

Biophysical Journal, Volume 118

Supplemental Information

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Table S1

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Table S1. CG beads types and bond parameters of polymyxin B, POPE and Re LPS.

i	type	residue	bond	Length (nm)	K_{bond} (KJ nm ⁻² mol ⁻¹)	angle	θ (degree)	K_{angle} (KJmol ⁻¹)
polymyxin B								
1	C1	AMO	1-2	0.367	5000	1-2-3	177.1	25
2	C1	AMO	2-3	0.362	5000	2-3-4	147.3	25
3	Na	AMO	3-4	0.305	5000	3-4-6	154.7	25
4	P5	DAB	4-5	0.321	5000	4-6-8	156.1	25
5	Qd	DAB	4-6	0.342	200	6-8-10	69.9	25
6	P5	THR	6-8	0.351	200	8-10-13	80.4	25
7	P1	THR	8-9	0.338	5000	10-13-14	134.9	25
8	P5	DAB	8-10	0.318	200	13-14-16	115.0	25
9	Qd	DAB	10-13	0.311	5000	14-16-18	108.4	25
10	P5	DABN	10-11	0.387	200	16-18-20	135.7	25
11	P5	DAB	11-12	0.348	5000	18-20-22	107.6	25
12	Qd	DAB	11-22	0.302	200	20-22-11	122.5	25
13	P1	DABN	22-23	0.332	7500	22-11-10	119.5	25
14	P5	THR	12-20	0.358	200	11-10-8	155.0	25
15	P1	THR	20-21	0.298	7500	11-10-13	98.4	25
16	P5	DAB	20-18	0.326	200	5-4-3	100.2	25

17	Qd	DAB	18-19	0.326	5000	5-4-6	102.9	25
18	P5	DAB	18-16	0.338	200	7-6-4	79.2	25
19	Qd	DAB	16-17	0.329	5000	7-6-8	102.3	25
20	P5	LEU	16-14	0.370	200	9-8-6	105.8	25
21	C1	LEU	14-13	0.305	5000	9-8-10	150.3	25
22	P5	DPHE	6-7	0.291	constraint	12-11-10	74.8	25
23	SC4	DPHE	14-15	0.231	constraint	12-11-22	162.6	25
24	SC4	DPHE	23-24	0.243	constraint	23-22-11	109.9	25
25	SC4	DPHE	23-25	0.289	constraint	23-22-20	121.4	25
			24-25	0.221	constraint	21-20-22	91.6	25
						21-20-18	139.6	25
						19-18-20	92.9	25
						19-18-16	124.0	25
						17-16-18	123.8	25
						17-16-14	112.3	25
						15-14-16	97.6	25
						15-14-13	126.6	25
						22-23-24	99.9	50
						22-23-25	133.3	50
						22-24-25-23	0	50

POPE

1	Qd	NH3	1-2	0.470	1250	2-3-4	120.0	25
2	Qa	PO4	2-3	0.470	1250	2-3-5	180.0	25
3	Na	GL1	3-4	0.370	1250	3-5-6	180.0	25
4	Na	GL2	3-5	0.470	1250	5-6-7	120.0	45
5	C1	C1A	5-6	0.470	1250	6-7-8	180.0	25
6	C3	D2A	6-7	0.470	1250	4-9-10	180.0	25
7	C1	C3A	7-8	0.470	1250	9-10-11	180.0	25
8	C1	C4A	4-9	0.470	1250	10-11-12	180.0	25
9	C1	C1B	9-10	0.470	1250			
10	C1	C2B	10-11	0.470	1250			
11	C1	C3B	11-12	0.470	1250			
12	C1	C4B						

