.0000000 0.0000000 3
158 157 160 161 1 0.0000000 0.6508444 3
158 157 160 162 1 0.0000000 0.6508444 3
158 157 160 163 1 0.0000000 1.0460000 1
158 157 160 163 1 0.0000000 0.0000000 3
159 157 160 161 1 0.0000000 0.6508444 3
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159 157 160 163 1 0.0000000 0.0000000 3
160 163 164 165 1 0.0000000 1.6038667 3
160 163 164 166 1 0.0000000 1.6038667 3
161 160 163 164 1 0.0000000 1.6038667 3
162 160 163 164 1 0.0000000 1.6038667 3
163 164 167 168 1 0.0000000 1.0460000 1
163 164 167 168 1 0.0000000 0.0000000 3
163 164 167 169 1 0.0000000 1.0460000 1
163 164 167 169 1 0.0000000 0.0000000 3
165 164 167 168 1 0.0000000 0.6508444 3
165 164 167 169 1 0.0000000 0.6508444 3
165 164 167 170 1 0.0000000 1.0460000 1
165 164 167 170 1 0.0000000 0.0000000 3
166 164 167 168 1 0.0000000 0.6508444 3
166 164 167 169 1 0.0000000 0.6508444 3
```

166 164 167 170 1 0.0000000 1.0460000 1
166 164 167 170 1 0.0000000 0.0000000 3
167 170 171 172 1 0.0000000 1.6038667 3
167 170 171 173 1 0.0000000 1.6038667 3
168 167 170 171 1 0.0000000 1.6038667 3
169 167 170 171 1 0.0000000 1.6038667 3
170 171 174 175 1 0.0000000 1.0460000 1
170 171 174 175 1 0.0000000 0.0000000 3
170 171 174 176 1 0.0000000 1.0460000 1
170 171 174 176 1 0.0000000 0.0000000 3
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172 171 174 176 1 0.0000000 0.6508444 3
172 171 174 177 1 0.0000000 1.0460000 1
172 171 174 177 1 0.0000000 0.0000000 3
173 171 174 175 1 0.0000000 0.6508444 3
173 171 174 176 1 0.0000000 0.6508444 3
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173 171 174 177 1 0.0000000 0.0000000 3
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174 177 178 180 1 0.0000000 1.6038667 3
175 174 177 178 1 0.0000000 1.6038667 3
176 174 177 178 1 0.0000000 1.6038667 3
177 178 181 182 1 0.0000000 1.0460000 1
177 178 181 182 1 0.0000000 0.0000000 3
177 178 181 183 1 0.0000000 1.0460000 1
177 178 181 183 1 0.0000000 0.0000000 3
179 178 181 182 1 0.0000000 0.6508444 3
179 178 181 183 1 0.0000000 0.6508444 3
179 178 181 184 1 0.0000000 1.0460000 1
179 178 181 184 1 0.0000000 0.0000000 3
180 178 181 182 1 0.0000000 0.6508444 3
180 178 181 183 1 0.0000000 0.6508444 3
180 178 181 184 1 0.0000000 1.0460000 1
180 178 181 184 1 0.0000000 0.0000000 3
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181 184 185 187 1 0.0000000 1.6038667 3
182 181 184 185 1 0.0000000 1.6038667 3
183 181 184 185 1 0.0000000 1.6038667 3
184 185 188 189 1 0.0000000 1.0460000 1
184 185 188 189 1 0.0000000 0.0000000 3
184 185 188 190 1 0.0000000 1.0460000 1
184 185 188 190 1 0.0000000 0.0000000 3
186 185 188 189 1 0.0000000 0.6508444 3
186 185 188 190 1 0.0000000 0.6508444 3
186 185 188 191 1 0.0000000 1.0460000 1
186 185 188 191 1 0.0000000 0.0000000 3
187 185 188 189 1 0.0000000 0.6508444 3
187 185 188 190 1 0.0000000 0.6508444 3
187 185 188 191 1 0.0000000 1.0460000 1
187 185 188 191 1 0.0000000 0.0000000 3
188 191 192 193 1 0.0000000 1.6038667 3
188 191 192 194 1 0.0000000 1.6038667 3
189 188 191 192 1 0.0000000 1.6038667 3
190 188 191 192 1 0.0000000 1.6038667 3
191 192 195 196 1 0.0000000 1.0460000 1
191 192 195 196 1 0.0000000 0.0000000 3

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191 192 195 197 1 0.0000000 1.0460000 1
191 192 195 197 1 0.0000000 0.0000000 3
193 192 195 196 1 0.0000000 0.6508444 3
193 192 195 197 1 0.0000000 0.6508444 3
193 192 195 198 1 0.0000000 1.0460000 1
193 192 195 198 1 0.0000000 0.0000000 3
194 192 195 196 1 0.0000000 0.6508444 3
194 192 195 197 1 0.0000000 0.6508444 3
194 192 195 198 1 0.0000000 1.0460000 1
194 192 195 198 1 0.0000000 0.0000000 3
195 198 199 200 1 0.0000000 1.6038667 3
195 198 199 201 1 0.0000000 1.6038667 3
196 195 198 199 1 0.0000000 1.6038667 3
197 195 198 199 1 0.0000000 1.6038667 3
198 199 202 203 1 0.0000000 1.0460000 1
198 199 202 203 1 0.0000000 0.0000000 3
198 199 202 204 1 0.0000000 1.0460000 1
198 199 202 204 1 0.0000000 0.0000000 3
200 199 202 203 1 0.0000000 0.6508444 3
200 199 202 204 1 0.0000000 0.6508444 3
200 199 202 205 1 0.0000000 1.0460000 1
200 199 202 205 1 0.0000000 0.0000000 3
201 199 202 203 1 0.0000000 0.6508444 3
201 199 202 204 1 0.0000000 0.6508444 3
201 199 202 205 1 0.0000000 1.0460000 1
201 199 202 205 1 0.0000000 0.0000000 3
202 205 206 207 1 0.0000000 1.6038667 3
202 205 206 208 1 0.0000000 1.6038667 3
203 202 205 206 1 0.0000000 1.6038667 3
204 202 205 206 1 0.0000000 1.6038667 3
205 206 209 210 1 0.0000000 1.0460000 1
205 206 209 210 1 0.0000000 0.0000000 3
205 206 209 211 1 0.0000000 1.0460000 1
205 206 209 211 1 0.0000000 0.0000000 3
207 206 209 210 1 0.0000000 0.6508444 3
207 206 209 211 1 0.0000000 0.6508444 3
207 206 209 212 1 0.0000000 1.0460000 1
207 206 209 212 1 0.0000000 0.0000000 3
208 206 209 210 1 0.0000000 0.6508444 3
208 206 209 211 1 0.0000000 0.6508444 3
208 206 209 212 1 0.0000000 1.0460000 1
208 206 209 212 1 0.0000000 0.0000000 3
209 212 213 214 1 0.0000000 1.6038667 3
209 212 213 215 1 0.0000000 1.6038667 3
