SUPPORTING INFORMATION FOR:

Biomembrane simulations of 12 lipid types using the general-amber force field in a tensionless
ensemble

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1. Testing the Molecular Dynamics Simulation Conditions:

- A. Tests on different initial bilayer structure configurations as a starting point for the MD simulations:

Although the initial bilayer starting structure is a lesser problem nowadays, due to the increase in computational power that lead to an increase in the simulations length, we have assessed if our parameters could reproduce the same results starting from different initial bilayer structures: a POPC system prepared using VMD's (Humphrey, Dalke & Schulten 1996) membrane builder plugin; a pre-equilibrated POPC biomembrane obtained by Heller *et al* (Heller, Schaefer & Schulten 1993); and two biomembrane systems (DOPC and DMPC) obtained by Rosso and Gould (Rosso & Gould 2008). We have compared this externally obtained systems and systems obtained with the VMD's membrane builder plugin, with the packmol (Martínez, Andrade, Birgin & Martínez 2009) generated bilayer main systems. Through Figure S1 we can observe that the values for the area per lipid structural parameter tend to be quite similar, despite the differences in the convergence time of each system. Hence, varying the initial structure for the simulation does not affect significantly the results.

Figure S1: Graphical representation of the area per lipid quantity versus the simulation time: **a)** DOPC/DMPC packmol constructed bilayers; DOPC/DMPC bilayers obtained by Rosso and Gould **b)** POPC packmol constructed bilayer; POPC bilayer constructed with VMD's membrane builder; and POPC bilayer obtained by Heller et al.

B. Tests on two different temperature schemes (Langevin and Berendsen) used in the MD simulations:

A comparison of the area per lipid structural parameter is also displayed taking into account the type of thermostat used. This was performed in order to check if the choice of thermostat could influence the structural parameters. However, when we compare the Berendsen and Langevin thermostats (study also conducted by Rosso and Gould) (Rosso & Gould 2008) we have found very similar results. Figure S2 displays the latter observation.

Figure S2: Graphical representation of the area per lipid quantity versus the simulation time for the different conditions: DOPC/DLPC MD simulations performed with the Berendsen thermostat; DOPC/DLPC MD simulations performed with the Langevin thermostat.

2. Complementary information for the comparison of RESP charges

Figure S3 provides the glycerophospholipids chemical partitioning performed, in the comparison of the RESP charges.

Figure S3: Schematic drawing of the partitioning of phospholipids into chemical groups, for the RESP charge comparisons.

3. AMBER topologies and files

The parameter files used in this study are provided with this article. The parameter files are compatible with the AMBER software: a) *.frcmod* files – list of parameters that were not present in the GAFF force field database; b) *.prepc* files – information on the connectivity and RESP charges of the different atoms of the glycerophospholipids.

Table S3: Information on the common abbreviated name of the glycerophospholipids used in this study, and the corresponding 3-letter code used in the corresponding parameter files (.frcmod and .prepc)

Common name	3-letter code
DLPC	DLC
DLPE	DLE
DMPC	DMC
DMPE	DME
DPPC	DPC
DPPE	DPE
DSPE	DSE
PLPC	PLC
PLPE	PLE
POPC	POC
POPE	POE
DOPC	DOC

DLPC glycerophospholipid:

.frcmod

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#DLPC Glycerophospholipid

IMPROPER

c3-o -c -os 10.5 180.0 2.0 General improper torsional angle (2 general atom types)

.prepc

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#JTS Coimbra; SF Sousa; PA Fernandes; M Rangel; MJ Ramos 2012
#DLPC Glycerophospholipid

0 0 2

This is a remark line

molecule.res

DLC XYZ 0

CHANGE OMIT DU BEG

0.0000

1	DUMM	DU	M	999.000	999.0	-999.0	.00000
2	DUMM	DU	M	999.000	-999.0	999.0	.00000
3	DUMM	DU	M	-999.000	999.0	999.0	.00000
4	C1	c3	M	-14.027000	7.740000	-0.221000	-0.37644
5	H1	hx	E	-14.643000	8.651000	-0.284000	0.17232
6	H2	hx	E	-14.306000	7.170000	0.675000	0.17232
7	H3	hx	E	-14.192000	7.125000	-1.116000	0.17232
8	N2	n4	M	-12.611000	8.118000	-0.142000	0.19496
9	C41	c3	3	-12.435000	8.967000	1.050000	-0.37644
10	H59	hx	E	-11.393000	9.295000	1.135000	0.17232
11	H60	hx	E	-12.718000	8.400000	1.948000	0.17232
12	H61	hx	E	-13.085000	9.852000	0.958000	0.17232
13	C42	c3	3	-12.284000	8.903000	-1.345000	-0.37644
14	H62	hx	E	-12.452000	8.284000	-2.237000	0.17232
15	H63	hx	E	-11.239000	9.229000	-1.315000	0.17232
16	H64	hx	E	-12.936000	9.788000	-1.385000	0.17232
17	C3	c3	M	-11.769000	6.837000	-0.069000	0.01713
18	H4	hx	E	-12.087000	6.269000	0.817000	0.08419
19	H5	hx	E	-11.985000	6.248000	-0.970000	0.08419
20	C4	c3	M	-10.194000	7.059000	0.015000	0.23957
21	H6	h1	E	-9.858000	7.623000	-0.863000	0.03824
22	H7	h1	E	-9.952000	7.626000	0.924000	0.03824
23	O5	os	M	-9.470000	5.780000	0.042000	-0.57090
24	P6	p5	M	-7.906000	6.048000	0.126000	1.32775
25	O39	o	E	-7.602000	6.762000	1.465000	-0.80266
26	O40	o	E	-7.541000	6.874000	-0.918000	-0.80266
27	O7	os	M	-7.042000	4.710000	0.050000	-0.49432
28	C8	c3	M	-5.606000	5.032000	0.148000	0.10242
29	H8	h1	E	-5.368000	5.684000	-0.694000	0.07868
30	H9	h1	E	-5.439000	5.568000	1.089000	0.07868
31	C9	c3	M	-4.702000	3.686000	0.152000	0.15833
32	O24	os	S	-3.653000	4.797000	0.524000	-0.53281
33	C25	c	B	-2.977000	5.625000	-0.540000	0.97141
34	C26	c3	3	-1.756000	6.484000	-0.209000	-0.39918
35	C27	c3	3	-0.497000	5.538000	-0.266000	0.06663
36	C28	c3	3	0.816000	6.328000	-0.022000	0.05026
37	C29	c3	3	2.063000	5.385000	-0.094000	-0.04225
38	C30	c3	3	3.341000	6.252000	0.076000	0.00960
39	C31	c3	3	4.648000	5.413000	-0.004000	0.05023
40	C32	c3	3	5.845000	6.394000	0.110000	0.05769
41	C33	c3	3	7.202000	5.660000	0.020000	-0.01460
42	C34	c3	3	8.330000	6.716000	0.096000	0.01556
43	C35	c3	3	9.708000	6.039000	-0.002000	0.15168
44	C36	c3	3	10.805000	7.121000	0.056000	-0.22766
45	H56	hc	E	11.796000	6.646000	-0.013000	0.04834
46	H57	hc	E	10.729000	7.672000	1.004000	0.04834
47	H58	hc	E	10.675000	7.818000	-0.785000	0.04834
48	H54	hc	E	9.835000	5.339000	0.835000	-0.02730
49	H55	hc	E	9.783000	5.494000	-0.953000	-0.02730
50	H52	hc	E	8.217000	7.421000	-0.740000	-0.00816

51	H53	hc	E	8.259000	7.262000	1.046000	-0.00816
52	H50	hc	E	7.299000	4.946000	0.851000	-0.01067
53	H51	hc	E	7.271000	5.124000	-0.936000	-0.01067
54	H48	hc	E	5.783000	7.116000	-0.715000	-0.02129
55	H49	hc	E	5.789000	6.930000	1.067000	-0.02129
56	H46	hc	E	4.677000	4.676000	0.814000	-0.01635
57	H47	hc	E	4.697000	4.892000	-0.970000	-0.01635
58	H44	hc	E	3.359000	6.996000	-0.731000	-0.01055
59	H45	hc	E	3.306000	6.768000	1.044000	-0.01055
60	H42	hc	E	2.007000	4.623000	0.699000	0.00795
61	H43	hc	E	2.094000	4.889000	-1.075000	0.00795
62	H40	hc	E	0.909000	7.095000	-0.803000	-0.00734
63	H41	hc	E	0.783000	6.811000	0.963000	-0.00734
64	H38	hc	E	-0.603000	4.751000	0.495000	-0.00144
65	H39	hc	E	-0.445000	5.075000	-1.261000	-0.00144
66	H36	hc	E	-1.626000	7.262000	-0.975000	0.10340
67	H37	hc	E	-1.823000	6.903000	0.803000	0.10340
68	O37	o	E	-3.284000	5.480000	-1.731000	-0.61937
69	H10	h1	E	-5.126000	3.188000	1.039000	0.13144
70	C10	c3	M	-3.220000	3.027000	0.162000	-0.03648
71	H11	h1	E	-2.630000	3.368000	-0.679000	0.10151
72	H12	h1	E	-2.743000	3.324000	1.106000	0.10151
73	O11	os	M	-3.099000	1.600000	0.069000	-0.44670
74	C12	c	M	-1.672000	1.417000	0.172000	0.85731
75	O38	o	E	-0.952000	2.407000	0.349000	-0.53773
76	C13	c3	M	-0.971000	0.091000	0.077000	-0.35463
77	H13	hc	E	-1.237000	-0.525000	0.947000	0.08883
78	H14	hc	E	-1.300000	-0.447000	-0.823000	0.08883
79	C14	c3	M	0.562000	0.399000	0.060000	0.10691
80	H15	hc	E	0.791000	1.028000	-0.813000	-0.00795
81	H16	hc	E	0.822000	0.946000	0.977000	-0.00795
82	C15	c3	M	1.418000	-0.876000	-0.003000	0.06518
83	H17	hc	E	1.207000	-1.500000	0.875000	-0.00773
84	H18	hc	E	1.188000	-1.438000	-0.919000	-0.00773
85	C16	c3	M	2.917000	-0.471000	0.001000	-0.04863
86	H19	hc	E	3.135000	0.150000	-0.881000	0.00522
87	H20	hc	E	3.139000	0.100000	0.914000	0.00522
88	C17	c3	M	3.790000	-1.739000	-0.028000	0.02691
89	H21	hc	E	3.563000	-2.348000	0.857000	-0.01515
90	H22	hc	E	3.566000	-2.316000	-0.935000	-0.01515
91	C18	c3	M	5.291000	-1.373000	-0.015000	0.04944
92	H23	hc	E	5.537000	-0.774000	-0.904000	-0.01439
93	H24	hc	E	5.527000	-0.798000	0.892000	-0.01439
94	C19	c3	M	6.104000	-2.681000	-0.023000	0.05036
95	H25	hc	E	5.845000	-3.269000	0.868000	-0.01877
96	H26	hc	E	5.856000	-3.257000	-0.924000	-0.01877
97	C20	c3	M	7.615000	-2.391000	-0.010000	-0.01383
98	H27	hc	E	7.890000	-1.813000	-0.904000	-0.00945
99	H28	hc	E	7.877000	-1.820000	0.892000	-0.00945
100	C21	c3	M	8.365000	-3.734000	-0.008000	0.01065
101	H29	hc	E	8.082000	-4.306000	0.887000	-0.00646
102	H30	hc	E	8.094000	-4.304000	-0.907000	-0.00646
103	C22	c3	M	9.880000	-3.492000	0.002000	0.14588
104	H31	hc	E	10.168000	-2.925000	-0.894000	-0.02479
105	H32	hc	E	10.156000	-2.925000	0.901000	-0.02479
106	C23	c3	M	10.603000	-4.851000	0.007000	-0.22809
107	H33	hc	E	11.691000	-4.690000	0.013000	0.04941
108	H34	hc	E	10.320000	-5.418000	-0.892000	0.04941
109	H35	hc	E	10.310000	-5.417000	0.904000	0.04941

LOOP

IMPROPER

C26 O37 C25 O24

C13 O38 C12 O11

DONE

STOP

DLPE glycerophospholipid:

.frcmod

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#DLPE Glycerophospholipid

BOND

c3-ha 337.30 1.092 same as c3-hc

ANGLE

n4-c3-ha 49.000 107.900 same as hc-c3-n4

c3-c3-ha 46.400 110.050 same as c3-c3-hc

ha-c3-ha 39.400 108.350 same as hc-c3-hc

ha-c3-os 41.404 109.295 Calculated with empirical approach

c -c3-ha 34.990 110.650 Calculated with empirical approach

IMPROPER

c3-o -c -os 10.5 180.0 2.0 General improper torsional angle (2 general atom types)

.prepc

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#DLPE Glycerophospholipid

0 0 2

This is a remark line

molecule.res

DLE XYZ 0

CHANGE OMIT DU BEG

0.0000

1	DUMM	DU	M	999.000	999.0	-999.0	.00000
2	DUMM	DU	M	999.000	-999.0	999.0	.00000
3	DUMM	DU	M	-999.000	999.0	999.0	.00000
4	N1	n4	M	-13.984000	7.979000	-0.080000	-0.75102
5	H1	hn	E	-14.547000	8.889000	-0.077000	0.42332
6	H2	hn	E	-14.306000	7.358000	0.730000	0.42332
7	H58	hn	E	-14.140000	7.467000	-1.006000	0.42332
8	C2	c3	M	-12.548000	8.288000	0.077000	0.20282
9	H3	ha	E	-12.220000	8.926000	-0.758000	0.07630
10	H4	ha	E	-12.396000	8.820000	1.025000	0.07630
11	C3	c3	M	-11.725000	6.975000	0.074000	0.14631
12	H5	ha	E	-12.074000	6.326000	0.891000	0.08042
13	H6	ha	E	-11.883000	6.464000	-0.887000	0.08042
14	O4	os	M	-10.304000	7.250000	0.255000	-0.54521
15	P5	p5	M	-9.494000	5.912000	0.110000	1.35161
16	O23	o	E	-10.101000	4.944000	0.886000	-0.86750
17	O24	o	E	-9.545000	5.464000	-1.371000	-0.86750
18	O6	os	M	-7.983000	6.045000	0.586000	-0.45050
19	C7	c3	M	-7.268000	4.857000	0.142000	-0.11209
20	H7	ha	E	-7.885000	3.983000	0.395000	0.13139
21	H8	ha	E	-7.145000	4.905000	-0.950000	0.13139
22	C8	c3	M	-5.867000	4.641000	0.844000	0.40753
23	O25	os	S	-4.806000	5.685000	0.683000	-0.59201
24	C26	c	B	-4.161000	5.930000	-0.575000	0.97425
25	C27	c3	3	-2.890000	6.801000	-0.558000	-0.62349
26	C28	c3	3	-1.620000	5.863000	-0.397000	0.16243
27	C29	c3	3	-0.287000	6.699000	-0.346000	-0.12703
28	C30	c3	3	0.976000	5.766000	-0.208000	-0.12097
29	C31	c3	3	2.283000	6.635000	-0.163000	0.08428
30	C32	c3	3	3.564000	5.742000	-0.065000	-0.01911
31	C33	c3	3	4.835000	6.648000	-0.042000	0.10014
32	C34	c3	3	6.126000	5.788000	0.018000	-0.05555
33	C35	c3	3	7.366000	6.716000	0.022000	0.03807
34	C36	c3	3	8.657000	5.872000	0.059000	0.17161
35	C37	c3	3	9.884000	6.808000	0.054000	-0.27308
36	H55	ha	E	10.806000	6.207000	0.077000	0.05727
37	H56	ha	E	9.851000	7.461000	0.938000	0.05727
38	H57	ha	E	9.871000	7.424000	-0.857000	0.05727
39	H53	ha	E	8.670000	5.257000	0.969000	-0.03105

