

Simulating Gram-Negative Bacterial Outer Membrane: A Coarse Grain Model

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Figure S1: Coarse grain (transparent beads) mapping of individual residues in the LPS molecule overlaid on atomistic (ball and stick model).

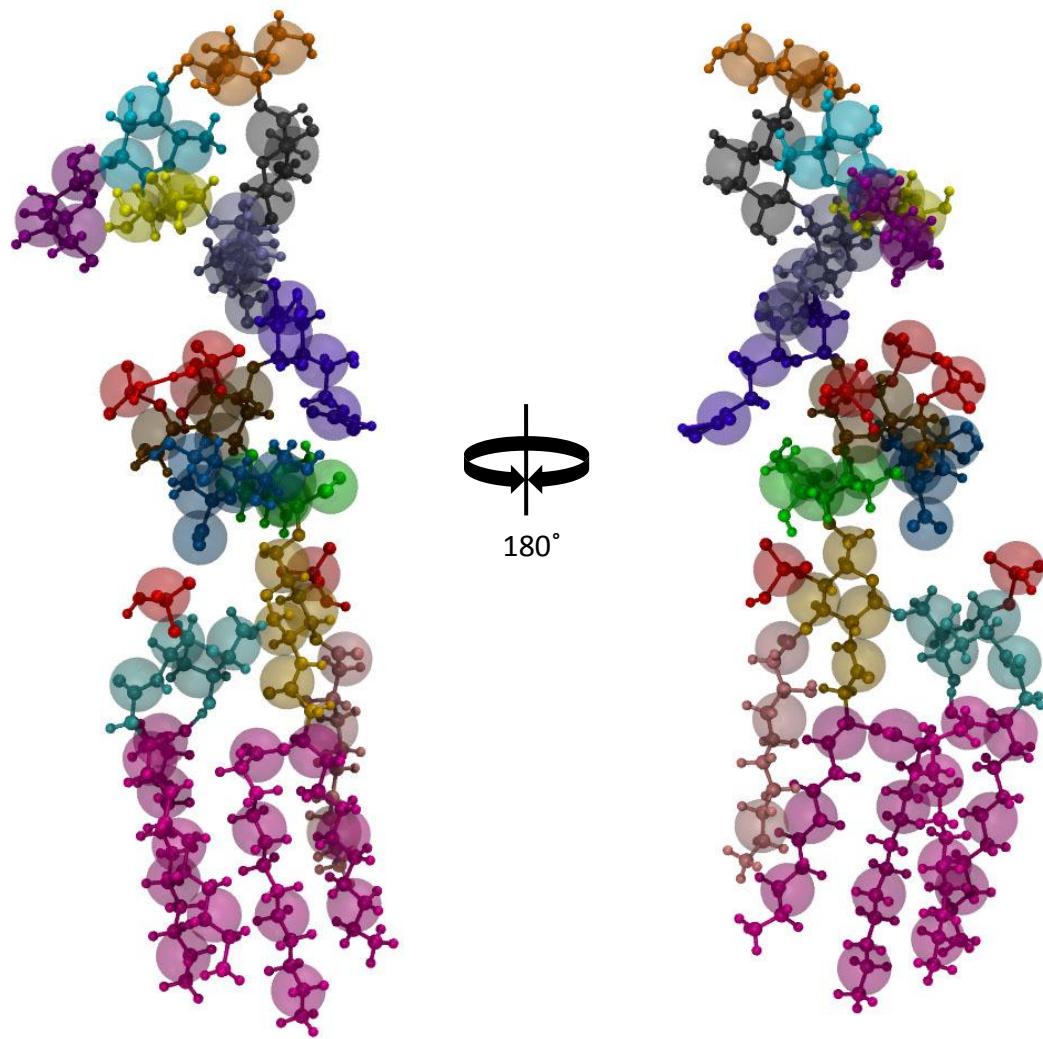


Table S1. Benchmarking data of time-averaged bond distances (nm) and standard deviation of coarse grained LPS and the underlying atomistic structure. Percent error is calculated based on Equation 3.

