SUPPORTING INFORMATION

CHARMM Drude Polarizable Force Field for Aldopentofuranoses and Methyl-aldopentofuranosides

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Table S1: Upper and lower bounds used for the optimization of the electrostatic parameters in the aldopentoses.

Atoms	Charges		Alpha		Thole	
	Upper	Lower	Upper	Lower	Upper	Lower
C1	0.173	0.073	-1.0	-2.10	2.4	0.3
O1	-0.15	-0.25	-0.5	-1.3	2.4	0.3
HO1	0.37	0.27	--	--	--	--
C4	0.142	0.042	-1.0	-2.10	2.4	0.3
O4	-0.087	-0.187	-0.5	-1.3	2.4	0.3
C5	-0.01	-0.11	-1.0	-2.10	2.4	0.3
O5	-0.18	-0.28	-0.5	-1.3	2.4	0.3
HO5	0.41	0.31	--	--	--	--
C2/C3	0.06	-0.04	-1.0/-1.0	-2.10/-2.10	2.4/2.4	0.3/0.3
O2/O3	-0.15	-0.25	-0.5/-0.5	-1.3/-1.3	2.4/2.4	0.3/0.3
HO2/HO3	0.37	0.27	--	--	--	--

Table S2. QM, Drude (Globalfit parameters) and Additive ARIB–Water Minimum Interaction Energies (kcal/mol).

Arib	Type	E_{QM}	E_{MM} (Drude)	ΔE (Drude MM-QM)	E_{MM} (Add)	ΔE (Add MM-QM)
HO1	D	-6.29	-5.14	1.15	-6.93	-0.64
HO2	D	-0.38	-0.37	0.01	0.81	1.19
HO5	D	-5.96	-5.69	0.27	-7.37	-1.41
H5	D	-1.53	-0.81	0.72	-1.07	0.46
H5	D	-1.32	-1.22	0.10	-1.39	0.08
O4	LP	-5.60	-5.66	-0.06	-5.14	0.46
O4	BIS	-4.65	-4.14	0.51	-3.81	0.84
O1	LP	-2.30	-3.09	-0.79	-3.54	-1.25
O2	LP	-4.88	-6.24	-1.36	-6.41	-1.54
O2	BIS	-4.34	-6.23	-1.89	-5.99	-1.65
O3	BIS	-5.96	-6.07	-0.11	-6.81	-0.85
O5	LP	-4.86	-5.11	-0.25	-5.55	-0.69
O5	BIS	-4.81	-5.14	-0.33	-5.94	-1.13
Average difference			-0.16		-0.48	

D represents the donor sites, BIS and LP represents Acceptor sites

Table S3. QM, Drude (Globalfit parameters) and Additive ARIB–Water Minimum Distances (Å).

Arib	Type	R_{QM}	R_{MM} (Drude)	ΔR (Drude MM-QM)	R_{MM} (Add)	ΔR (Add MM-QM)
HO1	D	1.85	1.87	0.02	1.82	-0.03
HO2	D	3.62	2.70	-0.92	4.50	0.88
HO5	D	1.89	1.88	-0.01	1.82	-0.07
H5	D	2.41	2.79	0.38	2.84	0.33
H5	D	2.44	2.72	0.28	2.68	0.24
O4	LP	1.89	1.79	-0.10	1.73	-0.16
O4	BIS	1.95	1.88	-0.07	1.77	-0.18
O1	LP	3.93	4.02	-0.09	4.11	0.08
O2	LP	1.96	1.79	-0.17	1.88	-0.08
O2	BIS	1.99	1.76	-0.23	1.87	-0.12
O3	BIS	1.90	1.81	-0.09	1.88	-0.02
O5	LP	1.96	1.83	-0.13	1.88	-0.08
O5	BIS	1.97	1.86	-0.11	1.87	-0.10
Average difference			-0.09		0.05	

D represents the donor sites, BIS and LP represents Acceptor sites

Table S4. QM, Drude (Globalfit parameters) and Additive BRIB–Water Minimum Interaction Energies (kcal/mol).

Brib	Type	E_{QM}	E_{MM} (Drude)	ΔE (Drude MM-QM)	E_{MM} (Add)	ΔE (Add MM-QM)
HO1	D	-5.26	-4.78	0.48	-6.66	-1.40
HO3	D	-0.02	-0.44	-0.42	0.07	0.09
HO5	D	-6.68	-6.00	0.68	-8.28	-1.60
H5	D	-1.74	-1.11	0.63	-1.33	0.41
H5	D	-1.97	-1.61	0.36	-1.99	-0.02
O4	LP	-5.39	-6.10	-0.71	-4.82	0.57
O4	BIS	-5.35	-4.82	0.53	-5.05	0.30
O1	LP	-4.17	-4.38	-0.21	-4.23	-0.07
O1	BIS	-4.58	-5.09	-0.51	-4.96	-0.38
O2	LP	-4.89	-5.66	-0.77	-5.27	-0.38
O2	BIS	-5.17	-6.06	-0.89	-6.04	-0.87
O3	BIS	-4.31	-4.97	-0.66	-4.68	-0.37
O5	LP	-4.15	-4.30	-0.15	-4.84	-0.69
O5	BIS	-3.79	-4.44	-0.65	-4.86	-1.07
Average difference			-0.16		-0.39	

D represents the donor sites, BIS and LP represents Acceptor sites

Table S5. QM, Drude (Globalfit parameters) and Additive BRIB–Water Minimum Distances (Å).

Brib	Type	R_{QM}	R_{MM} (Drude)	ΔR (Drude MM-QM)	R_{MM} (Add)	ΔR (Add MM-QM)
HO1	D	1.88	1.87	0.01	1.82	-0.06
HO2	D	4.35	4.49	0.14	4.49	0.14
HO5	D	1.87	1.87	0.00	1.82	-0.05
H5	D	2.29	2.71	0.42	2.67	0.38
H5	D	2.37	2.68	0.31	2.64	0.27
O4	LP	1.90	1.82	0.08	1.78	-0.12
O4	BIS	1.93	1.84	0.09	1.74	-0.19
O1	LP	1.98	1.82	-0.16	1.91	-0.07
O1	BIS	1.95	1.82	-0.13	1.89	-0.06
O2	LP	1.95	1.78	-0.17	1.89	-0.06
O2	BIS	1.94	1.79	-0.15	1.87	-0.07
O3	BIS	1.97	1.80	-0.17	1.90	-0.07
O5	LP	1.98	1.86	-0.12	1.90	-0.08
O5	BIS	1.96	1.83	-0.13	1.86	-0.10
Average difference			0.00		-0.01	

D represents the donor sites, BIS and LP represents Acceptor sites

Table S6: Furanose conformations used to fit QM energies at the RIMP2/cc-pVQZ//MP2/6-31G(d) level for different dihedral types. The subscripts R, E and H indicate ring, exocyclic and hydroxyl atoms, respectively.

Compounds	No. of conformations	Type of dihedrals
aarb	263	$C_{R/E}$-C_R-C_R-O_H, C_R-C_R-C_R-O_R C_R-C_R-O_H-H, C_R-C_E-O_H-H C_R-O_R-C_R-$C_{R/E}$, C_R-O_R-C_R-O_H O_R-C_R-C_R-O_H, C_R-C_R-C_R-C_R O_H-C_R-C_R-O_H, O_R-C_R-O_H-H, C_R-C_R-C_E-O_H
barb	279	
arib	276	
brib	278	

Table S6b. List of specific targeted dihedrals for the aldopentofuranoses

Type of dihedral	Specific dihedral
C_R-C_R-C_R-C_R	C1C2C3C4
C_R-C_R-C_R-O_R	C2C3C4O4, C3C2C1O4,
$C_{R/E}$-C_R-C_R-O_H	C3C2C1O1, C4C3C2O2, C5C4C3O3, C1C2C3O3
C_R-C_R-O_H-H	C1C2O2HO2, C2C3O3HO3, C3C2O2HO2, C4C3O3HO3, C2C1O1HO1
C_R-C_E-O_H-H	C4C5O5HO5
C_R-O_R-C_R-$C_{R/E}$	C1O4C4C3, C4O4C1C2, C4O4C1O1, C1O4C4C5
C_R-O_R-C_R-O_H	C4O4C1O1
O_R-C_R-C_R-O_H	O2C2C1O4, O3C3C4O4
O_H-C_R-C_R-O_H	O2C2C3O3, O1C1C2O2
O_R-C_R-O_H-H	O4C1O1HO1
C_R-C_R-C_E-O_H	C3C4C5O5

Figure S1. Convergence of the RMSD between MM and QM total dipole moments for methyl-furanosides using the MCSA approach.

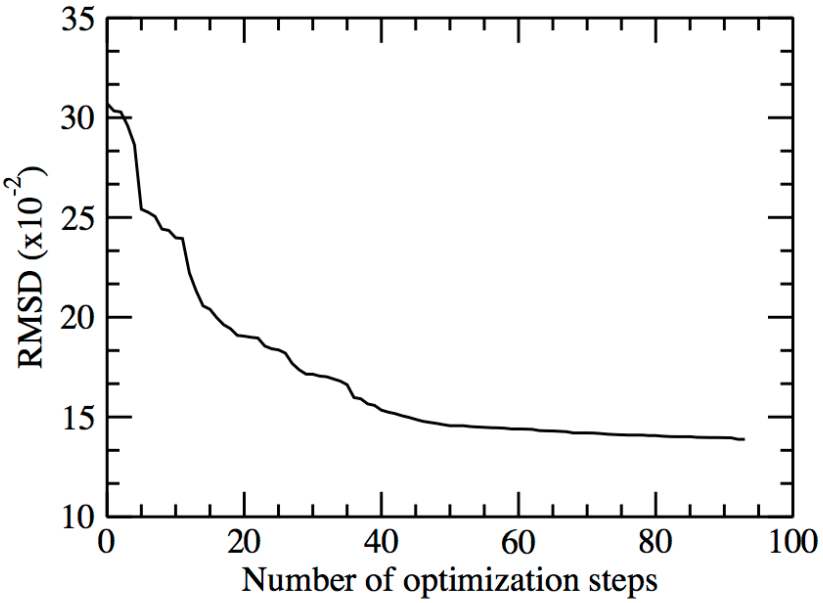

Figure S2. Relative QM (red) and Drude MM energies before (green) and after (blue) dihedral fit for conformations of α-methyl-arabinofuranoside, β-methyl-arabinofuranoside, α-methyl-lyxofuranoside.

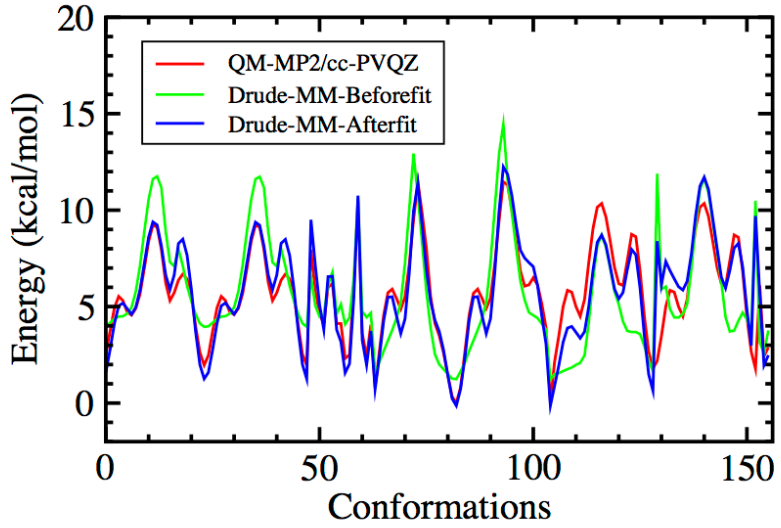

Figure S3. Interaction geometries of methyl-α-D-arabinofuranoside-water (left) and methyl-β-D-arabinofuranoside–water (right) interactions.

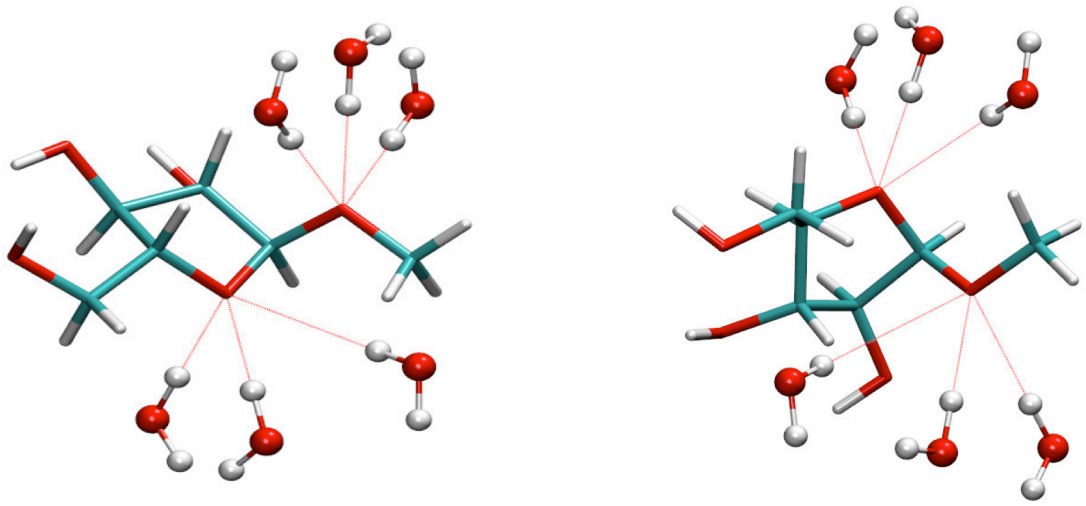

Table S7. Summary of the OME-AARB-water and OME-BARB-water interaction energies (kcal/mol) for the Drude FF and the CHARMM additive FF.