210 209 212 213 1 0.0000000 1.6038667 3
211 209 212 213 1 0.0000000 1.6038667 3
212 213 216 217 1 0.0000000 1.0460000 1
212 213 216 217 1 0.0000000 0.0000000 3
212 213 216 218 1 0.0000000 1.0460000 1
212 213 216 218 1 0.0000000 0.0000000 3
214 213 216 217 1 0.0000000 0.6508444 3
214 213 216 218 1 0.0000000 0.6508444 3
214 213 216 219 1 0.0000000 1.0460000 1
214 213 216 219 1 0.0000000 0.0000000 3
215 213 216 217 1 0.0000000 0.6508444 3
215 213 216 218 1 0.0000000 0.6508444 3
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215 213 216 219 1 0.0000000 1.0460000 1
215 213 216 219 1 0.0000000 0.0000000 3
216 219 220 221 1 0.0000000 1.6038667 3
216 219 220 222 1 0.0000000 1.6038667 3
217 216 219 220 1 0.0000000 1.6038667 3
218 216 219 220 1 0.0000000 1.6038667 3
219 220 223 224 1 0.0000000 1.0460000 1
219 220 223 224 1 0.0000000 0.0000000 3
219 220 223 225 1 0.0000000 1.0460000 1
219 220 223 225 1 0.0000000 0.0000000 3
221 220 223 224 1 0.0000000 0.6508444 3
221 220 223 225 1 0.0000000 0.6508444 3
221 220 223 226 1 0.0000000 1.0460000 1
221 220 223 226 1 0.0000000 0.0000000 3
222 220 223 224 1 0.0000000 0.6508444 3
222 220 223 225 1 0.0000000 0.6508444 3
222 220 223 226 1 0.0000000 1.0460000 1
222 220 223 226 1 0.0000000 0.0000000 3
223 226 227 228 1 0.0000000 1.6038667 3
223 226 227 229 1 0.0000000 1.6038667 3
224 223 226 227 1 0.0000000 1.6038667 3
225 223 226 227 1 0.0000000 1.6038667 3
226 227 230 231 1 0.0000000 1.0460000 1
226 227 230 231 1 0.0000000 0.0000000 3
226 227 230 232 1 0.0000000 1.0460000 1
226 227 230 232 1 0.0000000 0.0000000 3
228 227 230 231 1 0.0000000 0.6508444 3
228 227 230 232 1 0.0000000 0.6508444 3
228 227 230 233 1 0.0000000 1.0460000 1
228 227 230 233 1 0.0000000 0.0000000 3
229 227 230 231 1 0.0000000 0.6508444 3
229 227 230 232 1 0.0000000 0.6508444 3
229 227 230 233 1 0.0000000 1.0460000 1
229 227 230 233 1 0.0000000 0.0000000 3
230 233 234 235 1 0.0000000 1.6038667 3
230 233 234 236 1 0.0000000 1.6038667 3
231 230 233 234 1 0.0000000 1.6038667 3
232 230 233 234 1 0.0000000 1.6038667 3
233 234 237 238 1 0.0000000 1.0460000 1
233 234 237 238 1 0.0000000 0.0000000 3
233 234 237 239 1 0.0000000 1.0460000 1
233 234 237 239 1 0.0000000 0.0000000 3
235 234 237 238 1 0.0000000 0.6508444 3
235 234 237 239 1 0.0000000 0.6508444 3
235 234 237 240 1 0.0000000 1.0460000 1
235 234 237 240 1 0.0000000 0.0000000 3
236 234 237 238 1 0.0000000 0.6508444 3
236 234 237 239 1 0.0000000 0.6508444 3
236 234 237 240 1 0.0000000 1.0460000 1
236 234 237 240 1 0.0000000 0.0000000 3
237 240 241 242 1 0.0000000 1.6038667 3
237 240 241 243 1 0.0000000 1.6038667 3
238 237 240 241 1 0.0000000 1.6038667 3
239 237 240 241 1 0.0000000 1.6038667 3
240 241 244 245 1 0.0000000 1.0460000 1
240 241 244 245 1 0.0000000 0.0000000 3
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240 241 244 246 1 0.0000000 1.0460000 1
240 241 244 246 1 0.0000000 0.0000000 3
242 241 244 245 1 0.0000000 0.6508444 3
242 241 244 246 1 0.0000000 0.6508444 3
242 241 244 247 1 0.0000000 1.0460000 1
242 241 244 247 1 0.0000000 0.0000000 3
243 241 244 245 1 0.0000000 0.6508444 3
243 241 244 246 1 0.0000000 0.6508444 3
243 241 244 247 1 0.0000000 1.0460000 1
243 241 244 247 1 0.0000000 0.0000000 3
244 247 248 249 1 0.0000000 1.6038667 3
244 247 248 250 1 0.0000000 1.6038667 3
245 244 247 248 1 0.0000000 1.6038667 3
246 244 247 248 1 0.0000000 1.6038667 3
247 248 251 252 1 0.0000000 1.0460000 1
247 248 251 252 1 0.0000000 0.0000000 3
247 248 251 253 1 0.0000000 1.0460000 1
247 248 251 253 1 0.0000000 0.0000000 3
249 248 251 252 1 0.0000000 0.6508444 3
249 248 251 253 1 0.0000000 0.6508444 3
249 248 251 254 1 0.0000000 1.0460000 1
249 248 251 254 1 0.0000000 0.0000000 3
250 248 251 252 1 0.0000000 0.6508444 3
250 248 251 253 1 0.0000000 0.6508444 3
250 248 251 254 1 0.0000000 1.0460000 1
250 248 251 254 1 0.0000000 0.0000000 3
251 254 255 256 1 0.0000000 1.6038667 3
251 254 255 257 1 0.0000000 1.6038667 3
252 251 254 255 1 0.0000000 1.6038667 3
253 251 254 255 1 0.0000000 1.6038667 3
254 255 258 259 1 0.0000000 1.0460000 1
254 255 258 259 1 0.0000000 0.0000000 3
254 255 258 260 1 0.0000000 1.0460000 1
254 255 258 260 1 0.0000000 0.0000000 3
256 255 258 259 1 0.0000000 0.6508444 3
256 255 258 260 1 0.0000000 0.6508444 3
256 255 258 261 1 0.0000000 1.0460000 1
256 255 258 261 1 0.0000000 0.0000000 3
257 255 258 259 1 0.0000000 0.6508444 3
257 255 258 260 1 0.0000000 0.6508444 3
257 255 258 261 1 0.0000000 1.0460000 1
257 255 258 261 1 0.0000000 0.0000000 3
258 261 262 263 1 0.0000000 1.6038667 3
258 261 262 264 1 0.0000000 1.6038667 3
259 258 261 262 1 0.0000000 1.6038667 3
260 258 261 262 1 0.0000000 1.6038667 3
261 262 265 266 1 0.0000000 1.0460000 1
261 262 265 266 1 0.0000000 0.0000000 3
261 262 265 267 1 0.0000000 1.0460000 1
261 262 265 267 1 0.0000000 0.0000000 3
263 262 265 266 1 0.0000000 0.6508444 3
263 262 265 267 1 0.0000000 0.6508444 3
263 262 265 268 1 0.0000000 1.0460000 1
263 262 265 268 1 0.0000000 0.0000000 3