Re LPS

1	Qa	PO1	1-2	0.417	5074	1-2-3	89.5	8
2	P2	GM1	2-4	0.213	21824	1-2-4	82.7	12
3	Nda	GM2	2-6	0.418	5448	1-2-6	158.9	10
4	P1	GM3	3-9	0.320	6057	2-3-9	126.1	8
5	P2	GM4	3-17	0.339	5275	2-3-17	129.6	11
6	P1	GM5	5-8	0.398	7231	2-4-33	137.1	10
7	Nda	GM6	6-5	0.211	17769	2-6-5	151.0	10
8	Qa	PO2	7-25	0.289	5308	3-2-4	162.0	10
9	Na	GL1	7-29	0.296	7684	3-2-6	95.3	11
10	Na	GL2	9-10	0.312	1359	3-9-10	109.8	10
11	C1	C1A	9-14	0.448	1732	3-9-14	118.0	11
12	C1	C2A	10-11	0.400	1613	3-17-18	119.1	10

13	C1	C3A	11-12	0.468	1830	3-17-22	142.0	12
14	C1	C1B	12-13	0.460	1618	4-2-6	96.4	10
15	C1	C2B	14-15	0.468	1820	4-34-33	81.1	15
16	C1	C3B	15-16	0.409	2215	4-34-35	111.1	10
17	Na	GL3	17-18	0.342	1155	5-7-25	110.1	11
18	Na	GL4	17-22	0.437	1274	5-7-29	142.5	23
19	C1	C1C	18-19	0.398	1589	6-5-7	143.6	11
20	C1	C2C	19-20	0.353	3151	6-5-8	101.7	10
21	C1	C3C	20-21	0.408	2193	7-5-8	94.6	10
22	C1	C1D	22-23	0.465	1638	7-25-26	129.4	9
23	C1	C2D	23-24	0.408	2199	7-29-30	136.3	12
24	C1	C3D	25-26	0.305	4607	9-3-17	101.0	11
25	Na	GL5	26-27	0.463	2041	9-14-15	150.9	11
26	Nda	GL6	27-28	0.516	1210	9-10-11	150.9	10
27	C1	C1E	29-30	0.293	3803	10-11-12	150.1	11
28	C1	C2E	30-31	0.464	1848	10-9-14	66.5	11
29	Na	GL7	31-32	0.516	1205	11-12-13	152.4	9
30	Nda	GL8	4-34	0.336	14595	14-15-16	154.1	9
31	C1	C1F	35-36	0.157	13867	17-18-19	145.2	10
32	C1	C2F	35-37	0.347	3108	17-22-23	155.5	9
33	Qa	S01	35-38	0.397	14156	18-17-22	67.8	11
34	SC1	S02	39-40	0.157	24430	18-19-20	149.8	11
35	P2	S03	39-41	0.357	2563	19-20-21	154.5	9
36	SN0	S04	2-3	0.190	constraint	22-23-24	152.3	11
37	P4	S05	5-7	0.197	constraint	25-7-29	104.7	11
38	SC1	S06	33-34	0.224	constraint	25-26-27	142.0	11
39	P2	S07	34-35	0.165	constraint	26-27-28	154.7	9
40	SN0	S08	38-39	0.165	constraint	29-30-31	125.9	10
41	P4	S09	38-42	0.222	constraint	30-31-32	153.9	11
42	Qa	S10				33-34-35	145.5	8
						34-35-36	131.9	9
						34-35-37	118.4	11
						34-35-38	106.4	10
						35-38-42	77.1	12
						36-35-38	86.9	11
						37-35-38	132.6	11
						38-39-40	129.8	11
						38-39-41	118.9	12
						40-39-41	69.5	10