Beads		Coarse grained		Atomistic		% error
<i>i</i>	<i>j</i>	$\langle R_{CG} \rangle$	Std. Dev	$\langle R_{Atm} \rangle$	Std. Dev	
L1	L2	0.368	± 0.012	0.3632	± 0.0081	1.345
L1	L3	0.287	± 0.013	0.2945	± 0.0053	2.340
L2	L3	0.293	± 0.011	0.2861	± 0.0022	2.454
L1	L4	0.322	± 0.010	0.3114	± 0.0121	3.414
L4	L5	0.274	± 0.012	0.2650	± 0.0084	3.488
L4	L6	0.304	± 0.012	0.3050	± 0.0042	0.322
L5	L6	0.261	± 0.013	0.2705	± 0.0025	3.491
L4	L9	0.332	± 0.013	0.3264	± 0.0052	1.725
L7	L8	0.281	± 0.013	0.2800	± 0.0071	0.359
L7	L9	0.370	± 0.012	0.3787	± 0.0056	2.287
L8	L9	0.269	± 0.011	0.2772	± 0.0027	2.949
L7	L19	0.354	± 0.012	0.3439	± 0.0054	2.936
L10	L11	0.276	± 0.013	0.2717	± 0.0068	1.573
L10	L12	0.367	± 0.012	0.3752	± 0.0012	2.176
L11	L12	0.325	± 0.013	0.3216	± 0.0012	1.044
L10	L14	0.336	± 0.013	0.3450	± 0.0084	2.606
L13	L14	0.363	± 0.012	0.3745	± 0.0045	3.078
L13	L15	0.277	± 0.013	0.2792	± 0.0025	0.781
L14	L15	0.295	± 0.012	0.2920	± 0.0087	1.038
L13	L19	0.364	± 0.011	0.3738	± 0.0056	2.611
L19	L20	0.317	± 0.013	0.3127	± 0.0078	1.366
L16	L17	0.320	± 0.010	0.3240	± 0.0047	1.235
L16	L19	0.245	± 0.012	0.2480	± 0.0089	1.210
L16	L20	0.323	± 0.013	0.3159	± 0.0056	2.249
L17	L18	0.246	± 0.011	0.2510	± 0.0078	1.992
L16	L22	0.317	± 0.012	0.3100	± 0.0045	2.258
L21	L22	0.271	± 0.013	0.2753	± 0.0056	1.549
L21	L23	0.331	± 0.012	0.3236	± 0.0078	2.272
L22	L23	0.302	± 0.014	0.2971	± 0.0094	1.640
L23	L24	0.382	± 0.013	0.3758	± 0.0078	1.656
L21	L36	0.396	± 0.012	0.3887	± 0.0074	1.884
L36	L37	0.277	± 0.011	0.2820	± 0.0011	1.773
L36	L41	0.308	± 0.012	0.3152	± 0.0042	2.278
L36	L35	0.261	± 0.012	0.2690	± 0.0056	2.974
L37	L40	0.301	± 0.012	0.2929	± 0.0082	2.761
L37	L35	0.264	± 0.011	0.2562	± 0.0031	3.064

L37	L38	0.326	± 0.012	0.3164	± 0.0087	3.041
L38	L39	0.285	± 0.013	0.2922	± 0.0056	2.476
L35	L27	0.280	± 0.011	0.2751	± 0.0045	1.781
L27	L25	0.267	± 0.011	0.2604	± 0.0087	2.535
L27	L28	0.271	± 0.012	0.2786	± 0.0091	2.742
L28	L29	0.232	± 0.012	0.2354	± 0.0047	1.461
L25	L26	0.266	± 0.010	0.2740	± 0.0056	2.920
L25	L28	0.240	± 0.011	0.2333	± 0.0078	2.881
L27	L30	0.368	± 0.011	0.3590	± 0.0065	2.507
L30	L31	0.262	± 0.010	0.2590	± 0.0074	1.158
L30	L32	0.252	± 0.012	0.2547	± 0.0056	1.045
L30	L33	0.231	± 0.011	0.2260	± 0.0047	2.212
L32	L33	0.241	± 0.012	0.2456	± 0.0036	1.885
L33	L34	0.288	± 0.011	0.2834	± 0.0014	1.612
L25	L55	0.328	± 0.011	0.3325	± 0.0056	1.346
L55	L54	0.321	± 0.011	0.3202	± 0.0023	0.259
L55	L56	0.301	± 0.010	0.3066	± 0.0087	1.826
L54	L56	0.281	± 0.012	0.2856	± 0.0047	1.611
L54	L57	0.276	± 0.011	0.2793	± 0.0096	1.182
L56	L58	0.311	± 0.012	0.3182	± 0.0021	2.247
L56	L66	0.316	± 0.011	0.3120	± 0.0072	1.282
L66	L67	0.387	± 0.011	0.3824	± 0.0087	1.205
L67	L68	0.566	± 0.011	0.5799	± 0.0095	2.389
L57	L59	0.391	± 0.010	0.4026	± 0.0078	2.881
L59	L62	0.310	± 0.012	0.3119	± 0.0056	0.593
L59	L60	0.459	± 0.011	0.4673	± 0.0023	1.766
L60	L61	0.398	± 0.012	0.4053	± 0.0045	1.801
L62	L63	0.369	± 0.011	0.3725	± 0.0036	0.941
L63	L64	0.457	± 0.011	0.4466	± 0.0071	2.334
L64	L65	0.393	± 0.013	0.3901	± 0.0096	0.732
L54	L45	0.378	± 0.010	0.3891	± 0.0045	2.860
L45	L42	0.338	± 0.012	0.3438	± 0.0023	1.698
L45	L44	0.269	± 0.011	0.2720	± 0.0091	1.103
L42	L44	0.293	± 0.012	0.2852	± 0.0560	2.719
L42	L46	0.279	± 0.013	0.2843	± 0.0036	1.868
L42	L43	0.323	± 0.011	0.3310	± 0.0063	2.417
L43	L47	0.379	± 0.011	0.3720	± 0.0054	1.869
L47	L50	0.294	± 0.010	0.2898	± 0.0023	1.457
L50	L51	0.398	± 0.012	0.4099	± 0.0074	2.908
L51	L52	0.451	± 0.013	0.4416	± 0.0051	2.120
L52	L53	0.384	± 0.012	0.3810	± 0.0024	0.787
L47	L48	0.459	± 0.011	0.4491	± 0.0094	2.204

L48	L49	0.396 \pm 0.010	0.4035 \pm 0.0058	1.864
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Table S2. Benchmarking data of time-averaged bond angles (degrees) and standard deviation of coarse grained LPS and the underlying atomistic structure. Percent error is calculated based on Equation 3.