264 262 265 266 1 0.0000000 0.6508444 3
264 262 265 267 1 0.0000000 0.6508444 3
```

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264 262 265 268 1 0.0000000 1.0460000 1
264 262 265 268 1 0.0000000 0.0000000 3
265 268 269 270 1 0.0000000 1.6038667 3
265 268 269 271 1 0.0000000 1.6038667 3
266 265 268 269 1 0.0000000 1.6038667 3
267 265 268 269 1 0.0000000 1.6038667 3
268 269 272 273 1 0.0000000 1.0460000 1
268 269 272 273 1 0.0000000 0.0000000 3
268 269 272 274 1 0.0000000 1.0460000 1
268 269 272 274 1 0.0000000 0.0000000 3
270 269 272 273 1 0.0000000 0.6508444 3
270 269 272 274 1 0.0000000 0.6508444 3
270 269 272 275 1 0.0000000 1.0460000 1
270 269 272 275 1 0.0000000 0.0000000 3
271 269 272 273 1 0.0000000 0.6508444 3
271 269 272 274 1 0.0000000 0.6508444 3
271 269 272 275 1 0.0000000 1.0460000 1
271 269 272 275 1 0.0000000 0.0000000 3
272 275 276 277 1 0.0000000 1.6038667 3
272 275 276 278 1 0.0000000 1.6038667 3
273 272 275 276 1 0.0000000 1.6038667 3
274 272 275 276 1 0.0000000 1.6038667 3
275 276 279 280 1 0.0000000 1.0460000 1
275 276 279 280 1 0.0000000 0.0000000 3
275 276 279 281 1 0.0000000 1.0460000 1
275 276 279 281 1 0.0000000 0.0000000 3
277 276 279 280 1 0.0000000 0.6508444 3
277 276 279 281 1 0.0000000 0.6508444 3
277 276 279 282 1 0.0000000 1.0460000 1
277 276 279 282 1 0.0000000 0.0000000 3
278 276 279 280 1 0.0000000 0.6508444 3
278 276 279 281 1 0.0000000 0.6508444 3
278 276 279 282 1 0.0000000 1.0460000 1
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279 282 283 285 1 0.0000000 1.6038667 3
280 279 282 283 1 0.0000000 1.6038667 3
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282 283 286 287 1 0.0000000 0.0000000 3
282 283 286 288 1 0.0000000 1.0460000 1
282 283 286 288 1 0.0000000 0.0000000 3
284 283 286 287 1 0.0000000 0.6508444 3
284 283 286 288 1 0.0000000 0.6508444 3
284 283 286 289 1 0.0000000 1.0460000 1
284 283 286 289 1 0.0000000 0.0000000 3
285 283 286 287 1 0.0000000 0.6508444 3
285 283 286 288 1 0.0000000 0.6508444 3
285 283 286 289 1 0.0000000 1.0460000 1
285 283 286 289 1 0.0000000 0.0000000 3
286 289 290 291 1 0.0000000 1.6038667 3
286 289 290 292 1 0.0000000 1.6038667 3
287 286 289 290 1 0.0000000 1.6038667 3
288 286 289 290 1 0.0000000 1.6038667 3
289 290 293 294 1 0.0000000 1.0460000 1
289 290 293 294 1 0.0000000 0.0000000 3
```

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289 290 293 295 1 0.0000000 1.0460000 1
289 290 293 295 1 0.0000000 0.0000000 3
291 290 293 294 1 0.0000000 0.6508444 3
291 290 293 295 1 0.0000000 0.6508444 3
291 290 293 296 1 0.0000000 1.0460000 1
291 290 293 296 1 0.0000000 0.0000000 3
292 290 293 294 1 0.0000000 0.6508444 3
292 290 293 295 1 0.0000000 0.6508444 3
292 290 293 296 1 0.0000000 1.0460000 1
292 290 293 296 1 0.0000000 0.0000000 3
293 296 297 298 1 0.0000000 1.6038667 3
293 296 297 299 1 0.0000000 1.6038667 3
294 293 296 297 1 0.0000000 1.6038667 3
295 293 296 297 1 0.0000000 1.6038667 3
296 297 300 301 1 0.0000000 1.0460000 1
296 297 300 301 1 0.0000000 0.0000000 3
296 297 300 302 1 0.0000000 1.0460000 1
296 297 300 302 1 0.0000000 0.0000000 3
298 297 300 301 1 0.0000000 0.6508444 3
298 297 300 302 1 0.0000000 0.6508444 3
298 297 300 303 1 0.0000000 1.0460000 1
298 297 300 303 1 0.0000000 0.0000000 3
299 297 300 301 1 0.0000000 0.6508444 3
299 297 300 302 1 0.0000000 0.6508444 3
299 297 300 303 1 0.0000000 1.0460000 1
299 297 300 303 1 0.0000000 0.0000000 3
300 303 304 305 1 0.0000000 1.6038667 3
300 303 304 306 1 0.0000000 1.6038667 3
301 300 303 304 1 0.0000000 1.6038667 3
302 300 303 304 1 0.0000000 1.6038667 3
303 304 307 308 1 0.0000000 1.0460000 1
303 304 307 308 1 0.0000000 0.0000000 3
303 304 307 309 1 0.0000000 1.0460000 1
303 304 307 309 1 0.0000000 0.0000000 3
305 304 307 308 1 0.0000000 0.6508444 3
305 304 307 309 1 0.0000000 0.6508444 3
305 304 307 310 1 0.0000000 1.0460000 1
305 304 307 310 1 0.0000000 0.0000000 3
306 304 307 308 1 0.0000000 0.6508444 3
306 304 307 309 1 0.0000000 0.6508444 3
306 304 307 310 1 0.0000000 1.0460000 1
306 304 307 310 1 0.0000000 0.0000000 3
307 310 311 312 1 0.0000000 1.6038667 3
307 310 311 313 1 0.0000000 1.6038667 3
308 307 310 311 1 0.0000000 1.6038667 3
309 307 310 311 1 0.0000000 1.6038667 3
310 311 314 315 1 0.0000000 1.0460000 1
310 311 314 315 1 0.0000000 0.0000000 3
310 311 314 316 1 0.0000000 1.0460000 1
310 311 314 316 1 0.0000000 0.0000000 3
311 314 317 318 1 0.0000000 1.0460000 1
311 314 317 318 1 0.0000000 0.6694400 3
312 311 314 315 1 0.0000000 0.6508444 3
312 311 314 316 1 0.0000000 0.6508444 3
312 311 314 317 1 0.0000000 1.0460000 1
312 311 314 317 1 0.0000000 0.0000000 3
```

```
313 311 314 315 1 0.0000000 0.6508444 3
313 311 314 316 1 0.0000000 0.6508444 3
313 311 314 317 1 0.0000000 1.0460000 1
313 311 314 317 1 0.0000000 0.0000000 3
315 314 317 318 1 0.0000000 0.6973333 3
316 314 317 318 1 0.0000000 0.6973333 3
```

S5.7 Top level topology for PEG2000 in water. G54A7

```
; Top level topology for PolyEthylene system in water.