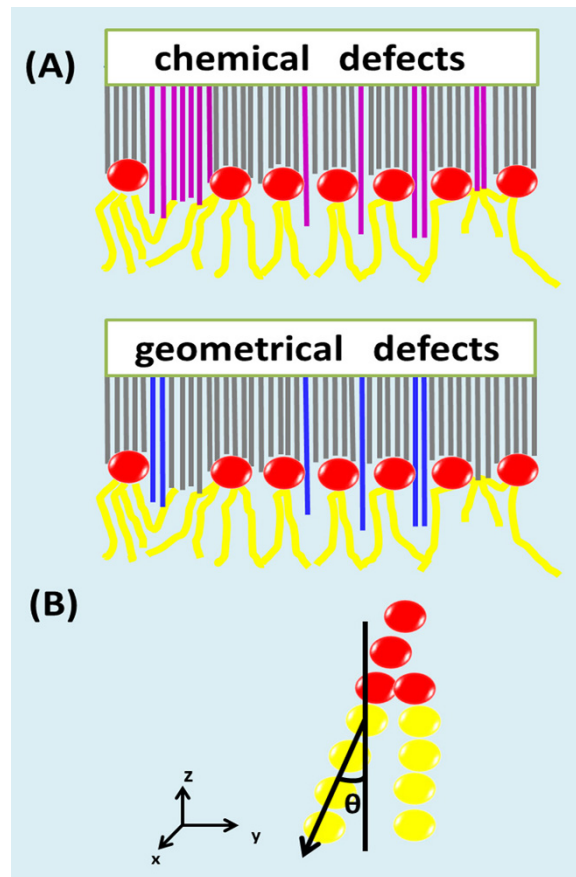


Figure S1. Schematic illustrations of the method for detecting lipid packing defects (A) and the definition of the lipid tail tilt angle (B). The planar bilayer normal is in the z direction. In (A), the chemical defects are represented by magenta lines, geometrical defects are represented by blue lines, and the gray lines are not defects.

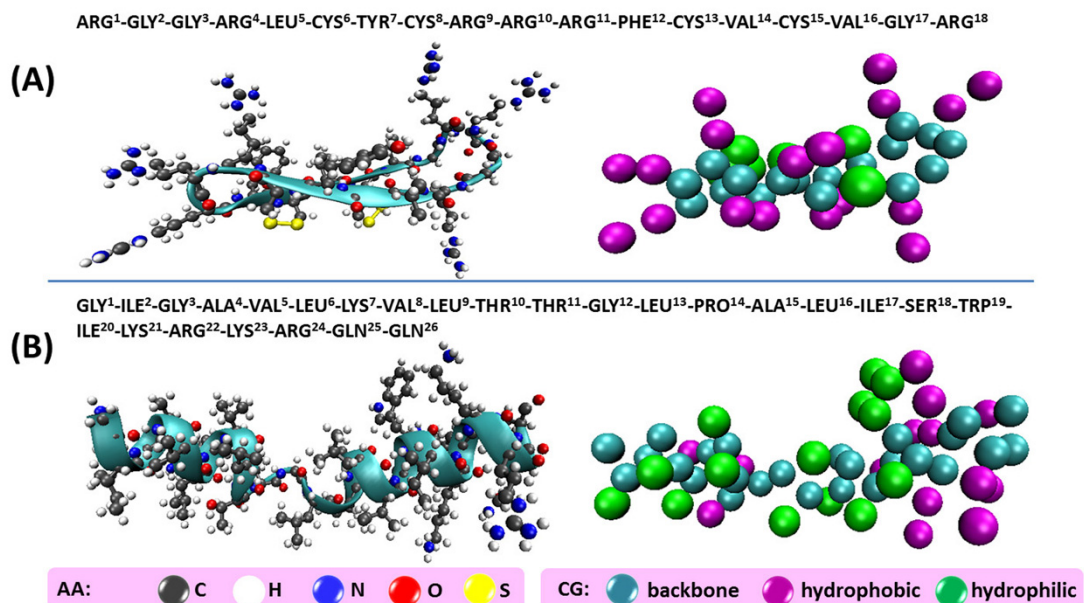


Figure S2. Molecular structures of protegrin-1 (A) and melittin (B) and their corresponding coarse-grained mappings.

