E. coli Outer Membrane and Interactions with OmpLA

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Table S1: System information.

Systems	Lipid composition	# Lipids		System Size ($Å^3$)	# Atom	# Water
		Top	Bottom			
OmpLA-LPS-PL	LPS0[#]/PPPE/ PVPG/PVCL2	37	75:20:5	87×87×101	~80,000	~43,600
LPS-PL[36,100]	LPS0[#]/PPPE/ PVPG/PVCL2	36	75:20:5	80×80×96	~66,000	~33,400
LPS-PL[37,100]	LPS0[#]/PPPE/ PVPG/PVCL2	37	75:20:5	81×81×95	~66,000	~32,900
PL-only	PPPE/PVPG/ PVCL2	75:20:5	75:20:5	80×80×90	~59,000	~11,100
OmpLA-DLPC	DLPC	77	75	76×76×81	~48,000	~9,300
DLPC-only	DLPC	64	64	63×63×70	~29,000	~5,100

[#]LPS0 is for a LPS with lipid A and R1 core.

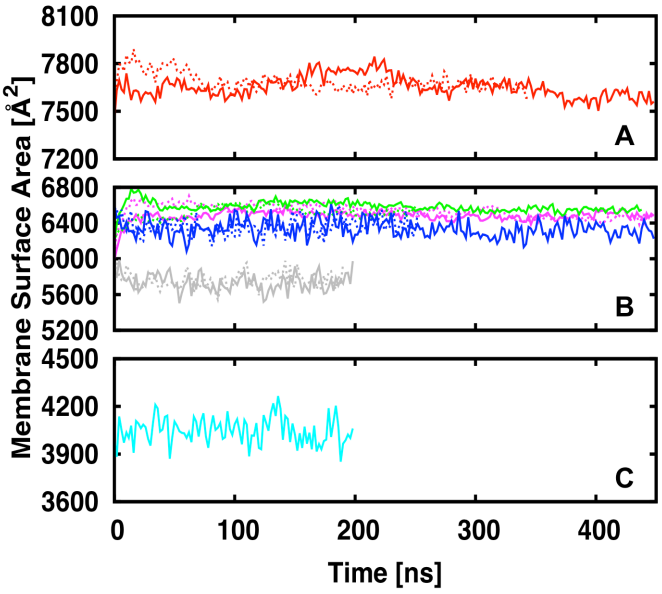

Figure S1: Time-series of the overall membrane surface area in two independent systems (one replica with solid line and the other replica with dotted line) for OmpLA-LPS-PL (red), LPS-PL[36,100] (magenta), LPS-PL[37,100] (green), PL-only (blue), OmpLA-DLPC (grey), and DLPC-only (cyan).

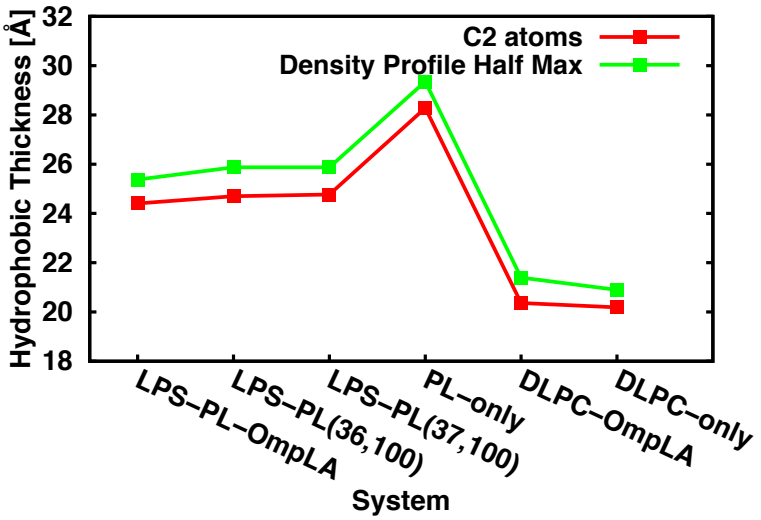

Figure S2**.** Average hydrophobic thickness of each lipid bilayer system calculated with C2 atoms (red) and number density profile (green).