40	H54	ha	E	8.694000	5.220000	-0.826000	-0.03105
41	H51	ha	E	7.364000	7.330000	-0.890000	-0.00715
42	H52	ha	E	7.333000	7.371000	0.904000	-0.00715
43	H49	ha	E	6.124000	5.175000	0.931000	-0.00173
44	H50	ha	E	6.168000	5.133000	-0.863000	-0.00173
45	H47	ha	E	4.859000	7.256000	-0.956000	-0.02958
46	H48	ha	E	4.797000	7.309000	0.836000	-0.02958
47	H45	ha	E	3.529000	5.136000	0.852000	-0.00093
48	H46	ha	E	3.611000	5.080000	-0.940000	-0.00093
49	H43	ha	E	2.345000	7.234000	-1.081000	-0.01391
50	H44	ha	E	2.243000	7.307000	0.707000	-0.01391
51	H41	ha	E	0.902000	5.172000	0.715000	0.02869
52	H42	ha	E	1.022000	5.090000	-1.074000	0.02869
53	H39	ha	E	-0.194000	7.284000	-1.271000	0.05163
54	H40	ha	E	-0.324000	7.383000	0.514000	0.05163
55	H37	ha	E	-1.711000	5.286000	0.536000	0.04877
56	H38	ha	E	-1.577000	5.168000	-1.248000	0.04877
57	H35	ha	E	-2.780000	7.339000	-1.509000	0.16647
58	H36	ha	E	-2.914000	7.486000	0.301000	0.16647
59	O38	o	E	-4.499000	5.361000	-1.619000	-0.60147
60	H9	ha	E	-6.038000	4.546000	1.925000	0.07523
61	C9	c3	M	-5.270000	3.324000	0.301000	-0.13738
62	H10	ha	E	-5.920000	2.463000	0.516000	0.13497
63	H11	ha	E	-5.149000	3.420000	-0.783000	0.13497
64	O10	os	M	-3.974000	3.192000	0.862000	-0.50466
65	C11	c	M	-3.277000	2.152000	0.268000	0.87763
66	O39	o	E	-3.815000	1.426000	-0.575000	-0.61370
67	C12	c3	M	-1.792000	2.153000	0.434000	-0.20625
68	H12	ha	E	-1.394000	2.819000	-0.345000	0.04988
69	H13	ha	E	-1.527000	2.586000	1.408000	0.04988
70	C13	c3	M	-1.133000	0.796000	0.227000	-0.00213
71	H14	ha	E	-1.461000	0.089000	1.002000	0.01433
72	H15	ha	E	-1.381000	0.400000	-0.768000	0.01433
73	C14	c3	M	0.382000	1.052000	0.312000	0.05908
74	H16	ha	E	0.664000	1.761000	-0.481000	-0.00658
75	H17	ha	E	0.625000	1.487000	1.290000	-0.00658
76	C15	c3	M	1.173000	-0.242000	0.130000	0.03356
77	H18	ha	E	0.915000	-0.944000	0.935000	-0.00997
78	H19	ha	E	0.935000	-0.694000	-0.843000	-0.00997
79	C16	c3	M	2.675000	0.092000	0.187000	-0.05123
80	H20	ha	E	2.926000	0.783000	-0.632000	-0.00544
81	H21	ha	E	2.911000	0.564000	1.150000	-0.00544
82	C17	c3	M	3.486000	-1.200000	0.041000	0.13362
83	H22	ha	E	3.232000	-1.875000	0.869000	-0.03297
84	H23	ha	E	3.244000	-1.684000	-0.914000	-0.03297
85	C18	c3	M	4.989000	-0.884000	0.087000	0.02604
86	H24	ha	E	5.254000	-0.221000	-0.750000	-0.01578
87	H25	ha	E	5.237000	-0.392000	1.037000	-0.01578
88	C19	c3	M	5.764000	-2.203000	-0.023000	-0.04023
89	H26	ha	E	5.489000	-2.851000	0.820000	-0.00349
90	H27	ha	E	5.509000	-2.702000	-0.967000	-0.00349
91	C20	c3	M	7.273000	-1.935000	0.019000	0.02413
92	H28	ha	E	7.560000	-1.297000	-0.830000	-0.00300
93	H29	ha	E	7.535000	-1.433000	0.961000	-0.00300
94	C21	c3	M	8.010000	-3.279000	-0.070000	0.17615
95	H30	ha	E	7.717000	-3.909000	0.782000	-0.02888
96	H31	ha	E	7.742000	-3.783000	-1.008000	-0.02888
97	C22	c3	M	9.527000	-3.039000	-0.031000	-0.29880
98	H32	ha	E	10.051000	-4.005000	-0.090000	0.06327
99	H33	ha	E	9.793000	-2.533000	0.908000	0.06327
100	H34	ha	E	9.819000	-2.410000	-0.883000	0.06327

LOOP

IMPROPER

C27 O38 C26 O25

C12 O39 C11 O10

DONE

STOP

DMPC glycerophospholipid:

.frcmod

#REQUIMTE, Dept Quim e Bioquim, FCUP, Univ Porto, Portugal;
#JTS Coimbra; SF Sousa; PA Fernandes; M Rangel; MJ Ramos 2012
#DMPC Glycerophospholipid

IMPROPER

c3-o -c -os 10.5 180.0 2.0 General improper torsional angle (2 general atom types)

.prepc

#REQUIMTE, Dept Quim e Bioquim, FCUP, Univ Porto, Portugal;
#JTS Coimbra; SF Sousa; PA Fernandes; M Rangel; MJ Ramos 2012
#DMPC Glycerophospholipid

0 0 2

This is a remark line

molecule.res

DMC XYZ 0

CHANGE OMIT DU BEG

0.0000

1	DUMM	DU	M	999.000	999.0	-999.0	.00000
2	DUMM	DU	M	999.000	-999.0	999.0	.00000
3	DUMM	DU	M	-999.000	999.0	999.0	.00000
4	C1	c3	M	-13.909000	7.643000	0.056000	-0.40920
5	H1	hx	E	-14.470000	8.572000	0.244000	0.18960
6	H2	hx	E	-14.140000	6.910000	0.841000	0.18960
7	H3	hx	E	-14.191000	7.236000	-0.923000	0.18960
8	N2	n4	M	-12.473000	7.935000	0.072000	0.17283
9	C45	c3	3	-12.201000	8.944000	-0.970000	-0.40920
10	H67	hx	E	-11.139000	9.210000	-0.976000	0.18960
11	H68	hx	E	-12.799000	9.845000	-0.759000	0.18960
12	H69	hx	E	-12.487000	8.539000	-1.950000	0.18960
13	C46	c3	3	-12.142000	8.509000	1.391000	-0.40920
14	H70	hx	E	-12.376000	7.779000	2.176000	0.18960
15	H71	hx	E	-12.744000	9.418000	1.546000	0.18960
16	H72	hx	E	-11.079000	8.772000	1.437000	0.18960
17	C3	c3	M	-11.707000	6.626000	-0.193000	-0.10162
18	H4	hx	E	-12.001000	5.903000	0.580000	0.12479
19	H5	hx	E	-12.014000	6.246000	-1.177000	0.12479
20	C4	c3	M	-10.124000	6.756000	-0.160000	0.15553
21	H6	h1	E	-9.796000	7.484000	-0.914000	0.11142
22	H7	h1	E	-9.823000	7.109000	0.833000	0.11142
23	O5	os	M	-9.439000	5.473000	-0.418000	-0.49122
24	P6	p5	M	-7.893000	5.723000	-0.208000	1.31043
25	O43	o	E	-7.527000	6.805000	-0.982000	-0.87183
26	O44	o	E	-7.684000	6.094000	1.282000	-0.87183
27	O7	os	M	-6.915000	4.497000	-0.570000	-0.45716
28	C8	c3	M	-5.588000	4.976000	-0.185000	-0.06022
29	H8	h1	E	-5.438000	5.933000	-0.700000	0.12618
30	H9	h1	E	-5.606000	5.156000	0.897000	0.12618
31	C9	c3	M	-4.304000	4.085000	-0.504000	0.41098
32	O10	os	S	-4.392000	2.714000	0.176000	-0.51165
33	C11	c	B	-3.295000	1.653000	0.277000	0.64352
34	C12	c3	3	-1.781000	1.802000	-0.082000	0.09415
35	C13	c3	3	-0.932000	0.473000	0.049000	-0.18885
36	C14	c3	3	0.617000	0.775000	-0.167000	0.00571
37	C15	c3	3	1.488000	-0.539000	-0.020000	0.06203
38	C16	c3	3	3.038000	-0.239000	-0.153000	-0.06197
39	C17	c3	3	3.867000	-1.575000	-0.018000	0.06473
40	C18	c3	3	5.418000	-1.317000	-0.105000	0.00018
41	C19	c3	3	6.191000	-2.678000	0.004000	0.02793
42	C20	c3	3	7.738000	-2.462000	-0.060000	0.04578
43	C21	c3	3	8.462000	-3.838000	0.024000	-0.03330
44	C22	c3	3	10.000000	-3.651000	-0.028000	0.01888
45	C23	c3	3	10.687000	-5.035000	0.040000	0.16840
46	C24	c3	3	12.220000	-4.863000	-0.005000	-0.27947
47	H35	hc	E	12.702000	-5.852000	0.041000	0.05925
48	H36	hc	E	12.547000	-4.258000	0.853000	0.05925
49	H37	hc	E	12.507000	-4.359000	-0.939000	0.05925
50	H33	hc	E	10.406000	-5.539000	0.975000	-0.02797

51	H34	hc	E	10.365000	-5.644000	-0.816000	-0.02797
52	H31	hc	E	10.281000	-3.152000	-0.965000	-0.00187
53	H32	hc	E	10.325000	-3.039000	0.825000	-0.00187
54	H29	hc	E	8.192000	-4.338000	0.964000	-0.00311
55	H30	hc	E	8.147000	-4.462000	-0.824000	-0.00311
56	H27	hc	E	8.004000	-1.971000	-1.006000	-0.01737
57	H28	hc	E	8.054000	-1.829000	0.782000	-0.01737
58	H25	hc	E	5.940000	-3.165000	0.956000	-0.00832
59	H26	hc	E	5.887000	-3.327000	-0.829000	-0.00832
60	H23	hc	E	5.661000	-0.841000	-1.065000	-0.00575
61	H24	hc	E	5.723000	-0.655000	0.719000	-0.00575
62	H21	hc	E	3.644000	-2.043000	0.950000	-0.01869
63	H22	hc	E	3.572000	-2.257000	-0.827000	-0.01869
64	H19	hc	E	3.245000	0.217000	-1.131000	0.00329
65	H20	hc	E	3.337000	0.456000	0.645000	0.00329
66	H17	hc	E	1.306000	-0.980000	0.970000	-0.00113
67	H18	hc	E	1.186000	-1.254000	-0.797000	-0.00113
68	H15	hc	E	0.777000	1.208000	-1.165000	-0.00525
69	H16	hc	E	0.938000	1.500000	0.597000	-0.00525
70	H13	hc	E	-1.057000	0.069000	1.063000	0.05740
71	H14	hc	E	-1.284000	-0.266000	-0.684000	0.05740
72	H11	hc	E	-1.675000	2.254000	-1.079000	0.01673
73	H12	hc	E	-1.372000	2.526000	0.632000	0.01673
74	O42	o	E	-3.617000	0.589000	0.816000	-0.52501
75	H10	h1	E	-4.196000	3.937000	-1.589000	0.01939
76	C25	c3	M	-3.187000	5.051000	0.007000	-0.22147
77	H38	h1	E	-3.280000	6.005000	-0.531000	0.15668
78	H39	h1	E	-3.321000	5.227000	1.083000	0.15668
79	O26	os	M	-1.919000	4.545000	-0.238000	-0.45472
80	C27	c	M	-0.918000	5.391000	0.182000	0.90504
81	O41	o	E	-1.179000	6.482000	0.701000	-0.62359
82	C28	c3	M	0.489000	4.920000	0.050000	-0.31245
83	H40	hc	E	0.702000	4.261000	0.904000	0.11002
84	H41	hc	E	0.585000	4.312000	-0.862000	0.11002
85	C29	c3	M	1.480000	6.071000	0.068000	-0.03399
86	H42	hc	E	1.298000	6.739000	-0.786000	0.03908
87	H43	hc	E	1.379000	6.633000	1.006000	0.03908
88	C30	c3	M	2.881000	5.468000	-0.018000	-0.01114
89	H44	hc	E	3.040000	4.801000	0.840000	0.00209
90	H45	hc	E	2.980000	4.893000	-0.951000	0.00209
91	C31	c3	M	3.921000	6.581000	0.007000	0.06759
92	H46	hc	E	3.774000	7.246000	-0.855000	-0.01411
93	H47	hc	E	3.818000	7.156000	0.938000	-0.01411
94	C32	c3	M	5.316000	5.955000	-0.048000	0.01638
95	H48	hc	E	5.454000	5.294000	0.819000	-0.01269
96	H49	hc	E	5.426000	5.372000	-0.975000	-0.01269
97	C33	c3	M	6.360000	7.069000	-0.015000	0.03884
98	H50	hc	E	6.223000	7.727000	-0.883000	-0.01908
99	H51	hc	E	6.240000	7.652000	0.910000	-0.01908
100	C34	c3	M	7.764000	6.459000	-0.045000	0.02297
101	H52	hc	E	7.902000	5.807000	0.828000	-0.01488
102	H53	hc	E	7.894000	5.873000	-0.967000	-0.01488
103	C35	c3	M	8.789000	7.595000	-0.010000	0.04903
104	H54	hc	E	8.646000	8.243000	-0.885000	-0.01671
105	H55	hc	E	8.650000	8.183000	0.908000	-0.01671
106	C36	c3	M	10.205000	7.015000	-0.028000	0.05780
107	H56	hc	E	10.353000	6.372000	0.851000	-0.02366
108	H57	hc	E	10.352000	6.426000	-0.944000	-0.02366
109	C37	c3	M	11.207000	8.173000	0.003000	-0.02228
110	H58	hc	E	11.054000	8.812000	-0.876000	-0.00932
111	H59	hc	E	11.054000	8.764000	0.918000	-0.00932
112	C38	c3	M	12.633000	7.618000	-0.010000	0.02917
113	H60	hc	E	12.790000	6.982000	0.872000	-0.00695
114	H61	hc	E	12.789000	7.026000	-0.923000	-0.00695
115	C39	c3	M	13.620000	8.790000	0.017000	0.18572
116	H62	hc	E	13.459000	9.424000	-0.866000	-0.03472
117	H63	hc	E	13.460000	9.382000	0.929000	-0.03472
118	C40	c3	M	15.055000	8.244000	0.004000	-0.27879
119	H64	hc	E	15.766000	9.083000	0.023000	0.05695
120	H65	hc	E	15.211000	7.649000	-0.907000	0.05695
121	H66	hc	E	15.211000	7.609000	0.888000	0.05695

LOOP

IMPROPER

C12 O42 C11 O10

C28 O41 C27 O26

DONE

STOP

DMPE glycerophospholipid:

.frcmod

#REQUIMTE, Dept Quim e Bioquim, FCUP, Univ Porto, Portugal;
#JTS Coimbra; SF Sousa; PA Fernandes; M Rangel; MJ Ramos 2012
#DMPE Glycerophospholipid

BOND

c3-ha 337.30 1.092 same as c3-hc

ANGLE

n4-c3-ha 49.000 107.900 same as hc-c3-n4
c3-c3-ha 46.400 110.050 same as c3-c3-hc
ha-c3-ha 39.400 108.350 same as hc-c3-hc
ha-c3-os 41.404 109.295 Calculated with empirical approach
c -c3-ha 34.990 110.650 Calculated with empirical approach

IMPROPER

c3-o -c -os 10.5 180.0 2.0 General improper torsional angle (2 general atom types)

.prepc

#REQUIMTE, Dept Quim e Bioquim, FCUP, Univ Porto, Portugal;
#JTS Coimbra; SF Sousa; PA Fernandes; M Rangel; MJ Ramos 2012
#DMPE Glycerophospholipid