Angle	Coarse grained		Atomistic		% error
	$\langle \theta_{CG} \rangle$	Std. Dev	$\langle \theta_{Atm} \rangle$	Std. Dev	
L3-L1-L4	119.1	± 8.12	121.0	± 8.2	1.6
L3-L1-L2	51.3	± 3.01	50.3	± 2.9	2.0
L1-L3-L2	78.7	± 4.2	81.4	± 4.3	3.3
L2-L1-L4	51.7	± 6.9	52.4	± 7.0	1.3
L1-L4-L5	117.9	± 8	115.5	± 7.8	2.0
L1-L4-L6	124.7	± 10	126.7	± 10.2	1.6
L4-L5-L6	69.4	± 4.07	71.8	± 4.2	3.3
L1-L4-L9	123.5	± 9.4	122.0	± 9.3	1.2
L6-L4-L9	98.445	± 6.01	99.6	± 6.1	1.2
L4-L9-L8	124	± 12.3	126.0	± 12.5	1.6
L9-L8-L7	84.7	± 4.8	82.2	± 4.7	3.1
L9-L7-L19	87	± 7.0	89.3	± 7.2	2.5
L7-L19-L13	127.6	± 11.1	131.4	± 11.3	2.9
L10-L11-L12	74.6	± 4.9	75.0	± 4.0	0.6
L11-L12-L10	46.5	± 2.7	46.6	± 2.7	0.2
L11-L10-L14	120.9	± 13.5	122.5	± 13.7	1.3
L14-L15-L13	78.6	± 4.3	76.2	± 4.2	3.1
L14-L13-L19	93.2	± 7.6	93.4	± 7.6	0.2
L19-L20-L16	45	± 2.6	44.5	± 2.6	1.2
L19-L16-L17	116.2	± 6.7	113.7	± 6.6	2.2
L16-L17-L18	162.1	± 8.6	164.7	± 8.7	1.6
L16-L22-L21	124.4	± 11.7	127.6	± 12.0	2.5
L21-L22-L23	70.2	± 3.9	72.0	± 4.0	2.5
L22-L23-L24	132.4	± 10.8	129.2	± 10.5	2.5
L21-L36-L41	105.1	± 7.5	103.1	± 7.4	2.0
L23-L36-L41	121.2	± 8.1	124.4	± 8.3	2.5
L36-L37-L35	57.5	± 3.4	59.0	± 3.5	2.5
L36-L37-L40	117.1	± 7.3	118.9	± 7.1	1.5
L36-L35-L38	87.7	± 5.4	88.2	± 5.4	0.6
L35-L38-L39	139	± 15.3	142.6	± 15.7	2.5
L37-L38-L39	141.4	± 12.6	139.6	± 12.4	1.3
L35-L27-L28	119.1	± 7.1	121.0	± 7.2	1.6
L27-L28-L29	143.9	± 8.7	147.6	± 8.9	2.5
L27-L25-L26	130.2	± 6.6	134.1	± 6.8	2.9
L28-L25-L26	131.6	± 6.6	129.8	± 5.9	1.4
L28-L27-L25	54.5	± 2.9	55.9	± 3.0	2.5
L35-L27-L30	98.3	± 5.5	98.7	± 5.5	0.4
L30-L32-L33	55.9	± 3.5	56.1	± 3.5	0.4
L32-L33-L30	64.4	± 3.8	64.8	± 3.8	0.6