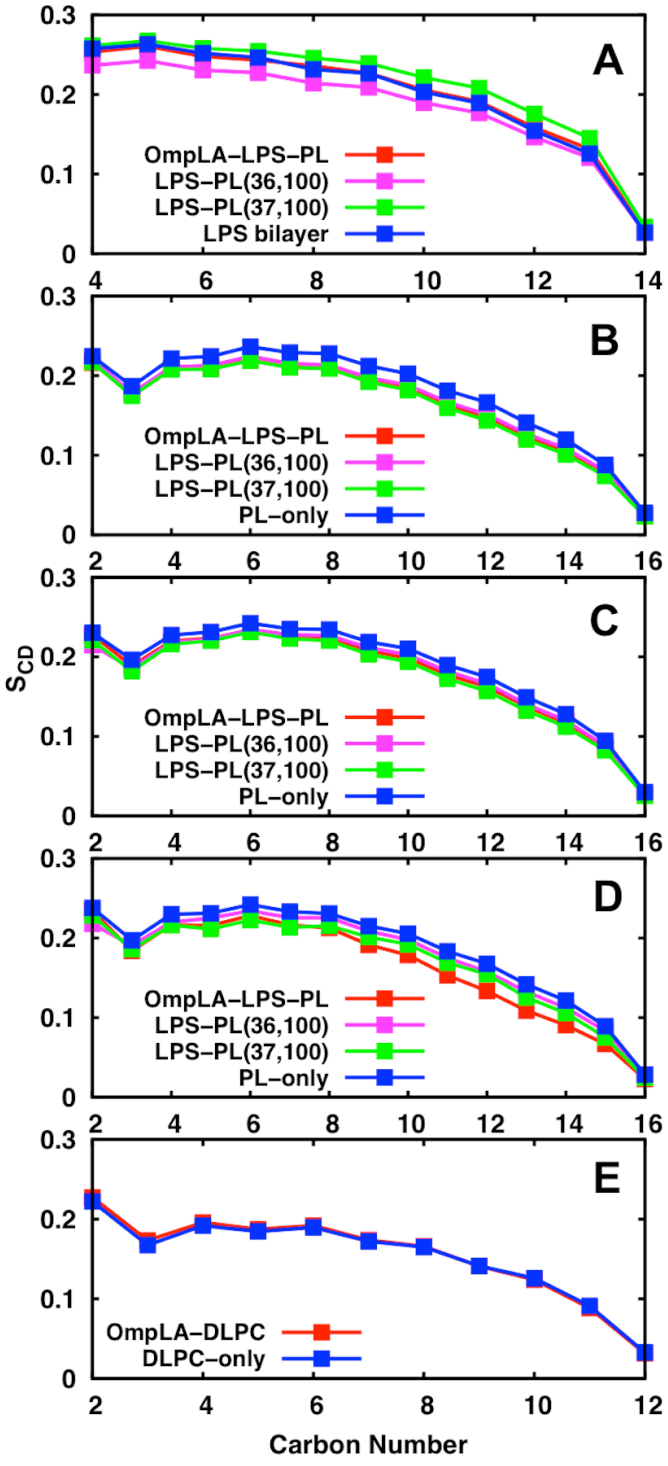

Figure S3: Deuterium order parameters for (A) Lipid A (chain 1), (B) PPPE, (C) PVPG, (D) PVCL2, and (E) DLPC *sn*-1 chains of each lipid bilayer system. The standard errors over two replicas are smaller than 0.02 for all the carbon atoms.