0 0 2

This is a remark line

molecule.res

DME XYZ 0

CHANGE OMIT DU BEG

0.0000

1	DUMM	DU	M	999.000	999.0	-999.0	.00000
2	DUMM	DU	M	999.000	-999.0	999.0	.00000
3	DUMM	DU	M	-999.000	999.0	999.0	.00000
4	N1	n4	M	-13.499000	7.987000	-0.090000	-0.72822
5	H1	hn	E	-14.027000	8.908000	0.038000	0.41660
6	H2	hn	E	-13.863000	7.266000	0.612000	0.41660
7	H36	hn	E	-13.652000	7.624000	-1.085000	0.41660
8	C2	c3	M	-12.063000	8.209000	0.135000	0.20501
9	H3	ha	E	-11.686000	8.946000	-0.588000	0.07435
10	H4	ha	E	-11.906000	8.581000	1.157000	0.07435
11	C3	c3	M	-11.316000	6.880000	-0.052000	0.13898
12	H5	ha	E	-11.708000	6.141000	0.662000	0.08398
13	H6	ha	E	-11.480000	6.518000	-1.077000	0.08398
14	O4	os	M	-9.906000	7.058000	0.175000	-0.52614
15	P5	p5	M	-9.207000	5.700000	-0.085000	1.32012
16	O46	o	E	-9.358000	5.333000	-1.582000	-0.86991
17	O47	o	E	-9.824000	4.731000	0.680000	-0.86991
18	O6	os	M	-7.692000	5.740000	0.297000	-0.43208
19	C7	c3	M	-7.152000	4.464000	-0.062000	-0.14357
20	H7	ha	E	-7.768000	3.686000	0.409000	0.15503
21	H8	ha	E	-7.196000	4.349000	-1.153000	0.15503
22	C8	c3	M	-5.699000	4.264000	0.423000	0.38200
23	O9	os	S	-5.302000	2.911000	0.026000	-0.56328
24	C10	c	B	-4.159000	2.460000	0.721000	0.83786
25	C11	c3	3	-3.492000	1.177000	0.369000	-0.33184
26	C12	c3	3	-1.977000	1.450000	0.375000	0.08198
27	C13	c3	3	-1.197000	0.170000	0.095000	-0.06077
28	C14	c3	3	0.302000	0.492000	0.149000	-0.13642
29	C15	c3	3	1.099000	-0.795000	-0.071000	0.16135
30	C16	c3	3	2.599000	-0.495000	0.021000	-0.02445
31	C17	c3	3	3.370000	-1.808000	-0.146000	0.02240

32	C18	c3	3	4.874000	-1.547000	-0.026000	0.04557
33	C19	c3	3	5.611000	-2.884000	-0.156000	0.06075
34	C20	c3	3	7.118000	-2.657000	-0.019000	-0.04064
35	C21	c3	3	7.831000	-4.008000	-0.127000	0.03874
36	C22	c3	3	9.341000	-3.800000	0.017000	0.17600
37	C23	c3	3	10.045000	-5.161000	-0.083000	-0.29263
38	H34	ha	E	11.130000	-5.021000	0.019000	0.06135
39	H35	ha	E	9.822000	-5.617000	-1.058000	0.06135
40	H37	ha	E	9.681000	-5.818000	0.721000	0.06135
41	H32	ha	E	9.698000	-3.139000	-0.785000	-0.03142
42	H33	ha	E	9.556000	-3.344000	0.993000	-0.03142
43	H30	ha	E	7.476000	-4.672000	0.675000	-0.00708
44	H31	ha	E	7.612000	-4.463000	-1.103000	-0.00708
45	H28	ha	E	7.467000	-1.987000	-0.817000	-0.00570
46	H29	ha	E	7.335000	-2.207000	0.960000	-0.00570
47	H26	ha	E	5.274000	-3.560000	0.642000	-0.02106
48	H27	ha	E	5.393000	-3.333000	-1.134000	-0.02106
49	H24	ha	E	5.200000	-0.859000	-0.819000	-0.01484
50	H25	ha	E	5.092000	-1.106000	0.957000	-0.01484
51	H22	ha	E	3.063000	-2.505000	0.646000	-0.01523
52	H23	ha	E	3.147000	-2.248000	-1.128000	-0.01523
53	H20	ha	E	2.889000	0.218000	-0.764000	-0.00370
54	H21	ha	E	2.824000	-0.068000	1.008000	-0.00370
55	H18	ha	E	0.830000	-1.517000	0.712000	-0.03340
56	H19	ha	E	0.863000	-1.219000	-1.057000	-0.03340
57	H16	ha	E	0.556000	1.232000	-0.625000	0.02491
58	H17	ha	E	0.547000	0.900000	1.139000	0.02491
59	H14	ha	E	-1.437000	-0.573000	0.867000	0.02654
60	H15	ha	E	-1.462000	-0.228000	-0.895000	0.02654
61	H12	ha	E	-1.736000	2.207000	-0.387000	0.04106
62	H13	ha	E	-1.687000	1.828000	1.365000	0.04106
63	H10	ha	E	-3.691000	0.440000	1.159000	0.09697
64	H11	ha	E	-3.844000	0.796000	-0.600000	0.09697
65	O45	o	E	-3.681000	3.133000	1.642000	-0.61136
66	H9	ha	E	-5.684000	4.340000	1.519000	0.06273
67	C26	c3	M	-4.715000	5.336000	-0.217000	0.00542
68	H41	ha	E	-4.757000	5.249000	-1.311000	0.08030
69	H42	ha	E	-4.998000	6.355000	0.084000	0.08030
70	O27	os	M	-3.391000	5.020000	0.226000	-0.43383
71	C28	c	M	-2.338000	5.757000	-0.288000	0.87373
72	O44	o	E	-2.516000	6.686000	-1.084000	-0.64508
73	C29	c3	M	-0.960000	5.236000	0.034000	-0.21528
74	H43	ha	E	-0.939000	4.925000	1.088000	0.05427
75	H44	ha	E	-0.819000	4.322000	-0.562000	0.05427
76	C30	c3	M	0.196000	6.188000	-0.279000	0.03855
77	H45	ha	E	0.193000	6.450000	-1.347000	0.00930
78	H46	ha	E	0.115000	7.099000	0.329000	0.00930
79	C31	c3	M	1.489000	5.414000	0.065000	-0.00908
80	H47	ha	E	1.470000	5.130000	1.126000	0.00504
81	H48	ha	E	1.532000	4.505000	-0.553000	0.00504
82	C32	c3	M	2.736000	6.261000	-0.206000	0.03846
83	H49	ha	E	2.766000	6.549000	-1.265000	-0.01001
84	H50	ha	E	2.712000	7.163000	0.421000	-0.01001
85	C33	c3	M	3.984000	5.420000	0.133000	0.01190
86	H51	ha	E	3.951000	5.121000	1.190000	-0.01549
87	H52	ha	E	4.003000	4.522000	-0.501000	-0.01549
88	C34	c3	M	5.243000	6.256000	-0.123000	0.07315
89	H53	ha	E	5.271000	6.562000	-1.177000	-0.02637
90	H54	ha	E	5.220000	7.149000	0.517000	-0.02637
91	C35	c3	M	6.502000	5.432000	0.199000	0.00681
92	H55	ha	E	6.484000	5.122000	1.254000	-0.01399
93	H56	ha	E	6.539000	4.542000	-0.446000	-0.01399
94	C36	c3	M	7.729000	6.315000	-0.058000	0.05803
95	H57	ha	E	7.734000	6.632000	-1.110000	-0.01779
96	H58	ha	E	7.675000	7.201000	0.589000	-0.01779
97	C37	c3	M	9.023000	5.549000	0.244000	0.04614
98	H59	ha	E	9.032000	5.232000	1.296000	-0.01993
99	H60	ha	E	9.097000	4.667000	-0.408000	-0.01993
100	C38	c3	M	10.202000	6.494000	-0.021000	-0.02687
101	H61	ha	E	10.182000	6.815000	-1.071000	-0.00675
102	H62	ha	E	10.113000	7.373000	0.632000	-0.00675
103	C39	c3	M	11.529000	5.786000	0.266000	0.02281
104	H63	ha	E	11.559000	5.465000	1.317000	-0.00460
105	H64	ha	E	11.632000	4.910000	-0.389000	-0.00460
106	C40	c3	M	12.672000	6.774000	-0.004000	0.18661
107	H65	ha	E	12.635000	7.096000	-1.054000	-0.03317
108	H66	ha	E	12.560000	7.649000	0.652000	-0.03317

109	C41	c3	M	14.019000	6.093000	0.276000	-0.29444
110	H67	ha	E	14.835000	6.804000	0.083000	0.06147
111	H68	ha	E	14.130000	5.218000	-0.380000	0.06147
112	H38	ha	E	14.053000	5.771000	1.327000	0.06147

LOOP

IMPROPER

C11 O45 C10 O9
C29 O44 C28 O27

DONE

STOP

DPPC glycerophospholipid:

.frcmod

#REQUIMTE, Dept Quim e Bioquim, FCUP, Univ Porto, Portugal;
#JTS Coimbra; SF Sousa; PA Fernandes; M Rangel; MJ Ramos 2012
#DPPC Glycerophospholipid

IMPROPER

c3-o -c -os 10.5 180.0 2.0 General improper torsional angle (2 general atom types)

.prepc

#REQUIMTE, Dept Quim e Bioquim, FCUP, Univ Porto, Portugal;
#JTS Coimbra; SF Sousa; PA Fernandes; M Rangel; MJ Ramos 2012
#DPPC Glycerophospholipid

0 0 2

This is a remark line

molecule.res

DPC XYZ 0

CHANGE OMIT DU BEG

0.0000

1	DUMM	DU	M	999.000	999.0	-999.0	.00000
2	DUMM	DU	M	999.000	-999.0	999.0	.00000
3	DUMM	DU	M	-999.000	999.0	999.0	.00000
4	C1	c3	M	-8.201000	-3.418000	-2.467000	-0.40610
5	H1	hx	E	-8.402000	-2.434000	-2.027000	0.18736
6	H2	hx	E	-9.151000	-3.955000	-2.595000	0.18736
7	H3	hx	E	-7.716000	-3.293000	-3.445000	0.18736
8	N2	n4	M	-7.319000	-4.206000	-1.584000	0.18665
9	C11	c3	3	-7.988000	-4.410000	-0.285000	-0.40610
10	H11	hx	E	-8.186000	-3.446000	0.200000	0.18736
11	H12	hx	E	-7.346000	-5.023000	0.362000	0.18736
12	H13	hx	E	-8.942000	-4.929000	-0.452000	0.18736
13	C12	c3	3	-7.100000	-5.511000	-2.198000	-0.40610
14	H14	hx	E	-6.456000	-6.117000	-1.546000	0.18736
15	H15	hx	E	-6.614000	-5.377000	-3.175000	0.18736
16	H16	hx	E	-8.067000	-6.016000	-2.334000	0.18736
17	C3	c3	M	-5.967000	-3.550000	-1.417000	-0.07285
18	H4	hx	E	-5.348000	-4.202000	-0.786000	0.10778
19	H5	hx	E	-5.505000	-3.464000	-2.410000	0.10778
20	C4	c3	M	-5.995000	-2.128000	-0.769000	0.21293
21	H6	h1	E	-6.588000	-1.442000	-1.388000	0.08927
22	H7	h1	E	-6.432000	-2.181000	0.236000	0.08927
23	O5	os	M	-4.662000	-1.627000	-0.668000	-0.48767
24	P6	p5	M	-4.716000	-0.223000	-0.025000	1.20503
25	O13	o	E	-5.474000	0.614000	-0.818000	-0.85744
26	O14	o	E	-5.368000	-0.330000	1.377000	-0.85744
27	O7	os	M	-3.290000	0.359000	0.120000	-0.43310
28	C8	c3	M	-3.399000	1.648000	0.722000	0.16442
29	H8	h1	E	-4.006000	2.296000	0.075000	0.10131
30	H9	h1	E	-3.889000	1.548000	1.700000	0.10131
31	C9	c3	M	-2.016000	2.290000	0.923000	0.17827

32	O10	os	S	-2.238000	3.606000	1.531000	-0.55192
33	C32	c	B	-1.139000	4.544000	1.622000	0.83438
34	C33	c3	3	0.242000	4.328000	1.014000	-0.17120
35	C34	c3	3	1.113000	5.570000	1.208000	-0.00306
36	C35	c3	3	2.491000	5.309000	0.601000	0.03420
37	C36	c3	3	3.369000	6.543000	0.809000	0.00782
38	C37	c3	3	4.752000	6.280000	0.214000	0.02316
39	C38	c3	3	5.628000	7.511000	0.437000	0.04006
40	C39	c3	3	7.017000	7.254000	-0.147000	0.03548
41	C40	c3	3	7.888000	8.486000	0.091000	0.02774
42	C41	c3	3	9.282000	8.235000	-0.484000	0.00806
43	C42	c3	3	10.148000	9.469000	-0.234000	0.05522
44	C43	c3	3	11.545000	9.225000	-0.802000	0.04810
45	C44	c3	3	12.407000	10.461000	-0.546000	-0.03535
46	C45	c3	3	13.806000	10.221000	-1.110000	0.02550
47	C46	c3	3	14.667000	11.459000	-0.850000	0.17497
48	C47	c3	3	16.073000	11.221000	-1.415000	-0.29093
49	H76	hc	E	16.698000	12.106000	-1.232000	0.06075
50	H77	hc	E	16.004000	11.036000	-2.497000	0.06075
51	H78	hc	E	16.520000	10.346000	-0.922000	0.06075
52	H74	hc	E	14.214000	12.331000	-1.343000	-0.02972
53	H75	hc	E	14.730000	11.640000	0.232000	-0.02972
54	H72	hc	E	14.258000	9.349000	-0.617000	-0.00361
55	H73	hc	E	13.741000	10.039000	-2.192000	-0.00361
56	H70	hc	E	11.955000	11.333000	-1.039000	-0.00471
57	H71	hc	E	12.473000	10.644000	0.536000	-0.00471
58	H68	hc	E	11.996000	8.353000	-0.309000	-0.01913
59	H69	hc	E	11.477000	9.041000	-1.883000	-0.01913
60	H66	hc	E	9.697000	10.341000	-0.728000	-0.01653
61	H67	hc	E	10.219000	9.655000	0.846000	-0.01653
62	H64	hc	E	9.733000	7.364000	0.011000	-0.01150
63	H65	hc	E	9.208000	8.047000	-1.564000	-0.01150
64	H62	hc	E	7.438000	9.357000	-0.403000	-0.01492
65	H63	hc	E	7.967000	8.675000	1.171000	-0.01492
66	H60	hc	E	7.468000	6.383000	0.349000	-0.01593
67	H61	hc	E	6.934000	7.061000	-1.226000	-0.01593
68	H58	hc	E	5.176000	8.382000	-0.058000	-0.01519
69	H59	hc	E	5.716000	7.707000	1.515000	-0.01519
70	H56	hc	E	5.206000	5.412000	0.711000	-0.01535
71	H57	hc	E	4.660000	6.081000	-0.863000	-0.01535
72	H54	hc	E	2.911000	7.410000	0.313000	-0.00241
73	H55	hc	E	3.466000	6.744000	1.885000	-0.00241
74	H52	hc	E	2.953000	4.445000	1.099000	-0.00793
75	H53	hc	E	2.390000	5.103000	-0.474000	-0.00793
76	H50	hc	E	0.647000	6.433000	0.712000	0.02435
77	H51	hc	E	1.220000	5.777000	2.281000	0.02435
78	H48	hc	E	0.715000	3.465000	1.493000	0.05075
79	H49	hc	E	0.134000	4.082000	-0.053000	0.05075
80	O50	o	E	-1.358000	5.629000	2.172000	-0.57832
81	H10	h1	E	-1.523000	2.407000	-0.052000	0.06283
82	C15	c3	M	-1.186000	1.348000	1.855000	-0.09520
83	H18	h1	E	-0.207000	1.788000	2.051000	0.12862
84	H19	h1	E	-1.720000	1.216000	2.806000	0.12862
85	O16	os	M	-0.986000	0.081000	1.234000	-0.43746
86	C17	c	M	-0.230000	-0.716000	2.085000	0.86062
87	O48	o	E	0.126000	-0.282000	3.187000	-0.61809
88	C18	c3	M	0.225000	-2.067000	1.645000	-0.36287
89	H20	hc	E	-0.003000	-2.815000	2.418000	0.10250
90	H21	hc	E	-0.215000	-2.340000	0.675000	0.10250
91	C19	c3	M	1.751000	-1.989000	1.541000	0.11107
92	H22	hc	E	2.025000	-1.225000	0.800000	-0.00441
93	H23	hc	E	2.164000	-1.711000	2.521000	-0.00441
94	C20	c3	M	2.338000	-3.335000	1.118000	0.03598
95	H24	hc	E	2.081000	-4.105000	1.859000	-0.00374
96	H25	hc	E	1.946000	-3.624000	0.133000	-0.00374
97	C21	c3	M	3.857000	-3.170000	1.048000	-0.01019
98	H26	hc	E	4.103000	-2.391000	0.313000	-0.00095
99	H27	hc	E	4.233000	-2.871000	2.036000	-0.00095
100	C22	c3	M	4.522000	-4.481000	0.635000	0.01270
101	H28	hc	E	4.289000	-5.265000	1.369000	-0.01338
102	H29	hc	E	4.162000	-4.787000	-0.358000	-0.01338
103	C23	c3	M	6.032000	-4.244000	0.592000	0.05221
104	H30	hc	E	6.256000	-3.454000	-0.138000	-0.01453
105	H31	hc	E	6.377000	-3.931000	1.587000	-0.01453
106	C24	c3	M	6.758000	-5.526000	0.188000	0.01976
107	H32	hc	E	6.544000	-6.319000	0.918000	-0.01179
108	H33	hc	E	6.426000	-5.844000	-0.810000	-0.01179