Compds	Energy	Drude	Additive
Me-aarb	Avg difference	0.278	0.553
	RMSD	0.486	0.746
	Avg abs difference	0.405	0.592
Me-barb	Avg difference	-0.09	0.09
	RMSD	0.499	0.764
	Avg abs difference	0.412	0.672

Table S8. Differences in average internal geometries of methyl-aldopentofuranoses as calculated from simulations of infinite crystals and experimental crystal data.

Compounds	methyl-α-arabinofuranoside	methyl-β-arabinofuranoside	methyl-α-xylofuranoside	methyl-α-lyxofuranoside	Average
Bonds					
O4-C1	0.01	0.03	0.02	0.01	0.02
C1-C2	0.00	-0.01	0.00	0.00	0.00
C2-C3	0.00	-0.01	0.00	0.00	0.00
C3-C4	-0.01	-0.01	0.00	0.01	0.00
O1-CM	-0.02	-0.01	-0.01	-0.02	-0.01
C2-O2	0.02	0.04	0.03	0.03	0.03
C3-O3	0.02	0.03	0.02	0.03	0.03
C4-C5	0.01	0.01	0.01	0.02	0.01
C5-O5	0.00	0.01	0.01	-0.01	0.00
C4-O4	-0.01	0.02	-0.02	-0.02	-0.02
C1-O1	0.03	0.03	0.03	0.04	0.03
Average diff.	0.01	0.01	0.01	0.01	0.01
Angles					
O4-C1-C2	-1.64	-1.27	-0.08	0.10	-0.77
C2-C1-O1	1.38	2.77	2.20	0.37	1.68
C1-C2-C3	0.10	-0.15	0.31	-0.57	-0.08
C2-C3-C4	-0.86	-1.10	-0.45	-0.02	-0.61
O4-C4-C5	-0.37	-4.35	0.14	-0.94	-1.38
C1-O1-CM	-1.96	-1.41	-1.47	-2.43	-1.82
C3-C2-O2	-4.86	-1.24	-2.17	0.06	-2.05
C4-C3-O3	-2.53	0.04	1.16	3.26	0.48
C4-C5-O5	1.02	-1.30	1.19	0.26	0.30
C3-C4-O4	-1.58	0.34	1.15	-0.60	-0.17
C4-O4-C1	0.27	0.48	-0.35	-0.21	0.05
O4-C1-O1	-1.28	-0.19	-0.72	0.08	-0.53
Average diff.	-1.03	-0.62	0.08	-0.05	-0.41
Dihedrals					
C4-O4-C1-C2	-1.35	-3.47	1.55	-2.83	-1.53
O4-C1-C2-C3	-1.56	-1.14	-1.41	1.66	-0.61
C1-C2-C3-C4	3.39	5.46	0.79	-0.29	2.34
C2-C3-C4-O4	-3.98	-7.05	0.13	-1.71	-3.15
C3-C4-O4-C1	3.65	6.53	-1.07	2.60	2.93
C2-C1-O1-CM	12.16	-5.92	6.43	4.11	4.19
C3-C2-O2-HO2	-2.88	-4.67	4.30	-3.70	-1.74
C4-C3-O3-HO3	-9.46	-3.15	4.79	4.36	-0.87
O4-C4-C5-O5	4.02	1.06	-0.43	3.35	2.00
C4-C5-O5-HO5	-3.64	1.05	-9.77	11.18	-0.30
C1-O4-C4-C5	-0.37	2.03	-0.24	-1.75	-0.08
Average diff.	0.00	0.84	0.46	1.54	0.29

Figure S4. Time evolution plot of pseudorotation angle for aarb, arib, axyf, alyf (left panel, top to bottom) and barb, brib, bxyf, blyf (right panel, top to bottom).

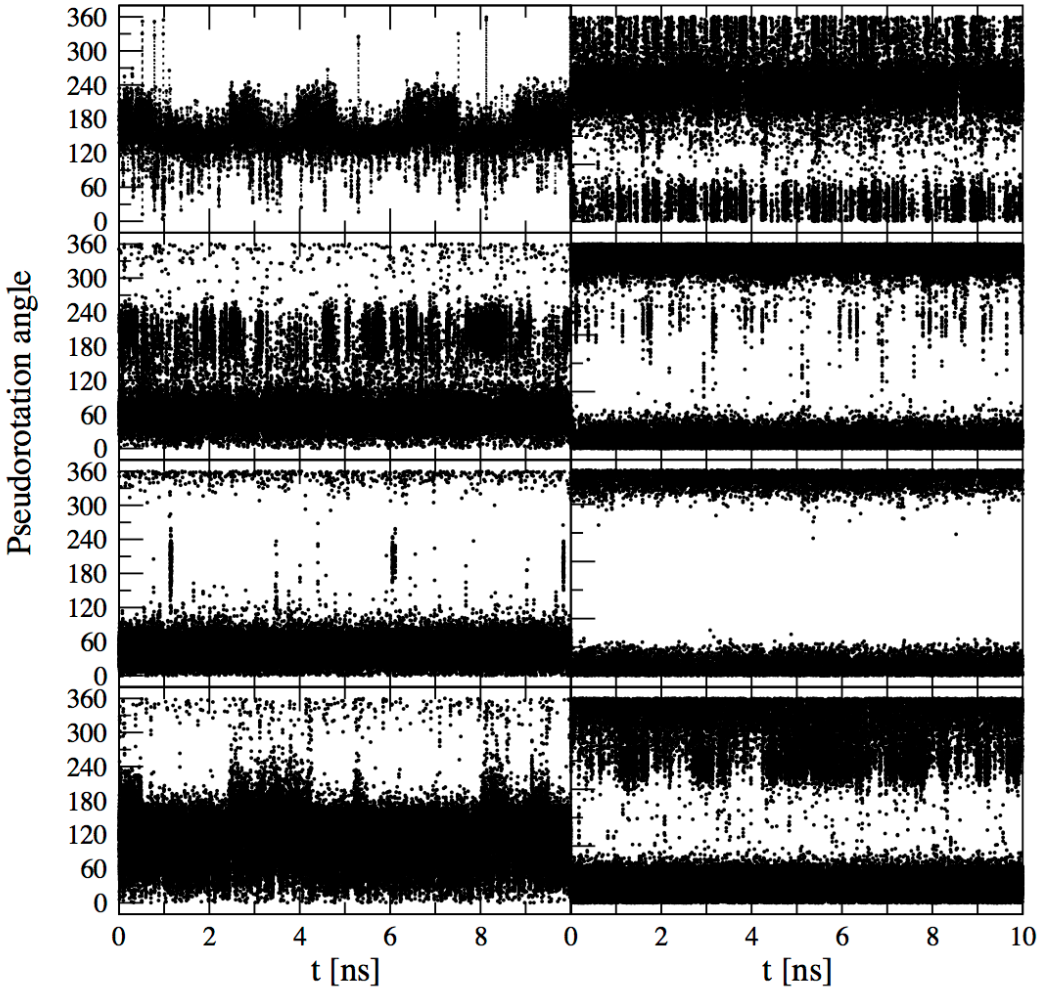

Figure S5. Distribution of pseudorotation angle for aarb, arib, axyf, alyf (a,c,e,g at left panel) and barb, brib, bxyf, blyf (b,d,f,h at right panel).

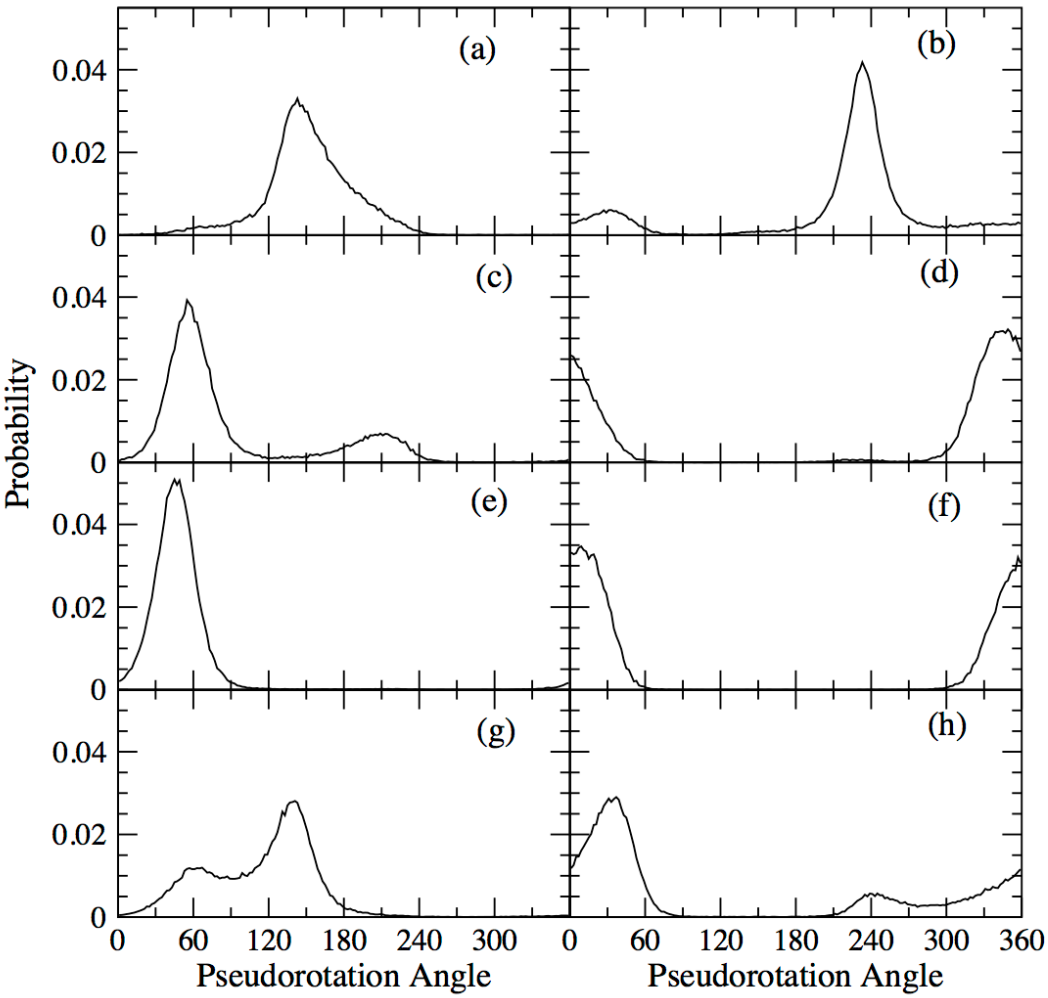

Table S9. Classical Drude oscillator based polarizable force field for furanose monosaccharides

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* DRUDE topology and parameter stream file
* Furanoses,
*

read rtf card append
* Drude Furanoses
*
38

!furanoses, rima
RESI ARIB           0.000  ! alpha-Ribose
!RING * 5 C1 C2 C3 C4 O4
!
!          HO5--O5
!                \       O4
!            H51--C5   /    \    H1
!                / \  /      \  /
!              H52   C4        C1
!                   / \        / \
!                 H4   \      /   O1--HO1
!                      C3----C2
!                     /  \   / \
!              HO3--O3  H3  O2 H2
!                           |
!                          HO2
GROUP
ATOM O4   OD305A   0.000  ALPHA -0.684 THOLE 2.074
ATOM C1   CD31FA   0.124  ALPHA -1.022 THOLE 0.462
ATOM H1   HDA1A    0.070
ATOM O1   OD31E    0.000  ALPHA -1.176 THOLE 1.559
ATOM HO1  HDP1A    0.333
ATOM C4   CD31FC   0.112  ALPHA -1.014 THOLE 0.820
ATOM H4   HDA2E    0.069
ATOM LP1A LPD     -0.202
ATOM LP1B LPD     -0.202
ATOM LP4A LPD     -0.152
ATOM LP4B LPD     -0.152
ATOM LPX4 LPD      0.000 !dummy for anisotropic polarizability
GROUP ! taken from ETOH
ATOM C5   CD32A   -0.086  ALPHA -1.805 THOLE 0.353
ATOM H51  HDA2A    0.080
ATOM H52  HDA2A    0.080
ATOM O5   OD31A    0.000  ALPHA -0.732 THOLE 1.027
ATOM HO5  HDP1A    0.328
ATOM LP5A LPD     -0.201
ATOM LP5B LPD     -0.201
GROUP ! taken from glycerol
ATOM C2   CD31FB  -0.006  ALPHA -1.438 THOLE 1.015
ATOM H2   HDA1A    0.070
ATOM O2   OD31E    0.000  ALPHA -0.940 THOLE 0.670
ATOM HO2  HDP1A    0.322
ATOM LP2A LPD     -0.193
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ATOM LP2B LPD     -0.193
GROUP ! taken from glycerol
ATOM C3   CD31FB  -0.006  ALPHA -1.127 THOLE 1.340
ATOM H3   HDA1A    0.070
ATOM O3   OD31E    0.000  ALPHA -0.881 THOLE 0.328
ATOM HO3  HDP1A    0.322
ATOM LP3A LPD     -0.193
ATOM LP3B LPD     -0.193
!
BOND O4 C1  C1 H1   C1 O1   O1 HO1
BOND C1 C2  C2 H2   C2 O2   O2 HO2
BOND C2 C3  C3 H3   C3 O3   O3 HO3
BOND C3 C4  C4 H4   C4 C5   C4 O4
BOND C5 H51 C5 H52  C5 O5   O5 HO5
BOND O1 LP1A O1 LP1B
BOND O2 LP2A O2 LP2B
BOND O3 LP3A O3 LP3B
BOND O4 LP4A O4 LP4B O4 LPX4
BOND O5 LP5A O5 LP5B

