Supplementary Information

Compatibility of GROMOS-Derived Atomic Parameters for Lipopolysaccharide Membranes with the SPC/E Water Model and Alternative Long-Range Electrostatic Treatments Using Single Nonbonded Cutoff and Atom-Based Charge Schemes

Manoela P. M. Lima,[a,#] Manuela Nader,[a] Denys E. S. Santos[a,#] and Thereza A. Soares *[,a]

[a]*Departamento de Química Fundamental, Universidade Federal de Pernambuco, 50740-560 Recife-PE, Brazil*

*e-mail: thereza.soares@ufpe.br
[#]These authors contributed equally.

Table S1. Topologies (atom type, bond, angle, torsion parameters) for the rough LPS from *P. aeruginosa*.[1,2] The GROMOS parameter set 54A7 was used.[3] Atomic parameters, topologies and atomic coordinates for the simulated OM models compatible with the GROMACS suite of programs are available for download at dqfnet.ufpe.br/biomat

Monosaccharide	Atom type	Atom charge
3-(Acetyl amino)-3-deoxy-D-glucose	CH1 or CH2	0.232
	C	0.108
	CH1	0.336
	CH1 aliphatic	0.376
	OA ether	–0.480
	OA pyranose ring	–0.642
	OA hydroxyl	–0.360
	O	-0.450
	N	-0.200
	H	0.310
3-Deoxy-D-manno-oct-2-ulosonic acid	CH1	0.232
	CH1 aliphatic	0.376
	C	0.360
Heptose	CH1	0.232
	CH1 aliphatic	0.376
	OA hydroxyl	–0.360
	OA pyranose ring	–0.642
	OA ether	–0.480
	H	0.41
Phosphate HPO_4^-	OM	–0.884
	OA	–0.733
	PA	1.346
	H	0.43
2-(2-L-Alanyl)-2-deoxy-D-galactosamine	CH1	0.232
	CH2 OR CH1 or CH3	0.000
	CH1 aliphatic	0.376

	OA pyranose ring	–0.642		C	0.270
	OM	–0.680		H	0.310
	OA hydroxyl	–0.360		N	–0.310
	OA ether	–0.480		OA hydroxyl	–0.360
	H	0.410		OM	–0.635
				OA ether	–0.480
Dodecanoyl acid(12:0-LP1)	C	–0.140	2-alpha-L-Rhamnose	CH2 or CH1	0.232
	CH2	0.000		CH1 aliphatic	0.376
	C	0.580		CH3	0.000
	OE	–0.360		OA ether	–0.480
				OA pyranose ring	–0.642
				H	0.232
3-Hydroxydecanoyl acid 10:0 (3-OH) (LP2)	CH1	0.232	L-Glycero-D-manno-heptose-7-formmamide	CH1	0.232
	CH2	0.000		CH1 aliphatic	0.376
	C	0.580		CH2	0.160

	H	0.410
	O	–0.380
	OA pyranose ring	–0.642
6-alpha-D-Glucose	CH1	0.232
	CH1 aliphatic	0.376
	OA ether	–0.480
	OA pyranose ring	–0.642
	H	0.41
	C	0.580
	OA ether	–0.480
	OA pyranose ring	–0.642
	OE	–0.360
	O	–0.380
	NT	–0.830
	H	0.415
	H	0.410

Bond-type	k_b / (× 10^6 kJ mol^{-1} nm^{-4})	b_o / nm	Bond-type	k_b / (× 10^6 kJ mol^{-1} nm^{-4})	b_o / nm
CHn−CHn	5.43	0.152	N−C	11.80	0.133
			C−HC	12.30	0.109
CHn−OA	8.18	0.143	OA−H	15.70	0.100
CHn−N or CHn−NL	8.71	0.147	C−O	16.60	0.123
OA−P	4.84	0.1630	H−OA	15.7	0.100
OM−P	8.60	0.148	C− NT	10.6	0.133
CHn−OA	6.1	0.1435	CR1−N,NR,CR1,C	11.80	0.133
N−H or NL−H	18.70	0.100	CHn−NR (6-ring)	7.64	0.148
CHn−C	7.15	0.1530			
Bond-angle type	k_θ / (kJ mol^{-1})	θ_o / degree	Bond-angle type	k_θ / (kJ mol^{-1})	θ_o / degree
C−NT−H H−NT−H	390	120.0	CHn−CHn−N CHn−CHn−OA CHn−CHn−C	520	109.5
OA−CH_1−CH_1 OA−CHn−OA	320	109.5	H−N−CHn	460	115