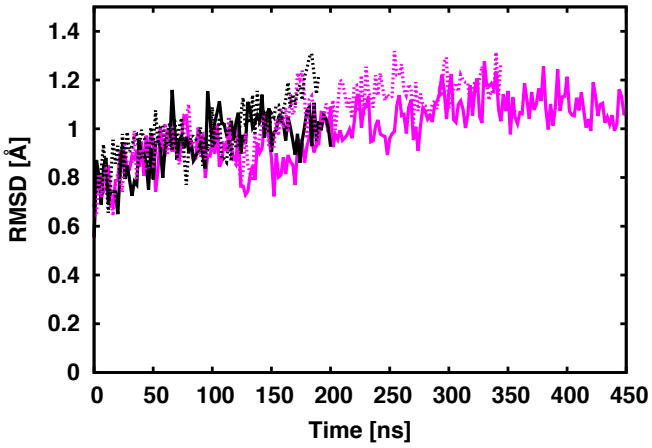

Figure S4. Time-series of the root-mean-square deviation (RMSD) of OmpLA β-barrel backbone atoms from the starting structure (1QD5) in two independent systems (replica 1 with solid line and replica 2 with dotted line) for OmpLA-LPS-PL (magenta) and OmpLA-DLPC (black).

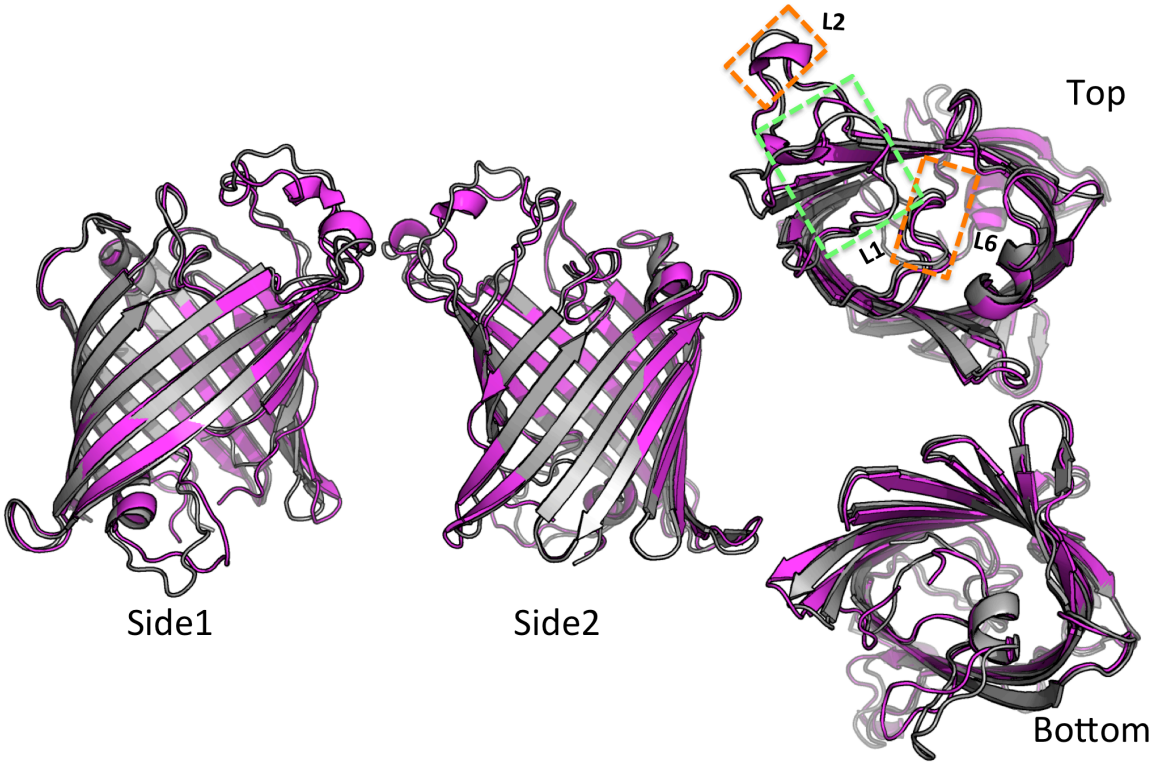

Figure S5: OmpLA average structures from the last 100 ns simulation of OmpLA-LPS-PL (magenta) and OmpLA-DLPC (grey) replica 1, viewed from the membrane (side), extracellular (top), and periplasmic (bottom) sides.