109	C25	c3	M	8.258000	-5.234000	0.167000	0.02080
110	H34	hc	E	8.465000	-4.436000	-0.559000	-0.01309
111	H35	hc	E	8.580000	-4.910000	1.167000	-0.01309
112	C26	c3	M	9.028000	-6.492000	-0.228000	0.02211
113	H36	hc	E	8.829000	-7.292000	0.499000	-0.01468
114	H37	hc	E	8.717000	-6.819000	-1.230000	-0.01468
115	C27	c3	M	10.521000	-6.162000	-0.234000	0.04707
116	H38	hc	E	10.716000	-5.359000	-0.958000	-0.01534
117	H39	hc	E	10.826000	-5.832000	0.769000	-0.01534
118	C28	c3	M	11.319000	-7.404000	-0.623000	0.06450
119	H40	hc	E	11.129000	-8.208000	0.102000	-0.02352
120	H41	hc	E	11.021000	-7.736000	-1.627000	-0.02352
121	C29	c3	M	12.807000	-7.051000	-0.619000	-0.04260
122	H42	hc	E	12.995000	-6.246000	-1.343000	-0.00426
123	H43	hc	E	13.102000	-6.718000	0.386000	-0.00426
124	C30	c3	M	13.620000	-8.286000	-1.005000	0.03150
125	H44	hc	E	13.433000	-9.091000	-0.281000	-0.00576
126	H45	hc	E	13.327000	-8.620000	-2.010000	-0.00576
127	C31	c3	M	15.107000	-7.923000	-0.997000	0.17616
128	H46	hc	E	15.291000	-7.116000	-1.721000	-0.03116
129	H47	hc	E	15.396000	-7.587000	0.009000	-0.03116
130	C49	c3	M	15.928000	-9.159000	-1.384000	-0.27644
131	H79	hc	E	16.998000	-8.905000	-1.380000	0.05684
132	H80	hc	E	15.633000	-9.493000	-2.389000	0.05684
133	H81	hc	E	15.738000	-9.964000	-0.660000	0.05684

LOOP

IMPROPER

C33 O50 C32 O10

C18 O48 C17 O16

DONE

STOP

DPPE glycerophospholipid:

.frcmod

#REQUIMTE, Dept Quim e Bioquim, FCUP, Univ Porto, Portugal;

#JTS Coimbra; SF Sousa; PA Fernandes; M Rangel; MJ Ramos 2012

#DPPE Glycerophospholipid

IMPROPER

c3-o -c -os 10.5 180.0 2.0 General improper torsional angle (2 general atom types)

.prepc

#REQUIMTE, Dept Quim e Bioquim, FCUP, Univ Porto, Portugal;

#JTS Coimbra; SF Sousa; PA Fernandes; M Rangel; MJ Ramos 2012

#DPPE Glycerophospholipid

0 0 2

This is a remark line

molecule.res

DPE XYZ 0

CHANGE OMIT DU BEG

0.0000

1	DUMM	DU	M	999.000	999.0	-999.0	.00000
2	DUMM	DU	M	999.000	-999.0	999.0	.00000
3	DUMM	DU	M	-999.000	999.0	999.0	.00000
4	N1	n4	M	-13.897000	7.763000	0.002000	-0.74542
5	H1	hn	E	-14.497000	8.600000	0.291000	0.41818
6	H2	hn	E	-14.269000	6.877000	0.473000	0.41818
7	H74	hn	E	-13.939000	7.645000	-1.061000	0.41818
8	C2	c3	M	-12.498000	7.992000	0.418000	0.28146
9	H3	hx	E	-12.119000	8.904000	-0.066000	0.04946
10	H4	hx	E	-12.464000	8.115000	1.509000	0.04946

11	C3	c3	M	-11.619000	6.783000	0.002000	0.16476
12	H5	h1	E	-12.018000	5.873000	0.475000	0.05653
13	H6	h1	E	-11.660000	6.671000	-1.091000	0.05653
14	O4	os	M	-10.236000	6.978000	0.426000	-0.54280
15	P5	p5	M	-9.359000	5.763000	-0.053000	1.39606
16	O46	o	E	-9.271000	5.786000	-1.430000	-0.87004
17	O47	o	E	-10.066000	4.454000	0.383000	-0.87004
18	O6	os	M	-7.900000	5.778000	0.585000	-0.49547
19	C7	c3	M	-7.156000	4.641000	0.058000	-0.15044
20	H7	h1	E	-7.777000	3.746000	0.200000	0.15490
21	H8	h1	E	-6.984000	4.790000	-1.018000	0.15490
22	C8	c3	M	-5.779000	4.370000	0.799000	0.41754
23	O27	os	S	-4.730000	5.436000	0.748000	-0.58182
24	C28	c	B	-4.077000	5.774000	-0.484000	0.94422
25	C29	c3	3	-2.820000	6.661000	-0.416000	-0.29190
26	C30	c3	3	-1.528000	5.737000	-0.317000	0.08576
27	C31	c3	3	-0.211000	6.607000	-0.242000	-0.12918
28	C32	c3	3	1.095000	5.714000	-0.161000	-0.09276
29	C33	c3	3	2.377000	6.638000	-0.103000	0.07014
30	C34	c3	3	3.715000	5.804000	-0.051000	-0.02260
31	C35	c3	3	4.954000	6.778000	-0.018000	0.05832
32	C36	c3	3	6.312000	5.991000	0.007000	0.00979
33	C37	c3	3	7.517000	6.995000	0.020000	0.01282
34	C38	c3	3	8.879000	6.231000	0.025000	0.02842
35	C39	c3	3	10.062000	7.245000	0.026000	0.06282
36	C40	c3	3	11.416000	6.488000	0.020000	-0.03748
37	C41	c3	3	12.587000	7.500000	0.015000	0.02366
38	C42	c3	3	13.928000	6.737000	0.005000	0.17696
39	C43	c3	3	15.097000	7.743000	-0.001000	-0.28001
40	H71	hc	E	16.053000	7.196000	-0.008000	0.05897
41	H72	hc	E	15.043000	8.373000	0.898000	0.05897
42	H73	hc	E	15.031000	8.377000	-0.897000	0.05897
43	H69	hc	E	13.996000	6.104000	0.901000	-0.03139
44	H70	hc	E	13.985000	6.108000	-0.894000	-0.03139
45	H67	hc	E	12.522000	8.133000	-0.881000	-0.00396
46	H68	hc	E	12.532000	8.130000	0.914000	-0.00396
47	H65	hc	E	11.486000	5.856000	0.915000	-0.00405
48	H66	hc	E	11.479000	5.859000	-0.879000	-0.00405
49	H63	hc	E	9.999000	7.878000	-0.871000	-0.02073
50	H64	hc	E	10.002000	7.877000	0.923000	-0.02073
51	H61	hc	E	8.942000	5.598000	0.921000	-0.01118
52	H62	hc	E	8.945000	5.602000	-0.873000	-0.01118
53	H59	hc	E	7.467000	7.628000	-0.877000	-0.00928
54	H60	hc	E	7.454000	7.627000	0.916000	-0.00928
55	H57	hc	E	6.355000	5.357000	0.904000	-0.00924
56	H58	hc	E	6.381000	5.360000	-0.890000	-0.00924
57	H55	hc	E	4.931000	7.412000	-0.915000	-0.01811
58	H56	hc	E	4.890000	7.414000	0.877000	-0.01811
59	H53	hc	E	3.723000	5.170000	0.847000	-0.00224
60	H54	hc	E	3.781000	5.171000	-0.947000	-0.00224
61	H51	hc	E	2.395000	7.269000	-1.001000	-0.01149
62	H52	hc	E	2.318000	7.277000	0.789000	-0.01149
63	H49	hc	E	1.056000	5.082000	0.739000	0.02811
64	H50	hc	E	1.150000	5.075000	-1.054000	0.02811
65	H47	hc	E	-0.152000	7.235000	-1.141000	0.05249
66	H48	hc	E	-0.259000	7.251000	0.648000	0.05249
67	H45	hc	E	-1.599000	5.110000	0.586000	0.03627
68	H46	hc	E	-1.482000	5.088000	-1.204000	0.03627
69	H43	hc	E	-2.726000	7.254000	-1.335000	0.06963
70	H44	hc	E	-2.852000	7.295000	0.481000	0.06963
71	O45	o	E	-4.413000	5.282000	-1.569000	-0.60932
72	H9	h1	E	-5.991000	4.191000	1.862000	0.07403
73	C9	c3	M	-5.143000	3.099000	0.186000	-0.19937
74	H10	h1	E	-5.793000	2.221000	0.315000	0.14982
75	H11	h1	E	-4.981000	3.270000	-0.883000	0.14982
76	O10	os	M	-3.862000	2.928000	0.789000	-0.51182
77	C11	c	M	-3.145000	1.917000	0.158000	0.87728
78	O44	o	E	-3.662000	1.245000	-0.741000	-0.61095
79	C12	c3	M	-1.657000	1.883000	0.371000	-0.17433
80	H12	hc	E	-1.221000	2.539000	-0.397000	0.04829
81	H13	hc	E	-1.409000	2.304000	1.354000	0.04829
82	C13	c3	M	-1.024000	0.500000	0.173000	-0.00039
83	H14	hc	E	-1.393000	-0.199000	0.937000	0.01200
84	H15	hc	E	-1.264000	0.116000	-0.828000	0.01200
85	C14	c3	M	0.507000	0.698000	0.288000	0.02906
86	H16	hc	E	0.826000	1.399000	-0.496000	-0.00363
87	H17	hc	E	0.748000	1.122000	1.273000	-0.00363

88	C15	c3	M	1.265000	-0.631000	0.114000	0.03963
89	H18	hc	E	0.973000	-1.325000	0.913000	-0.00665
90	H19	hc	E	1.023000	-1.072000	-0.864000	-0.00665
91	C16	c3	M	2.789000	-0.350000	0.183000	-0.03263
92	H20	hc	E	3.066000	0.334000	-0.632000	-0.00464
93	H21	hc	E	3.032000	0.115000	1.149000	-0.00464
94	C17	c3	M	3.579000	-1.670000	0.044000	0.06588
95	H22	hc	E	3.305000	-2.339000	0.871000	-0.02044
96	H23	hc	E	3.329000	-2.150000	-0.913000	-0.02044
97	C18	c3	M	5.102000	-1.389000	0.090000	0.03379
98	H24	hc	E	5.381000	-0.736000	-0.750000	-0.01439
99	H25	hc	E	5.356000	-0.896000	1.038000	-0.01439
100	C19	c3	M	5.872000	-2.728000	-0.009000	0.02402
101	H26	hc	E	5.589000	-3.364000	0.840000	-0.01367
102	H27	hc	E	5.611000	-3.234000	-0.949000	-0.01367
103	C20	c3	M	7.399000	-2.480000	0.029000	-0.00114
104	H28	hc	E	7.694000	-1.857000	-0.828000	-0.00880
105	H29	hc	E	7.666000	-1.967000	0.963000	-0.00880
106	C21	c3	M	8.135000	-3.838000	-0.033000	0.05061
107	H30	hc	E	7.836000	-4.448000	0.830000	-0.01431
108	H31	hc	E	7.864000	-4.361000	-0.961000	-0.01431
109	C22	c3	M	9.663000	-3.623000	0.001000	0.04615
110	H32	hc	E	9.971000	-3.025000	-0.867000	-0.01822
111	H33	hc	E	9.940000	-3.098000	0.926000	-0.01822
112	C23	c3	M	10.369000	-4.994000	-0.035000	-0.02940
113	H34	hc	E	10.059000	-5.585000	0.838000	-0.00575
114	H35	hc	E	10.090000	-5.527000	-0.955000	-0.00575
115	C24	c3	M	11.894000	-4.798000	-0.003000	0.01757
116	H36	hc	E	12.209000	-4.214000	-0.878000	-0.00276
117	H37	hc	E	12.178000	-4.265000	0.916000	-0.00276
118	C25	c3	M	12.582000	-6.174000	-0.027000	0.18367
119	H38	hc	E	12.267000	-6.755000	0.851000	-0.03235
120	H39	hc	E	12.296000	-6.710000	-0.943000	-0.03235
121	C26	c3	M	14.108000	-5.986000	0.003000	-0.28737
122	H40	hc	E	14.600000	-6.971000	-0.013000	0.06012
123	H41	hc	E	14.393000	-5.448000	0.919000	0.06012
124	H42	hc	E	14.422000	-5.405000	-0.876000	0.06012

LOOP

IMPROPER

C29 O45 C28 O27
C12 O44 C11 O10

DONE

STOP

DSPE glycerophospholipid:

.frcmod

#REQUIMTE, Dept Quim e Bioquim, FCUP, Univ Porto, Portugal;
#JTS Coimbra; SF Sousa; PA Fernandes; M Rangel; MJ Ramos 2012
#DSPE Glycerophospholipid

IMPROPER

c3-o -c -os 10.5 180.0 2.0 General improper torsional angle (2 general atom types)

.prepc

#REQUIMTE, Dept Quim e Bioquim, FCUP, Univ Porto, Portugal;
#JTS Coimbra; SF Sousa; PA Fernandes; M Rangel; MJ Ramos 2012
#DSPE Glycerophospholipid