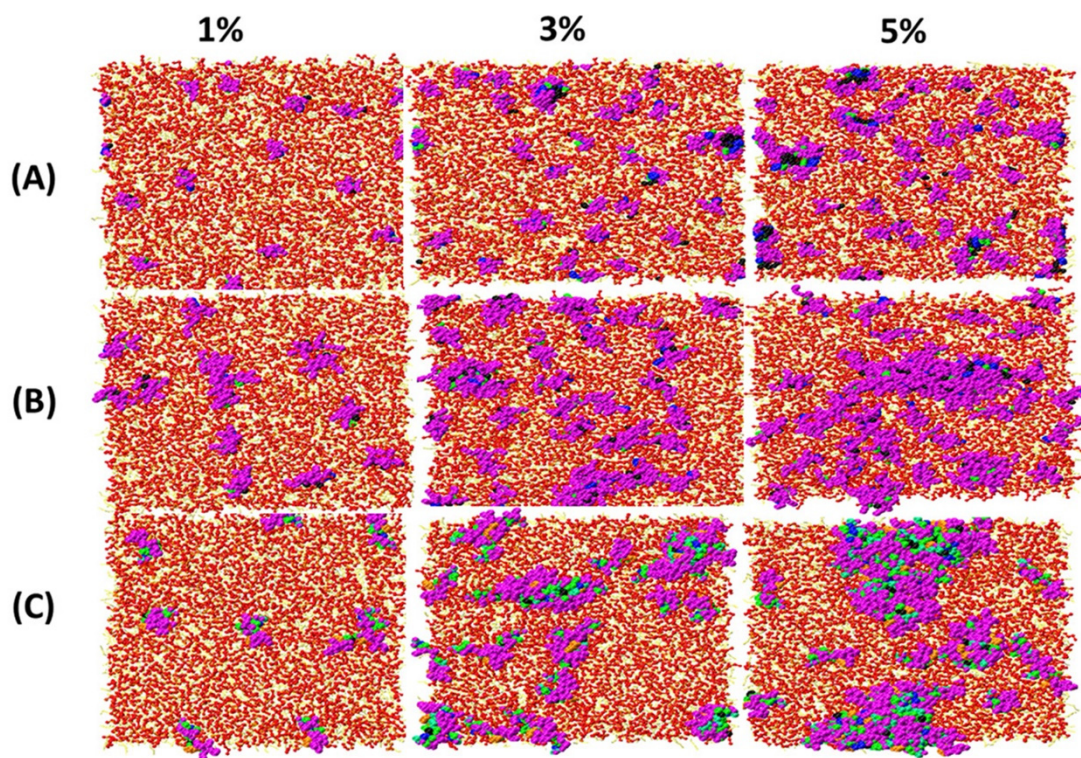


Figure S3. Top view of the snapshots of PmB (A), Pg1 (B) and Mel (C) binding to the inner membrane model.