; Gromos 54A7
; Include all relevant .itp files here then list and number the molecules.

; Include forcefield parameters
#include "./gromos54a7.ff/forcefield.itp"
#include "peg2000.itp"
#include "./gromos54a7.ff/spce.itp"

; Include Position restraint file
#ifdef POSRES
#include "posre.itp"
#endif

[ system ]
; Name
Polyethylene Glycol 2000 in Water in water

[ molecules ]
; Compound #mols
PEG2000 1
SOL 33327
```

S5.8 Top level topology for PEG2000 in water with Ethanol. G54A7 FF

```
; Top level topology for PolyEthylene system in water with Ethanol.
; Gromos 54A7 FF
; Include all relevant .itp files here then list and number the molecules.

; Include forcefield parameters
#include "./gromos54a7.ff/forcefield.itp"
#include "peg2000.itp"
#include "Ethanol.itp"
#include "./gromos54a7.ff/spce.itp"

; Include Position restraint file
#ifdef POSRES
#include "posre.itp"
#endif
```

```
[ system ]
; Name
Polyethylene Glycol 2000 in Water with Ethanol in water

[ molecules ]
; Compound #mols
PEG2000 1
_U1K 516
SOL 31715
```

S5.9 Top level topology for PEG2000 in water with Ethyl Acetate. G54A7 FF

```
; Top level topology for PolyEthylene system in Ethyl Acetate
; Gromos 54A7 FF
; Include all relevant .itp files here then list and number the molecules.

; Include forcefield parameters
#include "./gromos54a7.ff/forcefield.itp"
#include "peg2000.itp"
#include "acetate.itp"
#include "./gromos54a7.ff/spce.itp"

; Include Position restraint file
#ifdef POSRES
#include "posre.itp"
#endif

[ system ]
; Name
Polyethylene Glycol 2000 in Water with Ethyl Acetate

[ molecules ]
; Compound #mols
PEG2000 1
SF92 6106
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S5.10 Topology include file .itp for PEG2000. G54A7 FF

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; Topology include file .itp for PEG2000
; gromos G54A7 FF

[ moleculetype ]
; Name nrexcl
PEG2000 3

[ atoms ]
; nr type resnr residue atom cgnr charge mass typeB chargeB massB
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; residue 1 LIB rtp LIB q 0.0
1 H 1 LIB H21 1 0.309155 1.008
2 OA 1 LIB OO2 1 -0.556721 15.9994
3 C 1 LIB C1 1 0.415512 12.011
4 HC 1 LIB H11 1 -0.085219 1.008
5 HC 1 LIB H12 1 -0.085219 1.008
; residue 2 LIG rtp LIG q 0.0
6 C 2 LIG C3 2 0.222619 12.011
7 HC 2 LIG H31 2 -0.033074 1.008
8 HC 2 LIG H32 2 -0.033074 1.008
9 OE 2 LIG OO2 2 -0.409851 15.9994
10 C 2 LIG C1 2 0.021588 12.011
11 HC 2 LIG H11 2 0.096565 1.008
12 HC 2 LIG H12 2 0.096565 1.008
; residue 3 LIG rtp LIG q 0.0
13 C 3 LIG C3 3 -0.142658 12.011
14 HC 3 LIG H31 3 0.111514 1.008
15 HC 3 LIG H32 3 0.111514 1.008
16 OE 3 LIG OO2 3 -0.190007 15.9994
17 C 3 LIG C1 3 -0.001527 12.011
18 HC 3 LIG H11 3 0.050159 1.008
19 HC 3 LIG H12 3 0.050159 1.008
; residue 4 LIG rtp LIG q 0.0
20 C 4 LIG C3 4 0.157535 12.011
21 HC 4 LIG H31 4 0.017621 1.008
22 HC 4 LIG H32 4 0.017621 1.008
23 OE 4 LIG OO2 4 -0.393443 15.9994
24 C 4 LIG C1 4 0.222579 12.011
25 HC 4 LIG H11 4 0.003457 1.008
26 HC 4 LIG H12 4 0.003457 1.008
; residue 5 LIG rtp LIG q 0.0
27 C 5 LIG C3 5 0.135372 12.011
28 HC 5 LIG H31 5 0.012441 1.008
29 HC 5 LIG H32 5 0.012441 1.008
30 OE 5 LIG OO2 5 -0.360778 15.9994
31 C 5 LIG C1 5 -0.014461 12.011
32 HC 5 LIG H11 5 0.100645 1.008
33 HC 5 LIG H12 5 0.100645 1.008
; residue 6 LIG rtp LIG q 0.0
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35 HC 6 LIG H31 6 0.039656 1.008
36 HC 6 LIG H32 6 0.039656 1.008
37 OE 6 LIG OO2 6 -0.395231 15.9994
38 C 6 LIG C1 6 0.065690 12.011
39 HC 6 LIG H11 6 0.058576 1.008
40 HC 6 LIG H12 6 0.058576 1.008
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44 OE 7 LIG OO2 7 -0.275991 15.9994
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47 HC 7 LIG H12 7 0.071718 1.008
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52 C 8 LIG C1 8 0.262235 12.011
53 HC 8 LIG H11 8 0.000882 1.008
54 HC 8 LIG H12 8 0.000882 1.008
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58 OE 9 LIG OO2 9 -0.412384 15.9994
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60 HC 9 LIG H11 9 0.026371 1.008
61 HC 9 LIG H12 9 0.026371 1.008
; residue 10 LIG rtp LIG q 0.0
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63 HC 10 LIG H31 10 0.025977 1.008
64 HC 10 LIG H32 10 0.025977 1.008
65 OE 10 LIG OO2 10 -0.390006 15.9994
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67 HC 10 LIG H11 10 0.042283 1.008
68 HC 10 LIG H12 10 0.042283 1.008
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71 HC 11 LIG H32 11 0.045593 1.008
72 OE 11 LIG OO2 11 -0.358554 15.9994
73 C 11 LIG C1 11 0.053041 12.011
74 HC 11 LIG H11 11 0.058802 1.008
75 HC 11 LIG H12 11 0.058802 1.008