0 0 2

This is a remark line
molecule.res
DSE XYZ 0

CHANGE OMIT DU BEG

```

0.0000
1 DUMM DU M 999.000 999.0 -999.0 .00000
2 DUMM DU M 999.000 -999.0 999.0 .00000
3 DUMM DU M -999.000 999.0 999.0 .00000
4 N1 n4 M -14.426000 8.218000 0.015000 -0.75024
5 H1 hn E -15.020000 9.054000 0.319000 0.41927
6 H2 hn E -14.808000 7.327000 0.468000 0.41927
7 H82 hn E -14.466000 8.121000 -1.050000 0.41927
8 C2 c3 M -13.026000 8.427000 0.439000 0.28595
9 H3 hx E -12.639000 9.345000 -0.025000 0.04942
10 H4 hx E -12.995000 8.528000 1.533000 0.04942
11 C3 c3 M -12.155000 7.219000 0.003000 0.15567
12 H5 h1 E -12.562000 6.303000 0.457000 0.05909
13 H6 h1 E -12.192000 7.129000 -1.092000 0.05909
14 O4 os M -10.770000 7.396000 0.436000 -0.54327
15 P5 p5 M -9.894000 6.185000 -0.061000 1.40100
16 O50 o E -9.800000 6.231000 -1.437000 -0.87076
17 O51 o E -10.607000 4.871000 0.350000 -0.87076
18 O6 os M -8.436000 6.186000 0.584000 -0.50084
19 C7 c3 M -7.684000 5.056000 0.043000 -0.13669
20 H7 h1 E -8.304000 4.157000 0.168000 0.15195
21 H8 h1 E -7.507000 5.222000 -1.029000 0.15195
22 C8 c3 M -6.307000 4.779000 0.790000 0.41351
23 O29 os S -5.268000 5.858000 0.760000 -0.57795
24 C30 c B -4.602000 6.217000 -0.462000 0.92966
25 C31 c3 3 -3.384000 7.160000 -0.381000 -0.25172
26 C32 c3 3 -2.037000 6.314000 -0.292000 0.06804
27 C33 c3 3 -0.779000 7.277000 -0.213000 -0.10167
28 C34 c3 3 0.593000 6.484000 -0.143000 -0.08935
29 C35 c3 3 1.809000 7.500000 -0.086000 0.07904
30 C36 c3 3 3.208000 6.763000 -0.042000 -0.00239
31 C37 c3 3 4.384000 7.819000 -0.011000 0.02166
32 C38 c3 3 5.795000 7.119000 0.008000 -0.00045
33 C39 c3 3 6.942000 8.196000 0.019000 0.03636
34 C40 c3 3 8.356000 7.516000 0.021000 0.01530
35 C41 c3 3 9.483000 8.602000 0.021000 0.00735
36 C42 c3 3 10.890000 7.929000 0.017000 0.03871
37 C43 c3 3 12.006000 9.014000 0.013000 0.05663
38 C44 c3 3 13.400000 8.338000 0.007000 -0.03707
39 C45 c3 3 14.510000 9.414000 0.004000 0.02503
40 C46 c3 3 15.891000 8.728000 -0.001000 0.17876
41 C47 c3 3 17.001000 9.797000 -0.004000 -0.28060
42 H79 hc E 17.986000 9.304000 -0.007000 0.05885
43 H80 hc E 16.909000 10.424000 0.894000 0.05885
44 H81 hc E 16.903000 10.425000 -0.901000 0.05885
45 H77 hc E 15.992000 8.100000 0.896000 -0.03184
46 H78 hc E 15.986000 8.101000 -0.899000 -0.03184
47 H75 hc E 14.412000 10.041000 -0.893000 -0.00429
48 H76 hc E 14.418000 10.041000 0.902000 -0.00429
49 H73 hc E 13.507000 7.711000 0.904000 -0.00423
50 H74 hc E 13.500000 7.712000 -0.890000 -0.00423
51 H71 hc E 11.904000 9.641000 -0.884000 -0.01965
52 H72 hc E 11.910000 9.641000 0.911000 -0.01965
53 H69 hc E 10.998000 7.303000 0.913000 -0.01293
54 H70 hc E 10.992000 7.304000 -0.881000 -0.01293
55 H67 hc E 9.382000 9.229000 -0.875000 -0.00888
56 H68 hc E 9.385000 9.229000 0.918000 -0.00888
57 H65 hc E 8.458000 6.888000 0.917000 -0.01009
58 H66 hc E 8.459000 6.891000 -0.876000 -0.01009
59 H63 hc E 6.853000 8.825000 -0.878000 -0.01173
60 H64 hc E 6.843000 8.823000 0.915000 -0.01173
61 H61 hc E 5.880000 6.488000 0.904000 -0.00468
62 H62 hc E 5.900000 6.494000 -0.890000 -0.00468
63 H59 hc E 4.317000 8.450000 -0.908000 -0.00907
64 H60 hc E 4.282000 8.447000 0.884000 -0.00907
65 H57 hc E 3.262000 6.129000 0.854000 -0.00435
66 H58 hc E 3.312000 6.138000 -0.939000 -0.00435
67 H55 hc E 1.777000 8.135000 -0.982000 -0.01618
68 H56 hc E 1.708000 8.131000 0.809000 -0.01618
69 H53 hc E 0.606000 5.846000 0.754000 0.02213
70 H54 hc E 0.692000 5.855000 -1.038000 0.02213
71 H51 hc E -0.769000 7.913000 -1.108000 0.04629
72 H52 hc E -0.871000 7.910000 0.680000 0.04629
73 H49 hc E -2.064000 5.676000 0.605000 0.03141
74 H50 hc E -1.951000 5.679000 -1.185000 0.03141
75 H47 hc E -3.323000 7.768000 -1.294000 0.05994

```

76	H48	hc	E	-3.451000	7.783000	0.521000	0.05994
77	O48	o	E	-4.912000	5.722000	-1.552000	-0.60450
78	H9	h1	E	-6.525000	4.583000	1.849000	0.07516
79	C9	c3	M	-5.665000	3.514000	0.161000	-0.21596
80	H10	h1	E	-6.321000	2.637000	0.275000	0.15358
81	H11	h1	E	-5.499000	3.699000	-0.904000	0.15358
82	O10	os	M	-4.384000	3.321000	0.766000	-0.50754
83	C11	c	M	-3.680000	2.300000	0.127000	0.88737
84	O49	o	E	-4.210000	1.643000	-0.776000	-0.61027
85	C12	c3	M	-2.190000	2.228000	0.345000	-0.21071
86	H12	hc	E	-1.736000	2.871000	-0.422000	0.05686
87	H13	hc	E	-1.936000	2.644000	1.329000	0.05686
88	C13	c3	M	-1.589000	0.821000	0.151000	0.03175
89	H14	hc	E	-1.980000	0.134000	0.915000	0.00572
90	H15	hc	E	-1.836000	0.442000	-0.850000	0.00572
91	C14	c3	M	-0.047000	0.973000	0.272000	0.02823
92	H16	hc	E	0.294000	1.664000	-0.513000	-0.00436
93	H17	hc	E	0.202000	1.393000	1.256000	-0.00436
94	C15	c3	M	0.683000	-0.381000	0.100000	0.02948
95	H18	hc	E	0.371000	-1.066000	0.901000	-0.00555
96	H19	hc	E	0.433000	-0.817000	-0.876000	-0.00555
97	C16	c3	M	2.222000	-0.141000	0.176000	-0.01730
98	H20	hc	E	2.517000	0.535000	-0.641000	-0.00524
99	H21	hc	E	2.473000	0.321000	1.139000	-0.00524
100	C17	c3	M	2.991000	-1.484000	0.038000	0.05080
101	H22	hc	E	2.701000	-2.145000	0.867000	-0.01614
102	H23	hc	E	2.733000	-1.960000	-0.917000	-0.01614
103	C18	c3	M	4.529000	-1.236000	0.089000	0.01531
104	H24	hc	E	4.821000	-0.589000	-0.752000	-0.00880
105	H25	hc	E	4.791000	-0.745000	1.036000	-0.00880
106	C19	c3	M	5.285000	-2.594000	-0.009000	0.01365
107	H26	hc	E	4.989000	-3.225000	0.842000	-0.00871
108	H27	hc	E	5.016000	-3.098000	-0.946000	-0.00871
109	C20	c3	M	6.826000	-2.373000	0.032000	0.02270
110	H28	hc	E	7.129000	-1.756000	-0.827000	-0.01175
111	H29	hc	E	7.099000	-1.862000	0.964000	-0.01175
112	C21	c3	M	7.553000	-3.748000	-0.030000	0.04191
113	H30	hc	E	7.247000	-4.352000	0.836000	-0.01573
114	H31	hc	E	7.274000	-4.269000	-0.955000	-0.01573
115	C22	c3	M	9.094000	-3.553000	0.005000	-0.01018
116	H32	hc	E	9.407000	-2.960000	-0.867000	-0.00672
117	H33	hc	E	9.377000	-3.028000	0.926000	-0.00672
118	C23	c3	M	9.796000	-4.937000	-0.031000	0.05540
119	H34	hc	E	9.484000	-5.523000	0.846000	-0.01640
120	H35	hc	E	9.511000	-5.470000	-0.947000	-0.01640
121	C24	c3	M	11.334000	-4.757000	-0.001000	0.04733
122	H36	hc	E	11.651000	-4.179000	-0.881000	-0.01819
123	H37	hc	E	11.624000	-4.222000	0.913000	-0.01819
124	C25	c3	M	12.018000	-6.142000	-0.023000	-0.03630
125	H38	hc	E	11.704000	-6.717000	0.861000	-0.00372
126	H39	hc	E	11.728000	-6.683000	-0.933000	-0.00372
127	C26	c3	M	13.550000	-5.969000	0.002000	0.02124
128	H40	hc	E	13.869000	-5.400000	-0.883000	-0.00286
129	H41	hc	E	13.847000	-5.429000	0.911000	-0.00286
130	C27	c3	M	14.222000	-7.355000	-0.013000	0.17686
131	H42	hc	E	13.905000	-7.924000	0.874000	-0.03136
132	H43	hc	E	13.925000	-7.897000	-0.921000	-0.03136
133	C28	c3	M	15.752000	-7.186000	0.007000	-0.27697
134	H44	hc	E	16.232000	-8.176000	-0.002000	0.05781
135	H45	hc	E	16.049000	-6.642000	0.915000	0.05781
136	H46	hc	E	16.069000	-6.618000	-0.880000	0.05781

LOOP

IMPROPER

C31 O48 C30 O29

C12 O49 C11 O10

DONE

STOP

PLPC glycerophospholipid:

.frcmod

#REQUIMTE, Dept Quim e Bioquim, FCUP, Univ Porto, Portugal;
#JTS Coimbra; SF Sousa; PA Fernandes; M Rangel; MJ Ramos 2012
#PLPC Glycerophospholipid

IMPROPER

c3-o -c -os	10.5	180.0	2.0	General improper torsional angle (2 general atom types)
c2-c3-c2-ha	1.1	180.0	2.0	Using default value

.prepc

#REQUIMTE, Dept Quim e Bioquim, FCUP, Univ Porto, Portugal;
#JTS Coimbra; SF Sousa; PA Fernandes; M Rangel; MJ Ramos 2012
#PLPC Glycerophospholipid

0 0 2

This is a remark line

molecule.res

PLC XYZ 0

CHANGE OMIT DU BEG

0.0000

1	DUMM	DU	M	999.000	999.0	-999.0	.00000
2	DUMM	DU	M	999.000	-999.0	999.0	.00000
3	DUMM	DU	M	-999.000	999.0	999.0	.00000
4	C1	c3	M	-13.964000	6.036000	1.016000	-0.46962
5	H104	hx	E	-14.687000	6.717000	1.426000	0.20810
6	H106	hx	E	-13.406000	5.573000	1.835000	0.20810
7	H108	hx	E	-14.461000	5.261000	0.429000	0.20810
8	N2	n4	M	-13.053000	6.794000	0.123000	0.15100
9	C54	c3	3	-13.936000	7.408000	-0.930000	-0.46962
10	H190	hx	E	-13.341000	8.006000	-1.632000	0.20810
11	H192	hx	E	-14.645000	8.042000	-0.447000	0.20810
12	H194	hx	E	-14.451000	6.611000	-1.476000	0.20810
13	C56	c3	3	-12.353000	7.873000	0.849000	-0.46962
14	H196	hx	E	-11.705000	8.420000	0.139000	0.20810
15	H198	hx	E	-11.723000	7.456000	1.649000	0.20810
16	H200	hx	E	-13.092000	8.557000	1.284000	0.20810
17	C3	c3	M	-11.977000	5.926000	-0.496000	-0.10436
18	H110	hx	E	-12.432000	5.148000	-1.120000	0.11223
19	H112	hx	E	-11.378000	6.592000	-1.134000	0.11223
20	C4	c3	M	-10.992000	5.205000	0.576000	0.29779
21	H114	h1	E	-10.555000	5.957000	1.237000	-0.00032
22	H116	h1	E	-11.581000	4.513000	1.177000	-0.00032
23	O5	os	M	-9.848000	4.460000	-0.009000	-0.45034
24	P6	p5	M	-8.866000	5.488000	-0.742000	1.23255
25	O58	o	E	-9.142000	6.692000	0.150000	-0.76069
26	O60	o	E	-9.727000	5.838000	-1.938000	-0.76069
27	O7	os	M	-7.386000	4.895000	-1.097000	-0.53473
28	C8	c3	M	-6.684000	4.115000	0.054000	0.20788
29	H118	h1	E	-6.237000	4.823000	0.765000	0.05820
30	H120	h1	E	-7.487000	3.566000	0.564000	0.05820
31	C9	c3	M	-5.589000	2.925000	-0.454000	0.24371
32	C10	c3	3	-5.012000	1.893000	0.840000	-0.11358
33	O11	os	S	-4.215000	0.656000	0.439000	-0.56313
34	C12	c	B	-2.897000	0.861000	0.090000	1.01062
35	C13	c3	3	-2.053000	-0.278000	-0.351000	-0.29735
36	C14	c3	3	-0.634000	-0.072000	0.194000	-0.00696
37	C15	c3	3	0.267000	-1.213000	-0.290000	0.04963
38	C16	c3	3	1.692000	-1.014000	0.253000	-0.07766
39	C17	c3	3	2.583000	-2.160000	-0.246000	-0.00277
40	C18	c3	3	4.009000	-1.984000	0.291000	0.02388
41	C19	c3	3	4.876000	-3.141000	-0.223000	0.00411
42	C20	c3	3	6.307000	-2.995000	0.308000	-0.00230
43	C21	c3	3	7.151000	-4.164000	-0.218000	-0.00746
44	C22	c3	3	8.586000	-4.042000	0.309000	0.01072
45	C23	c3	3	9.415000	-5.219000	-0.223000	0.02227
46	C24	c3	3	10.850000	-5.112000	0.304000	-0.04144
47	C25	c3	3	11.671000	-6.292000	-0.230000	-0.00709
48	C26	c3	3	13.107000	-6.189000	0.298000	0.13100
49	C27	c3	3	13.928000	-7.372000	-0.237000	-0.23241

50	H184	hc	E	14.959000	-7.303000	0.139000	0.04950
51	H186	hc	E	13.936000	-7.343000	-1.337000	0.04950
52	H188	hc	E	13.475000	-8.315000	0.102000	0.04950
53	H180	hc	E	13.556000	-5.245000	-0.041000	-0.01844
54	H182	hc	E	13.096000	-6.217000	1.397000	-0.01844
55	H176	hc	E	11.222000	-7.236000	0.110000	0.00592
56	H178	hc	E	11.681000	-6.264000	-1.329000	0.00592
57	H172	hc	E	11.299000	-4.168000	-0.036000	0.00456
58	H174	hc	E	10.841000	-5.139000	1.403000	0.00456
59	H168	hc	E	8.970000	-6.164000	0.118000	-0.00511
60	H170	hc	E	9.424000	-5.194000	-1.322000	-0.00511
61	H164	hc	E	9.027000	-3.096000	-0.033000	-0.00052
62	H166	hc	E	8.577000	-4.068000	1.409000	-0.00052
63	H160	hc	E	6.716000	-5.112000	0.126000	0.00038
64	H162	hc	E	7.162000	-4.142000	-1.317000	0.00038
65	H156	hc	E	6.736000	-2.044000	-0.038000	-0.00114
66	H158	hc	E	6.295000	-3.015000	1.407000	-0.00114
67	H152	hc	E	4.454000	-4.094000	0.125000	-0.00128
68	H154	hc	E	4.890000	-3.126000	-1.322000	-0.00128
69	H148	hc	E	4.423000	-1.028000	-0.059000	-0.00377
70	H150	hc	E	3.992000	-1.996000	1.391000	-0.00377
71	H144	hc	E	2.177000	-3.119000	0.107000	-0.00134
72	H146	hc	E	2.604000	-2.154000	-1.346000	-0.00134
73	H140	hc	E	2.094000	-0.055000	-0.104000	0.02419
74	H142	hc	E	1.669000	-1.016000	1.352000	0.02419
75	H136	hc	E	-0.131000	-2.172000	0.070000	0.00470
76	H138	hc	E	0.289000	-1.215000	-1.388000	0.00470
77	H132	hc	E	-0.239000	0.887000	-0.172000	0.01717
78	H134	hc	E	-0.664000	-0.059000	1.292000	0.01717
79	H128	hc	E	-2.489000	-1.236000	-0.026000	0.08605
80	H130	hc	E	-1.995000	-0.267000	-1.449000	0.08605
81	O62	o	E	-2.375000	1.960000	0.229000	-0.65465
82	H124	h1	E	-4.411000	2.472000	1.567000	0.14809
83	H126	h1	E	-5.903000	1.495000	1.357000	0.14809
84	H122	h1	E	-6.185000	2.293000	-1.119000	0.11099
85	O64	os	M	-4.345000	3.422000	-1.250000	-0.53149
86	C65	c	M	-3.473000	4.289000	-0.540000	0.76669
87	O78	o	E	-3.815000	4.623000	0.594000	-0.58026
88	C66	c3	M	-2.275000	4.901000	-1.209000	-0.34292
89	H202	hc	E	-2.146000	4.477000	-2.213000	0.09793
90	H204	hc	E	-2.397000	5.997000	-1.261000	0.09793
91	C67	c3	M	-1.050000	4.624000	-0.321000	0.12595
92	H206	hc	E	-1.220000	5.064000	0.671000	0.01652
93	H208	hc	E	-0.922000	3.540000	-0.219000	0.01652
94	C68	c3	M	0.232000	5.213000	-0.923000	-0.02047
95	H210	hc	E	0.421000	4.766000	-1.910000	0.01171
96	H212	hc	E	0.137000	6.300000	-1.023000	0.01171
97	C69	c3	M	1.377000	4.859000	0.041000	-0.01749
98	H214	hc	E	1.168000	5.306000	1.024000	-0.00031
99	H216	hc	E	1.425000	3.768000	0.143000	-0.00031
100	C70	c3	M	2.739000	5.364000	-0.467000	-0.04889
101	H218	hc	E	2.966000	4.906000	-1.441000	0.00056
102	H220	hc	E	2.729000	6.459000	-0.565000	0.00056
103	C80	c3	M	3.793000	4.934000	0.567000	0.15090
104	H222	hc	E	3.550000	5.389000	1.538000	-0.02448
105	H224	hc	E	3.769000	3.840000	0.663000	-0.02448
106	C82	c3	M	5.208000	5.365000	0.143000	0.05427
107	H226	hc	E	5.481000	4.926000	-0.828000	0.00834
108	H228	hc	E	5.261000	6.459000	0.050000	0.00834
109	C83	c2	M	6.180000	4.902000	1.209000	-0.25949
110	H230	ha	E	5.783000	4.552000	2.129000	0.12345
111	C86	c2	M	7.511000	4.890000	1.051000	-0.25900
112	H232	ha	E	8.105000	4.528000	1.852000	0.13670
113	C88	c3	M	8.219000	5.343000	-0.214000	0.22748
114	H234	hc	E	7.539000	5.225000	-1.066000	0.01900
115	H236	hc	E	8.506000	6.395000	-0.114000	0.01900
116	C90	c2	M	9.439000	4.445000	-0.389000	-0.26042
117	H238	ha	E	9.276000	3.401000	-0.484000	0.12674
118	C92	c2	M	10.707000	4.884000	-0.410000	-0.21125
119	H240	ha	E	11.481000	4.168000	-0.529000	0.10625
120	C94	c3	M	11.096000	6.334000	-0.267000	0.06288
121	H242	hc	E	10.666000	6.910000	-1.100000	0.01157
122	H244	hc	E	10.678000	6.735000	0.667000	0.01157
123	C96	c3	M	12.630000	6.444000	-0.269000	0.01996
124	H246	hc	E	13.037000	5.864000	0.572000	0.00938
125	H248	hc	E	13.024000	6.044000	-1.214000	0.00938
126	C98	c3	M	13.054000	7.909000	-0.123000	-0.09517