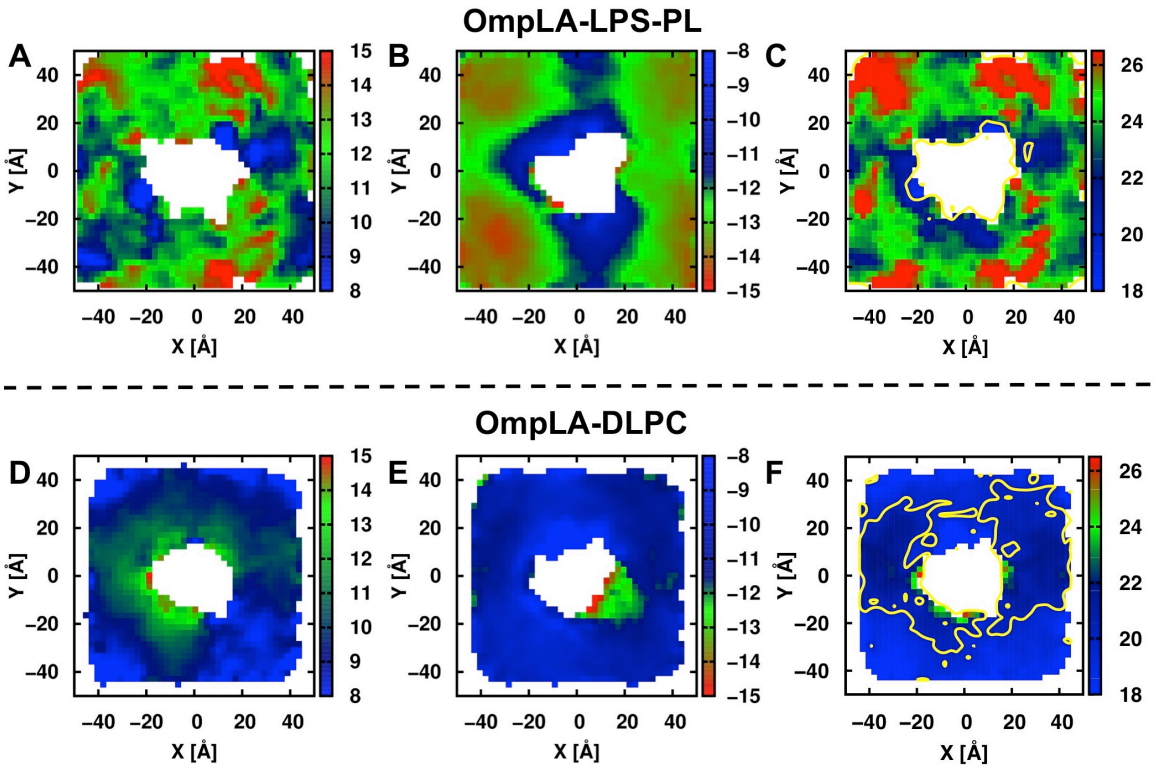

Figure S6: 2D *Z* position distributions of the C2 and C4 atoms of lipid A (A) and the acyl chain C2 atoms of phospholipids (B, D, and E), as well as the 2D thickness distribution of the full bilayer (C and F) for both OmpLA-LPS-PL (top row) and OmpLA-DLPC (bottom row). The color legends of panels A, B, D, and E indicate the distance from the bilayer center to C2 atoms along Z-axis: blue to red transition corresponds to close-to-far (thin-to-thick) position of the atoms within the bilayer with respect to its center. For panel C and F, the color legend refers to the total membrane thickness. Contours are drawn for 20 Å in yellow.