L33-L30-L31	137.1	± 7.8	134.4	± 7.6	2.0
L32-L33-L34	79.1	± 4.6	77.2	± 4.5	2.5
L25-L55-L56	139.3	± 8.21	137.3	± 8.1	1.4
L55-L56-L58	102.4	± 5.3	104.0	± 5.1	1.6
L55-L54-L56	59.5	± 3.2	60.5	± 3.3	1.6
L54-L56-L66	106.2	± 5.6	110.0	± 5.8	3.5
L56-L66-L67	142.1	± 14.1	142.4	± 14.1	0.2
L66-L67-L68	149.5	± 14.2	144.1	± 13.7	3.7
L55-L56-L54	65.8	± 3.4	66.2	± 3.5	0.6
L54-L57-L59	98.2	± 7.2	99.8	± 7.3	1.6
L57-L59-L62	93.8	± 5.9	94.4	± 5.9	0.6
L57-L59-L60	150.4	± 13.9	155.8	± 14.4	3.5
L59-L60-L61	149.8	± 13.9	150.1	± 13.9	0.2
L59-L62-L63	102.9	± 9.4	103.1	± 9.0	0.2
L62-L63-L64	146.8	± 13.9	147.8	± 14.0	0.7
L54-L45-L44	112.7	± 8.9	114.1	± 9.0	1.2
L45-L44-L42	68.7	± 4.3	69.8	± 4.4	1.6
L44-L42-L46	106.4	± 5.8	107.6	± 5.9	1.1
L44-L43-L47	100.5	± 9.4	101.1	± 9.5	0.6
L43-L47-L50	97.8	± 6.9	98.1	± 6.9	0.3
L47-L50-L51	117.8	± 11.6	112.6	± 11.1	4.6
L50-L51-L52	132.6	± 12.5	136.0	± 12.8	2.5
L51-L52-L53	147.9	± 14.1	149.8	± 14.3	1.3
L47-L48-L49	152.9	± 13.5	153.2	± 13.5	0.2
U1-U2-U3	58.7	± 3.5	59.3	± 3.5	1.1
U1-U3-U2	62.6	± 4.8	63.6	± 4.8	1.6
U1-U3-U4	118.1	± 9.2	115.3	± 9.0	2.5
U4-U3-U5	114.2	± 3.8	112.6	± 3.7	1.4
U3-U5-U6	117.9	± 5.8	119.0	± 5.8	0.9
U6-U5-U7	62.3	± 2.6	61.5	± 2.6	1.3
U5-U6-U7	59.8	± 3.2	57.9	± 3.2	3.2
U5-U7-U6	63.9	± 2.8	64.1	± 2.8	0.3
U7-U8-U9	113.9	± 9.5	116.3	± 9.7	2.1
U7-U8-15	117.3	± 7.8	118.6	± 7.8	1.1
U9-U8-U10	58.8	± 4.5	60.3	± 4.6	2.5
U8-U9-U10	62.6	± 5.3	61.8	± 5.3	1.3
U8-U10-U9	66.2	± 7.8	63.9	± 7.5	3.6
U8-U15-U17	118.5	± 5.8	116.8	± 5.7	1.4
U15-U16-U17	56.8	± 7.7	57.7	± 7.8	1.6
U16-U15-U17	63.9	± 4.5	65.6	± 4.6	2.5
U15-U17-U16	59.3	± 7.8	60.8	± 7.8	2.5
U10-U11-U12	118.3	± 4.6	116.8	± 4.5	1.3
U12-U11-U13	61.4	± 3.7	63.0	± 3.8	2.5
U11-U12-U13	65.3	± 5.6	64.0	± 5.5	2.0

U11-U13-U12	57.4	± 4.5	56.6	± 4.4	1.4
U11-U13-U14	112.6	± 6.9	114.4	± 7.0	1.6

Figure S2: Average values of key bond distances for CG LPS molecule over 2 microsecond trajectory.