127	H250	hc	E	12.656000	8.495000	-0.963000	0.02104
128	H252	hc	E	12.668000	8.314000	0.824000	0.02104
129	C100	c3	M	14.587000	7.979000	-0.125000	0.17180
130	H254	hc	E	14.981000	7.389000	0.715000	-0.03116
131	H256	hc	E	14.971000	7.571000	-1.071000	-0.03116
132	C102	c3	M	15.035000	9.441000	0.022000	-0.20698
133	H258	hc	E	16.134000	9.490000	0.021000	0.04344
134	H260	hc	E	14.651000	9.849000	0.968000	0.04344
135	H262	hc	E	14.640000	10.031000	-0.818000	0.04344

LOOP

IMPROPER

C13 O62 C12 O11
 C66 O78 C65 O64
 C86 C82 C83 H230
 C83 C88 C86 H232
 C92 C88 C90 H238
 C90 C94 C92 H240

DONE

STOP

PLPE glycerophospholipid:

.frcmod

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 #JTS Coimbra; SF Sousa; PA Fernandes; M Rangel; MJ Ramos 2012
 #PLPE Glycerophospholipid*

IMPROPER

c3-o -c -os	10.5	180.0	2.0	General improper torsional angle (2 general atom types)
c2-c3-c2-ha	1.1	180.0	2.0	Using default value

.prepc

*#REQUIMTE, Dept Quim e Bioquim, FCUP, Univ Porto, Portugal;
 #JTS Coimbra; SF Sousa; PA Fernandes; M Rangel; MJ Ramos 2012
 #PLPE Glycerophospholipid*

0 0 2

This is a remark line

molecule.res

PLE XYZ 0

CHANGE OMIT DU BEG

0.0000
1 DUMM DU M 999.000 999.0 -999.0 .00000
2 DUMM DU M 999.000 -999.0 999.0 .00000
3 DUMM DU M -999.000 999.0 999.0 .00000
4 N1 n4 M -14.065000 6.600000 0.066000 -0.39782
5 H98 hn E -14.938000 7.166000 0.036000 0.30852
6 H100 hn E -13.983000 6.072000 0.943000 0.30852
7 H102 hn E -14.019000 5.940000 -0.719000 0.30852
8 C2 c3 M -12.927000 7.383000 -0.021000 0.06015
9 H104 hx E -12.866000 7.926000 -0.973000 0.06759
10 H106 hx E -12.820000 8.060000 0.838000 0.06759
11 C3 c3 M -11.994000 6.306000 0.034000 -0.02712
12 H108 h1 E -12.157000 5.764000 0.964000 0.10859
13 H110 h1 E -12.206000 5.643000 -0.802000 0.10859
14 O4 os M -10.710000 6.695000 -0.025000 -0.45916
15 P5 p5 M -10.060000 5.367000 -0.012000 1.22262
16 O52 o E -10.664000 4.650000 1.178000 -0.72631
17 O54 o E -10.627000 4.622000 -1.226000 -0.72631
18 O6 os M -8.622000 5.593000 0.076000 -0.46906
19 C7 c3 M -7.923000 4.250000 -0.019000 0.02678
20 H112 h1 E -8.526000 3.595000 0.628000 0.10447
21 H114 h1 E -8.035000 3.902000 -1.052000 0.10447

22	C8	c3	M	-6.308000	4.026000	0.501000	-0.00108
23	C9	c3	3	-6.198000	2.391000	0.346000	0.10093
24	O10	os	S	-4.869000	1.700000	0.823000	-0.53014
25	C11	c	B	-3.878000	1.594000	-0.211000	0.82774
26	C12	c3	3	-2.381000	1.278000	0.092000	-0.16124
27	C13	c3	3	-1.883000	-0.197000	-0.092000	-0.01380
28	C14	c3	3	-0.312000	-0.138000	0.138000	0.10473
29	C15	c3	3	0.434000	-1.518000	-0.011000	-0.03340
30	C16	c3	3	1.994000	-1.288000	0.144000	0.05076
31	C17	c3	3	2.794000	-2.635000	0.016000	0.00915
32	C18	c3	3	4.345000	-2.381000	0.114000	0.11763
33	C19	c3	3	5.127000	-3.736000	0.011000	-0.05344
34	C20	c3	3	6.676000	-3.508000	0.073000	0.02384
35	C21	c3	3	7.417000	-4.880000	-0.005000	-0.00817
36	C22	c3	3	8.962000	-4.683000	0.039000	0.02948
37	C23	c3	3	9.663000	-6.068000	-0.019000	-0.05987
38	C24	c3	3	11.202000	-5.899000	0.016000	-0.00180
39	C25	c3	3	11.870000	-7.292000	-0.032000	0.12183
40	C26	c3	3	13.404000	-7.138000	0.000000	-0.24906
41	H178	hc	E	13.873000	-8.134000	-0.033000	0.05543
42	H180	hc	E	13.702000	-6.625000	0.926000	0.05543
43	H182	hc	E	13.734000	-6.549000	-0.867000	0.05543
44	H174	hc	E	11.545000	-7.885000	0.833000	-0.01365
45	H176	hc	E	11.577000	-7.806000	-0.960000	-0.01365
46	H170	hc	E	11.530000	-5.304000	-0.846000	0.00613
47	H172	hc	E	11.494000	-5.390000	0.947000	0.00613
48	H166	hc	E	9.345000	-6.674000	0.838000	0.00912
49	H168	hc	E	9.382000	-6.579000	-0.953000	0.00912
50	H162	hc	E	9.282000	-4.070000	-0.813000	-0.00405
51	H164	hc	E	9.241000	-4.179000	0.979000	-0.00405
52	H158	hc	E	7.107000	-5.506000	0.839000	0.00615
53	H160	hc	E	7.152000	-5.380000	-0.950000	0.00615
54	H154	hc	E	6.988000	-2.871000	-0.764000	-0.01176
55	H156	hc	E	6.935000	-3.017000	1.025000	-0.01176
56	H150	hc	E	4.822000	-4.390000	0.835000	0.00467
57	H152	hc	E	4.884000	-4.220000	-0.949000	0.00467
58	H146	hc	E	4.655000	-1.713000	-0.700000	-0.02793
59	H148	hc	E	4.579000	-1.909000	1.083000	-0.02793
60	H142	hc	E	2.481000	-3.318000	0.815000	-0.01036
61	H144	hc	E	2.578000	-3.092000	-0.962000	-0.01036
62	H138	hc	E	2.329000	-0.597000	-0.641000	-0.02643
63	H140	hc	E	2.203000	-0.846000	1.131000	-0.02643
64	H134	hc	E	0.075000	-2.220000	0.754000	0.00683
65	H136	hc	E	0.241000	-1.933000	-1.012000	0.00683
66	H130	hc	E	0.099000	0.556000	-0.605000	-0.02506
67	H132	hc	E	-0.114000	0.257000	1.146000	-0.02506
68	H126	hc	E	-2.374000	-0.870000	0.627000	0.00860
69	H128	hc	E	-2.082000	-0.538000	-1.119000	0.00860
70	H122	hc	E	-1.787000	1.868000	-0.620000	0.05811
71	H124	hc	E	-2.156000	1.569000	1.129000	0.05811
72	O56	o	E	-4.172000	1.947000	-1.356000	-0.57849
73	H118	h1	E	-7.022000	1.991000	0.960000	0.10938
74	H120	h1	E	-6.379000	2.106000	-0.696000	0.10938
75	H116	h1	E	-6.285000	4.295000	1.558000	0.23488
76	O58	os	M	-5.074000	4.838000	-0.204000	-0.46453
77	C59	c	M	-3.739000	4.703000	0.420000	0.91595
78	O96	o	E	-3.538000	3.949000	1.389000	-0.66513
79	C60	c3	M	-2.527000	5.548000	-0.055000	-0.45411
80	H184	hc	E	-2.668000	5.897000	-1.089000	0.12930
81	H186	hc	E	-2.458000	6.424000	0.605000	0.12930
82	C61	c3	M	-1.197000	4.730000	0.123000	0.10435
83	H188	hc	E	-1.122000	4.409000	1.172000	0.00137
84	H190	hc	E	-1.237000	3.846000	-0.524000	0.00137
85	C62	c3	M	0.088000	5.559000	-0.218000	-0.00690
86	H192	hc	E	0.047000	5.902000	-1.261000	0.02496
87	H194	hc	E	0.141000	6.426000	0.455000	0.02496
88	C63	c3	M	1.346000	4.632000	0.001000	0.02034
89	H196	hc	E	1.335000	4.271000	1.040000	-0.01165
90	H198	hc	E	1.262000	3.771000	-0.679000	-0.01165
91	C64	c3	M	2.737000	5.347000	-0.253000	-0.08273
92	H200	hc	E	2.799000	5.712000	-1.288000	0.00153
93	H202	hc	E	2.857000	6.187000	0.446000	0.00153
94	C65	c3	M	3.852000	4.275000	0.006000	0.20816
95	H204	hc	E	3.729000	3.903000	1.033000	-0.04112
96	H206	hc	E	3.683000	3.443000	-0.695000	-0.04112
97	C66	c3	M	5.361000	4.753000	-0.157000	0.06074
98	H208	hc	E	5.569000	5.105000	-1.178000	0.00712

99	H210	hc	E	5.616000	5.557000	0.549000	0.00712
100	C67	c2	M	6.168000	3.500000	0.148000	-0.23924
101	H212	ha	E	5.600000	2.628000	0.345000	0.09796
102	C78	c2	M	7.506000	3.344000	0.203000	-0.24698
103	H214	ha	E	7.832000	2.363000	0.432000	0.15337
104	C80	c3	M	8.637000	4.363000	-0.033000	0.15864
105	H216	hc	E	8.488000	4.935000	-0.962000	0.03370
106	H218	hc	E	8.730000	5.084000	0.795000	0.03370
107	C82	c2	M	9.858000	3.427000	-0.107000	-0.23335
108	H220	ha	E	9.630000	2.393000	-0.153000	0.11422
109	C84	c2	M	11.171000	3.718000	-0.108000	-0.21491
110	H222	ha	E	11.825000	2.884000	-0.158000	0.10979
111	C86	c3	M	11.847000	5.069000	-0.047000	0.06975
112	H224	hc	E	11.582000	5.672000	-0.928000	0.01059
113	H226	hc	E	11.549000	5.618000	0.859000	0.01059
114	C87	c3	M	13.377000	4.692000	-0.038000	0.00570
115	H228	hc	E	13.567000	4.061000	0.843000	0.01094
116	H230	hc	E	13.588000	4.108000	-0.945000	0.01094
117	C88	c3	M	14.374000	5.871000	-0.000000	-0.07890
118	H232	hc	E	14.245000	6.506000	-0.888000	0.01810
119	H234	hc	E	14.230000	6.468000	0.911000	0.01810
120	C89	c3	M	15.799000	5.234000	-0.003000	0.15719
121	H236	hc	E	15.906000	4.589000	0.882000	-0.02486
122	H238	hc	E	15.917000	4.623000	-0.910000	-0.02486
123	C90	c3	M	16.907000	6.306000	0.022000	-0.22614
124	H240	hc	E	17.892000	5.808000	0.019000	0.04994
125	H242	hc	E	16.812000	6.917000	0.929000	0.04994
126	H244	hc	E	16.822000	6.947000	-0.866000	0.04994

LOOP

IMPROPER

C12 O56 C11 O10
 C60 O96 C59 O58
 C78 C66 C67 H212
 C67 C80 C78 H214
 C84 C80 C82 H220
 C82 C86 C84 H222

DONE

STOP

POPC glycerophospholipid:

.frcmod

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 #JTS Coimbra; SF Sousa; PA Fernandes; M Rangel; MJ Ramos 2012
 #POPC Glycerophospholipid

IMPROPER

c3-o -c -os	10.5	180.0	2.0	General improper torsional angle (2 general atom types)
c2-c3-c2-ha	1.1	180.0	2.0	Using default value

.prepc

#REQUIMTE, Dept Quim e Bioquim, FCUP, Univ Porto, Portugal;
 #JTS Coimbra; SF Sousa; PA Fernandes; M Rangel; MJ Ramos 2012
 #POPC Glycerophospholipid