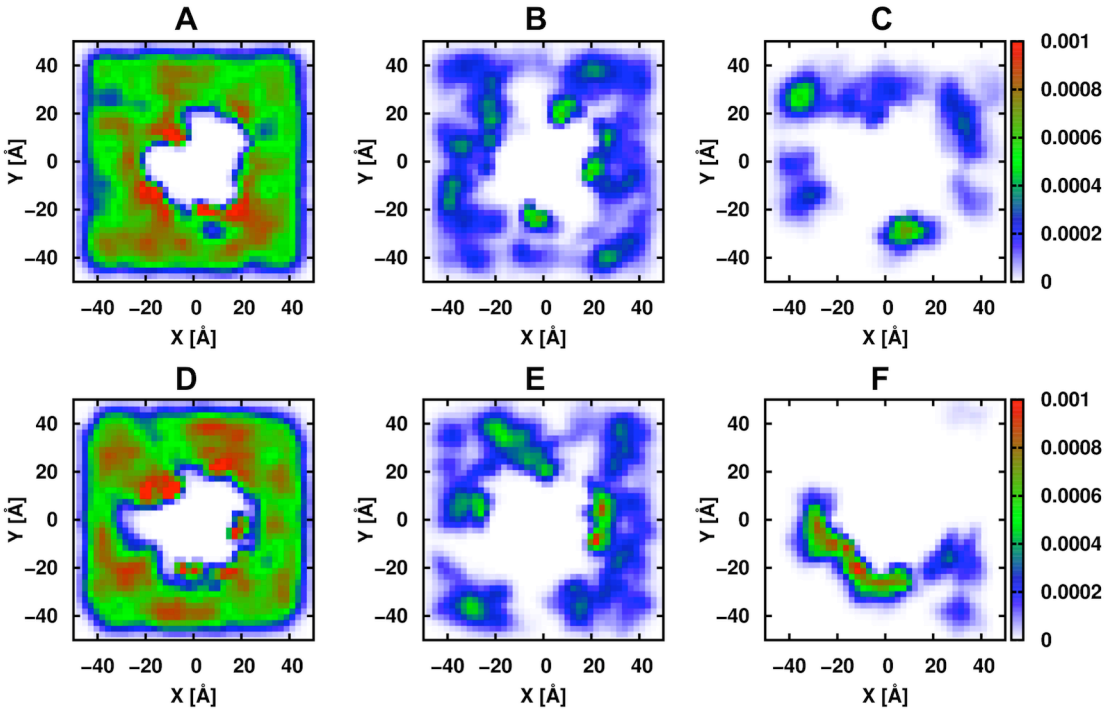

Figure S7: 2D number density plots of the C2 atoms of (A) and (D) PPPE, (B) and (E) PVPG, and (C) and (F) PVCL2 for two independent OmpLA-LPS-PL systems: top row for replica 1 and bottom row for replica 2. Note that PVPG and PVCL2 do not cover the entire system during the simulation simply because their numbers (20 PVPG and 5 PVCL2) in the system are small compared to 75 PPPE.