LONEPAIR relative LP1A O1 C1 HO1 distance 0.35 angle 110.0 dihe  91.0
LONEPAIR relative LP1B O1 C1 HO1 distance 0.35 angle 110.0 dihe 269.0
ANISOTROPY O1 C1 LP1A LP1B A11 0.8108 A22 1.2162

LONEPAIR relative LP2A O2 C2 HO2 distance 0.35 angle 110.0 dihe  91.0
LONEPAIR relative LP2B O2 C2 HO2 distance 0.35 angle 110.0 dihe 269.0
ANISOTROPY O2 C2 LP2A LP2B A11 0.8108 A22 1.2162

LONEPAIR relative LP3A O3 C3 HO3 distance 0.35 angle 110.0 dihe  91.0
LONEPAIR relative LP3B O3 C3 HO3 distance 0.35 angle 110.0 dihe 269.0
ANISOTROPY O3 C3 LP3A LP3B A11 0.8108 A22 1.2162

LONEPAIR bisector LP4A O4 C1 C4 distance 0.35 angle 110.0 dihe  90.0
LONEPAIR bisector LP4B O4 C1 C4 distance 0.35 angle 110.0 dihe 270.0
LONEPAIR bisector LPX4 O4 C1 C4 distance 0.10 angle   0.0 dihe   0.0
ANISOTROPY O4 LPX4 LP4A LP4B A11 0.8889  A22 1.2222

LONEPAIR relative LP5A O5 C5 HO5 distance 0.35 angle 110.0 dihe  91.0
LONEPAIR relative LP5B O5 C5 HO5 distance 0.35 angle 110.0 dihe 269.0
ANISOTROPY O5 C5 LP5A LP5B A11 0.8108 A22 1.2162


! IC table; from minimized geometry*
IC C4   O4   C1   C2   1.4343  107.06  -43.51  102.91   1.5564
IC O4   C1   C2   C3   1.4227  102.91   29.68  103.27   1.5615
IC C1   C2   C3   C4   1.5564  103.27   -6.90  103.97   1.5386
IC C3   O4  *C4   C5   1.5386  104.85  125.17  112.30   1.5446
IC C3   O4  *C4   H4   1.5386  104.85 -116.42  106.12   1.1143
IC O4   C4   C5   O5   1.4343  112.30 -178.59  110.88   1.4293
IC C4   C5   O5   HO5  1.5446  110.88  -86.85  110.49   0.9639
IC O5   C4  *C5   H51  1.4293  110.88  119.78  108.95   1.1027
IC O5   C4  *C5   H52  1.4293  110.88 -122.02  109.96   1.1020
IC C2   O4  *C1   O1   1.5564  102.91  122.54  109.76   1.4025
IC O4   C1   O1   HO1  1.4227  109.76   66.79  107.33   0.9584
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IC C2   O4  *C1   H1   1.5564  102.91 -117.68  108.69   1.1117
IC C3   C1  *C2   H2   1.5615  103.27 -113.35  106.87   1.1124
IC C3   C1  *C2   O2   1.5615  103.27  127.46  116.16   1.4278
IC C1   C2   O2   HO2  1.5564  116.16  -81.77  106.00   0.9665
IC C2   C4  *C3   O3   1.5615  103.97 -125.04  111.07   1.4263
IC C2   C4  *C3   H3   1.5615  103.97  115.28  109.94   1.1126
IC C4   C3   O3   HO3  1.5386  111.07  -77.15  108.40   0.9644
IC C2   C4  *C3   H4   1.5615  103.97  -95.69   28.61   2.1867

RESI BRIB           0.000  ! beta-Ribose
!RING * 5 C1 C2 C3 C4 O4
!
!          HO5--O5
!                \       O4
!            H51--C5   /    \    O1--HO1
!                / \  /      \  /
!             H52   C4        C1
!                  / \        / \
!               H4   \      /   H1
!                    C3----C2
!                   /  \   / \
!             HO3--O3  H3  O2 H2
!                          |
!                         HO2
GROUP
ATOM O4   OD305A   0.000  ALPHA -0.684 THOLE 2.074
ATOM C1   CD31FA   0.124  ALPHA -1.022 THOLE 0.462
ATOM H1   HDA1A    0.070
ATOM O1   OD31E    0.000  ALPHA -1.176 THOLE 1.559
ATOM HO1  HDP1A    0.333
ATOM C4   CD31FC   0.112  ALPHA -1.014 THOLE 0.820
ATOM H4   HDA2E    0.069
ATOM LP1A LPD     -0.202
ATOM LP1B LPD     -0.202
ATOM LP4A LPD     -0.152
ATOM LP4B LPD     -0.152
ATOM LPX4 LPD      0.000 !dummy for anisotropic polarizability
GROUP ! taken from ETOH
ATOM C5   CD32A   -0.086  ALPHA -1.805 THOLE 0.353
ATOM H51  HDA2A    0.080
ATOM H52  HDA2A    0.080
ATOM O5   OD31A    0.000  ALPHA -0.732 THOLE 1.027
ATOM HO5  HDP1A    0.328
ATOM LP5A LPD     -0.201
ATOM LP5B LPD     -0.201
GROUP ! taken from glycerol
ATOM C2   CD31FB  -0.006  ALPHA -1.438 THOLE 1.015
ATOM H2   HDA1A    0.070
ATOM O2   OD31E    0.000  ALPHA -0.940 THOLE 0.670
ATOM HO2  HDP1A    0.322
ATOM LP2A LPD     -0.193
ATOM LP2B LPD     -0.193
GROUP ! taken from glycerol
ATOM C3   CD31FB  -0.006  ALPHA -1.127 THOLE 1.340
```

```
ATOM H3   HDA1A    0.070
ATOM O3   OD31E    0.000  ALPHA -0.881 THOLE 0.328
ATOM HO3  HDP1A    0.322
ATOM LP3A LPD     -0.193
ATOM LP3B LPD     -0.193
!
BOND O4 C1  C1 H1   C1 O1   O1 HO1
BOND C1 C2  C2 H2   C2 O2   O2 HO2
BOND C2 C3  C3 H3   C3 O3   O3 HO3
BOND C3 C4  C4 H4   C4 C5   C4 O4
BOND C5 H51 C5 H52  C5 O5   O5 HO5
BOND O1 LP1A O1 LP1B
BOND O2 LP2A O2 LP2B
BOND O3 LP3A O3 LP3B
BOND O4 LP4A O4 LP4B O4 LPX4
BOND O5 LP5A O5 LP5B

LONEPAIR relative LP1A O1 C1 HO1 distance 0.35 angle 110.0 dihe  91.0
LONEPAIR relative LP1B O1 C1 HO1 distance 0.35 angle 110.0 dihe 269.0
ANISOTROPY O1 C1 LP1A LP1B A11 0.8108 A22 1.2162

LONEPAIR relative LP2A O2 C2 HO2 distance 0.35 angle 110.0 dihe  91.0
LONEPAIR relative LP2B O2 C2 HO2 distance 0.35 angle 110.0 dihe 269.0
ANISOTROPY O2 C2 LP2A LP2B A11 0.8108 A22 1.2162

LONEPAIR relative LP3A O3 C3 HO3 distance 0.35 angle 110.0 dihe  91.0
LONEPAIR relative LP3B O3 C3 HO3 distance 0.35 angle 110.0 dihe 269.0
ANISOTROPY O3 C3 LP3A LP3B A11 0.8108 A22 1.2162

LONEPAIR bisector LP4A O4 C1 C4 distance 0.35 angle 110.0 dihe  90.0
LONEPAIR bisector LP4B O4 C1 C4 distance 0.35 angle 110.0 dihe 270.0
LONEPAIR bisector LPX4 O4 C1 C4 distance 0.10 angle   0.0 dihe   0.0
ANISOTROPY O4 LPX4 LP4A LP4B A11 0.8889  A22 1.2222
LONEPAIR relative LP5A O5 C5 HO5 distance 0.35 angle 110.0 dihe  91.0
LONEPAIR relative LP5B O5 C5 HO5 distance 0.35 angle 110.0 dihe 269.0
ANISOTROPY O5 C5 LP5A LP5B A11 0.8108 A22 1.2162

! IC table; from minimized geometry*
IC C4   O4   C1   C2   1.4343  107.06  -43.51  102.91   1.5564
IC O4   C1   C2   C3   1.4227  102.91   29.68  103.27   1.5615
IC C1   C2   C3   C4   1.5564  103.27   -6.90  103.97   1.5386
IC C3   O4  *C4   C5   1.5386  104.85  125.17  112.30   1.5446
IC C3   O4  *C4   H4   1.5386  104.85 -116.42  106.12   1.1143
IC O4   C4   C5   O5   1.4343  112.30 -178.59  110.88   1.4293
IC C4   C5   O5   HO5  1.5446  110.88  -86.85  110.49   0.9639
IC O5   C4  *C5   H51  1.4293  110.88  119.78  108.95   1.1027
IC O5   C4  *C5   H52  1.4293  110.88 -122.02  109.96   1.1020
IC C2   O4  *C1   O1   1.5564  102.91 -122.54  109.76   1.4025
IC O4   C1   O1   HO1  1.4227  109.76   66.79  107.33   0.9584
IC C2   O4  *C1   H1   1.5564  102.91  117.68  108.69   1.1117
IC C3   C1  *C2   H2   1.5615  103.27 -113.35  106.87   1.1124
IC C3   C1  *C2   O2   1.5615  103.27  127.46  116.16   1.4278
IC C1   C2   O2   HO2  1.5564  116.16  -81.77  106.00   0.9665
IC C2   C4  *C3   O3   1.5615  103.97 -125.04  111.07   1.4263
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IC C2   C4  *C3   H3   1.5615  103.97  115.28  109.94   1.1126
IC C4   C3   O3   HO3  1.5386  111.07  -77.15  108.40   0.9644
IC C2   C4  *C3   H4   1.5615  103.97  -95.69   28.61   2.1867

RESI AARB           0.000  ! alpha-Arabinose
!RING * 5 C1 C2 C3 C4 O4
!          HO5--O5
!                \       O4
!            H51--C5   /    \    H1
!                / \  /      \  /
!             H52   C4        C1
!                  / \        / \
!                 H4   \      /   O1--HO1
!                      C3----C2
!                     /  \   / \
!              HO3--O3  H3  H2 O2
!                               |
!                              HO2
GROUP
ATOM O4   OD305A   0.000  ALPHA -0.684 THOLE 2.074
ATOM C1   CD31FA   0.124  ALPHA -1.022 THOLE 0.462
ATOM H1   HDA1A    0.070
ATOM O1   OD31E    0.000  ALPHA -1.176 THOLE 1.559
ATOM HO1  HDP1A    0.333
ATOM C4   CD31FC   0.112  ALPHA -1.014 THOLE 0.820
ATOM H4   HDA2E    0.069
ATOM LP1A LPD     -0.202
ATOM LP1B LPD     -0.202
ATOM LP4A LPD     -0.152
ATOM LP4B LPD     -0.152
ATOM LPX4 LPD      0.000 !dummy for anisotropic polarizability
GROUP ! taken from ETOH
ATOM C5   CD32A   -0.086  ALPHA -1.805 THOLE 0.353
ATOM H51  HDA2A    0.080
ATOM H52  HDA2A    0.080
ATOM O5   OD31A    0.000  ALPHA -0.732 THOLE 1.027
ATOM HO5  HDP1A    0.328
ATOM LP5A LPD     -0.201
ATOM LP5B LPD     -0.201
GROUP ! taken from glycerol
ATOM C2   CD31FB  -0.006  ALPHA -1.438 THOLE 1.015
ATOM H2   HDA1A    0.070
ATOM O2   OD31E    0.000  ALPHA -0.940 THOLE 0.670
ATOM HO2  HDP1A    0.322
ATOM LP2A LPD     -0.193
ATOM LP2B LPD     -0.193
GROUP ! taken from glycerol
ATOM C3   CD31FB  -0.006  ALPHA -1.127 THOLE 1.340
ATOM H3   HDA1A    0.070
ATOM O3   OD31E    0.000  ALPHA -0.881 THOLE 0.328
ATOM HO3  HDP1A    0.322
ATOM LP3A LPD     -0.193
ATOM LP3B LPD     -0.193
!
```

```
BOND O4 C1  C1 H1   C1 O1   O1 HO1
BOND C1 C2  C2 H2   C2 O2   O2 HO2
BOND C2 C3  C3 H3   C3 O3   O3 HO3
BOND C3 C4  C4 H4   C4 C5   C4 O4
BOND C5 H51 C5 H52  C5 O5   O5 HO5
BOND O1 LP1A O1 LP1B
BOND O2 LP2A O2 LP2B
BOND O3 LP3A O3 LP3B
BOND O4 LP4A O4 LP4B O4 LPX4
BOND O5 LP5A O5 LP5B

LONEPAIR relative LP1A O1 C1 HO1 distance 0.35 angle 110.0 dihe  91.0
LONEPAIR relative LP1B O1 C1 HO1 distance 0.35 angle 110.0 dihe 269.0
ANISOTROPY O1 C1 LP1A LP1B A11 0.8108 A22 1.2162

LONEPAIR relative LP2A O2 C2 HO2 distance 0.35 angle 110.0 dihe  91.0
LONEPAIR relative LP2B O2 C2 HO2 distance 0.35 angle 110.0 dihe 269.0
ANISOTROPY O2 C2 LP2A LP2B A11 0.8108 A22 1.2162

LONEPAIR relative LP3A O3 C3 HO3 distance 0.35 angle 110.0 dihe  91.0
LONEPAIR relative LP3B O3 C3 HO3 distance 0.35 angle 110.0 dihe 269.0
ANISOTROPY O3 C3 LP3A LP3B A11 0.8108 A22 1.2162

