

Supporting Information

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

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Protein/Membrane System

Download PDB File: Download Source: ▾

Upload PDB File: no file selected

PDB Format: RCSB CHARMM

Membrane Only System


Next Step: 
Select Model/Chain

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.

System Size Determination Options:

Homogeneous Lipid
 Heterogeneous Lipid

1. Box Type:

2. Length of Z based on:
 Water thickness (Minimum water height on top and bottom of the system)

3. Length of XY based on:
 Numbers of lipid components

XY Dimension Ratio:
 (The system size along the X and Y must be the same)

click this once you fill the following table:

Lipid Type	# of Lipid on Upperleaflet	# of Lipid on Lowerleaflet	Surface Area
▼ Standard Lipids			
DLPC [Image]	<input type="text" value="60"/>	<input type="text" value="60"/>	<input type="text" value="57.2"/>
DLPE [Image]	<input type="text" value="0"/>	<input type="text" value="0"/>	<input type="text" value="55.0"/>
DPPC [Image]	<input type="text" value="0"/>	<input type="text" value="0"/>	<input type="text" value="63.0"/>
DPPE [Image]	<input type="text" value="0"/>	<input type="text" value="0"/>	<input type="text" value="63.0"/>
DSPC [Image]	<input type="text" value="0"/>	<input type="text" value="0"/>	<input type="text" value="63.0"/>
DSPE [Image]	<input type="text" value="0"/>	<input type="text" value="0"/>	<input type="text" value="63.0"/>
POPC [Image]	<input type="text" value="0"/>	<input type="text" value="0"/>	<input type="text" value="68.3"/>
POPE [Image]	<input type="text" value="0"/>	<input type="text" value="0"/>	<input type="text" value="63.0"/>
DOPC [Image]	<input type="text" value="0"/>	<input type="text" value="0"/>	<input type="text" value="67.4"/>
DOPE [Image]	<input type="text" value="0"/>	<input type="text" value="0"/>	<input type="text" value="67.4"/>
► PUFA (polyunsaturated Fatty Acid) Lipids			

Calculated XY System Size:		
	Upperleaflet	Lowerleaflet
Protein Area	190.188	176.45
Lipid Area	3432	3432
# of Lipids	60	60
Total Area	3622.188	3608.45
Protein X Extent	15.78	
Protein Y Extent	14.84	
Average Area	3615.32	
A	60.13	
B	60.13	

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


Determined System Size:			
# of Atoms			
Crystal Type	TETRAGONAL		
System Size	A	60.1275	Dimension along the A (X) axis
	B	60.1275	Dimension along the B (Y) axis
	C	85.504	Dimension along the C (Z) axis
Crystal Angle	Alpha	90.0	Angle between the axis B and C
	Beta	90.0	Angle between the axis A and C
	Gamma	90.0	Angle between the axis A and B
Lipid			
# of Lipids	on Top	60	
	on Bottom	60	
# of Water	0		
# of NA Ion	16		
# of CL Ion	15		
Z Center	5.221	Center of the system along the Z axis	
Equilibration Options:			
<input checked="" type="radio"/> NPT ensemble			
Temperature:	<input type="text" value="303.15"/>	K	
			Next Step:  Equilibrate Membrane

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.

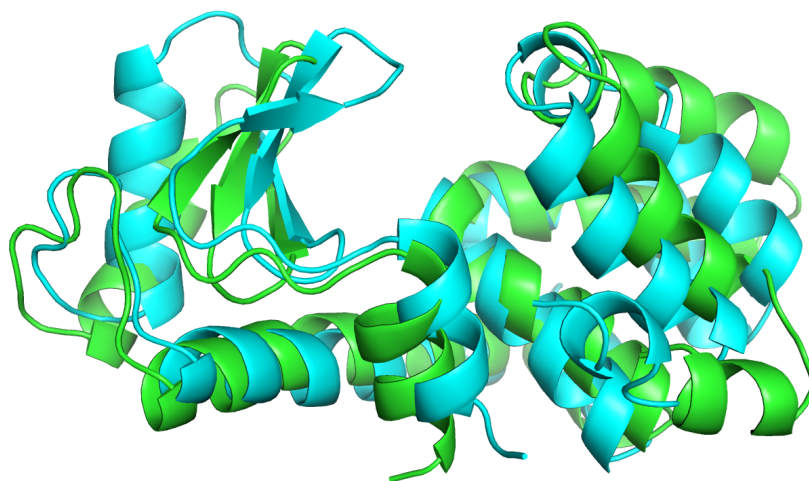


Figure S4. Comparison of the last snapshot from MD (green) to the crystal structure of lysozyme (cyan) shows the displacement of helices.