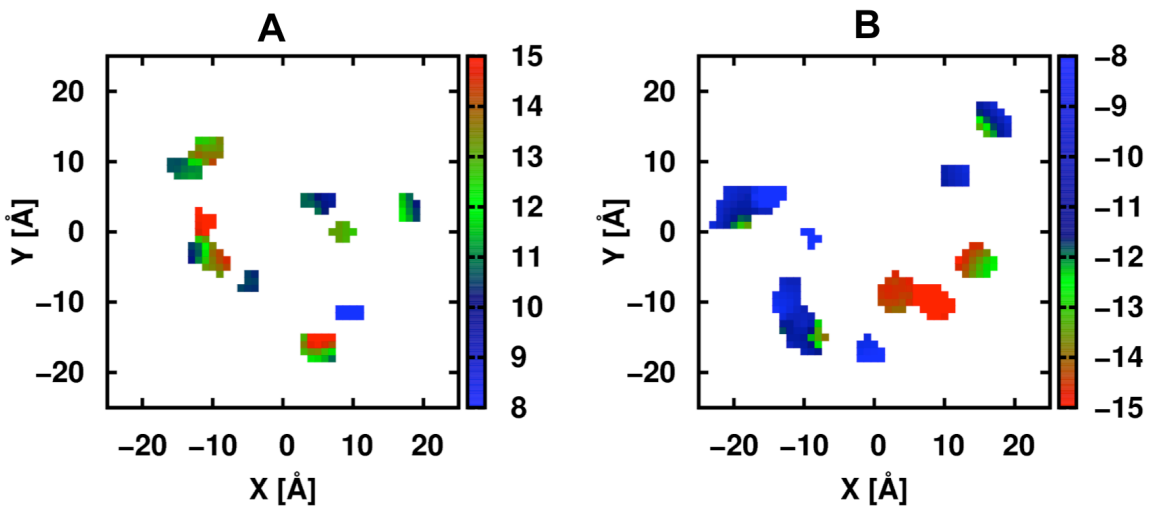

Figure S8: 2D *Z* position distributions of the sidechain center of mass of the hydrophobic residues on the rim of each β-strand for (A) upper leaflet and (B) lower leaflet in OmpLA-LPS-PL. The 2D plots were constructed with a grid spacing of 2.4 Å.

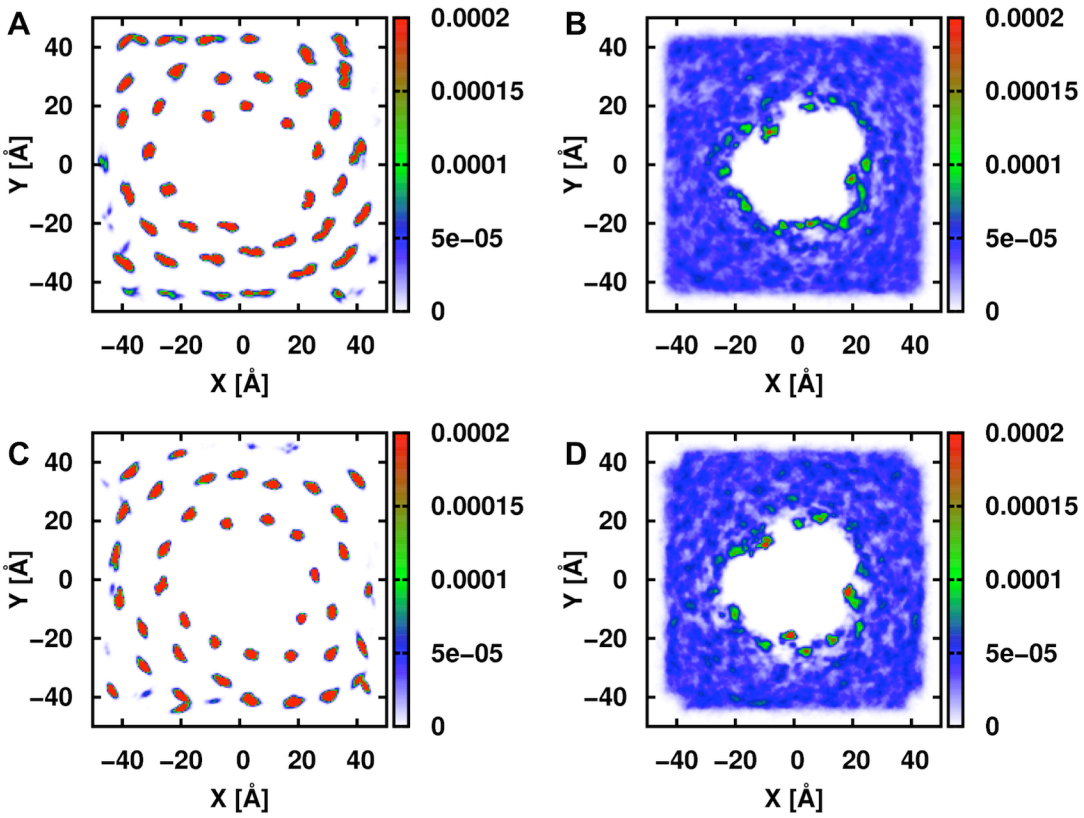

Figure S9: 2D number density plots of the center of mass of (A) and (C) lipid A and (B) and (D) PPPE, PVPE, and PVCL2 for two independent OmpLA-LPS-PL systems: top row for replica 1 and bottom row for replica 2. The 2D plots were constructed with a grid spacing of 0.5 Å.