0 0 2

This is a remark line

molecule.res

POC XYZ 0

CHANGE OMIT DU BEG

0.0000

1	DUMM	DU	M	999.000	999.0	-999.0	.00000
2	DUMM	DU	M	999.000	-999.0	999.0	.00000

3	DUMM	DU	M	-999.000	999.0	999.0	.00000
4	C1	c3	M	-13.476000	4.360000	-0.300000	-0.46111
5	H104	hx	E	-14.475000	4.222000	-0.750000	0.20512
6	H106	hx	E	-13.479000	3.966000	0.728000	0.20512
7	H108	hx	E	-12.727000	3.809000	-0.898000	0.20512
8	N2	n4	M	-13.153000	5.813000	-0.272000	0.14773
9	C54	c3	3	-14.138000	6.467000	0.527000	-0.46111
10	H190	hx	E	-13.912000	7.542000	0.563000	0.20512
11	H192	hx	E	-14.128000	6.058000	1.554000	0.20512
12	H194	hx	E	-15.124000	6.315000	0.088000	0.20512
13	C56	c3	3	-13.193000	6.338000	-1.649000	-0.46111
14	H196	hx	E	-13.029000	7.430000	-1.645000	0.20512
15	H198	hx	E	-14.162000	6.127000	-2.062000	0.20512
16	H200	hx	E	-12.432000	5.846000	-2.276000	0.20512
17	C3	c3	M	-11.848000	6.071000	0.375000	-0.07311
18	H110	hx	E	-11.643000	7.145000	0.428000	0.11661
19	H112	hx	E	-11.890000	5.656000	1.394000	0.11661
20	C4	c3	M	-10.752000	5.417000	-0.349000	0.18874
21	H114	h1	E	-10.988000	4.385000	-0.417000	0.02150
22	H116	h1	E	-10.615000	5.790000	-1.367000	0.02150
23	O5	os	M	-9.581000	5.572000	0.357000	-0.38727
24	P6	p5	M	-8.856000	4.373000	-0.115000	1.20597
25	O58	o	E	-9.256000	4.346000	-1.578000	-0.75488
26	O60	o	E	-9.840000	3.304000	0.516000	-0.75488
27	O7	os	M	-7.328000	4.355000	0.348000	-0.50163
28	C8	c3	M	-6.771000	3.141000	-0.228000	0.18984
29	H118	h1	E	-7.545000	2.383000	-0.039000	0.05361
30	H120	h1	E	-6.707000	3.290000	-1.314000	0.05361
31	C9	c3	M	-5.382000	2.451000	0.338000	0.18407
32	C10	c3	3	-5.397000	1.131000	-0.535000	-0.07471
33	O11	os	S	-4.349000	0.048000	-0.177000	-0.54965
34	C12	c	B	-2.953000	0.253000	-0.416000	0.95465
35	C13	c3	3	-1.980000	-0.869000	-0.037000	-0.21661
36	C14	c3	3	-0.514000	-0.556000	-0.449000	-0.01770
37	C15	c3	3	0.382000	-1.740000	-0.010000	0.02019
38	C16	c3	3	1.861000	-1.496000	-0.406000	-0.04046
39	C17	c3	3	2.716000	-2.703000	0.058000	-0.00434
40	C18	c3	3	4.194000	-2.502000	-0.340000	0.02315
41	C19	c3	3	5.015000	-3.720000	0.129000	0.00160
42	C20	c3	3	6.490000	-3.549000	-0.281000	0.00006
43	C21	c3	3	7.293000	-4.778000	0.181000	-0.00945
44	C22	c3	3	8.763000	-4.626000	-0.244000	0.01332
45	C23	c3	3	9.553000	-5.865000	0.208000	0.02172
46	C24	c3	3	11.018000	-5.726000	-0.229000	-0.04125
47	C25	c3	3	11.799000	-6.970000	0.215000	-0.00754
48	C26	c3	3	13.262000	-6.836000	-0.230000	0.13351
49	C27	c3	3	14.042000	-8.085000	0.211000	-0.23249
50	H184	hc	E	15.091000	-7.994000	-0.106000	0.04951
51	H186	hc	E	13.595000	-8.977000	-0.252000	0.04951
52	H188	hc	E	13.996000	-8.178000	1.305000	0.04951
53	H180	hc	E	13.306000	-6.744000	-1.325000	-0.01909
54	H182	hc	E	13.706000	-5.943000	0.233000	-0.01909
55	H176	hc	E	11.754000	-7.064000	1.309000	0.00560
56	H178	hc	E	11.357000	-7.864000	-0.249000	0.00560
57	H172	hc	E	11.067000	-5.635000	-1.323000	0.00468
58	H174	hc	E	11.458000	-4.831000	0.234000	0.00468
59	H168	hc	E	9.501000	-5.957000	1.302000	-0.00535
60	H170	hc	E	9.119000	-6.762000	-0.257000	-0.00535
61	H164	hc	E	8.820000	-4.537000	-1.337000	-0.00113
62	H166	hc	E	9.191000	-3.726000	0.221000	-0.00113
63	H160	hc	E	7.232000	-4.870000	1.275000	0.00046
64	H162	hc	E	6.874000	-5.681000	-0.287000	0.00046
65	H156	hc	E	6.557000	-3.460000	-1.374000	-0.00076
66	H158	hc	E	6.902000	-2.643000	0.188000	-0.00076
67	H152	hc	E	4.945000	-3.814000	1.221000	-0.00129
68	H154	hc	E	4.615000	-4.630000	-0.343000	-0.00129
69	H148	hc	E	4.268000	-2.409000	-1.432000	-0.00347
70	H150	hc	E	4.585000	-1.590000	0.134000	-0.00347
71	H144	hc	E	2.643000	-2.805000	1.150000	-0.00281
72	H146	hc	E	2.339000	-3.619000	-0.421000	-0.00281
73	H140	hc	E	1.935000	-1.391000	-1.498000	0.01471
74	H142	hc	E	2.229000	-0.579000	0.077000	0.01471
75	H136	hc	E	0.312000	-1.857000	1.080000	0.00673
76	H138	hc	E	0.027000	-2.659000	-0.498000	0.00673
77	H132	hc	E	-0.458000	-0.428000	-1.538000	0.02098
78	H134	hc	E	-0.171000	0.362000	0.046000	0.02098
79	H128	hc	E	-2.043000	-1.028000	1.050000	0.06859

80	H130	hc	E	-2.323000	-1.802000	-0.507000	0.06859
81	O62	o	E	-2.512000	1.280000	-0.943000	-0.65930
82	H124	h1	E	-6.386000	0.677000	-0.379000	0.13609
83	H126	h1	E	-5.305000	1.401000	-1.592000	0.13609
84	H122	h1	E	-5.543000	2.189000	1.382000	0.12017
85	O64	os	M	-3.946000	3.113000	0.201000	-0.55652
86	C65	c	M	-3.528000	4.043000	1.232000	0.87770
87	O102	o	E	-4.294000	4.252000	2.172000	-0.62016
88	C66	c3	M	-2.211000	4.755000	1.213000	-0.38882
89	H202	hc	E	-2.290000	5.636000	0.552000	0.10301
90	H204	hc	E	-1.986000	5.107000	2.233000	0.10301
91	C67	c3	M	-1.080000	3.854000	0.673000	0.06434
92	H206	hc	E	-0.996000	2.960000	1.305000	0.05396
93	H208	hc	E	-1.302000	3.553000	-0.361000	0.05396
94	C68	c3	M	0.253000	4.642000	0.728000	-0.06877
95	H210	hc	E	0.175000	5.545000	0.108000	0.03069
96	H212	hc	E	0.444000	4.928000	1.769000	0.03069
97	C69	c3	M	1.418000	3.760000	0.227000	-0.02380
98	H214	hc	E	1.472000	2.858000	0.849000	0.01057
99	H216	hc	E	1.240000	3.473000	-0.820000	0.01057
100	C70	c3	M	2.772000	4.518000	0.334000	-0.02493
101	H218	hc	E	2.752000	5.423000	-0.290000	-0.00215
102	H220	hc	E	2.955000	4.795000	1.382000	-0.00215
103	C71	c3	M	3.888000	3.567000	-0.145000	0.04718
104	H222	hc	E	3.874000	2.666000	0.483000	-0.00040
105	H224	hc	E	3.694000	3.284000	-1.190000	-0.00040
106	C72	c3	M	5.296000	4.211000	-0.050000	0.10680
107	H226	hc	E	5.367000	5.113000	-0.675000	0.00774
108	H228	hc	E	5.530000	4.497000	0.987000	0.00774
109	C73	c2	M	6.290000	3.176000	-0.523000	-0.27640
110	H230	ha	E	5.915000	2.237000	-0.839000	0.13694
111	C84	c2	M	7.614000	3.369000	-0.565000	-0.28428
112	H232	ha	E	8.221000	2.571000	-0.913000	0.13367
113	C86	c3	M	8.302000	4.647000	-0.151000	0.15613
114	H234	hc	E	7.984000	5.467000	-0.812000	-0.00435
115	H236	hc	E	8.025000	4.912000	0.880000	-0.00435
116	C87	c3	M	9.822000	4.392000	-0.283000	0.01891
117	H238	hc	E	10.100000	3.561000	0.381000	0.00081
118	H240	hc	E	10.042000	4.113000	-1.323000	0.00081
119	C88	c3	M	10.671000	5.621000	0.080000	-0.02997
120	H242	hc	E	10.426000	6.457000	-0.592000	-0.00088
121	H244	hc	E	10.491000	5.917000	1.123000	-0.00088
122	C89	c3	M	12.146000	5.210000	-0.108000	0.05096
123	H246	hc	E	12.372000	4.368000	0.560000	-0.01300
124	H248	hc	E	12.299000	4.897000	-1.151000	-0.01300
125	C90	c3	M	13.103000	6.370000	0.203000	-0.03022
126	H250	hc	E	12.897000	7.213000	-0.472000	0.00398
127	H252	hc	E	12.977000	6.693000	1.246000	0.00398
128	C91	c3	M	14.541000	5.868000	-0.018000	-0.02140
129	H254	hc	E	14.739000	5.023000	0.656000	0.00894
130	H256	hc	E	14.653000	5.537000	-1.061000	0.00894
131	C92	c3	M	15.545000	6.992000	0.265000	0.13124
132	H258	hc	E	15.354000	7.835000	-0.413000	-0.01881
133	H260	hc	E	15.442000	7.325000	1.307000	-0.01881
134	C100	c3	M	16.969000	6.456000	0.032000	-0.23359
135	H262	hc	E	17.699000	7.254000	0.230000	0.05092
136	H264	hc	E	17.067000	6.120000	-1.011000	0.05092
137	H266	hc	E	17.157000	5.610000	0.709000	0.05092

LOOP

IMPROPER

C13 O62 C12 O11
 C66 O102 C65 O64
 C84 C72 C73 H230
 C73 C86 C84 H232

DONE

STOP

POPE glycerophospholipid:

.frcmod

#REQUIMTE, Dept Quim e Bioquim, FCUP, Univ Porto, Portugal;
#JTS Coimbra; SF Sousa; PA Fernandes; M Rangel; MJ Ramos 2012
#POPE Glycerophospholipid

IMPROPER

c3-o -c -os	10.5	180.0	2.0	General improper torsional angle (2 general atom types)
c2-c3-c2-ha	1.1	180.0	2.0	Using default value

.prepc

#REQUIMTE, Dept Quim e Bioquim, FCUP, Univ Porto, Portugal;
#JTS Coimbra; SF Sousa; PA Fernandes; M Rangel; MJ Ramos 2012
#POPE Glycerophospholipid

0 0 2

This is a remark line

molecule.res

POE XYZ 0

CHANGE OMIT DU BEG

0.0000

1	DUMM	DU	M	999.000	999.0	-999.0	.00000
2	DUMM	DU	M	999.000	-999.0	999.0	.00000
3	DUMM	DU	M	-999.000	999.0	999.0	.00000
4	N1	n4	M	-12.466000	5.436000	0.187000	-0.58494
5	H98	hn	E	-13.256000	6.074000	0.186000	0.36159
6	H100	hn	E	-12.422000	4.942000	1.089000	0.36159
7	H102	hn	E	-12.578000	4.746000	-0.569000	0.36159
8	C2	c3	M	-11.202000	6.152000	-0.018000	0.04362
9	H104	hx	E	-11.184000	6.654000	-0.991000	0.08537
10	H106	hx	E	-11.012000	6.866000	0.790000	0.08537
11	C3	c3	M	-10.215000	5.092000	0.011000	0.08289
12	H108	h1	E	-10.298000	4.595000	0.974000	0.07981
13	H110	h1	E	-10.481000	4.393000	-0.772000	0.07981
14	O4	os	M	-8.868000	5.532000	-0.177000	-0.48150
15	P5	p5	M	-8.149000	4.224000	-0.053000	1.31887
16	O52	o	E	-8.675000	3.723000	1.271000	-0.75348
17	O54	o	E	-8.940000	3.334000	-1.071000	-0.75348
18	O6	os	M	-6.567000	4.346000	-0.244000	-0.54702
19	C7	c3	M	-6.099000	2.985000	-0.040000	0.16960
20	H112	h1	E	-6.281000	2.728000	1.013000	0.03953
21	H114	h1	E	-6.791000	2.384000	-0.655000	0.03953
22	C8	c3	M	-4.575000	2.504000	-0.500000	0.30445
23	C9	c3	3	-4.634000	0.932000	-0.252000	-0.08106
24	O10	os	S	-3.351000	0.278000	-0.744000	-0.50543
25	C11	c	B	-2.306000	0.367000	0.207000	0.97471
26	C12	c3	3	-0.847000	0.145000	-0.162000	-0.58244
27	C13	c3	3	-0.322000	-1.292000	0.085000	0.21748
28	C14	c3	3	1.229000	-1.241000	-0.192000	0.01398
29	C15	c3	3	1.961000	-2.614000	0.012000	-0.08463
30	C16	c3	3	3.515000	-2.407000	-0.179000	0.00767
31	C17	c3	3	4.304000	-3.753000	-0.007000	0.02253
32	C18	c3	3	5.854000	-3.509000	-0.134000	-0.01632
33	C19	c3	3	6.636000	-4.861000	0.004000	-0.00170
34	C20	c3	3	8.184000	-4.631000	-0.082000	-0.01000
35	C21	c3	3	8.933000	-5.999000	0.020000	0.00608
36	C22	c3	3	10.478000	-5.798000	-0.042000	0.01882
37	C23	c3	3	11.188000	-7.179000	0.031000	-0.04294
38	C24	c3	3	12.726000	-7.003000	-0.018000	-0.01177
39	C25	c3	3	13.403000	-8.392000	0.038000	0.12294
40	C26	c3	3	14.937000	-8.231000	-0.003000	-0.24201
41	H178	hc	E	15.411000	-9.224000	0.034000	0.05317
42	H180	hc	E	15.267000	-7.637000	0.862000	0.05317
43	H182	hc	E	15.229000	-7.720000	-0.932000	0.05317
44	H174	hc	E	13.117000	-8.903000	0.968000	-0.01475
45	H176	hc	E	13.077000	-8.992000	-0.825000	-0.01475
46	H170	hc	E	13.012000	-6.497000	-0.950000	0.00843
47	H172	hc	E	13.055000	-6.401000	0.842000	0.00843
48	H166	hc	E	10.913000	-7.685000	0.967000	0.00577
49	H168	hc	E	10.868000	-7.793000	-0.824000	0.00577