LONEPAIR bisector LP4A O4 C1 C4 distance 0.35 angle 110.0 dihe  90.0
LONEPAIR bisector LP4B O4 C1 C4 distance 0.35 angle 110.0 dihe 270.0
LONEPAIR bisector LPX4 O4 C1 C4 distance 0.10 angle   0.0 dihe   0.0
ANISOTROPY O4 LPX4 LP4A LP4B A11 0.8889  A22 1.2222

LONEPAIR relative LP5A O5 C5 HO5 distance 0.35 angle 110.0 dihe  91.0
LONEPAIR relative LP5B O5 C5 HO5 distance 0.35 angle 110.0 dihe 269.0
ANISOTROPY O5 C5 LP5A LP5B A11 0.8108 A22 1.2162

! IC table; from minimized geometry*
IC C4   O4   C1   C2   1.4319  108.67  -17.05  106.71   1.5578
IC O4   C1   C2   C3   1.4302  106.71  -10.12  102.15   1.5355
IC C1   C2   C3   C4   1.5578  102.15   31.25  101.91   1.5267
IC C3   O4  *C4   C5   1.5267  102.62  124.20  112.49   1.5454
IC C3   O4  *C4   H4   1.5267  102.62 -115.89  106.69   1.1135
IC O4   C4   C5   O5   1.4319  112.49 -179.23  111.10   1.4305
IC C4   C5   O5   HO5  1.5454  111.10  -93.06  110.47   0.9646
IC O5   C4  *C5   H51  1.4305  111.10  119.95  108.87   1.1029
IC O5   C4  *C5   H52  1.4305  111.10 -122.01  109.82   1.1021
IC C2   O4  *C1   O1   1.5578  106.71  122.01  110.02   1.3992
IC O4   C1   O1   HO1  1.4302  110.02   65.19  106.88   0.9590
IC C2   O4  *C1   H1   1.5578  106.71 -118.66  107.16   1.1129
IC C3   C1  *C2   H2   1.5355  102.15  115.71  109.19   1.1138
IC C3   C1  *C2   O2   1.5355  102.15 -121.95  114.37   1.4285
IC C1   C2   O2   HO2  1.5578  114.37 -171.75  108.32   0.9638
IC C2   C4  *C3   O3   1.5355  101.91 -122.00  112.32   1.4206
IC C2   C4  *C3   H3   1.5355  101.91  116.42  109.37   1.1143
IC C4   C3   O3   HO3  1.5267  112.32  -53.24  107.21   0.9692
IC C2   C4  *C3   H4   1.5355  101.91  -71.04   28.67   2.1783
!
RESI BARB           0.000  ! beta-Arabinose
```

```
!RING * 5 C1 C2 C3 C4 O4
!
!          HO5--O5
!                \       O4
!             H51--C5   /    \    O1--HO1
!                  / \  /      \  /
!              H52   C4         C1
!                   / \         / \
!                 H4   \       /   H1
!                       C3----C2
!                      /  \   / \
!              HO3--O3  H3  H2 O2
!                               |
!                              HO2
!
!
GROUP
ATOM O4   OD305A   0.000  ALPHA -0.684 THOLE 2.074
ATOM C1   CD31FA   0.124  ALPHA -1.022 THOLE 0.462
ATOM H1   HDA1A    0.070
ATOM O1   OD31E    0.000  ALPHA -1.176 THOLE 1.559
ATOM HO1  HDP1A    0.333
ATOM C4   CD31FC   0.112  ALPHA -1.014 THOLE 0.820
ATOM H4   HDA2E    0.069
ATOM LP1A LPD     -0.202
ATOM LP1B LPD     -0.202
ATOM LP4A LPD     -0.152
ATOM LP4B LPD     -0.152
ATOM LPX4 LPD      0.000 !dummy for anisotropic polarizability
GROUP ! taken from ETOH
ATOM C5   CD32A   -0.086  ALPHA -1.805 THOLE 0.353
ATOM H51  HDA2A    0.080
ATOM H52  HDA2A    0.080
ATOM O5   OD31A    0.000  ALPHA -0.732 THOLE 1.027
ATOM HO5  HDP1A    0.328
ATOM LP5A LPD     -0.201
ATOM LP5B LPD     -0.201
GROUP ! taken from glycerol
ATOM C2   CD31FB  -0.006  ALPHA -1.438 THOLE 1.015
ATOM H2   HDA1A    0.070
ATOM O2   OD31E    0.000  ALPHA -0.940 THOLE 0.670
ATOM HO2  HDP1A    0.322
ATOM LP2A LPD     -0.193
ATOM LP2B LPD     -0.193
GROUP ! taken from glycerol
ATOM C3   CD31FB  -0.006  ALPHA -1.127 THOLE 1.340
ATOM H3   HDA1A    0.070
ATOM O3   OD31E    0.000  ALPHA -0.881 THOLE 0.328
ATOM HO3  HDP1A    0.322
ATOM LP3A LPD     -0.193
ATOM LP3B LPD     -0.193
!
BOND O4 C1  C1 H1   C1 O1   O1 HO1
BOND C1 C2  C2 H2   C2 O2   O2 HO2
```

```
BOND C2 C3  C3 H3   C3 O3   O3 HO3
BOND C3 C4  C4 H4   C4 C5   C4 O4
BOND C5 H51 C5 H52  C5 O5   O5 HO5
BOND O1 LP1A O1 LP1B
BOND O2 LP2A O2 LP2B
BOND O3 LP3A O3 LP3B
BOND O4 LP4A O4 LP4B O4 LPX4
BOND O5 LP5A O5 LP5B

LONEPAIR relative LP1A O1 C1 HO1 distance 0.35 angle 110.0 dihe  91.0
LONEPAIR relative LP1B O1 C1 HO1 distance 0.35 angle 110.0 dihe 269.0
ANISOTROPY O1 C1 LP1A LP1B A11 0.8108 A22 1.2162

LONEPAIR relative LP2A O2 C2 HO2 distance 0.35 angle 110.0 dihe  91.0
LONEPAIR relative LP2B O2 C2 HO2 distance 0.35 angle 110.0 dihe 269.0
ANISOTROPY O2 C2 LP2A LP2B A11 0.8108 A22 1.2162

LONEPAIR relative LP3A O3 C3 HO3 distance 0.35 angle 110.0 dihe  91.0
LONEPAIR relative LP3B O3 C3 HO3 distance 0.35 angle 110.0 dihe 269.0
ANISOTROPY O3 C3 LP3A LP3B A11 0.8108 A22 1.2162

LONEPAIR bisector LP4A O4 C1 C4 distance 0.35 angle 110.0 dihe  90.0
LONEPAIR bisector LP4B O4 C1 C4 distance 0.35 angle 110.0 dihe 270.0
LONEPAIR bisector LPX4 O4 C1 C4 distance 0.10 angle   0.0 dihe   0.0
ANISOTROPY O4 LPX4 LP4A LP4B A11 0.8889  A22 1.2222

LONEPAIR relative LP5A O5 C5 HO5 distance 0.35 angle 110.0 dihe  91.0
LONEPAIR relative LP5B O5 C5 HO5 distance 0.35 angle 110.0 dihe 269.0
ANISOTROPY O5 C5 LP5A LP5B A11 0.8108 A22 1.2162

! IC table; from minimized geometry*
IC C4   O4   C1   C2   1.4319  108.67  -17.05  106.71   1.5578
IC O4   C1   C2   C3   1.4302  106.71  -10.12  102.15   1.5355
IC C1   C2   C3   C4   1.5578  102.15   31.25  101.91   1.5267
IC C3   O4  *C4   C5   1.5267  102.62  124.20  112.49   1.5454
IC C3   O4  *C4   H4   1.5267  102.62 -115.89  106.69   1.1135
IC O4   C4   C5   O5   1.4319  112.49 -179.23  111.10   1.4305
IC C4   C5   O5   HO5  1.5454  111.10  -93.06  110.47   0.9646
IC O5   C4  *C5   H51  1.4305  111.10  119.95  108.87   1.1029
IC O5   C4  *C5   H52  1.4305  111.10 -122.01  109.82   1.1021
IC C2   O4  *C1   O1   1.5578  106.71 -122.01  110.02   1.3992
IC O4   C1   O1   HO1  1.4302  110.02   65.19  106.88   0.9590
IC C2   O4  *C1   H1   1.5578  106.71  118.66  107.16   1.1129
IC C3   C1  *C2   H2   1.5355  102.15  115.71  109.19   1.1138
IC C3   C1  *C2   O2   1.5355  102.15 -121.95  114.37   1.4285
IC C1   C2   O2   HO2  1.5578  114.37 -171.75  108.32   0.9638
IC C2   C4  *C3   O3   1.5355  101.91 -122.00  112.32   1.4206
IC C2   C4  *C3   H3   1.5355  101.91  116.42  109.37   1.1143
IC C4   C3   O3   HO3  1.5267  112.32  -53.24  107.21   0.9692
IC C2   C4  *C3   H4   1.5355  101.91  -71.04   28.67   2.1783

RESI AXYF           0.000  ! alpha-Xylofuranose
!RING * 5 C1 C2 C3 C4 O4
!          HO5--O5
```

```
!                \       O4
!            H51--C5   /    \    H1
!                / \  /      \  /
!             H52   C4        C1
!                  / \        / \
!                 H4   \      /   O1--HO1
!                      C3----C2
!                     /  \   / \
!                    H3  O3 O2 H2
!                        |   |
!                       HO3   HO2
GROUP
ATOM O4   OD305A   0.000  ALPHA -0.684 THOLE 2.074
ATOM C1   CD31FA   0.124  ALPHA -1.022 THOLE 0.462
ATOM H1   HDA1A    0.070
ATOM O1   OD31E    0.000  ALPHA -1.176 THOLE 1.559
ATOM HO1  HDP1A    0.333
ATOM C4   CD31FC   0.112  ALPHA -1.014 THOLE 0.820
ATOM H4   HDA2E    0.069
ATOM LP1A LPD     -0.202
ATOM LP1B LPD     -0.202
ATOM LP4A LPD     -0.152
ATOM LP4B LPD     -0.152
ATOM LPX4 LPD      0.000 !dummy for anisotropic polarizability
GROUP ! taken from ETOH
ATOM C5   CD32A   -0.086  ALPHA -1.805 THOLE 0.353
ATOM H51  HDA2A    0.080
ATOM H52  HDA2A    0.080
ATOM O5   OD31A    0.000  ALPHA -0.732 THOLE 1.027
ATOM HO5  HDP1A    0.328
ATOM LP5A LPD     -0.201
ATOM LP5B LPD     -0.201
GROUP ! taken from glycerol
ATOM C2   CD31FB  -0.006  ALPHA -1.438 THOLE 1.015
ATOM H2   HDA1A    0.070
ATOM O2   OD31E    0.000  ALPHA -0.940 THOLE 0.670
ATOM HO2  HDP1A    0.322
ATOM LP2A LPD     -0.193
ATOM LP2B LPD     -0.193
GROUP ! taken from glycerol
ATOM C3   CD31FB  -0.006  ALPHA -1.127 THOLE 1.340
ATOM H3   HDA1A    0.070
ATOM O3   OD31E    0.000  ALPHA -0.881 THOLE 0.328
ATOM HO3  HDP1A    0.322
ATOM LP3A LPD     -0.193
ATOM LP3B LPD     -0.193
!
BOND O4 C1  C1 H1   C1 O1   O1 HO1
BOND C1 C2  C2 H2   C2 O2   O2 HO2
BOND C2 C3  C3 H3   C3 O3   O3 HO3
BOND C3 C4  C4 H4   C4 C5   C4 O4
BOND C5 H51 C5 H52  C5 O5   O5 HO5
BOND O1 LP1A O1 LP1B
BOND O2 LP2A O2 LP2B
```

```
BOND O3 LP3A O3 LP3B
BOND O4 LP4A O4 LP4B O4 LPX4
BOND O5 LP5A O5 LP5B

LONEPAIR relative LP1A O1 C1 HO1 distance 0.35 angle 110.0 dihe  91.0
LONEPAIR relative LP1B O1 C1 HO1 distance 0.35 angle 110.0 dihe 269.0
ANISOTROPY O1 C1 LP1A LP1B A11 0.8108 A22 1.2162

LONEPAIR relative LP2A O2 C2 HO2 distance 0.35 angle 110.0 dihe  91.0
LONEPAIR relative LP2B O2 C2 HO2 distance 0.35 angle 110.0 dihe 269.0
ANISOTROPY O2 C2 LP2A LP2B A11 0.8108 A22 1.2162

LONEPAIR relative LP3A O3 C3 HO3 distance 0.35 angle 110.0 dihe  91.0
LONEPAIR relative LP3B O3 C3 HO3 distance 0.35 angle 110.0 dihe 269.0
ANISOTROPY O3 C3 LP3A LP3B A11 0.8108 A22 1.2162

LONEPAIR bisector LP4A O4 C1 C4 distance 0.35 angle 110.0 dihe  90.0
LONEPAIR bisector LP4B O4 C1 C4 distance 0.35 angle 110.0 dihe 270.0
LONEPAIR bisector LPX4 O4 C1 C4 distance 0.10 angle   0.0 dihe   0.0
ANISOTROPY O4 LPX4 LP4A LP4B A11 0.8889  A22 1.2222

LONEPAIR relative LP5A O5 C5 HO5 distance 0.35 angle 110.0 dihe  91.0
LONEPAIR relative LP5B O5 C5 HO5 distance 0.35 angle 110.0 dihe 269.0
ANISOTROPY O5 C5 LP5A LP5B A11 0.8108 A22 1.2162