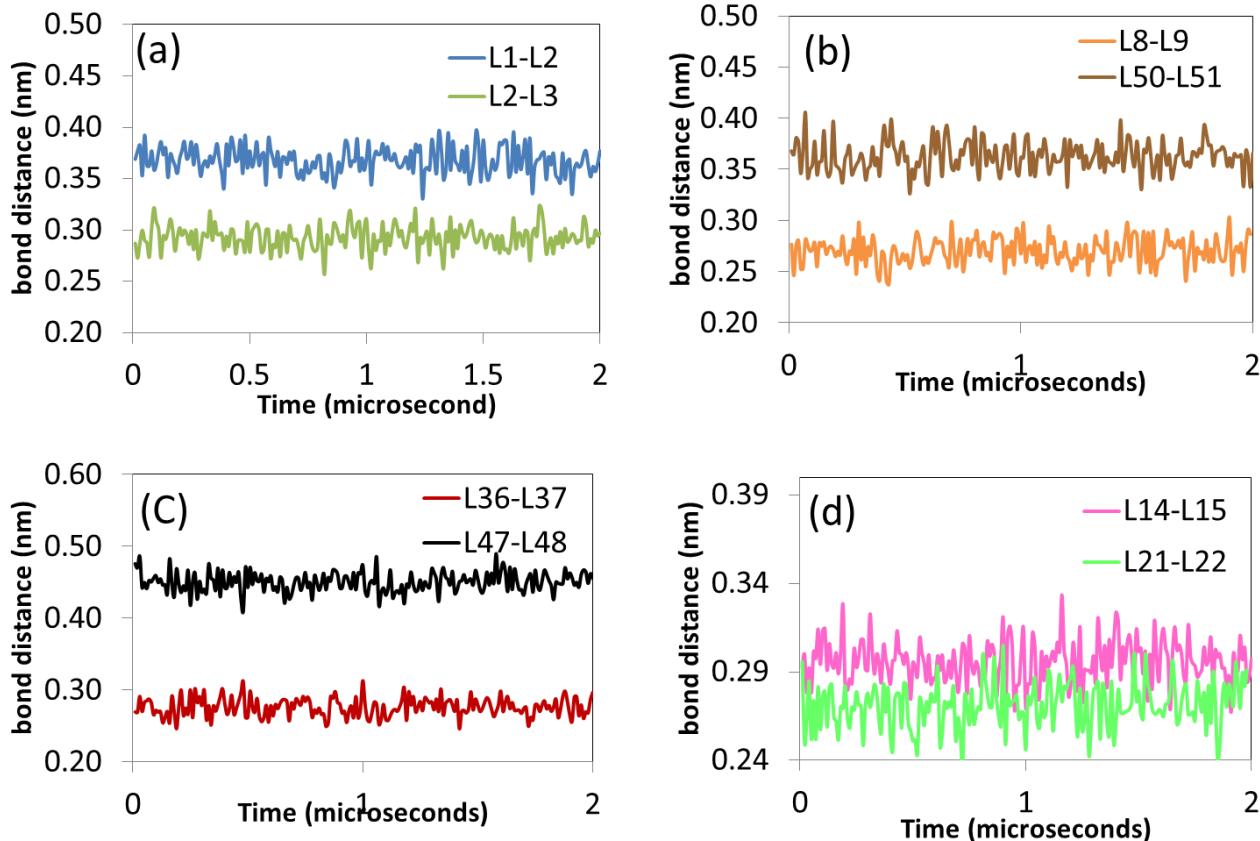


Figure S3: Comparison of bond angle distributions for (a) L1-L3-L4 (b) L10-L11-L12 (c) L56-L66-L67, (d) L16-L22-L21, and (e) L30-L32-L33 for CG (blue) and atomistic (red) LPS molecules.

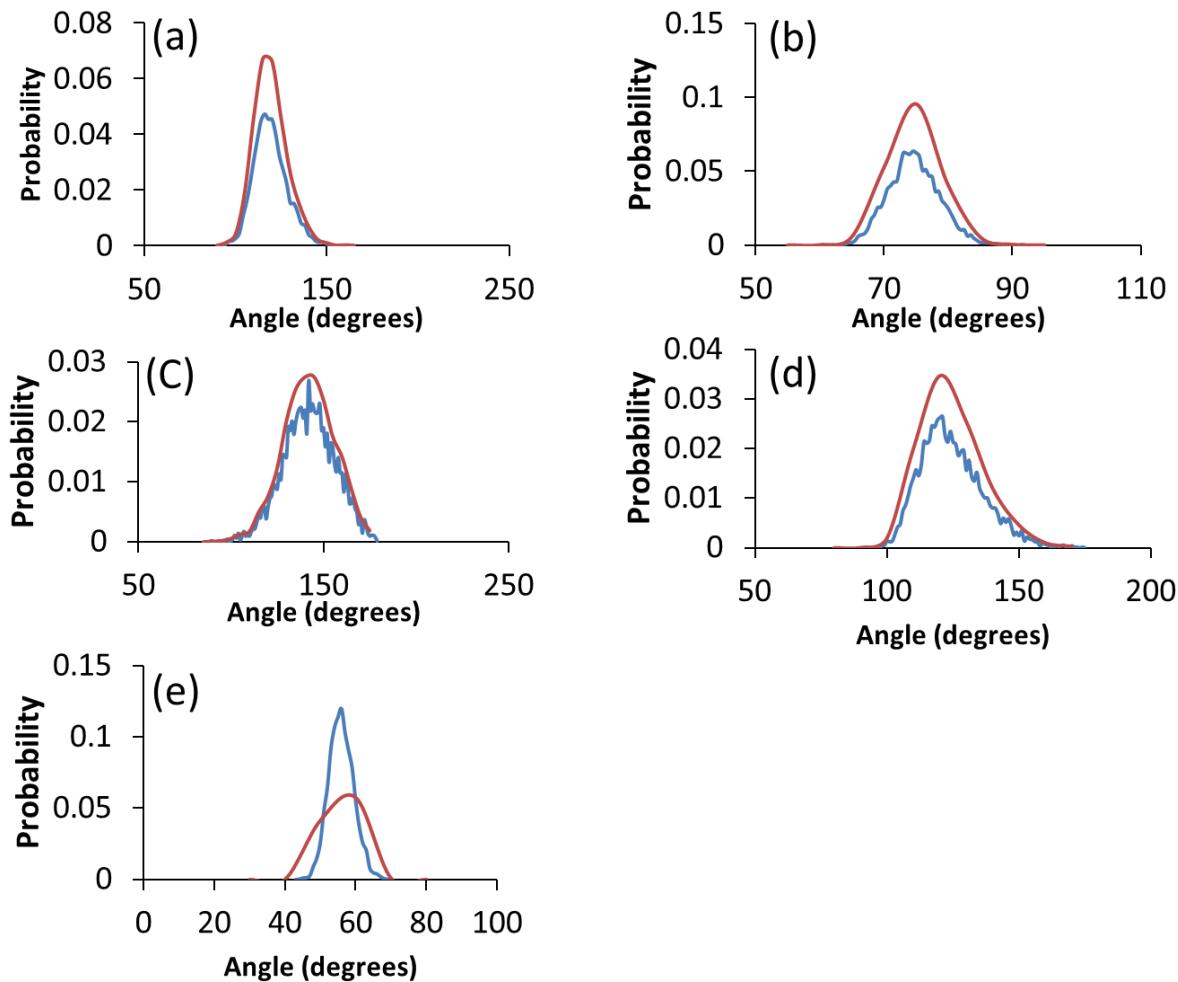


Figure S4. A_L values of CG (solid line) and atomistic (dashed line). Color scheme: LPS (blue) and DPPE (red). Inset plot shows the comparison of the CG and atomistic data in the initial 10 ns of the simulation.