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78 HC 12 LIG H32 12 0.084271 1.008
79 OE 12 LIG OO2 12 -0.363350 15.9994
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81 HC 12 LIG H11 12 0.060837 1.008
82 HC 12 LIG H12 12 0.060837 1.008
; residue 13 LIG rtp LIG q 0.0
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84 HC 13 LIG H31 13 -0.029136 1.008
85 HC 13 LIG H32 13 -0.029136 1.008
86 OE 13 LIG OO2 13 -0.466633 15.9994
87 C 13 LIG C1 13 0.237342 12.011
88 HC 13 LIG H11 13 -0.011644 1.008
89 HC 13 LIG H12 13 -0.011644 1.008
; residue 14 LIG rtp LIG q 0.0
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91 HC 14 LIG H31 14 0.041698 1.008
92 HC 14 LIG H32 14 0.041698 1.008
93 OE 14 LIG OO2 14 -0.380275 15.9994
94 C 14 LIG C1 14 0.160553 12.011
95 HC 14 LIG H11 14 0.014015 1.008
96 HC 14 LIG H12 14 0.014015 1.008
; residue 15 LIG rtp LIG q 0.0
97 C 15 LIG C3 15 0.080822 12.011
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99 HC 15 LIG H32 15 0.050953 1.008
100 OE 15 LIG OO2 15 -0.400943 15.9994
101 C 15 LIG C1 15 0.241410 12.011
102 HC 15 LIG H11 15 0.004755 1.008
103 HC 15 LIG H12 15 0.004755 1.008
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104 C 16 LIG C3 16 0.019878 12.011
105 HC 16 LIG H31 16 0.056132 1.008
106 HC 16 LIG H32 16 0.056132 1.008
107 OE 16 LIG OO2 16 -0.345307 15.9994
108 C 16 LIG C1 16 0.161663 12.011
109 HC 16 LIG H11 16 0.041876 1.008
110 HC 16 LIG H12 16 0.041876 1.008
; residue 17 LIG rtp LIG q 0.0
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112 HC 17 LIG H31 17 0.054452 1.008
113 HC 17 LIG H32 17 0.054452 1.008
114 OE 17 LIG OO2 17 -0.235373 15.9994
115 C 17 LIG C1 17 0.009932 12.011
116 HC 17 LIG H11 17 0.059877 1.008
117 HC 17 LIG H12 17 0.059877 1.008
; residue 18 LIG rtp LIG q 0.0
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119 HC 18 LIG H31 18 0.009670 1.008
120 HC 18 LIG H32 18 0.009670 1.008
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122 C 18 LIG C1 18 0.225572 12.011
123 HC 18 LIG H11 18 0.007691 1.008
124 HC 18 LIG H12 18 0.007691 1.008
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126 HC 19 LIG H31 19 0.050109 1.008
127 HC 19 LIG H32 19 0.050109 1.008
128 OE 19 LIG OO2 19 -0.289322 15.9994
129 C 19 LIG C1 19 0.101127 12.011
130 HC 19 LIG H11 19 0.047075 1.008
131 HC 19 LIG H12 19 0.047075 1.008
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133 HC 20 LIG H31 20 0.091034 1.008
134 HC 20 LIG H32 20 0.091034 1.008
135 OE 20 LIG OO2 20 -0.342085 15.9994
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137 HC 20 LIG H11 20 0.026753 1.008
138 HC 20 LIG H12 20 0.026753 1.008
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140 HC 21 LIG H31 21 0.000417 1.008
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142 OE 21 LIG OO2 21 -0.401586 15.9994
143 C 21 LIG C1 21 0.087744 12.011
144 HC 21 LIG H11 21 0.031700 1.008
145 HC 21 LIG H12 21 0.031700 1.008
; residue 22 LIG rtp LIG q 0.0
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148 HC 22 LIG H32 22 0.018197 1.008
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150 C 22 LIG C1 22 -0.011056 12.011
151 HC 22 LIG H11 22 0.120215 1.008
152 HC 22 LIG H12 22 0.120215 1.008
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156 OE 23 LIG OO2 23 -0.306789 15.9994
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158 HC 23 LIG H11 23 0.131733 1.008
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163 OE 24 LIG OO2 24 -0.306789 15.9994
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166 HC 24 LIG H12 24 0.125303 1.008
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168 HC 25 LIG H31 25 0.120215 1.008
169 HC 25 LIG H32 25 0.120215 1.008
170 OE 25 LIG OO2 25 -0.310271 15.9994
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176 HC 26 LIG H32 26 0.031700 1.008
177 OE 26 LIG OO2 26 -0.401586 15.9994
178 C 26 LIG C1 26 0.208035 12.011
179 HC 26 LIG H11 26 0.000417 1.008
180 HC 26 LIG H12 26 0.000417 1.008
; residue 27 LIG rtp LIG q 0.0
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182 HC 27 LIG H31 27 0.026753 1.008
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184 OE 27 LIG OO2 27 -0.342085 15.9994
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186 HC 27 LIG H11 27 0.091034 1.008
187 HC 27 LIG H12 27 0.091034 1.008
; residue 28 LIG rtp LIG q 0.0
188 C 28 LIG C3 28 0.101127 12.011
189 HC 28 LIG H31 28 0.047075 1.008
190 HC 28 LIG H32 28 0.047075 1.008
191 OE 28 LIG OO2 28 -0.289322 15.9994
192 C 28 LIG C1 28 -0.009025 12.011
193 HC 28 LIG H11 28 0.050109 1.008
194 HC 28 LIG H12 28 0.050109 1.008
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195 C 29 LIG C3 29 0.225572 12.011