! IC table; from minimized geometry*
IC C4   O4   C1   C2   1.4368  109.21    7.17  106.92   1.5609
IC O4   C1   C2   C3   1.4288  106.92  -29.31  100.61   1.5256
IC C1   C2   C3   C4   1.5609  100.61   38.33  101.22   1.5366
IC C3   O4  *C4   C5   1.5366  105.95  126.07  111.10   1.5466
IC C3   O4  *C4   H4   1.5366  105.95 -115.62  106.41   1.1129
IC O4   C4   C5   O5   1.4368  111.10 -170.12  111.17   1.4292
IC C4   C5   O5   HO5  1.5466  111.17  -86.81  110.69   0.9637
IC O5   C4  *C5   H51  1.4292  111.17  119.44  108.73   1.1031
IC O5   C4  *C5   H52  1.4292  111.17 -122.76  110.12   1.1017
IC C2   O4  *C1   O1   1.5609  106.92  123.12  110.19   1.4024
IC O4   C1   O1   HO1  1.4288  110.19   60.16  106.38   0.9603
IC C2   O4  *C1   H1   1.5609  106.92 -117.24  106.84   1.1130
IC C3   C1  *C2   H2   1.5256  100.61 -119.80  111.22   1.1086
IC C3   C1  *C2   O2   1.5256  100.61  116.99  113.84   1.4299
IC C1   C2   O2   HO2  1.5609  113.84   25.15  106.11   0.9678
IC C2   C4  *C3   O3   1.5256  101.22  116.82  111.32   1.4223
IC C2   C4  *C3   H3   1.5256  101.22 -120.45  112.39   1.1104
IC C4   C3   O3   HO3  1.5366  111.32   68.17  107.50   0.9664
IC C2   C4  *C3   H4   1.5256  101.22  -77.82   29.09   2.1676

RESI BXYF          0.000  ! beta-Xylofuranose
!RING * 5 C1 C2 C3 C4 O4
!          HO5--O5
!                \       O4
!            H51--C5   /    \    O1--HO1
!                / \  /      \  /
!              H52   C4        C1
!                   / \        / \
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```
!                H4   \      /   H1
!                     C3----C2
!                    /  \   / \
!                   H3  O3 O2 H2
!                       |   |
!                      HO3   HO2
GROUP
ATOM O4   OD305A   0.000  ALPHA -0.684 THOLE 2.074
ATOM C1   CD31FA   0.124  ALPHA -1.022 THOLE 0.462
ATOM H1   HDA1A    0.070
ATOM O1   OD31E    0.000  ALPHA -1.176 THOLE 1.559
ATOM HO1  HDP1A    0.333
ATOM C4   CD31FC   0.112  ALPHA -1.014 THOLE 0.820
ATOM H4   HDA2E    0.069
ATOM LP1A LPD     -0.202
ATOM LP1B LPD     -0.202
ATOM LP4A LPD     -0.152
ATOM LP4B LPD     -0.152
ATOM LPX4 LPD      0.000 !dummy for anisotropic polarizability
GROUP ! taken from ETOH
ATOM C5   CD32A   -0.086  ALPHA -1.805 THOLE 0.353
ATOM H51  HDA2A    0.080
ATOM H52  HDA2A    0.080
ATOM O5   OD31A    0.000  ALPHA -0.732 THOLE 1.027
ATOM HO5  HDP1A    0.328
ATOM LP5A LPD     -0.201
ATOM LP5B LPD     -0.201
GROUP ! taken from glycerol
ATOM C2   CD31FB  -0.006  ALPHA -1.438 THOLE 1.015
ATOM H2   HDA1A    0.070
ATOM O2   OD31E    0.000  ALPHA -0.940 THOLE 0.670
ATOM HO2  HDP1A    0.322
ATOM LP2A LPD     -0.193
ATOM LP2B LPD     -0.193
GROUP ! taken from glycerol
ATOM C3   CD31FB  -0.006  ALPHA -1.127 THOLE 1.340
ATOM H3   HDA1A    0.070
ATOM O3   OD31E    0.000  ALPHA -0.881 THOLE 0.328
ATOM HO3  HDP1A    0.322
ATOM LP3A LPD     -0.193
ATOM LP3B LPD     -0.193
!
BOND O4 C1  C1 H1   C1 O1   O1 HO1
BOND C1 C2  C2 H2   C2 O2   O2 HO2
BOND C2 C3  C3 H3   C3 O3   O3 HO3
BOND C3 C4  C4 H4   C4 C5   C4 O4
BOND C5 H51 C5 H52  C5 O5   O5 HO5
BOND O1 LP1A O1 LP1B
BOND O2 LP2A O2 LP2B
BOND O3 LP3A O3 LP3B
BOND O4 LP4A O4 LP4B O4 LPX4
BOND O5 LP5A O5 LP5B

LONEPAIR relative LP1A O1 C1 HO1 distance 0.35 angle 110.0 dihe  91.0
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LONEPAIR relative LP1B O1 C1 HO1 distance 0.35 angle 110.0 dihe 269.0
ANISOTROPY O1 C1 LP1A LP1B A11 0.8108 A22 1.2162

LONEPAIR relative LP2A O2 C2 HO2 distance 0.35 angle 110.0 dihe  91.0
LONEPAIR relative LP2B O2 C2 HO2 distance 0.35 angle 110.0 dihe 269.0
ANISOTROPY O2 C2 LP2A LP2B A11 0.8108 A22 1.2162

LONEPAIR relative LP3A O3 C3 HO3 distance 0.35 angle 110.0 dihe  91.0
LONEPAIR relative LP3B O3 C3 HO3 distance 0.35 angle 110.0 dihe 269.0
ANISOTROPY O3 C3 LP3A LP3B A11 0.8108 A22 1.2162

LONEPAIR bisector LP4A O4 C1 C4 distance 0.35 angle 110.0 dihe  90.0
LONEPAIR bisector LP4B O4 C1 C4 distance 0.35 angle 110.0 dihe 270.0
LONEPAIR bisector LPX4 O4 C1 C4 distance 0.10 angle   0.0 dihe   0.0
ANISOTROPY O4 LPX4 LP4A LP4B A11 0.8889  A22 1.2222

LONEPAIR relative LP5A O5 C5 HO5 distance 0.35 angle 110.0 dihe  91.0
LONEPAIR relative LP5B O5 C5 HO5 distance 0.35 angle 110.0 dihe 269.0
ANISOTROPY O5 C5 LP5A LP5B A11 0.8108 A22 1.2162

! IC table; from minimized geometry*
IC C4   O4   C1   C2   1.4368  109.21    7.17  106.92   1.5609
IC O4   C1   C2   C3   1.4288  106.92  -29.31  100.61   1.5256
IC C1   C2   C3   C4   1.5609  100.61   38.33  101.22   1.5366
IC C3   O4  *C4   C5   1.5366  105.95  126.07  111.10   1.5466
IC C3   O4  *C4   H4   1.5366  105.95 -115.62  106.41   1.1129
IC O4   C4   C5   O5   1.4368  111.10 -170.12  111.17   1.4292
IC C4   C5   O5   HO5  1.5466  111.17  -86.81  110.69   0.9637
IC O5   C4  *C5   H51  1.4292  111.17  119.44  108.73   1.1031
IC O5   C4  *C5   H52  1.4292  111.17 -122.76  110.12   1.1017
IC C2   O4  *C1   O1   1.5609  106.92 -123.12  110.19   1.4024
IC O4   C1   O1   HO1  1.4288  110.19   60.16  106.38   0.9603
IC C2   O4  *C1   H1   1.5609  106.92  117.24  106.84   1.1130
IC C3   C1  *C2   H2   1.5256  100.61 -119.80  111.22   1.1086
IC C3   C1  *C2   O2   1.5256  100.61  116.99  113.84   1.4299
IC C1   C2   O2   HO2  1.5609  113.84   25.15  106.11   0.9678
IC C2   C4  *C3   O3   1.5256  101.22  116.82  111.32   1.4223
IC C2   C4  *C3   H3   1.5256  101.22 -120.45  112.39   1.1104
IC C4   C3   O3   HO3  1.5366  111.32   68.17  107.50   0.9664
IC C2   C4  *C3   H4   1.5256  101.22  -77.82   29.09   2.1676

RESI ALYF           0.000  ! alpha-lyxofuranose
!RING * 5 C1 C2 C3 C4 O4
!          HO5--O5
!                \       O4
!            H51--C5   /    \    H1
!                / \  /      \  /
!             H52   C4        C1
!                  / \        / \
!                H4   \      /   O1--HO1
!                     C3----C2
!                    /  \   / \
!                   H3  O3  H2 O2
!                       |      |
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!                       HO3    HO2
GROUP
ATOM O4   OD305A   0.000  ALPHA -0.684 THOLE 2.074
ATOM C1   CD31FA   0.124  ALPHA -1.022 THOLE 0.462
ATOM H1   HDA1A    0.070
ATOM O1   OD31E    0.000  ALPHA -1.176 THOLE 1.559
ATOM HO1  HDP1A    0.333
ATOM C4   CD31FC   0.112  ALPHA -1.014 THOLE 0.820
ATOM H4   HDA2E    0.069
ATOM LP1A LPD     -0.202
ATOM LP1B LPD     -0.202
ATOM LP4A LPD     -0.152
ATOM LP4B LPD     -0.152
ATOM LPX4 LPD      0.000 !dummy for anisotropic polarizability
GROUP ! taken from ETOH
ATOM C5   CD32A   -0.086  ALPHA -1.805 THOLE 0.353
ATOM H51  HDA2A    0.080
ATOM H52  HDA2A    0.080
ATOM O5   OD31A    0.000  ALPHA -0.732 THOLE 1.027
ATOM HO5  HDP1A    0.328
ATOM LP5A LPD     -0.201
ATOM LP5B LPD     -0.201
GROUP ! taken from glycerol
ATOM C2   CD31FB  -0.006  ALPHA -1.438 THOLE 1.015
ATOM H2   HDA1A    0.070
ATOM O2   OD31E    0.000  ALPHA -0.940 THOLE 0.670
ATOM HO2  HDP1A    0.322
ATOM LP2A LPD     -0.193
ATOM LP2B LPD     -0.193
GROUP ! taken from glycerol
ATOM C3   CD31FB  -0.006  ALPHA -1.127 THOLE 1.340
ATOM H3   HDA1A    0.070
ATOM O3   OD31E    0.000  ALPHA -0.881 THOLE 0.328
ATOM HO3  HDP1A    0.322
ATOM LP3A LPD     -0.193
ATOM LP3B LPD     -0.193
!
BOND O4 C1  C1 H1   C1 O1   O1 HO1
BOND C1 C2  C2 H2   C2 O2   O2 HO2
BOND C2 C3  C3 H3   C3 O3   O3 HO3
BOND C3 C4  C4 H4   C4 C5   C4 O4
BOND C5 H51 C5 H52  C5 O5   O5 HO5
BOND O1 LP1A O1 LP1B
BOND O2 LP2A O2 LP2B
BOND O3 LP3A O3 LP3B
BOND O4 LP4A O4 LP4B O4 LPX4
BOND O5 LP5A O5 LP5B

LONEPAIR relative LP1A O1 C1 HO1 distance 0.35 angle 110.0 dihe  91.0
LONEPAIR relative LP1B O1 C1 HO1 distance 0.35 angle 110.0 dihe 269.0
ANISOTROPY O1 C1 LP1A LP1B A11 0.8108 A22 1.2162

LONEPAIR relative LP2A O2 C2 HO2 distance 0.35 angle 110.0 dihe  91.0
LONEPAIR relative LP2B O2 C2 HO2 distance 0.35 angle 110.0 dihe 269.0
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ANISOTROPY O2 C2 LP2A LP2B A11 0.8108 A22 1.2162

LONEPAIR relative LP3A O3 C3 HO3 distance 0.35 angle 110.0 dihe  91.0
LONEPAIR relative LP3B O3 C3 HO3 distance 0.35 angle 110.0 dihe 269.0
ANISOTROPY O3 C3 LP3A LP3B A11 0.8108 A22 1.2162

LONEPAIR bisector LP4A O4 C1 C4 distance 0.35 angle 110.0 dihe  90.0
LONEPAIR bisector LP4B O4 C1 C4 distance 0.35 angle 110.0 dihe 270.0
LONEPAIR bisector LPX4 O4 C1 C4 distance 0.10 angle   0.0 dihe   0.0
ANISOTROPY O4 LPX4 LP4A LP4B A11 0.8889  A22 1.2222

LONEPAIR relative LP5A O5 C5 HO5 distance 0.35 angle 110.0 dihe  91.0
LONEPAIR relative LP5B O5 C5 HO5 distance 0.35 angle 110.0 dihe 269.0
ANISOTROPY O5 C5 LP5A LP5B A11 0.8108 A22 1.2162

! IC table; from minimized geometry*
IC C4   O4   C1   C2   1.4315  107.76  -22.45  106.42   1.5606
IC O4   C1   C2   C3   1.4298  106.42   -6.06  102.41   1.5494
IC C1   C2   C3   C4   1.5606  102.41   29.67  101.01   1.5315
IC C3   O4  *C4   C5   1.5315  102.23  127.07  113.37   1.5469
IC C3   O4  *C4   H4   1.5315  102.23 -114.55  106.16   1.1145
IC O4   C4   C5   O5   1.4315  113.37  172.78  110.88   1.4279
IC C4   C5   O5   HO5  1.5469  110.88  -89.23  111.11   0.9627
IC O5   C4  *C5   H51  1.4279  110.88  120.67  109.96   1.1012
IC O5   C4  *C5   H52  1.4279  110.88 -120.92  109.55   1.1021
IC C2   O4  *C1   O1   1.5606  106.42  121.62  109.95   1.3992
IC O4   C1   O1   HO1  1.4298  109.95   66.51  107.28   0.9594
IC C2   O4  *C1   H1   1.5606  106.42 -119.08  107.39   1.1123
IC C3   C1  *C2   H2   1.5494  102.41  115.35  109.45   1.1122
IC C3   C1  *C2   O2   1.5494  102.41 -123.37  114.05   1.4282
IC C1   C2   O2   HO2  1.5606  114.05  104.03  106.69   0.9675
IC C2   C4  *C3   O3   1.5494  101.01  118.58  111.21   1.4279
IC C2   C4  *C3   H3   1.5494  101.01 -119.18  112.30   1.1095
IC C4   C3   O3   HO3  1.5315  111.21  -32.26  108.53   0.9635
IC C2   C4  *C3   H4   1.5494  101.01  -68.34   28.96   2.1721