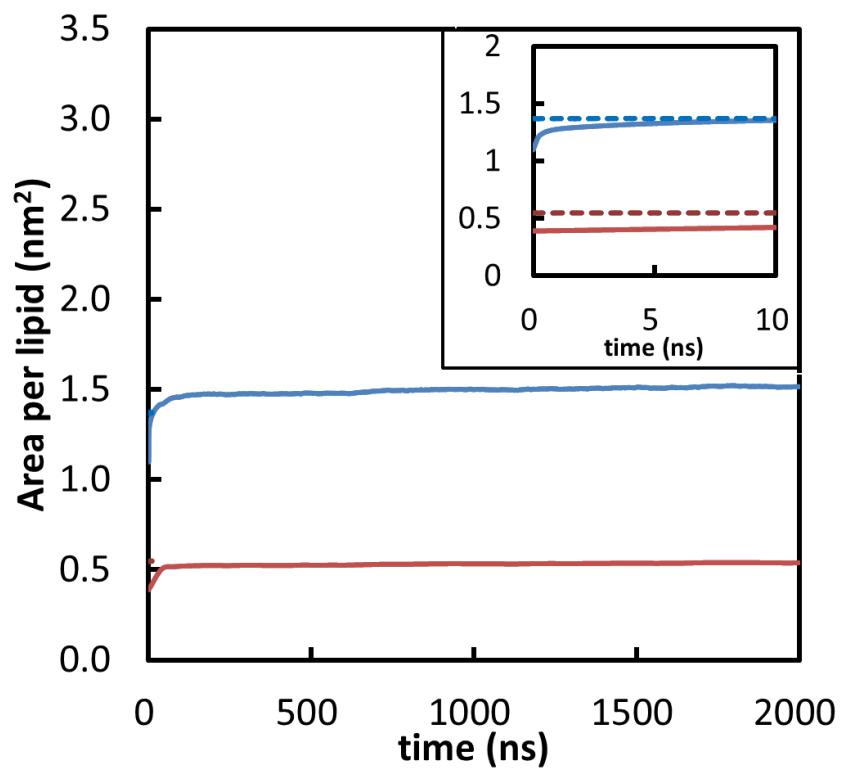


Figure S5. Density profiles of DPPE lipids (gray) and water (red) along the direction normal to the membrane (z-axis). The atomistic (dashed) and CG (solid) system are shown for increasing LPS (LIPO+OLIP) concentration starting from (a) 10%, (b) 20%, (c) 30%, (d) 50%, (e) 70%, (f) 90%, and (g) 100% in the outer leaflet. The inner leaflet is 100 % DPPE in all cases. In each plot, the membrane mid-plane is indicated by the green bar for reference.