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197 HC 29 LIG H32 29 0.007691 1.008
198 OE 29 LIG OO2 29 -0.430798 15.9994
199 C 29 LIG C1 29 0.198660 12.011
200 HC 29 LIG H11 29 0.009670 1.008
201 HC 29 LIG H12 29 0.009670 1.008
; residue 30 LIG rtp LIG q 0.0
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203 HC 30 LIG H31 30 0.059877 1.008
204 HC 30 LIG H32 30 0.059877 1.008
205 OE 30 LIG OO2 30 -0.235373 15.9994
206 C 30 LIG C1 30 -0.032288 12.011
207 HC 30 LIG H11 30 0.054452 1.008
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215 HC 31 LIG H12 31 0.056132 1.008
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217 HC 32 LIG H31 32 0.004755 1.008
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219 OE 32 LIG OO2 32 -0.400943 15.9994
220 C 32 LIG C1 32 0.080822 12.011
221 HC 32 LIG H11 32 0.050953 1.008
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226 OE 33 LIG OO2 33 -0.380275 15.9994
227 C 33 LIG C1 33 0.085420 12.011
228 HC 33 LIG H11 33 0.041698 1.008
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; residue 34 LIG rtp LIG q 0.0
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231 HC 34 LIG H31 34 -0.011644 1.008
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233 OE 34 LIG OO2 34 -0.466633 15.9994
234 C 34 LIG C1 34 0.329150 12.011
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238 HC 35 LIG H31 35 0.060837 1.008
239 HC 35 LIG H32 35 0.060837 1.008
240 OE 35 LIG OO2 35 -0.363350 15.9994
241 C 35 LIG C1 35 0.011060 12.011
242 HC 35 LIG H11 35 0.084271 1.008
243 HC 35 LIG H12 35 0.084271 1.008
; residue 36 LIG rtp LIG q 0.0
244 C 36 LIG C3 36 0.053041 12.011
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245 HC 36 LIG H31 36 0.058802 1.008
246 HC 36 LIG H32 36 0.058802 1.008
247 OE 36 LIG OO2 36 -0.358554 15.9994
248 C 36 LIG C1 36 0.068832 12.011
249 HC 36 LIG H11 36 0.045593 1.008
250 HC 36 LIG H12 36 0.045593 1.008
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251 C 37 LIG C3 37 0.120195 12.011
252 HC 37 LIG H31 37 0.042283 1.008
253 HC 37 LIG H32 37 0.042283 1.008
254 OE 37 LIG OO2 37 -0.390006 15.9994
255 C 37 LIG C1 37 0.107414 12.011
256 HC 37 LIG H11 37 0.025977 1.008
257 HC 37 LIG H12 37 0.025977 1.008
; residue 38 LIG rtp LIG q 0.0
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259 HC 38 LIG H31 38 0.026371 1.008
260 HC 38 LIG H32 38 0.026371 1.008
261 OE 38 LIG OO2 38 -0.412384 15.9994
262 C 38 LIG C1 38 0.012234 12.011
263 HC 38 LIG H11 38 0.058578 1.008
264 HC 38 LIG H12 38 0.058578 1.008
; residue 39 LIG rtp LIG q 0.0
265 C 39 LIG C3 39 0.262235 12.011
266 HC 39 LIG H31 39 0.000882 1.008
267 HC 39 LIG H32 39 0.000882 1.008
268 OE 39 LIG OO2 39 -0.439920 15.9994
269 C 39 LIG C1 39 0.249790 12.011
270 HC 39 LIG H11 39 0.028561 1.008
271 HC 39 LIG H12 39 0.028561 1.008
; residue 40 LIG rtp LIG q 0.0
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273 HC 40 LIG H31 40 0.071718 1.008
274 HC 40 LIG H32 40 0.071718 1.008
275 OE 40 LIG OO2 40 -0.275991 15.9994
276 C 40 LIG C1 40 0.045985 12.011
277 HC 40 LIG H11 40 0.052913 1.008
278 HC 40 LIG H12 40 0.052913 1.008
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279 C 41 LIG C3 41 0.065690 12.011
280 HC 41 LIG H31 41 0.058576 1.008
281 HC 41 LIG H32 41 0.058576 1.008
282 OE 41 LIG OO2 41 -0.395231 15.9994
283 C 41 LIG C1 41 0.139294 12.011
284 HC 41 LIG H11 41 0.039656 1.008
285 HC 41 LIG H12 41 0.039656 1.008
; residue 42 LIG rtp LIG q 0.0
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287 HC 42 LIG H31 42 0.100645 1.008
288 HC 42 LIG H32 42 0.100645 1.008
289 OE 42 LIG OO2 42 -0.360778 15.9994
290 C 42 LIG C1 42 0.135372 12.011
291 HC 42 LIG H11 42 0.012441 1.008
292 HC 42 LIG H12 42 0.012441 1.008
; residue 43 LIG rtp LIG q 0.0
293 C 43 LIG C3 43 0.222579 12.011
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294 HC 43 LIG H31 43 0.003457 1.008
295 HC 43 LIG H32 43 0.003457 1.008
296 OE 43 LIG OO2 43 -0.393443 15.9994
297 C 43 LIG C1 43 0.157535 12.011
298 HC 43 LIG H11 43 0.017621 1.008
299 HC 43 LIG H12 43 0.017621 1.008
; residue 44 LIG rtp LIG q 0.0
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301 HC 44 LIG H31 44 0.050159 1.008
302 HC 44 LIG H32 44 0.050159 1.008
303 OE 44 LIG OO2 44 -0.190007 15.9994
304 C 44 LIG C1 44 -0.142658 12.011
305 HC 44 LIG H11 44 0.111514 1.008
306 HC 44 LIG H12 44 0.111514 1.008
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308 HC 45 LIG H31 45 0.096565 1.008
309 HC 45 LIG H32 45 0.096565 1.008
310 OE 45 LIG OO2 45 -0.409851 15.9994
311 C 45 LIG C1 45 0.222619 12.011
312 HC 45 LIG H11 45 -0.033074 1.008