RESI BLYF           0.000  ! beta-lyxofuranose
!RING * 5 C1 C2 C3 C4 O4
!          HO5--O5
!                \       O4
!            H51--C5   /    \    O1--HO1
!                / \  /      \  /
!             H52   C4        C1
!                  / \        / \
!                H4   \      /   H1
!                     C3----C2
!                   /  \   / \
!                  H3  O3  H2 O2
!                      |      |
!                     HO3    HO2
!
GROUP
ATOM O4   OD305A   0.000  ALPHA -0.684 THOLE 2.074
ATOM C1   CD31FA   0.124  ALPHA -1.022 THOLE 0.462
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ATOM H1   HDA1A    0.070
ATOM O1   OD31E    0.000  ALPHA -1.176 THOLE 1.559
ATOM HO1  HDP1A    0.333
ATOM C4   CD31FC   0.112  ALPHA -1.014 THOLE 0.820
ATOM H4   HDA2E    0.069
ATOM LP1A LPD     -0.202
ATOM LP1B LPD     -0.202
ATOM LP4A LPD     -0.152
ATOM LP4B LPD     -0.152
ATOM LPX4 LPD      0.000 !dummy for anisotropic polarizability
GROUP ! taken from ETOH
ATOM C5   CD32A   -0.086  ALPHA -1.805 THOLE 0.353
ATOM H51  HDA2A    0.080
ATOM H52  HDA2A    0.080
ATOM O5   OD31A    0.000  ALPHA -0.732 THOLE 1.027
ATOM HO5  HDP1A    0.328
ATOM LP5A LPD     -0.201
ATOM LP5B LPD     -0.201
GROUP ! taken from glycerol
ATOM C2   CD31FB  -0.006  ALPHA -1.438 THOLE 1.015
ATOM H2   HDA1A    0.070
ATOM O2   OD31E    0.000  ALPHA -0.940 THOLE 0.670
ATOM HO2  HDP1A    0.322
ATOM LP2A LPD     -0.193
ATOM LP2B LPD     -0.193
GROUP ! taken from glycerol
ATOM C3   CD31FB  -0.006  ALPHA -1.127 THOLE 1.340
ATOM H3   HDA1A    0.070
ATOM O3   OD31E    0.000  ALPHA -0.881 THOLE 0.328
ATOM HO3  HDP1A    0.322
ATOM LP3A LPD     -0.193
ATOM LP3B LPD     -0.193
!
BOND O4 C1  C1 H1   C1 O1   O1 HO1
BOND C1 C2  C2 H2   C2 O2   O2 HO2
BOND C2 C3  C3 H3   C3 O3   O3 HO3
BOND C3 C4  C4 H4   C4 C5   C4 O4
BOND C5 H51 C5 H52  C5 O5   O5 HO5
BOND O1 LP1A O1 LP1B
BOND O2 LP2A O2 LP2B
BOND O3 LP3A O3 LP3B
BOND O4 LP4A O4 LP4B O4 LPX4
BOND O5 LP5A O5 LP5B

LONEPAIR relative LP1A O1 C1 HO1 distance 0.35 angle 110.0 dihe  91.0
LONEPAIR relative LP1B O1 C1 HO1 distance 0.35 angle 110.0 dihe 269.0
ANISOTROPY O1 C1 LP1A LP1B A11 0.8108 A22 1.2162

LONEPAIR relative LP2A O2 C2 HO2 distance 0.35 angle 110.0 dihe  91.0
LONEPAIR relative LP2B O2 C2 HO2 distance 0.35 angle 110.0 dihe 269.0
ANISOTROPY O2 C2 LP2A LP2B A11 0.8108 A22 1.2162

LONEPAIR relative LP3A O3 C3 HO3 distance 0.35 angle 110.0 dihe  91.0
LONEPAIR relative LP3B O3 C3 HO3 distance 0.35 angle 110.0 dihe 269.0
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ANISOTROPY O3 C3 LP3A LP3B A11 0.8108 A22 1.2162

LONEPAIR bisector LP4A O4 C1 C4 distance 0.35 angle 110.0 dihe  90.0
LONEPAIR bisector LP4B O4 C1 C4 distance 0.35 angle 110.0 dihe 270.0
LONEPAIR bisector LPX4 O4 C1 C4 distance 0.10 angle   0.0 dihe   0.0
ANISOTROPY O4 LPX4 LP4A LP4B A11 0.8889  A22 1.2222

LONEPAIR relative LP5A O5 C5 HO5 distance 0.35 angle 110.0 dihe  91.0
LONEPAIR relative LP5B O5 C5 HO5 distance 0.35 angle 110.0 dihe 269.0
ANISOTROPY O5 C5 LP5A LP5B A11 0.8108 A22 1.2162

! IC table; from minimized geometry*
IC C4   O4   C1   C2   1.4315  107.76  -22.45  106.42   1.5606
IC O4   C1   C2   C3   1.4298  106.42   -6.06  102.41   1.5494
IC C1   C2   C3   C4   1.5606  102.41   29.67  101.01   1.5315
IC C3   O4  *C4   C5   1.5315  102.23  127.07  113.37   1.5469
IC C3   O4  *C4   H4   1.5315  102.23 -114.55  106.16   1.1145
IC O4   C4   C5   O5   1.4315  113.37  172.78  110.88   1.4279
IC C4   C5   O5   HO5  1.5469  110.88  -89.23  111.11   0.9627
IC O5   C4  *C5   H51  1.4279  110.88  120.67  109.96   1.1012
IC O5   C4  *C5   H52  1.4279  110.88 -120.92  109.55   1.1021
IC C2   O4  *C1   O1   1.5606  106.42 -121.62  109.95   1.3992
IC O4   C1   O1   HO1  1.4298  109.95   66.51  107.28   0.9594
IC C2   O4  *C1   H1   1.5606  106.42  119.08  107.39   1.1123
IC C3   C1  *C2   H2   1.5494  102.41  115.35  109.45   1.1122
IC C3   C1  *C2   O2   1.5494  102.41 -123.37  114.05   1.4282
IC C1   C2   O2   HO2  1.5606  114.05  104.03  106.69   0.9675
IC C2   C4  *C3   O3   1.5494  101.01  118.58  111.21   1.4279
IC C2   C4  *C3   H3   1.5494  101.01 -119.18  112.30   1.1095
IC C4   C3   O3   HO3  1.5315  111.21  -32.26  108.53   0.9635
IC C2   C4  *C3   H4   1.5494  101.01  -68.34   28.96   2.1721

RESI ADEO           0.000  ! alpha-Deoxy-Ribose
!RING * 5 C1 C2 C3 C4 O4
!
!           HO5--O5
!                \       O4
!             H51--C5   /    \    H1
!                 / \  /      \  /
!              H52   C4        C1
!                   / \        / \
!                 H4   \      /   O1--HO1
!                      C3----C2
!                     /  \   / \
!               HO3--O3  H3  H21 H22
!
GROUP
ATOM O4   OD305A   0.000  ALPHA -0.684 THOLE 2.074
ATOM C1   CD31FA   0.124  ALPHA -1.022 THOLE 0.462
ATOM H1   HDA1A    0.070
ATOM O1   OD31E    0.000  ALPHA -1.176 THOLE 1.559
ATOM HO1  HDP1A    0.333
ATOM C4   CD31FC   0.112  ALPHA -1.014 THOLE 0.820
ATOM H4   HDA2E    0.069
```

```
ATOM LP1A LPD     -0.202
ATOM LP1B LPD     -0.202
ATOM LP4A LPD     -0.152
ATOM LP4B LPD     -0.152
ATOM LPX4 LPD      0.000 !dummy for anisotropic polarizability
GROUP ! taken from ETOH
ATOM C5   CD32A   -0.086  ALPHA -1.805 THOLE 0.353
ATOM H51  HDA2A    0.080
ATOM H52  HDA2A    0.080
ATOM O5   OD31A    0.000  ALPHA -0.732 THOLE 1.027
ATOM HO5  HDP1A    0.328
ATOM LP5A LPD     -0.201
ATOM LP5B LPD     -0.201
GROUP ! taken from THF
ATOM C2   CD325B  -0.142  ALPHA -1.617  THOLE 1.103! ALPHA @ALPHA1 THOLE
@THOLE1  !ALPHA -1.617  THOLE 1.103
ATOM H21  HDA2R5   0.071
ATOM H22  HDA2R5   0.071
GROUP ! taken from glycerol
ATOM C3   CD31FB  -0.006  ALPHA -1.127 THOLE 1.340
ATOM H3   HDA1A    0.070
ATOM O3   OD31E    0.000  ALPHA -0.881 THOLE 0.328
ATOM HO3  HDP1A    0.322
ATOM LP3A LPD     -0.193
ATOM LP3B LPD     -0.193
!
BOND O4 C1  C1 H1   C1 O1   O1 HO1
BOND C1 C2  C2 H21  C2 H22  C2 C3
BOND C3 H3  C3 O3   O3 HO3  C3 C4
BOND C4 H4  C4 O4   C4 C5   C5 H51
BOND C5 H52  C5 O5  O5 HO5
BOND O1 LP1A O1 LP1B
BOND O3 LP3A O3 LP3B
BOND O4 LP4A O4 LP4B O4 LPX4
BOND O5 LP5A O5 LP5B

LONEPAIR relative LP1A O1 C1 HO1 distance 0.35 angle 110.0 dihe  91.0
LONEPAIR relative LP1B O1 C1 HO1 distance 0.35 angle 110.0 dihe 269.0
ANISOTROPY O1 C1 LP1A LP1B A11 0.8108 A22 1.2162

LONEPAIR relative LP3A O3 C3 HO3 distance 0.35 angle 110.0 dihe  91.0
LONEPAIR relative LP3B O3 C3 HO3 distance 0.35 angle 110.0 dihe 269.0
ANISOTROPY O3 C3 LP3A LP3B A11 0.8108 A22 1.2162

LONEPAIR bisector LP4A O4 C1 C4 distance 0.35 angle 110.0 dihe  90.0
LONEPAIR bisector LP4B O4 C1 C4 distance 0.35 angle 110.0 dihe 270.0
LONEPAIR bisector LPX4 O4 C1 C4 distance 0.10 angle   0.0 dihe   0.0
ANISOTROPY O4 LPX4 LP4A LP4B A11 0.8889  A22 1.2222

LONEPAIR relative LP5A O5 C5 HO5 distance 0.35 angle 110.0 dihe  91.0
LONEPAIR relative LP5B O5 C5 HO5 distance 0.35 angle 110.0 dihe 269.0
ANISOTROPY O5 C5 LP5A LP5B A11 0.8108 A22 1.2162

! IC table; from minimized geometry*
```

```
IC C4   O4   C1   C2   1.4309  108.67  -19.01  106.25   1.5278
IC O4   C1   C2   C3   1.4258  106.25   -8.82  103.23   1.5178
IC C1   C2   C3   C4   1.5278  103.23   31.05  101.83   1.5232
IC C3   O4  *C4   C5   1.5232  101.44  124.05  113.01   1.5448
IC C3   O4  *C4   H4   1.5232  101.44 -115.42  106.74   1.1134
IC O4   C4   C5   O5   1.4309  113.01 -178.27  111.12   1.4304
IC C4   C5   O5   HO5  1.5448  111.12  -87.73  110.40   0.9643
IC O4   C4  *C5   H51  2.4824   32.04   59.71  109.84   1.1020
IC O4   C4  *C5   H52  2.4824   32.04  -58.37  108.86   1.1027
IC C2   O4  *C1   O1   1.5278  106.25  119.87  110.66   1.3905
IC O4   C1   O1   HO1  1.4258  110.66   60.11  106.63   0.9584
IC C2   O4  *C1   H1   1.5278  106.25 -119.86  107.45   1.1137
IC C3   C1  *C2   H21  1.5178  103.23  118.42  111.24   1.1030
IC C3   C1  *C2   H22  1.5178  103.23 -122.05  112.95   1.0962
IC C2   C4  *C3   O3   1.5178  101.83 -120.07  112.49   1.4116
IC C4   C3   O3   HO3  1.5232  112.49  -53.93  107.21   0.9673
IC C2   C4  *C3   H3   1.5178  101.83  117.41  109.93   1.1144

