Supporting Information

CHARMM-GUI PACE CG Builder for Solution, Micelle, and Bilayer Coarse-Grained Simulations

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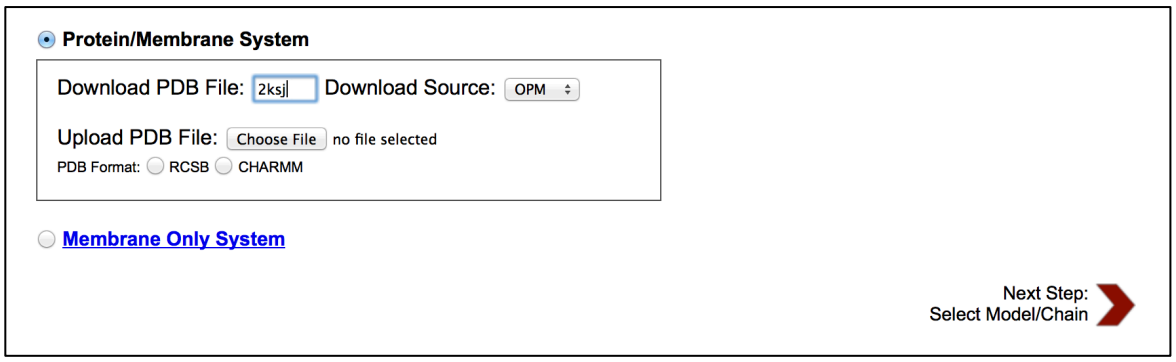

Figure S1. Screenshot of STEP 1 in Bilayer Builder. The builder can build membrane-only or protein/membrane systems. Users can upload the PDB file or specify the PDB ID to be downloaded from the OPM database or the PDB.

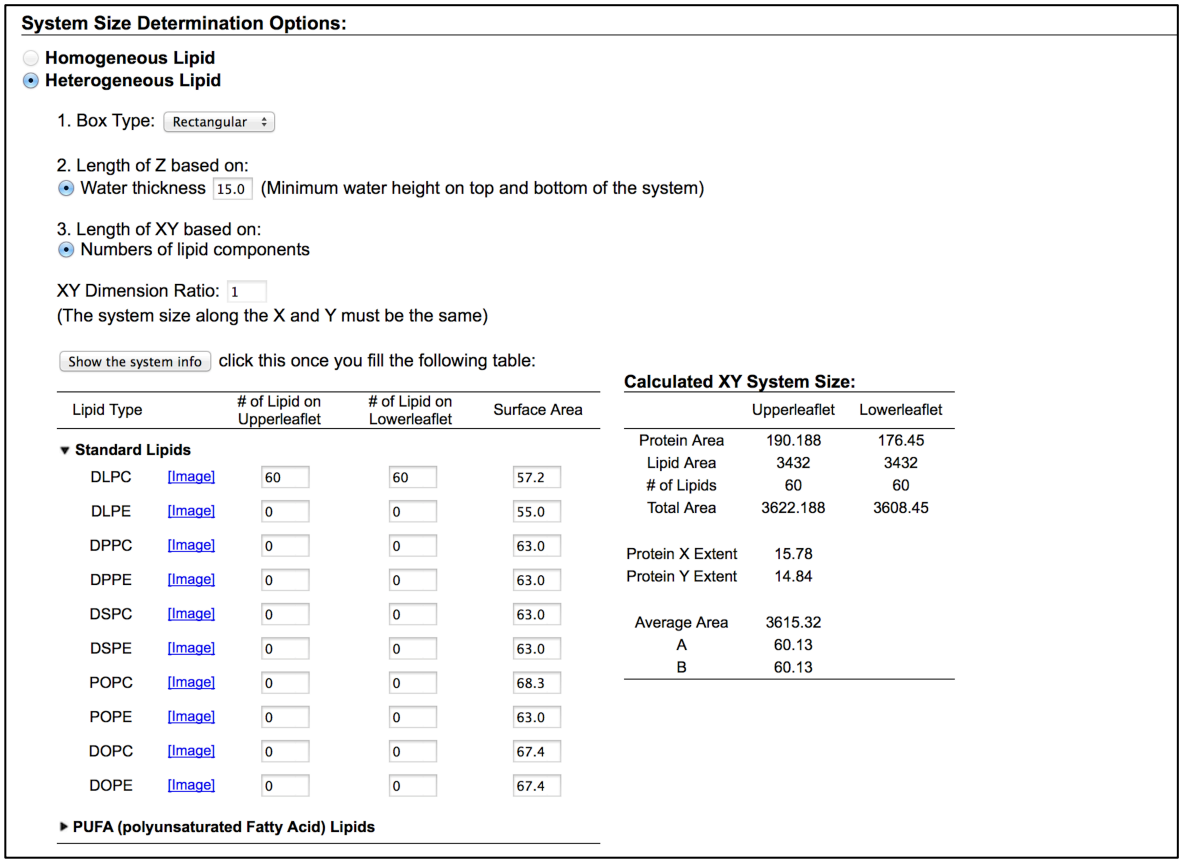

Figure S2. Screenshot of system size determination (STEP 3) in Bilayer Builder. Users can specify the number of lipids in each leaflet.