313 HC 45 LIG H12 45 -0.033074 1.008
; residue 46 LIE rtp LIE q 0.0
314 C 46 LIE C3 46 0.415512 12.011
315 HC 46 LIE H31 46 -0.085219 1.008
316 HC 46 LIE H32 46 -0.085219 1.008
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318 H 46 LIE H11 46 0.309155 1.008

[ bonds ]
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[ dihedrals ]
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3 6 9 10 1 gd_23
6 9 10 13 1 gd_23
9 10 13 16 1 gd_25
10 13 16 17 1 gd_23
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34 37 38 41 1 gd_23
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44 45 48 51 1 gd_25
45 48 51 52 1 gd_23
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80 83 86 87 1 gd_23
83 86 87 90 1 gd_23
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; Topology include file .itp for Ethanol
; Gromos 54A7 FF
;
[ moleculetype ]
; Name nrexcl
_U1K 3
[ atoms ]
; nr type resnr resid atom cgnr charge mass total_charge
1 H 1 _U1K H9 1 0.399 1.0080
2 OA 1 _U1K O3 1 -0.691 15.9994
3 C 1 _U1K C2 1 0.342 12.0110
4 HC 1 _U1K H7 1 -0.025 1.0080
5 HC 1 _U1K H8 1 -0.025 1.0080 ; 0.000
6 C 1 _U1K C1 2 -0.231 12.0110
7 HC 1 _U1K H4 2 0.077 1.0080
8 HC 1 _U1K H5 2 0.077 1.0080
9 HC 1 _U1K H6 2 0.077 1.0080 ; -0.000
; total charge of the molecule:  0.000
[ bonds ]
; ai aj funct c0 c1
1 2 2 0.1000 1.5700e+07
2 3 2 0.1430 8.1800e+06
3 4 2 0.1100 1.2100e+07
3 5 2 0.1100 1.2100e+07
3 6 2 0.1520 5.4300e+06
6 7 2 0.1100 1.2100e+07
6 8 2 0.1100 1.2100e+07
6 9 2 0.1100 1.2100e+07
[ pairs ]
; ai aj funct ; all 1-4 pairs but the ones excluded in GROMOS itp
1 4 1
1 5 1
1 6 1
2 7 1
2 8 1
2 9 1
4 7 1
4 8 1
```

```
4 9 1
5 7 1
5 8 1
5 9 1
[ angles ]
; ai aj ak funct angle fc
1 2 3 2 108.53 443.00
2 3 4 2 111.30 632.00
2 3 5 2 110.30 524.00
2 3 6 2 109.50 520.00
4 3 5 2 103.00 741.00
4 3 6 2 109.50 618.00
5 3 6 2 110.30 524.00
3 6 7 2 111.00 530.00
3 6 8 2 111.30 632.00
3 6 9 2 109.50 285.00
7 6 8 2 108.00 740.00
7 6 9 2 109.50 285.00
8 6 9 2 109.50 285.00
[ dihedrals ]
; GROMOS improper dihedrals
; ai aj ak al funct angle fc
[ dihedrals ]
; ai aj ak al funct ph0 cp mult
1 2 3 6 1 0.00 1.26 3
2 3 6 7 1 0.00 5.92 3
[ exclusions ]
; ai aj funct ; GROMOS 1-4 exclusions
```

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; Topology include .itp file for Ethyl Acetate
; Gromos 54A7 FF
;
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; Name nrexcl
SF92 3
[ atoms ]
; nr type resnr resid atom cgnr charge mass total_charge
1 HC 1 SF92 H3 1 0.168 1.0080
2 C 1 SF92 C1 1 -0.504 12.0110
3 HC 1 SF92 H1 1 0.168 1.0080
4 HC 1 SF92 H2 1 0.168 1.0080 ; 0.000
5 C 1 SF92 C2 2 0.829 12.0110
6 O 1 SF92 OA 2 -0.633 15.9994
7 OE 1 SF92 OB 2 -0.497 15.9994
8 C 1 SF92 C3 2 0.322 12.0110
9 HC 1 SF92 H4 2 0.011 1.0080
10 HC 1 SF92 H5 2 0.011 1.0080 ; 0.043
11 C 1 SF92 C4 3 -0.349 12.0110
12 HC 1 SF92 H6 3 0.102 1.0080
13 HC 1 SF92 H7 3 0.102 1.0080
14 HC 1 SF92 H8 3 0.102 1.0080 ; -0.043
; total charge of the molecule:  -0.000
[ bonds ]
; ai aj funct c0 c1
1 2 2 0.1100 1.2100e+07
2 3 2 0.1090 1.2300e+07
```

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2 4 2 0.1100 1.2100e+07
2 5 2 0.1520 5.4300e+06
5 6 2 0.1230 1.6600e+07
5 7 2 0.1360 1.0200e+07
7 8 2 0.1435 6.1000e+06
8 9 2 0.1090 1.2300e+07
8 10 2 0.1090 1.2300e+07
8 11 2 0.1520 5.4300e+06
11 12 2 0.1100 1.2100e+07
11 13 2 0.1100 1.2100e+07
11 14 2 0.1100 1.2100e+07
[ pairs ]
; ai aj funct ; all 1-4 pairs but the ones excluded in GROMOS itp
1 6 1
1 7 1
2 8 1
3 6 1
3 7 1
4 6 1
4 7 1
5 9 1
5 10 1
5 11 1
6 8 1
7 12 1
7 13 1
7 14 1
9 12 1
9 13 1
9 14 1
10 12 1
10 13 1
10 14 1
[ angles ]
; ai aj ak funct angle fc
1 2 3 2 109.60 450.00
1 2 4 2 106.00 848.00
1 2 5 2 109.50 618.00
3 2 4 2 109.50 285.00
3 2 5 2 109.50 285.00
4 2 5 2 109.50 618.00
2 5 6 2 121.00 685.00
2 5 7 2 115.00 610.00
6 5 7 2 124.00 730.00
5 7 8 2 120.00 780.00
7 8 9 2 107.60 507.00
7 8 10 2 109.50 520.00
7 8 11 2 109.50 520.00
9 8 10 2 106.00 848.00
9 8 11 2 111.30 632.00
10 8 11 2 111.30 632.00
8 11 12 2 111.30 632.00
8 11 13 2 111.30 632.00
8 11 14 2 109.50 285.00
12 11 13 2 113.00 921.00
12 11 14 2 109.50 285.00
```

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13 11 14 2 109.50 285.00
[ dihedrals ]
; GROMOS improper dihedrals
; ai aj ak al funct angle fc
5 2 6 7 2 0.00 167.36
[ dihedrals ]
; ai aj ak al funct ph0 cp mult
3 2 5 6 1 180.00 1.00 6
2 5 7 8 1 180.00 24.00 2
5 7 8 11 1 0.00 1.26 3
7 8 11 12 1 0.00 5.92 3
[ exclusions ]
; ai aj funct ; GROMOS 1-4 exclusions
```

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    ; This is a standalone topology file
; Convert into a .itp file to be included in other .top files.