RESI BDEO           0.000  ! beta-Deoxy-Ribose
!RING * 5 C1 C2 C3 C4 O4
!
!          HO5--O5
!                \       O4
!             H51--C5   /    \    O1--HO1
!                 / \  /      \  /
!              H52   C4         C1
!                   / \         / \
!                 H4   \       /   H1
!                      C3----C2
!                     /  \   / \
!               HO3--O3  H3  H21 H22
!
!
GROUP
ATOM O4   OD305A   0.000  ALPHA -0.684 THOLE 2.074
ATOM C1   CD31FA   0.124  ALPHA -1.022 THOLE 0.462
ATOM H1   HDA1A    0.070
ATOM O1   OD31E    0.000  ALPHA -1.176 THOLE 1.559
ATOM HO1  HDP1A    0.333
ATOM C4   CD31FC   0.112  ALPHA -1.014 THOLE 0.820
ATOM H4   HDA2E    0.069
ATOM LP1A LPD     -0.202
ATOM LP1B LPD     -0.202
ATOM LP4A LPD     -0.152
ATOM LP4B LPD     -0.152
ATOM LPX4 LPD      0.000 !dummy for anisotropic polarizability
GROUP ! taken from ETOH
ATOM C5   CD32A   -0.086  ALPHA -1.805 THOLE 0.353
ATOM H51  HDA2A    0.080
ATOM H52  HDA2A    0.080
ATOM O5   OD31A    0.000  ALPHA -0.732 THOLE 1.027
ATOM HO5  HDP1A    0.328
ATOM LP5A LPD     -0.201
ATOM LP5B LPD     -0.201
```

```
GROUP ! taken from THF
ATOM C2   CD325B  -0.142  ALPHA -1.617  THOLE 1.103! ALPHA @ALPHA1 THOLE
@THOLE1  !ALPHA -1.617  THOLE 1.103
ATOM H21  HDA2R5   0.071
ATOM H22  HDA2R5   0.071
GROUP ! taken from glycerol
ATOM C3   CD31FB  -0.006  ALPHA -1.127 THOLE 1.340
ATOM H3   HDA1A    0.070
ATOM O3   OD31E    0.000  ALPHA -0.881 THOLE 0.328
ATOM HO3  HDP1A    0.322
ATOM LP3A LPD     -0.193
ATOM LP3B LPD     -0.193
!
BOND O4 C1  C1 H1   C1 O1   O1 HO1
BOND C1 C2  C2 H21  C2 H22  C2 C3
BOND C3 H3  C3 O3   O3 HO3  C3 C4
BOND C4 H4  C4 O4   C4 C5   C5 H51
BOND C5 H52  C5 O5  O5 HO5
BOND O1 LP1A O1 LP1B
BOND O3 LP3A O3 LP3B
BOND O4 LP4A O4 LP4B O4 LPX4
BOND O5 LP5A O5 LP5B

LONEPAIR relative LP1A O1 C1 HO1 distance 0.35 angle 110.0 dihe  91.0
LONEPAIR relative LP1B O1 C1 HO1 distance 0.35 angle 110.0 dihe 269.0
ANISOTROPY O1 C1 LP1A LP1B A11 0.8108 A22 1.2162

LONEPAIR relative LP3A O3 C3 HO3 distance 0.35 angle 110.0 dihe  91.0
LONEPAIR relative LP3B O3 C3 HO3 distance 0.35 angle 110.0 dihe 269.0
ANISOTROPY O3 C3 LP3A LP3B A11 0.8108 A22 1.2162

LONEPAIR bisector LP4A O4 C1 C4 distance 0.35 angle 110.0 dihe  90.0
LONEPAIR bisector LP4B O4 C1 C4 distance 0.35 angle 110.0 dihe 270.0
LONEPAIR bisector LPX4 O4 C1 C4 distance 0.10 angle   0.0 dihe   0.0
ANISOTROPY O4 LPX4 LP4A LP4B A11 0.8889  A22 1.2222

LONEPAIR relative LP5A O5 C5 HO5 distance 0.35 angle 110.0 dihe  91.0
LONEPAIR relative LP5B O5 C5 HO5 distance 0.35 angle 110.0 dihe 269.0
ANISOTROPY O5 C5 LP5A LP5B A11 0.8108 A22 1.2162

! IC table; from minimized geometry*
IC C4   O4   C1   C2   1.4309  108.67  -19.01  106.25   1.5278
IC O4   C1   C2   C3   1.4258  106.25   -8.82  103.23   1.5178
IC C1   C2   C3   C4   1.5278  103.23   31.05  101.83   1.5232
IC C3   O4  *C4   C5   1.5232  101.44  124.05  113.01   1.5448
IC C3   O4  *C4   H4   1.5232  101.44 -115.42  106.74   1.1134
IC O4   C4   C5   O5   1.4309  113.01 -178.27  111.12   1.4304
IC C4   C5   O5   HO5  1.5448  111.12  -87.73  110.40   0.9643
IC O4   C4  *C5   H51  2.4824   32.04   59.71  109.84   1.1020
IC O4   C4  *C5   H52  2.4824   32.04  -58.37  108.86   1.1027
IC C2   O4  *C1   O1   1.5278  106.25 -119.87  110.66   1.3905
IC O4   C1   O1   HO1  1.4258  110.66   60.11  106.63   0.9584
IC C2   O4  *C1   H1   1.5278  106.25  119.86  107.45   1.1137
IC C3   C1  *C2   H21  1.5178  103.23  118.42  111.24   1.1030
```

```
IC C3   C1  *C2   H22  1.5178  103.23 -122.05  112.95   1.0962
IC C2   C4  *C3   O3   1.5178  101.83 -120.07  112.49   1.4116
IC C4   C3   O3   HO3  1.5232  112.49  -53.93  107.21   0.9673
IC C2   C4  *C3   H3   1.5178  101.83  117.41  109.93   1.1144

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
! O-alkyl patches for furanose !
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
PRES FOMA           0.000  ! adding alpha O-methyl to C1 on aldopentose
dele atom HO1
dele atom LP1A
dele atom LP1B
GROUP
ATOM O4   OD305A   0.000  ALPHA -0.505 THOLE 0.807
ATOM C1   CD31FA   0.152  ALPHA -1.000 THOLE 0.487
ATOM H1   HDA1A    0.070
ATOM O1   OD30A    0.000  ALPHA -0.503 THOLE 0.443
ATOM CM   CD33E   -0.053  ALPHA -1.038 THOLE 0.667
ATOM HM1  HDA3A    0.069
ATOM HM2  HDA3A    0.069
ATOM HM3  HDA3A    0.069
ATOM C4   CD31FC   0.131  ALPHA -1.029 THOLE 0.909
ATOM H4   HDA2E    0.069
ATOM LPMA LPD     -0.121
ATOM LPMB LPD     -0.121
ATOM LP4A LPD     -0.167
ATOM LP4B LPD     -0.167
ATOM LPX4 LPD      0.000 !dummy for anisotropic polarizability
ATOM LPX1 LPD      0.000 !dummy for anisotropic polarizability
BOND O1 CM
BOND CM HM1  CM HM2  CM HM3
BOND O1 LPMA O1 LPMB O1 LPX1

LONEPAIR bisector LPMA O1 C1 CM distance 0.35 angle 110.0 dihe  90.0
LONEPAIR bisector LPMB O1 C1 CM distance 0.35 angle 110.0 dihe 270.0
LONEPAIR bisector LPX1 O1 C1 CM distance 0.10 angle   0.0 dihe   0.0
ANISOTROPY O1 LPX1 LPMA LPMB A11 0.8889  A22 1.2222

!    I    J    K    L      R(IK)   T(IKJ)    PHI   T(JKL)   R(KL)
IC   O4   C1   O1   CM     1.4477  109.89   66.08  108.74   1.4244
IC   C1   O1   CM   HM1    1.4355  108.74   59.11  111.44   1.0883
IC   HM1  O1  *CM   HM2    1.0883  111.44  119.69  113.64   1.0586
IC   HM3  O1  *CM   HM2    1.1131  110.64 -122.99  113.64   1.0586

PRES FOMB           0.000  ! adding beta O-methyl to C1 on aldopentose
dele atom HO1
dele atom LP1A
dele atom LP1B
GROUP
ATOM O4   OD305A   0.000  ALPHA -0.505 THOLE 0.807
ATOM C1   CD31FA   0.152  ALPHA -1.000 THOLE 0.487
ATOM H1   HDA1A    0.070
ATOM O1   OD30A    0.000  ALPHA -0.503 THOLE 0.443
ATOM CM   CD33E   -0.053  ALPHA -1.038 THOLE 0.667
```

```
ATOM HM1  HDA3A    0.069
ATOM HM2  HDA3A    0.069
ATOM HM3  HDA3A    0.069
ATOM C4   CD31FC   0.131  ALPHA -1.029 THOLE 0.909
ATOM H4   HDA2E    0.069
ATOM LPMA LPD     -0.121
ATOM LPMB LPD     -0.121
ATOM LP4A LPD     -0.167
ATOM LP4B LPD     -0.167
ATOM LPX4 LPD      0.000 !dummy for anisotropic polarizability
ATOM LPX1 LPD      0.000 !dummy for anisotropic polarizability
BOND O1 CM
BOND CM HM1  CM HM2  CM HM3
BOND O1 LPMA O1 LPMB O1 LPX1

LONEPAIR bisector LPMA O1 C1 CM distance 0.35 angle 110.0 dihe  90.0
LONEPAIR bisector LPMB O1 C1 CM distance 0.35 angle 110.0 dihe 270.0
LONEPAIR bisector LPX1 O1 C1 CM distance 0.10 angle   0.0 dihe   0.0
ANISOTROPY O1 LPX1 LPMA LPMB A11 0.8889  A22 1.2222

!    I    J    K    L      R(IK)   T(IKJ)    PHI   T(JKL)   R(KL)
IC   O4   C1   O1   CM     1.4138  114.30  -66.36  108.55   1.4077
IC   C1   O1   CM   HM1    1.4353  108.55   41.11  109.39   1.0734
IC   HM1  O1  *CM   HM2    1.0734  109.39  129.90  119.45   1.0441
IC   HM3  O1  *CM   HM2    1.1148  107.24 -121.74  119.45   1.0441
!furanoses, rima

end

read para card append
* Drude polarizable FF parameters
*

BONDS
!atom type      Kb       b0
!============================================
OD305A   CD31FA   280.0       1.430 !
CD31FC   OD305A   280.0       1.415 !
CD31FA   HDA1A    309.0       1.093 !
OD31E    CD31FA   350.0       1.400 !
CD31FA   CD31FB   222.5       1.520 !
CD31FB   HDA1A    309.0       1.093 !
CD31FB   OD31E    350.0       1.440 !
CD31FB   CD31FB   222.5       1.520 !
CD31FB   CD31FC   222.5       1.520 !
CD31FC   HDA2E    307.0       1.100 !
CD31FC   CD32A    222.5       1.510 !
CD31FA   CD325B   222.5       1.520 !
CD325B   CD31FB   222.5       1.520 !
OD30A   CD31FA    280.0       1.430 !

ANGLES
!atom types     Ktheta  Theta0   Kub     S0
!================================================
```

```
CD31FA   OD305A   CD31FC    95.00    111.00 !
OD305A   CD31FA   HDA1A     70.00    107.30 !
OD305A   CD31FA   OD31E     90.00    111.50 !
OD305A   CD31FA   CD31FB    45.00    111.10 !
OD305A   CD31FC   HDA2E     70.00    107.30 !
OD305A   CD31FC   CD32A     75.00    106.50 !
OD305A   CD31FC   CD31FB    45.00    111.50 !
OD31E    CD31FA   HDA1A     47.00    110.50 !
CD31FB   CD31FA   HDA1A     35.00    111.40   22.53   2.179 !
CD31FA   CD31FB   HDA1A     35.00    111.40   22.53   2.179 !
CD31FA   OD31E    HDP1A     59.00    108.00 !
CD31FB   OD31E    HDP1A     59.00    108.00 !
HDA1A    CD31FB   OD31E     47.00    110.50 !
CD31FB   CD31FB   OD31E     65.30    109.00 !
CD31FC   CD32A    HDA2A     34.60    110.10   22.53   2.179  !
CD31FB   CD31FB   HDA1A     35.00    111.40   22.53   2.179  !
CD31FC   CD31FB   OD31E     65.30    109.00 !
CD31FC   CD31FB   HDA1A     35.00    111.40   22.53   2.179  !
CD31FC   CD31FB   CD31FB    58.00    109.50   11.16   2.561  !
CD31FC   CD32A    OD31A     63.00    111.00 !
HDA2E    CD31FC   CD32A     34.50    110.10   22.53   2.179  !
CD31FA   CD31FB   CD31FB    58.00    109.50   11.16   2.561  !
CD31FA   CD31FB   OD31E     65.30    109.00 !
CD32A    CD31FC   CD31FB    58.00    109.50   11.16   2.561  !
HDA2E    CD31FC   CD31FB    35.00    111.40   22.53   2.179  !
CD31FB   CD31FA   OD31E     65.30    109.00 !
OD305A   CD31FA   CD325B    45.00    111.10 !
HDA1A    CD31FA   CD325B    35.00    111.40   22.53   2.179 !
OD31E    CD31FA   CD325B    65.30    109.00 !
CD31FA   CD325B   HDA2R5    35.00    111.40   22.53   2.179 !
CD31FB   CD325B   HDA2R5    35.00    111.40   22.53   2.179 !
CD31FA   CD325B   CD31FB    58.00    109.50   11.16   2.561 !
CD31FC   CD31FB   CD325B    58.00    109.50   11.16   2.561  !
CD325B   CD31FB   HDA1A     35.00    111.40   22.53   2.179  !
CD325B   CD31FB   OD31E     65.30    109.00 !
OD305A   CD31FA   OD30A     90.00    111.50 !
HDA1A    CD31FA   OD30A     47.00    110.50 !
OD30A    CD31FA   CD31FB    65.30    109.00 !
CD31FA   OD30A    CD33E     95.00    109.70 !