50	H162	hc	E	10.749000	-5.301000	-0.983000	-0.00384
51	H164	hc	E	10.799000	-5.175000	0.807000	-0.00384
52	H158	hc	E	8.674000	-6.490000	0.968000	0.00149
53	H160	hc	E	8.620000	-6.638000	-0.819000	0.00149
54	H154	hc	E	8.436000	-4.153000	-1.038000	0.00262
55	H156	hc	E	8.499000	-3.979000	0.748000	0.00262
56	H150	hc	E	6.399000	-5.326000	0.970000	-0.00012
57	H152	hc	E	6.326000	-5.532000	-0.811000	-0.00012
58	H146	hc	E	6.080000	-3.061000	-1.110000	0.00391
59	H148	hc	E	6.172000	-2.822000	0.666000	0.00391
60	H142	hc	E	4.093000	-4.178000	0.983000	-0.00067
61	H144	hc	E	3.978000	-4.458000	-0.785000	-0.00067
62	H138	hc	E	3.714000	-2.002000	-1.181000	-0.00262
63	H140	hc	E	3.864000	-1.689000	0.579000	-0.00262
64	H134	hc	E	1.778000	-2.983000	1.031000	0.01786
65	H136	hc	E	1.582000	-3.346000	-0.719000	0.01786
66	H130	hc	E	1.405000	-0.895000	-1.220000	0.00990
67	H132	hc	E	1.658000	-0.513000	0.510000	0.00990
68	H126	hc	E	-0.491000	-1.574000	1.132000	-0.01975
69	H128	hc	E	-0.833000	-2.002000	-0.581000	-0.01975
70	H122	hc	E	-0.685000	0.382000	-1.222000	0.14316
71	H124	hc	E	-0.251000	0.799000	0.489000	0.14316
72	O56	o	E	-2.530000	0.730000	1.365000	-0.62460
73	H118	h1	E	-4.796000	0.700000	0.806000	0.14919
74	H120	h1	E	-5.491000	0.556000	-0.838000	0.14919
75	H116	h1	E	-4.492000	2.665000	-1.573000	0.12910
76	O58	os	M	-3.206000	3.030000	0.158000	-0.53903
77	C59	c	M	-2.609000	4.123000	-0.558000	0.84430
78	O96	o	E	-3.236000	4.535000	-1.533000	-0.61932
79	C60	c3	M	-1.280000	4.788000	-0.211000	-0.39121
80	H184	hc	E	-1.103000	5.596000	-0.932000	0.09857
81	H186	hc	E	-1.321000	5.186000	0.812000	0.09857
82	C61	c3	M	-0.091000	3.753000	-0.266000	0.16705
83	H188	hc	E	-0.257000	2.976000	0.494000	-0.01499
84	H190	hc	E	-0.071000	3.291000	-1.262000	-0.01499
85	C62	c3	M	1.304000	4.466000	-0.024000	0.00871
86	H192	hc	E	1.439000	5.219000	-0.813000	0.00657
87	H194	hc	E	1.301000	4.963000	0.956000	0.00657
88	C63	c3	M	2.511000	3.429000	-0.089000	-0.02543
89	H196	hc	E	2.387000	2.688000	0.716000	0.01308
90	H198	hc	E	2.488000	2.915000	-1.061000	0.01308
91	C64	c3	M	3.934000	4.143000	0.056000	-0.05834
92	H200	hc	E	4.058000	4.859000	-0.770000	0.00412
93	H202	hc	E	3.988000	4.678000	1.014000	0.00412
94	C65	c3	M	5.095000	3.068000	-0.010000	0.03939
95	H204	hc	E	4.957000	2.364000	0.825000	0.00046
96	H206	hc	E	5.012000	2.519000	-0.959000	0.00046
97	C66	c3	M	6.569000	3.682000	0.081000	0.12888
98	H208	hc	E	6.766000	4.375000	-0.751000	0.00369
99	H210	hc	E	6.704000	4.236000	1.021000	0.00369
100	C67	c2	M	7.568000	2.512000	0.034000	-0.26100
101	H212	ha	E	7.156000	1.535000	0.043000	0.12651
102	C78	c2	M	8.917000	2.601000	-0.016000	-0.27335
103	H214	ha	E	9.454000	1.686000	-0.041000	0.12864
104	C80	c3	M	9.756000	3.887000	-0.042000	0.14160
105	H216	hc	E	9.494000	4.482000	-0.929000	-0.00152
106	H218	hc	E	9.541000	4.494000	0.850000	-0.00152
107	C81	c3	M	11.281000	3.441000	-0.082000	0.00881
108	H220	hc	E	11.488000	2.836000	0.813000	0.00447
109	H222	hc	E	11.437000	2.821000	-0.977000	0.00447
110	C82	c3	M	12.311000	4.623000	-0.123000	-0.04521
111	H224	hc	E	12.144000	5.231000	-1.023000	0.00399
112	H226	hc	E	12.197000	5.250000	0.773000	0.00399
113	C83	c3	M	13.764000	4.014000	-0.159000	0.05799
114	H228	hc	E	13.916000	3.400000	0.740000	-0.01146
115	H230	hc	E	13.862000	3.379000	-1.052000	-0.01146
116	C84	c3	M	14.867000	5.118000	-0.206000	-0.04353
117	H232	hc	E	14.736000	5.733000	-1.108000	0.00790
118	H234	hc	E	14.790000	5.755000	0.686000	0.00790
119	C85	c3	M	16.276000	4.449000	-0.240000	-0.02415
120	H236	hc	E	16.410000	3.834000	0.662000	0.01099
121	H238	hc	E	16.356000	3.811000	-1.132000	0.01099
122	C86	c3	M	17.384000	5.530000	-0.288000	0.12527
123	H240	hc	E	17.259000	6.145000	-1.190000	-0.01641
124	H242	hc	E	17.313000	6.169000	0.604000	-0.01641
125	C87	c3	M	18.776000	4.854000	-0.321000	-0.23337
126	H244	hc	E	19.560000	5.628000	-0.355000	0.05118

127	H246	hc	E	18.855000	4.216000	-1.213000	0.05118
128	H248	hc	E	18.909000	4.240000	0.582000	0.05118

LOOP

IMPROPER

C12 O56 C11 O10
C60 O96 C59 O58
C78 C66 C67 H212
C67 C80 C78 H214

DONE

STOP

DOPC glycerophospholipid:

.frcmod

#REQUIMTE, Dept Quim e Bioquim, FCUP, Univ Porto, Portugal;
#JTS Coimbra; SF Sousa; PA Fernandes; M Rangel; MJ Ramos 2012
#DOPC Glycerophospholipid

IMPROPER

c3-o -c -os	10.5	180.0	2.0	General improper torsional angle (2 general atom types)
c2-c3-c2-ha	1.1	180.0	2.0	Using default value

.prepc

#REQUIMTE, Dept Quim e Bioquim, FCUP, Univ Porto, Portugal;
#JTS Coimbra; SF Sousa; PA Fernandes; M Rangel; MJ Ramos 2012
#DOPC Glycerophospholipid

0 0 2

This is a remark line

molecule.res

DOC XYZ 0

CHANGE OMIT DU BEG

0.0000
1 DUMM DU M 999.000 999.0 -999.0 .00000
2 DUMM DU M 999.000 -999.0 999.0 .00000
3 DUMM DU M -999.000 999.0 999.0 .00000
4 C1 c3 M -14.217000 6.726000 -0.403000 -0.32361
5 H108 hx E -14.698000 7.710000 -0.296000 0.16487
6 H110 hx E -14.659000 6.025000 0.323000 0.16487
7 H112 hx E -14.386000 6.347000 -1.424000 0.16487
8 N2 n4 M -12.766000 6.852000 -0.154000 0.04830
9 C40 c3 3 -12.566000 7.407000 1.209000 -0.32361
10 H162 hx E -11.491000 7.518000 1.415000 0.16487
11 H164 hx E -13.023000 6.743000 1.961000 0.16487
12 H166 hx E -13.046000 8.386000 1.264000 0.16487
13 C42 c3 3 -12.224000 7.847000 -1.123000 -0.32361
14 H168 hx E -12.416000 7.516000 -2.162000 0.16487
15 H170 hx E -11.140000 7.966000 -0.966000 0.16487
16 H172 hx E -12.719000 8.805000 -0.963000 0.16487
17 C3 c3 M -12.134000 5.413000 -0.321000 -0.05605
18 H114 hx E -12.630000 4.743000 0.394000 0.10409
19 H116 hx E -12.351000 5.067000 -1.340000 0.10409
20 C4 c3 M -10.600000 5.238000 -0.099000 0.23101
21 H118 h1 E -10.028000 5.852000 -0.804000 0.04274
22 H120 h1 E -10.321000 5.514000 0.927000 0.04274
23 O5 os M -10.253000 3.848000 -0.311000 -0.48392
24 P6 p5 M -8.704000 3.766000 -0.030000 1.19458
25 O44 o E -8.270000 4.801000 -0.814000 -0.73865
26 O46 o E -8.609000 4.296000 1.357000 -0.73865
27 O7 os M -8.039000 2.474000 -0.263000 -0.50922
28 C8 c3 M -6.712000 2.682000 0.142000 0.16309
29 H122 h1 E -6.357000 3.595000 -0.365000 0.06668
30 H124 h1 E -6.698000 2.857000 1.227000 0.06668

31	C9	c3	M	-5.790000	1.480000	-0.264000	0.20153
32	O50	os	S	-6.098000	0.145000	0.328000	-0.51406
33	C51	c	B	-7.353000	-0.370000	-0.109000	0.85385
34	C52	c3	3	-7.500000	-1.887000	0.112000	-0.30564
35	C56	c3	3	-6.040000	-2.408000	0.026000	0.04435
36	C57	c3	3	-5.880000	-3.942000	0.171000	-0.19146
37	C58	c3	3	-4.349000	-4.215000	0.061000	0.08811
38	C59	c3	3	-3.920000	-5.716000	0.145000	-0.15272
39	C66	c3	3	-2.370000	-5.682000	0.032000	0.10877
40	C67	c3	3	-1.626000	-7.060000	0.076000	0.01048
41	C68	c2	B	-0.159000	-6.678000	-0.032000	-0.32282
42	C74	c2	B	0.894000	-7.511000	-0.071000	-0.16072
43	C76	c3	3	0.859000	-9.025000	-0.012000	0.04410
44	C80	c3	3	2.369000	-9.442000	-0.026000	0.01360
45	C81	c3	3	2.651000	-10.963000	0.017000	-0.01352
46	C82	c3	3	4.204000	-11.105000	-0.011000	0.05808
47	C83	c3	3	4.684000	-12.573000	0.022000	-0.03967
48	C84	c3	3	6.235000	-12.566000	-0.005000	-0.02189
49	C85	c3	3	6.789000	-14.003000	0.017000	0.12226
50	C86	c3	3	8.332000	-13.951000	-0.001000	-0.23705
51	H240	hc	E	8.735000	-14.975000	0.009000	0.05259
52	H242	hc	E	8.688000	-13.410000	0.890000	0.05259
53	H244	hc	E	8.674000	-13.430000	-0.906000	0.05259
54	H236	hc	E	6.448000	-14.521000	0.920000	-0.01484
55	H238	hc	E	6.434000	-14.542000	-0.875000	-0.01484
56	H232	hc	E	6.587000	-12.054000	-0.905000	0.01035
57	H234	hc	E	6.603000	-12.031000	0.889000	0.01035
58	H228	hc	E	4.324000	-13.076000	0.923000	0.00623
59	H230	hc	E	4.308000	-13.101000	-0.874000	0.00623
60	H224	hc	E	4.593000	-10.623000	-0.911000	-0.01417
61	H226	hc	E	4.611000	-10.592000	0.880000	-0.01417
62	H220	hc	E	2.235000	-11.413000	0.923000	-0.00400
63	H222	hc	E	2.217000	-11.449000	-0.876000	-0.00400
64	H216	hc	E	2.830000	-9.035000	-0.932000	0.00409
65	H218	hc	E	2.851000	-8.989000	0.857000	0.00409
66	H208	hc	E	0.341000	-9.369000	0.892000	0.02627
67	H210	hc	E	0.328000	-9.424000	-0.892000	0.02627
68	H206	ha	E	1.851000	-7.062000	-0.145000	0.11629
69	H202	ha	E	0.056000	-5.645000	-0.083000	0.14333
70	H198	hc	E	-1.812000	-7.591000	1.023000	0.03223
71	H200	hc	E	-1.921000	-7.716000	-0.756000	0.03223
72	H194	hc	E	-2.114000	-5.195000	-0.921000	0.00577
73	H196	hc	E	-1.991000	-5.069000	0.858000	0.00577
74	H190	hc	E	-4.222000	-6.152000	1.111000	0.02997
75	H192	hc	E	-4.360000	-6.292000	-0.680000	0.02997
76	H186	hc	E	-4.003000	-3.823000	-0.907000	-0.00094
77	H188	hc	E	-3.846000	-3.668000	0.869000	-0.00094
78	H182	hc	E	-6.259000	-4.273000	1.146000	0.06013
79	H184	hc	E	-6.422000	-4.452000	-0.635000	0.06013
80	H178	hc	E	-5.635000	-2.111000	-0.952000	0.04619
81	H180	hc	E	-5.454000	-1.916000	0.816000	0.04619
82	H174	hc	E	-7.894000	-2.100000	1.117000	0.11044
83	H176	hc	E	-8.155000	-2.330000	-0.652000	0.11044
84	O64	o	E	-8.069000	0.200000	-0.933000	-0.67377
85	H126	h1	E	-5.826000	1.377000	-1.356000	0.09960
86	C10	c3	M	-4.342000	1.781000	0.180000	0.12566
87	H128	h1	E	-3.989000	2.707000	-0.299000	0.04783
88	H130	h1	E	-4.334000	1.911000	1.266000	0.04783
89	O11	os	M	-3.486000	0.564000	-0.197000	-0.52953
90	C12	c	M	-2.063000	0.609000	0.164000	0.86965
91	O48	o	E	-1.623000	1.617000	0.718000	-0.55770
92	C13	c3	M	-1.172000	-0.696000	-0.015000	-0.27008
93	H132	hc	E	-1.455000	-1.377000	0.802000	0.08864
94	H134	hc	E	-1.467000	-1.194000	-0.951000	0.08864
95	C14	c3	M	0.420000	-0.514000	0.049000	-0.04978
96	H136	hc	E	0.750000	0.136000	-0.776000	0.01863
97	H138	hc	E	0.695000	-0.053000	1.009000	0.01863
98	C15	c3	M	1.148000	-1.954000	-0.063000	0.08637
99	H140	hc	E	0.798000	-2.577000	0.771000	-0.00811
100	H142	hc	E	0.856000	-2.424000	-1.012000	-0.00811
101	C16	c3	M	2.754000	-1.854000	0.001000	-0.05109
102	H144	hc	E	3.101000	-1.235000	-0.840000	0.02054
103	H146	hc	E	3.038000	-1.368000	0.946000	0.02054
104	C17	c3	M	3.498000	-3.293000	-0.072000	-0.07415
105	H148	hc	E	3.178000	-3.913000	0.778000	0.00881
106	H150	hc	E	3.237000	-3.798000	-1.013000	0.00881
107	C18	c3	M	5.082000	-3.090000	-0.007000	-0.00715

108	H152	hc	E	5.376000	-2.460000	-0.859000	0.01695
109	H154	hc	E	5.321000	-2.562000	0.926000	0.01695
110	C19	c3	M	5.974000	-4.436000	-0.054000	0.10951
111	H156	hc	E	5.749000	-5.098000	0.796000	0.01887
112	H158	hc	E	5.796000	-5.001000	-0.981000	0.01887
113	C20	c2	M	7.455000	-3.991000	0.005000	-0.27178
114	H160	ha	E	7.626000	-2.946000	0.030000	0.12488
115	C72	c2	M	8.560000	-4.776000	0.027000	-0.24250
116	H204	ha	E	9.492000	-4.269000	0.067000	0.11262
117	C78	c3	M	8.631000	-6.314000	0.002000	0.15274
118	H212	hc	E	8.121000	-6.725000	0.885000	-0.00877
119	H214	hc	E	8.127000	-6.701000	-0.896000	-0.00877
120	C94	c3	M	10.183000	-6.688000	0.007000	-0.01176
121	H246	hc	E	10.648000	-6.234000	-0.880000	0.00976
122	H248	hc	E	10.637000	-6.254000	0.909000	0.00976
123	C95	c3	M	10.515000	-8.225000	-0.006000	-0.04366
124	H250	hc	E	10.092000	-8.707000	0.887000	0.00425
125	H252	hc	E	10.101000	-8.692000	-0.911000	0.00425
126	C96	c3	M	12.087000	-8.379000	0.001000	0.05500
127	H254	hc	E	12.496000	-7.880000	-0.890000	-0.01314
128	H256	hc	E	12.487000	-7.892000	0.902000	-0.01314
129	C97	c3	M	12.554000	-9.871000	-0.006000	-0.01878
130	H258	hc	E	12.171000	-10.384000	0.887000	0.00139
131	H260	hc	E	12.178000	-10.374000	-0.908000	0.00139
132	C98	c3	M	14.115000	-9.920000	-0.000000	-0.03267
133	H262	hc	E	14.499000	-9.407000	-0.894000	0.01081
134	H264	hc	E	14.492000	-9.415000	0.900000	0.01081
135	C99	c3	M	14.618000	-11.386000	-0.005000	0.13725
136	H266	hc	E	14.246000	-11.905000	0.890000	-0.01887
137	H268	hc	E	14.252000	-11.898000	-0.905000	-0.01887
138	C100	c3	M	16.165000	-11.407000	0.000000	-0.24446
139	H270	hc	E	16.520000	-12.450000	-0.003000	0.05384
140	H272	hc	E	16.538000	-10.898000	0.901000	0.05384
141	H274	hc	E	16.544000	-10.891000	-0.895000	0.05384

LOOP

IMPROPER

C52 O64 C51 O50
C74 C67 C68 H202
C68 C76 C74 H206
C13 O48 C12 O11
C72 C19 C20 H160
C20 C78 C72 H204

DONE

STOP

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