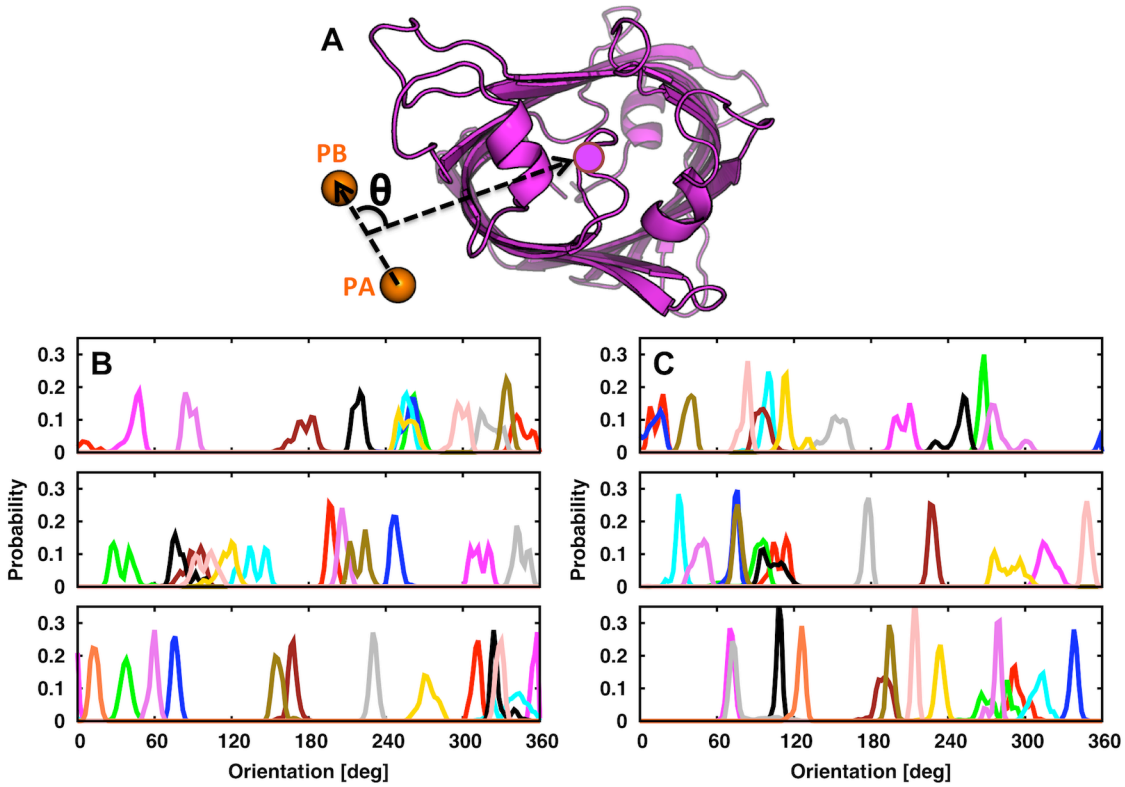

Figure S10: (A) The LPS orientation to OmpLA is defined by the angle (θ) between the vector connecting lipid A phosphate PA and PB atoms (orange spheres) and the vector connecting the geometry center of PA and PB and the center of OmpLA backbone atoms (magenta sphere). (B) and (C) The θ distributions for LPS residue 1-12 (top, in contact with OmpLA), residue 13-24 (middle), and residue 25-37 (bottom) for two independent OmpLA-LPS-PL systems. Each color represents one LPS molecule.