DIHEDRALS
!atom types            Kchi     n     delta
!================================================
!
!furanoses, rima
OD305A   CD31FA   CD31FB   HDA1A   0.190    3     0.00 !
OD305A   CD31FC   CD32A    HDA2A   0.200    3     0.00 !
OD305A   CD31FC   CD31FB   HDA1A   0.190    3     0.00 !
CD31FA   OD305A   CD31FC   HDA2E   0.300    3     0.00 !
HDA1A    CD31FA   OD305A   CD31FC  0.300    3     0.00 !
CD31FA   CD31FB   CD31FB   HDA1A   0.190    3     0.00 !
HDP1A    OD31E    CD31FA   HDA1A   0.060    1     0.00 !
HDP1A    OD31E    CD31FA   HDA1A   0.060    2     0.00 !
HDP1A    OD31E    CD31FA   HDA1A   0.000    3     0.00 !
```

```
HDA1A    CD31FA   CD31FB   HDA1A   0.190    3     0.00 !
OD31E    CD31FB   CD31FA   HDA1A   0.270    1     0.00 !
OD31E    CD31FB   CD31FA   HDA1A   0.050    2     0.00 !
OD31E    CD31FB   CD31FA   HDA1A   0.120    3     0.00 !
CD31FB   CD31FB   CD31FA   HDA1A   0.190    3     0.00 !
OD31E    CD31FA   CD31FB   HDA1A   0.270    1     0.00 !
OD31E    CD31FA   CD31FB   HDA1A   0.050    2     0.00 !
OD31E    CD31FA   CD31FB   HDA1A   0.120    3     0.00 !
CD31FC   CD31FB   CD31FB   HDA1A   0.190    3     0.00 !
HDA2E    CD31FC   CD32A    HDA2A   0.190    3     0.00 !
HDA2E    CD31FC   CD32A    OD31A   0.175    3     0.00 !
HDA2E    CD31FC   CD31FB   CD31FB  0.190    3     0.00 !
HDA2E    CD31FC   CD31FB   HDA1A   0.190    3     0.00 !
HDA2E    CD31FC   CD31FB   OD31E   0.270    1     0.00 !
HDA2E    CD31FC   CD31FB   OD31E   0.050    2     0.00 !
HDA2E    CD31FC   CD31FB   OD31E   0.120    3     0.00 !
CD31FB   CD31FB   CD31FC   CD32A   0.410    3   180.00 !
HDA1A    CD31FB   CD31FC   CD32A   0.190    3     0.00 !
CD31FB   CD31FC   CD32A    HDA2A   0.190    3     0.00 !
HDA1A    CD31FB   OD31E    HDP1A   0.060    1     0.00 !
HDA1A    CD31FB   OD31E    HDP1A   0.060    2     0.00 !
HDA1A    CD31FB   OD31E    HDP1A   0.000    3     0.00 !
HDA1A    CD31FB   CD31FB   HDA1A   0.190    3     0.00 !
OD31E    CD31FB   CD31FB   HDA1A   0.270    1     0.00 !
OD31E    CD31FB   CD31FB   HDA1A   0.050    2     0.00 !
OD31E    CD31FB   CD31FB   HDA1A   0.120    3     0.00 !
!fitdih furanoses
CD31FA   CD31FB   CD31FB   CD31FC      1.0392  1     0.00 !
CD31FA   CD31FB   CD31FB   CD31FC      0.9303  2     0.00 !
CD31FA   CD31FB   CD31FB   CD31FC      0.7483  3     0.00 !
CD31FA   CD31FB   CD31FB   OD31E       0.2742  1     0.00 !
CD31FA   CD31FB   CD31FB   OD31E       0.0453  2     0.00 !
CD31FA   CD31FB   CD31FB   OD31E       0.5903  3   180.00 !
CD31FA   CD31FB   OD31E    HDP1A       0.2611  1     0.00 !
CD31FA   CD31FB   OD31E    HDP1A       0.5154  2     0.00 !
CD31FA   CD31FB   OD31E    HDP1A       0.1830  3     0.00 !
CD31FB   CD31FC   OD305A   CD31FA      0.6882  1     0.00 !
CD31FB   CD31FC   OD305A   CD31FA      0.7079  2     0.00 !
CD31FB   CD31FC   OD305A   CD31FA      0.7433  3     0.00 !
CD32A    CD31FC   OD305A   CD31FA      0.9269  1   180.00 !
CD32A    CD31FC   OD305A   CD31FA      0.5245  2     0.00 !
CD32A    CD31FC   OD305A   CD31FA      0.2728  3     0.00 !
CD31FB   CD31FA   OD31E    HDP1A       0.3772  1     0.00 !
CD31FB   CD31FA   OD31E    HDP1A       0.4430  2     0.00 !
CD31FB   CD31FA   OD31E    HDP1A       0.1763  3   180.00 !
CD31FB   CD31FB   CD31FC   OD305A      0.5081  1     0.00 !
CD31FB   CD31FB   CD31FC   OD305A      0.4468  2     0.00 !
CD31FB   CD31FB   CD31FC   OD305A      0.3245  3     0.00 !
CD31FB   CD31FB   OD31E    HDP1A       0.4056  1     0.00 !
CD31FB   CD31FB   OD31E    HDP1A       0.4316  2     0.00 !
CD31FB   CD31FB   OD31E    HDP1A       0.2648  3     0.00 !
OD31E    CD31FA   CD31FB   CD31FB      0.1215  1     0.00 !
OD31E    CD31FA   CD31FB   CD31FB      0.6332  2   180.00 !
OD31E    CD31FA   CD31FB   CD31FB      0.3012  3   180.00 !
```

```
OD305A   CD31FA   CD31FB   CD31FB       0.4187  1     0.00 !
OD305A   CD31FA   CD31FB   CD31FB       0.2784  2     0.00 !
OD305A   CD31FA   CD31FB   CD31FB       0.0200  3     0.00 !
CD31FB   CD31FC   CD32A    OD31A        0.5003  1   180.00 !
CD31FB   CD31FC   CD32A    OD31A        0.2096  2     0.00 !
CD31FB   CD31FC   CD32A    OD31A        0.0681  3     0.00 !
CD31FC   CD31FB   CD31FB   OD31E        0.3659  1   180.00 !
CD31FC   CD31FB   CD31FB   OD31E        0.2749  2     0.00 !
CD31FC   CD31FB   CD31FB   OD31E        0.8934  3     0.00 !
CD31FC   CD31FB   OD31E    HDP1A        0.3741  1     0.00 !
CD31FC   CD31FB   OD31E    HDP1A        0.0242  2     0.00 !
CD31FC   CD31FB   OD31E    HDP1A        0.1025  3     0.00 !
CD31FC   CD32A    OD31A    HDP1A        0.3581  1     0.00 !
CD31FC   CD32A    OD31A    HDP1A        0.4874  2     0.00 !
CD31FC   CD32A    OD31A    HDP1A        0.1880  3     0.00 !
CD31FB   CD31FA   OD305A   CD31FC       0.8201  1     0.00 !
CD31FB   CD31FA   OD305A   CD31FC       0.5947  2     0.00 !
CD31FB   CD31FA   OD305A   CD31FC       0.2261  3     0.00 !
OD31E    CD31FA   OD305A   CD31FC       1.1409  1   180.00 !
OD31E    CD31FA   OD305A   CD31FC       1.0488  2     0.00 !
OD31E    CD31FA   OD305A   CD31FC       0.3135  3     0.00 !
OD31E    CD31FB   CD31FC   CD32A        0.1541  1     0.00 !
OD31E    CD31FB   CD31FC   CD32A        0.3485  2   180.00 !
OD31E    CD31FB   CD31FC   CD32A        0.0817  3     0.00 !
OD31E    CD31FA   CD31FB   OD31E        0.2182  1   180.00 !
OD31E    CD31FA   CD31FB   OD31E        0.1501  2   180.00 !
OD31E    CD31FA   CD31FB   OD31E        0.0060  3     0.00 !
OD305A   CD31FA   CD31FB   OD31E        0.4388  1     0.00 !
OD305A   CD31FA   CD31FB   OD31E        0.4009  2   180.00 !
OD305A   CD31FA   CD31FB   OD31E        0.3834  3     0.00 !
OD31E    CD31FB   CD31FB   OD31E        0.4307  1   180.00 !
OD31E    CD31FB   CD31FB   OD31E        0.6208  2   180.00 !
OD31E    CD31FB   CD31FB   OD31E        0.4495  3   180.00 !
OD31E    CD31FB   CD31FC   OD305A       0.7740  1   180.00 !
OD31E    CD31FB   CD31FC   OD305A       0.0201  2     0.00 !
OD31E    CD31FB   CD31FC   OD305A       0.5125  3     0.00 !
OD305A   CD31FA   OD31E    HDP1A        0.7166  1     0.00 !
OD305A   CD31FA   OD31E    HDP1A        1.0359  2     0.00 !
OD305A   CD31FA   OD31E    HDP1A        0.6708  3     0.00 !
OD305A   CD31FC   CD32A    OD31A        0.9708  1   180.00 !
OD305A   CD31FC   CD32A    OD31A        0.7860  2     0.00 !
OD305A   CD31FC   CD32A    OD31A        0.0222  3   180.00 !
OD305A   CD31FA   CD325B   HDA2R5       0.190    3     0.00 !
CD31FA   CD325B   CD31FB   CD31FC       1.0392   1     0.00 !
CD31FA   CD325B   CD31FB   CD31FC       0.9303   2     0.00 !
CD31FA   CD325B   CD31FB   CD31FC       0.7483   3     0.00 !
CD31FA   CD325B   CD31FB   HDA1A        0.190    3     0.00 !
HDA1A    CD31FA   CD325B   HDA2R5       0.190    3     0.00 !
HDA1A    CD31FA   CD325B   CD31FB       0.190    3     0.00 !
OD31E    CD31FA   CD325B   HDA2R5       0.270    1     0.00 !
OD31E    CD31FA   CD325B   HDA2R5       0.050    2     0.00 !
OD31E    CD31FA   CD325B   HDA2R5       0.120    3     0.00 !
CD31FC   CD31FB   CD325B   HDA2R5       0.190    3     0.00 !
HDA2E    CD31FC   CD31FB   CD325B       0.190    3     0.00 !
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CD32A    CD31FC   CD31FB   CD325B       0.410    3   180.00 !
HDA2R5   CD325B   CD31FB   HDA1A        0.190    3     0.00 !
HDA2R5   CD325B   CD31FB   OD31E        0.270    1     0.00 !
HDA2R5   CD325B   CD31FB   OD31E        0.050    2     0.00 !
HDA2R5   CD325B   CD31FB   OD31E        0.120    3     0.00 !
OD31E    CD31FB   CD325B   CD31FA       1.6826   1     0.00 !
OD31E    CD31FB   CD325B   CD31FA       0.3708   2   180.00 !
OD31E    CD31FB   CD325B   CD31FA       1.0478   3   180.00 !
CD325B   CD31FA   OD31E    HDP1A        0.5210   1     0.00 !
CD325B   CD31FA   OD31E    HDP1A        0.2497   2     0.00 !
CD325B   CD31FA   OD31E    HDP1A        0.2382   3     0.00 !
CD325B   CD31FB   CD31FC   OD305A       0.4277   1   180.00 !
CD325B   CD31FB   CD31FC   OD305A       0.3937   2   180.00 !
CD325B   CD31FB   CD31FC   OD305A       0.3030   3   180.00 !
CD325B   CD31FB   OD31E    HDP1A        0.9384   1     0.00 !
CD325B   CD31FB   OD31E    HDP1A        0.0104   2     0.00 !
CD325B   CD31FB   OD31E    HDP1A        0.2568   3     0.00 !
OD31E    CD31FA   CD325B   CD31FB       0.2311   1     0.00 !
OD31E    CD31FA   CD325B   CD31FB       0.3468   2   180.00 !
OD31E    CD31FA   CD325B   CD31FB       0.0532   3     0.00 !
OD305A   CD31FA   CD325B   CD31FB       0.2237   1     0.00 !
OD305A   CD31FA   CD325B   CD31FB       0.1834   2     0.00 !
OD305A   CD31FA   CD325B   CD31FB       0.1093   3     0.00 !
CD325B   CD31FA   OD305A   CD31FC       0.3531   1     0.00 !
CD325B   CD31FA   OD305A   CD31FC       0.1220   2     0.00 !
CD325B   CD31FA   OD305A   CD31FC       0.2640   3   180.00 !
CD31FA   OD30A    CD33E    HDA3A        0.000    3     0.00 !
HDA1A    CD31FA   OD30A    CD33E        0.000    3     0.00 !
OD30A    CD31FA   CD31FB   HDA1A        0.000    3     0.00 !
OD30A    CD31FA   CD31FB   CD31FB       1.3664   1     0.00 !
OD30A    CD31FA   CD31FB   CD31FB       1.0474   2     0.00 !
OD30A    CD31FA   CD31FB   CD31FB       1.8077   3   180.00 !
CD31FB   CD31FA   OD30A    CD33E        1.3198   1   180.00 !
CD31FB   CD31FA   OD30A    CD33E        0.5302   2   180.00 !
CD31FB   CD31FA   OD30A    CD33E        0.0701   3     0.00 !
OD30A    CD31FA   CD31FB   OD31E        0.2039   1   180.00 !
OD30A    CD31FA   CD31FB   OD31E        1.6691   2   180.00 !
OD30A    CD31FA   CD31FB   OD31E        1.6110   3     0.00 !
OD30A    CD31FA   OD305A   CD31FC       0.8447   1     0.00 !
OD30A    CD31FA   OD305A   CD31FC       1.8332   2     0.00 !
OD30A    CD31FA   OD305A   CD31FC       0.6738   3     0.00 !
OD305A   CD31FA   OD30A    CD33E        0.4818   1   180.00 !
OD305A   CD31FA   OD30A    CD33E        1.2301   2     0.00 !
OD305A   CD31FA   OD30A    CD33E        1.0062   3     0.00 !

NBFIX
!
OD31A   ODW    -0.17790  3.52190 !
OD31E   ODW    -0.17990  3.48690 !
END
```