[ moleculetype ]
; Name nrexcl
PEG2000 3

[ atoms ]
; nr type resnr residue atom cgnr charge mass typeB chargeB massB
; residue 1 LIB rtp LIB q 0.0
1 H 1 LIB H21 1 0.309155 1.008
2 OA 1 LIB OO2 1 -0.556721 15.9994
3 C 1 LIB C1 1 0.415512 12.011
4 HC 1 LIB H11 1 -0.085219 1.008
5 HC 1 LIB H12 1 -0.085219 1.008
; residue 2 LIG rtp LIG q 0.0
6 C 2 LIG C3 2 0.222619 12.011
7 HC 2 LIG H31 2 -0.033074 1.008
8 HC 2 LIG H32 2 -0.033074 1.008
9 OE 2 LIG OO2 2 -0.409851 15.9994
10 C 2 LIG C1 2 0.021588 12.011
11 HC 2 LIG H11 2 0.096565 1.008
12 HC 2 LIG H12 2 0.096565 1.008
; residue 3 LIG rtp LIG q 0.0
13 C 3 LIG C3 3 -0.142658 12.011
14 HC 3 LIG H31 3 0.111514 1.008
15 HC 3 LIG H32 3 0.111514 1.008
16 OE 3 LIG OO2 3 -0.190007 15.9994
17 C 3 LIG C1 3 -0.001527 12.011
18 HC 3 LIG H11 3 0.050159 1.008
19 HC 3 LIG H12 3 0.050159 1.008
; residue 4 LIG rtp LIG q 0.0
20 C 4 LIG C3 4 0.157535 12.011
21 HC 4 LIG H31 4 0.017621 1.008
22 HC 4 LIG H32 4 0.017621 1.008
23 OE 4 LIG OO2 4 -0.393443 15.9994
24 C 4 LIG C1 4 0.222579 12.011
25 HC 4 LIG H11 4 0.003457 1.008
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26 HC 4 LIG H12 4 0.003457 1.008
; residue 5 LIG rtp LIG q 0.0
27 C 5 LIG C3 5 0.135372 12.011
28 HC 5 LIG H31 5 0.012441 1.008
29 HC 5 LIG H32 5 0.012441 1.008
30 OE 5 LIG OO2 5 -0.360778 15.9994
31 C 5 LIG C1 5 -0.014461 12.011
32 HC 5 LIG H11 5 0.100645 1.008
33 HC 5 LIG H12 5 0.100645 1.008
; residue 6 LIG rtp LIG q 0.0
34 C 6 LIG C3 6 0.139294 12.011
35 HC 6 LIG H31 6 0.039656 1.008
36 HC 6 LIG H32 6 0.039656 1.008
37 OE 6 LIG OO2 6 -0.395231 15.9994
38 C 6 LIG C1 6 0.065690 12.011
39 HC 6 LIG H11 6 0.058576 1.008
40 HC 6 LIG H12 6 0.058576 1.008
; residue 7 LIG rtp LIG q 0.0
41 C 7 LIG C3 7 0.045985 12.011
42 HC 7 LIG H31 7 0.052913 1.008
43 HC 7 LIG H32 7 0.052913 1.008
44 OE 7 LIG OO2 7 -0.275991 15.9994
45 C 7 LIG C1 7 -0.081739 12.011
46 HC 7 LIG H11 7 0.071718 1.008
47 HC 7 LIG H12 7 0.071718 1.008
; residue 8 LIG rtp LIG q 0.0
48 C 8 LIG C3 8 0.249790 12.011
49 HC 8 LIG H31 8 0.028561 1.008
50 HC 8 LIG H32 8 0.028561 1.008
51 OE 8 LIG OO2 8 -0.439920 15.9994
52 C 8 LIG C1 8 0.262235 12.011
53 HC 8 LIG H11 8 0.000882 1.008
54 HC 8 LIG H12 8 0.000882 1.008
; residue 9 LIG rtp LIG q 0.0
55 C 9 LIG C3 9 0.012234 12.011
56 HC 9 LIG H31 9 0.058578 1.008
57 HC 9 LIG H32 9 0.058578 1.008
58 OE 9 LIG OO2 9 -0.412384 15.9994
59 C 9 LIG C1 9 0.193113 12.011
60 HC 9 LIG H11 9 0.026371 1.008
61 HC 9 LIG H12 9 0.026371 1.008
; residue 10 LIG rtp LIG q 0.0
62 C 10 LIG C3 10 0.107414 12.011
63 HC 10 LIG H31 10 0.025977 1.008
64 HC 10 LIG H32 10 0.025977 1.008
65 OE 10 LIG OO2 10 -0.390006 15.9994
66 C 10 LIG C1 10 0.120195 12.011
67 HC 10 LIG H11 10 0.042283 1.008
68 HC 10 LIG H12 10 0.042283 1.008
; residue 11 LIG rtp LIG q 0.0
69 C 11 LIG C3 11 0.068832 12.011
70 HC 11 LIG H31 11 0.045593 1.008
71 HC 11 LIG H32 11 0.045593 1.008
72 OE 11 LIG OO2 11 -0.358554 15.9994
73 C 11 LIG C1 11 0.053041 12.011
74 HC 11 LIG H11 11 0.058802 1.008
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75 HC 11 LIG H12 11 0.058802 1.008
; residue 12 LIG rtp LIG q 0.0
76 C 12 LIG C3 12 0.011060 12.011
77 HC 12 LIG H31 12 0.084271 1.008
78 HC 12 LIG H32 12 0.084271 1.008
79 OE 12 LIG OO2 12 -0.363350 15.9994
80 C 12 LIG C1 12 0.077337 12.011
81 HC 12 LIG H11 12 0.060837 1.008
82 HC 12 LIG H12 12 0.060837 1.008
; residue 13 LIG rtp LIG q 0.0
83 C 13 LIG C3 13 0.329150 12.011
84 HC 13 LIG H31 13 -0.029136 1.008
85 HC 13 LIG H32 13 -0.029136 1.008
86 OE 13 LIG OO2 13 -0.466633 15.9994
87 C 13 LIG C1 13 0.237342 12.011
88 HC 13 LIG H11 13 -0.011644 1.008
89 HC 13 LIG H12 13 -0.011644 1.008
; residue 14 LIG rtp LIG q 0.0
90 C 14 LIG C3 14 0.085420 12.011
91 HC 14 LIG H31 14 0.041698 1.008
92 HC 14 LIG H32 14 0.041698 1.008
93 OE 14 LIG OO2 14 -0.380275 15.9994
94 C 14 LIG C1 14 0.160553 12.011
95 HC 14 LIG H11 14 0.014015 1.008
96 HC 14 LIG H12 14 0.014015 1.008
; residue 15 LIG rtp LIG q 0.0
97 C 15 LIG C3 15 0.080822 12.011
98 HC 15 LIG H31 15 0.050953 1.008
99 HC 15 LIG H32 15 0.050953 1.008
100 OE 15 LIG OO2 15 -0.400943 15.9994
101 C 15 LIG C1 15 0.241410 12.011
102 HC 15 LIG H11 15 0.004755 1.008
103 HC 15 LIG H12 15 0.004755 1.008
; residue 16 LIG rtp LIG q 0.0
104 C 16 LIG C3 16 0.019878 12.011
105 HC 16 LIG H31 16 0.056132 1.008
106 HC 16 LIG H32 16 0.056132 1.008
107 OE 16 LIG OO2 16 -0.345307 15.9994
108 C 16 LIG C1 16 0.161663 12.011
109 HC 16 LIG H11 16 0.041876 1.008
110 HC 16 LIG H12 16 0.041876 1.008
; residue 17 LIG rtp LIG q 0.0
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