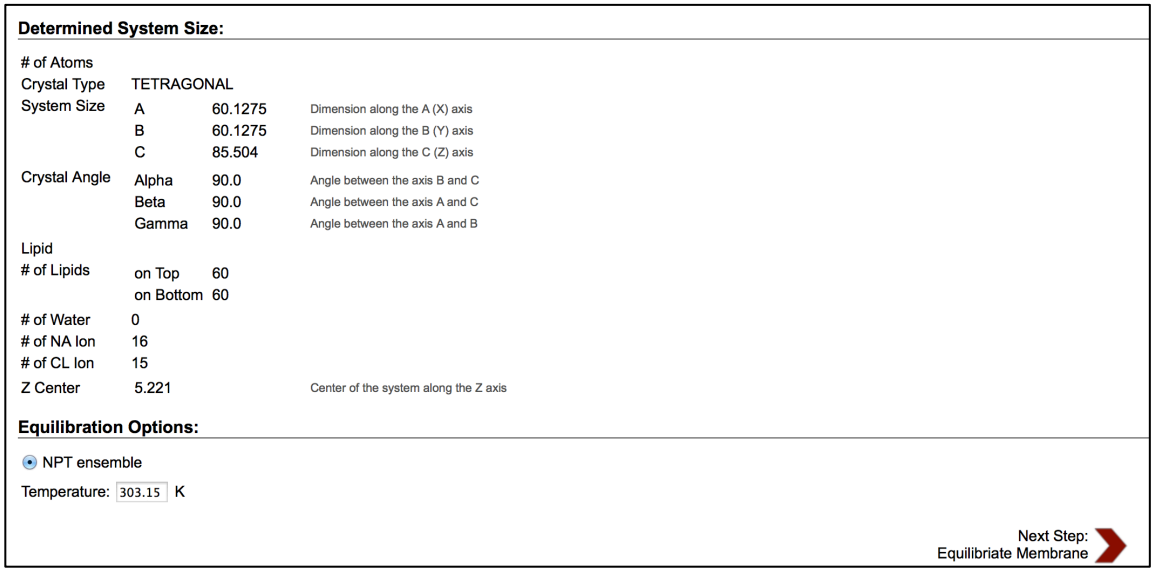

Figure S3. Screenshot of the determined system size (STEP 3) in Bilayer Builder. Based on the user input in **Figure S2**, the system size is determined. Users can specify the simulation temperature in this step.

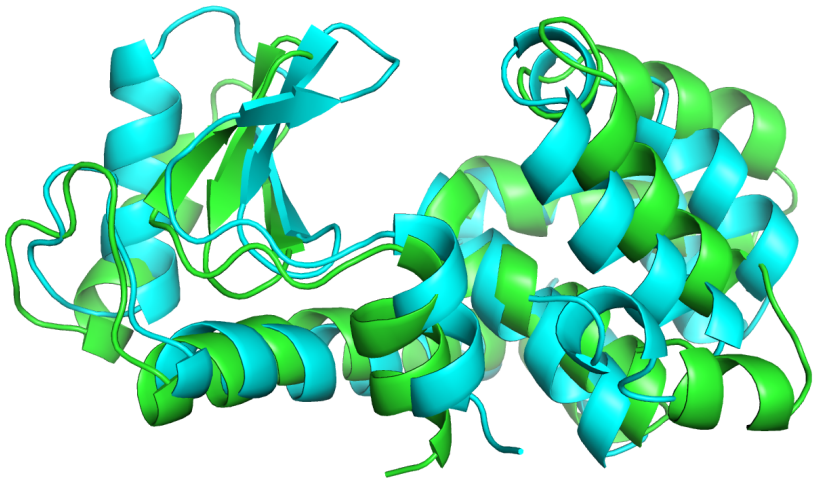

Figure S4. Comparison of the last snapshot from MD (green) to the crystal structure of lysozyme (cyan) shows the displacement of helices.