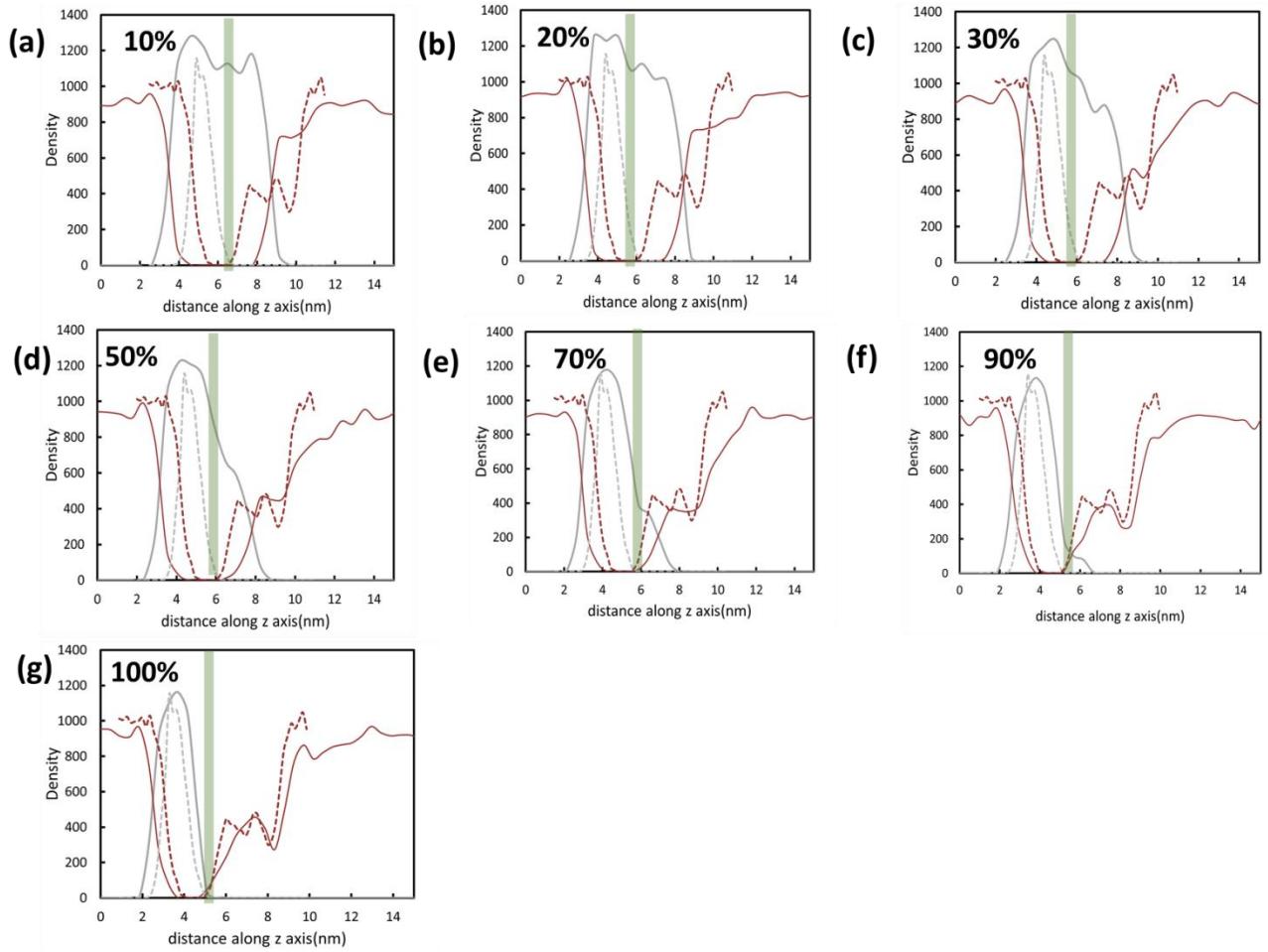
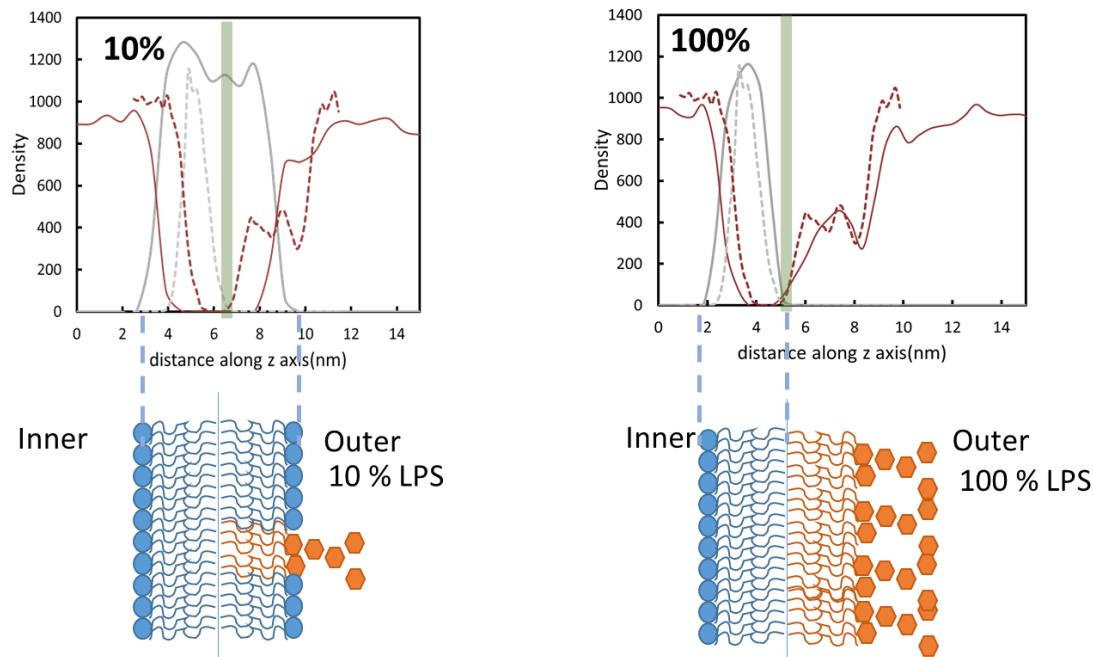


Figure S6. Comparison of CG (solid) and atomistic (dashed) density profiles of DPPE lipids (gray) and water (red) along the direction normal to the membrane (z-axis). Schematic on the left shows system with 10% LPS in the outer leaflet and the one on the right has 100% LPS.



In the 10% LPS, presents a broad DPPE profile of between 2.8-9.8 nm while 100% LPS has narrower DPPE profile between 2.0-5.1 nm.

Figure S7. Membrane thickness of CG membranes with Ca^{2+} (System I, blue) and Na^+ (System II, red).

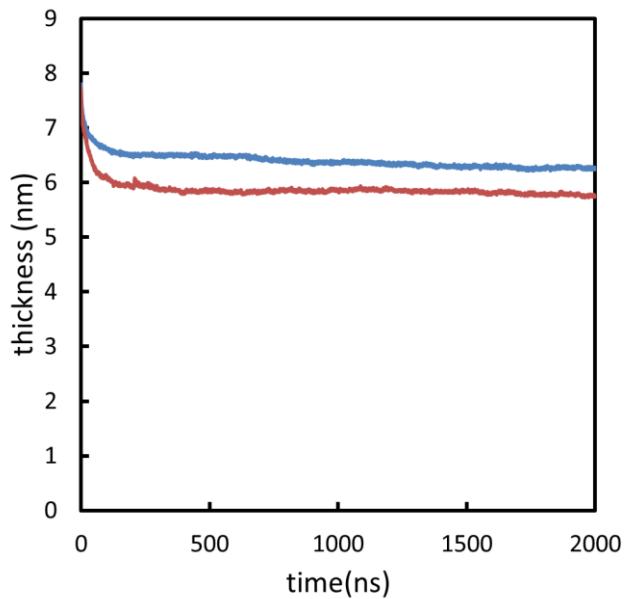


Figure S8. T_m (K) values determined from the heating scans of outer membrane systems differing in LPS:DPPE compositions. The area per lipid values are shown for the entire range of scanned temperature for systems with (a) 10%, (b) 20%, (c) 30%, (d) 50%, (e) 70%, (f) 90%, and (g) 100% LPS. The fits for lower and higher temperature domains are shown in blue and red lines, respectively. The change in slope marks the T_m value in each plot.