CHn−CHn−CHn	285	109.5	H−N−C	415	123.0
CHn−OA−P	530	120	N−C−O	730	124.0
OM−P−OA	450	109.5	N−C−CHn	610	115.0
OA−P−OA	420	103.0	C−CHn−CHn CHn−CHn−CHn CHn−CHn−N	530	111.0
OM−P−OM	780	120.0	CH_1−OA−CH_1	380	109.5
CHn−OE−C CHn−C−OM	635	117.0	CH_2−OA−H P−OA−H	450	109.5
OE−C−C OE−C−O CHn−N−C	700	122.0	OM−C−OM	770	126.0
OE−CHn−CHn	545	113.0			

Improper dihedral	k_ξ / (kJ mol^{-1} rad^{-2})	ξ_o / degree	Improper dihedral	k_ξ / (kJ mol^{-1} rad^{-2})	ξ_o / degree
CHn−CHn−OE−CHn	334.85	35.26	C−CHn−O−O	167.42	0
CHn−O−C−CH_2	334.85	35.26	C−CH_2−CH_1−H	167.42	0
CH_1−N−C−CH_3 (2-(2-L-alanyl)-2-deoxy-D-galactosamine)	334.85	35.26	C−CH_2−N−O	167.42	0
CH_1−OA−OA−CH_1	334.85	35.26	CH1−OM−OM−C (rhamnose)	167.42	0
			N−C−CH_1−H (acyl chain)	167.42	0

Dihedral angle	k_ϕ / (kJ mol^{-1})	δ	n	Dihedral angle	k_ϕ / (kJ mol^{-1})	δ	n
CH_1−CH_1−OA−P	3.77	0	3	OA−CH_1−CH_1−CH_1	0.7	180	6
OA−CH_1−CH_1−OE	2.09	0	2	CH_1−CH_1−CH_1−CH_1	5.92	0	3
OA−CH_1−CH_1−P	2.80	0	3	CH_1−OA−P−OA or OA−P−OA−H	3.14	0	2
CH_1−CH_1−OA−C	3.77	0	3	OA−CH_1−CH_1−N	0.418	0	2
CH_1−CH_1−CH_1−N	0	0	2	CH_1−OA−C−C	24.0	180	2

OA−C−C−C N−C−CH_1−CH_1	1.0	0	6	CH_1−CH_1−N−C	3.9	0	3
CH_1−N−C−CH_2	24.0	180	0	OA−CH_1−CH_1−OA	9.35	180	1
OA−CHn−CHn−OA	9.5	0	3	OA−CHn−OA−CHn	9.45	180	1
OA−CH_1−OA−CH_1	3.65	0	3	OA−CHn−OA−CHn	3.41	180	1
OA−CHn−OA−CHn	4.69	0	3	CHn−CHn−CHn−OA	2.67	180	1

Exclusion

OA−H	OM−H	within the phosphate group

k_b, k_θ, k_ξ, k_ϕ: force constants; b_o: bond-length distance reference value; θ_o: bond-angle reference value; ξ_o: improper-dihedral reference value; δ: associated phase shift; n: multiplicity of the term.

Table S2. Benchmarks for simulated systems (total of 220825 atoms *per* system) run on GPU and CPU cores

	ns/day	h/ns	cores	core.hours
GPU	15.576	1.541	12	1849.2
CPU	6.972	3.443	40	13772.0

References

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