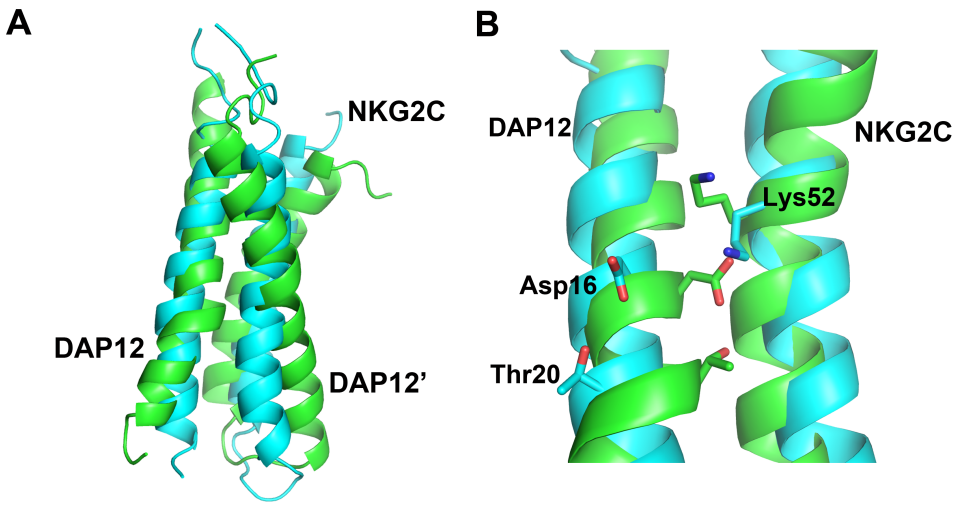

Figure S5. Comparison of the last snapshot from MD (green) to the NMR structure of DAP12-NKG2C (cyan). (A) One of the DAP12 protomers is distorted at the C terminus, and the other is rotated. (B) Asp16 and Thr20 from one of the DAP12 protomers move inwards during the simulation. For clarity, another DAP12 protomer is not shown in (B).

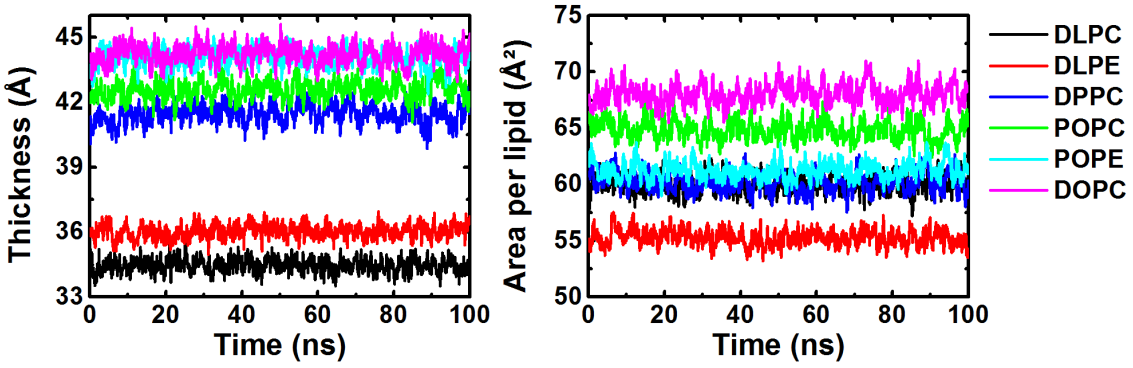

Figure S6. Time-series of the bilayer thickness and per-lipid area in the lipid-only bilayer systems.