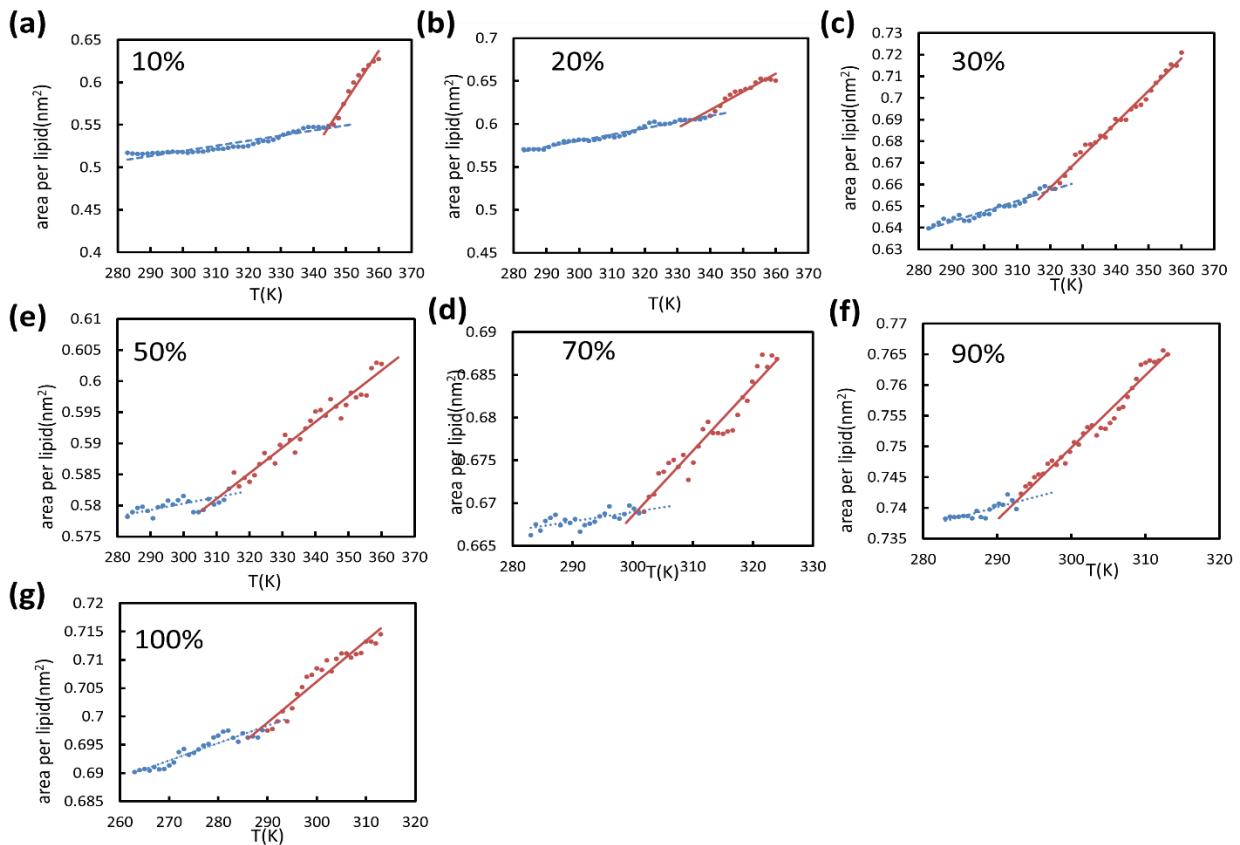


Table S3. Diffusion coefficients of membrane components of selected systems presented in Table V of the main article.

Systems	Temp (K)	Diffusion Coefficients ($1 \times 10^{-7} \text{ cm}^2\text{s}^{-1}$)				
		LIPO	OLIP	DPPE (outer)	DPPE (inner)	OccD1
I	310	0.15±0.09	0.14±0.01	0.15±0.06	0.24±0.11	-
II	310	0.14±0.08	0.14±0.05	0.14±0.08	0.22±0.12	-
III	310	0.12±0.07	0.13±0.04	0.21±0.10	3.95±0.45	0.12±0.05
IV	310	0.11±0.03	0.13±0.08	0.33±0.17	3.42±0.38	0.10±0.03
VII	283	0.02±0.01	0.02±0.01	0.02±0.03	0.20±0.09	-
VIII	350	0.41±0.11	0.47±0.06	0.43±0.11	3.88±0.59	-
X	310	0.35±0.04	-	-	0.99±0.09	-