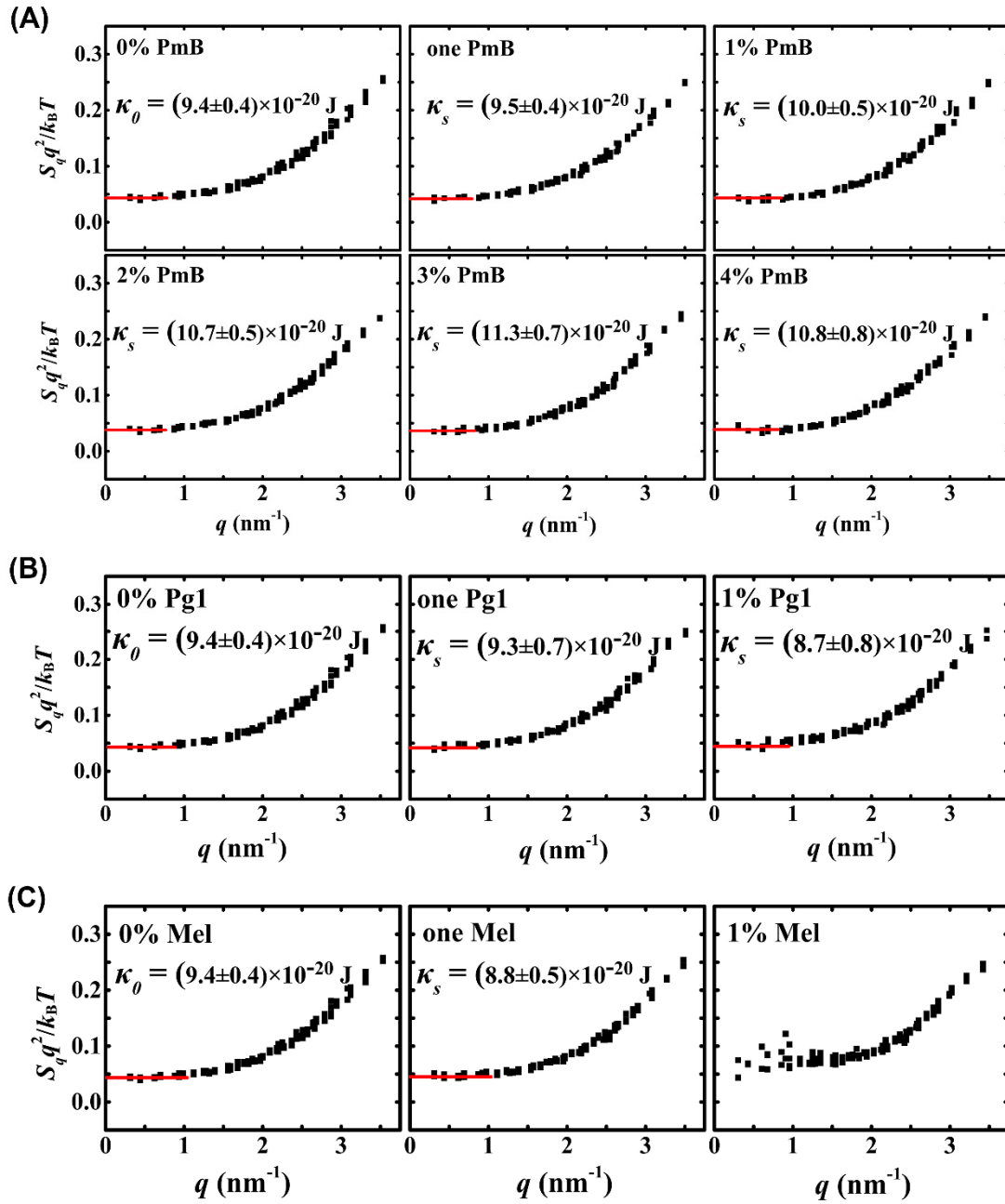


Figure S4. Spectra of the longitudinal lipid orientation fluctuations before and after PmB (A), Pg1 (B) and Mel (B) binding to the membrane. The converged κ_θ and κ_s values were obtained from the plateau regions extending over, at least, the smallest four wave vectors.

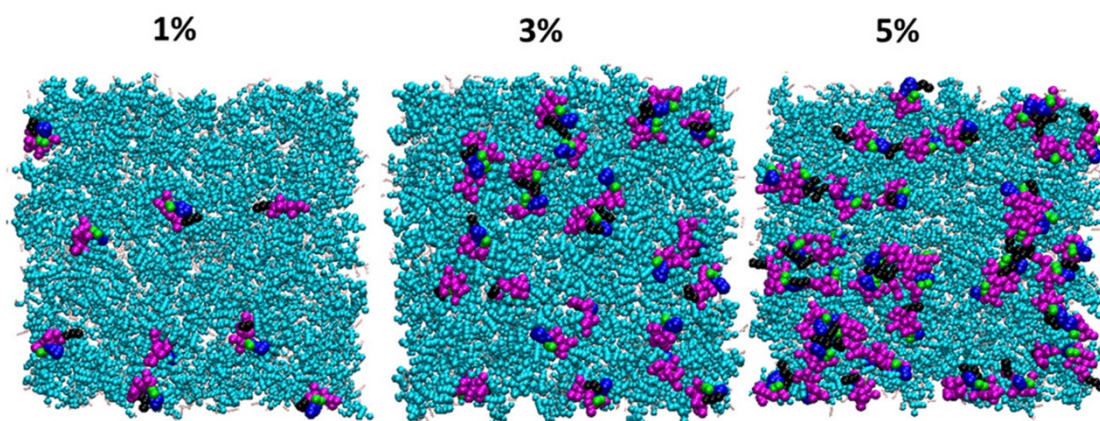


Figure S5. Top view of the snapshots of PmBs binding to the outer membrane model at different P/L ratios.