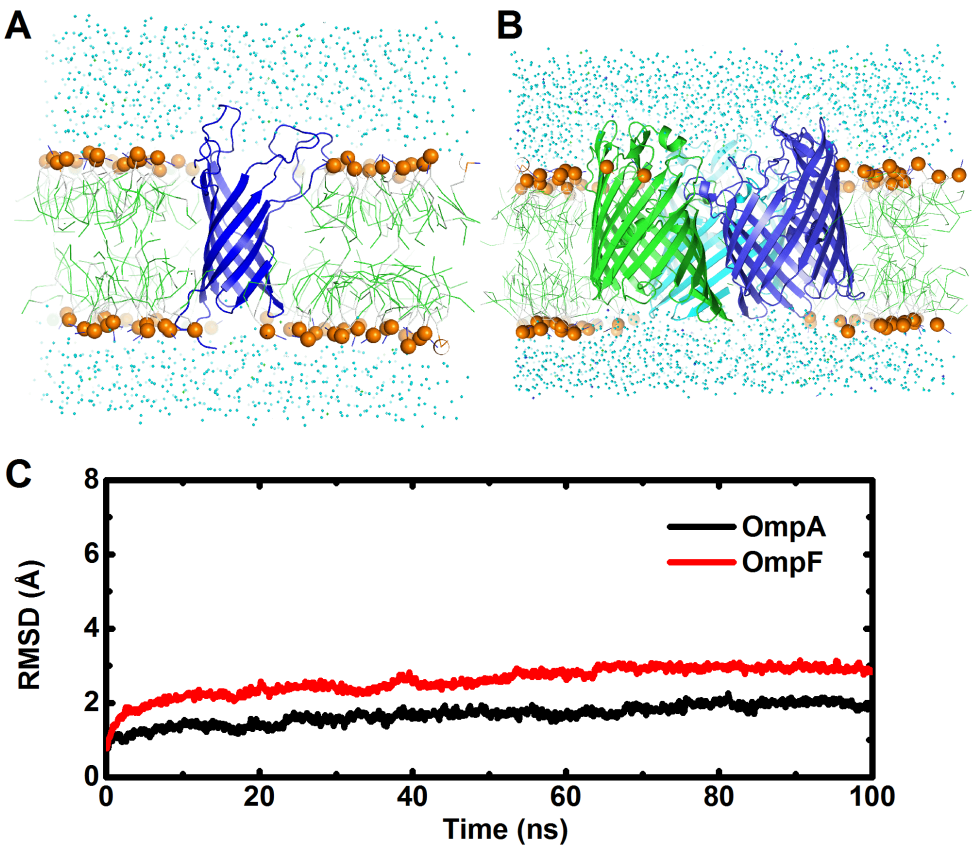

Figure S7. Bilayer systems: (A) OmpA, (B) OmpF, and (C) their RMSD time-series.

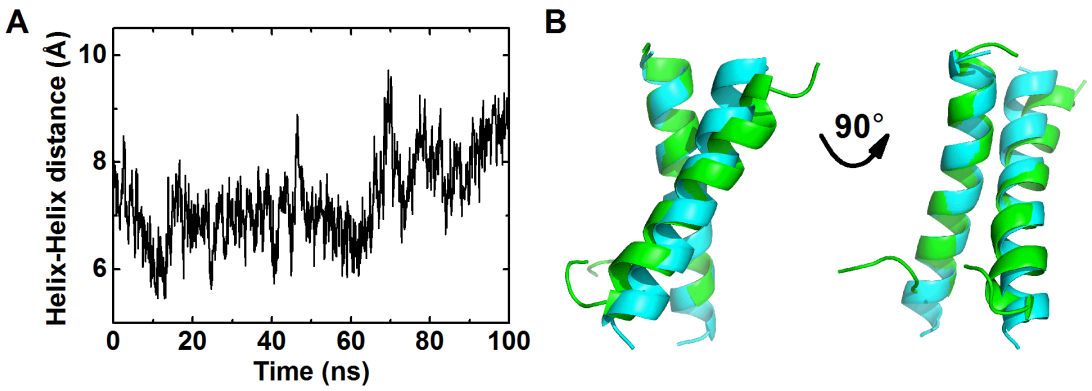

Figure S8. The GpA conformation during simulation. (A) The helix-helix distance shows that the helices do not dissociate. (B) Comparison of the last snapshot (green) to the crystal structure (cyan) shows about 10° change in the crossing angle.

Table S1. Validation of the converted MARTINI force field.[a]

	Bond	Angle	van der Waals	Electrostatic
	DHPC micelle			
GROMACS[b]	82.4951	31.7611	-15085.9478	-46.3831
NAMD	82.4951	31.7611	-15085.9447	-46.3831
Difference[c]	0	0	-2.0×10^{-7}	0
	POPE bilayer			
GROMACS[b]	590.8491	554.6695	-17420.5586	-140.3388
NAMD	590.8493	554.6690	-17420.5415	-140.3388
Difference[c]	3.3×10^{-7}	-9.0×10^{-7}	-9.8×10^{-7}	0
	POPC bilayer			
GROMACS[b]	310.9246	453.6337	-19442.9915	-207.4843
NAMD	310.9247	453.6338	-19443.0259	-207.4842
Difference[c]	3.2×10^{-7}	2.2×10^{-7}	1.9×10^{-6}	-4.8×10^{-7}
	DOPC bilayer			
GROMACS[b]	567.0872	592.4514	-19043.1872	-150.8735
NAMD	567.0876	592.4516	-19043.1971	-150.8734
Difference[c]	7.0×10^{-7}	3.4×10^{-7}	5.2×10^{-7}	-6.6×10^{-7}

[a]The validation was made by comparisons of bond, angle, van der Waals, and electrostatic energies (in kcal/mol) for the same DHPC-only micelle and lipid-only bilayer systems. [b]Energy calculated using GROMACS 4.5.5.[1] [c]Relative change of the NAMD energy compared to the GROMACS energy, i.e., Difference = (E_{NAMD} - $E_{GROMACS}$) / E_{NAMD}.

References:

1. Pronk, S.; Pall, S.; Schulz, R.; Larsson, P.; Bjelkmar, P.; Apostolov, R.; Shirts, M. R.; Smith, J. C.; Kasson, P. M.; van der Spoel, D.; Hess, B.; Lindahl, E. Gromacs 4.5: A High-Throughput and Highly Parallel Open Source Molecular Simulation Toolkit. *Bioinformatics* **2013**, *29*, 845-854.