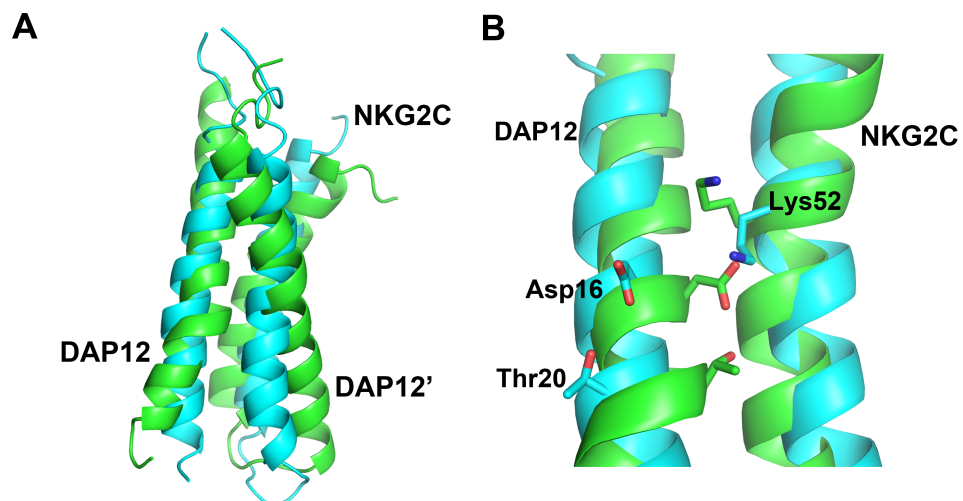


Figure S5. Comparison of the last snapshot from MD (green) to the NMR structure of DAP12-NKG2C (cyan). (A) One of the DAP12 protomers is distorted at the C terminus, and the other is rotated. (B) Asp16 and Thr20 from one of the DAP12 protomers move inwards during the simulation. For clarity, another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

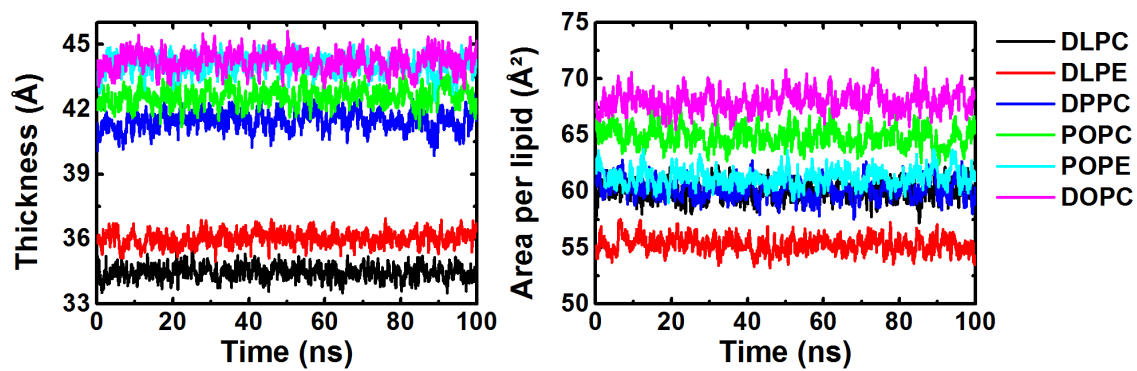


Figure S6. Time-series of the bilayer thickness and per-lipid area in the lipid-only bilayer systems.

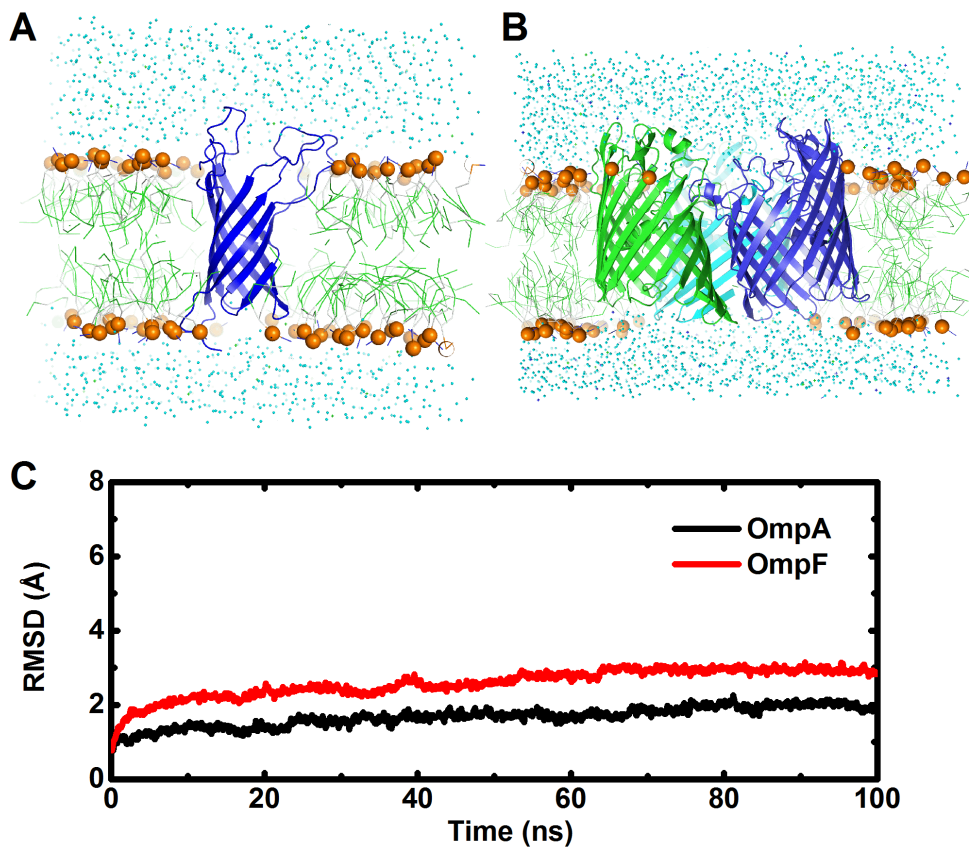


Figure S7. Bilayer systems: (A) OmpA, (B) OmpF, and (C) their RMSD time-series.

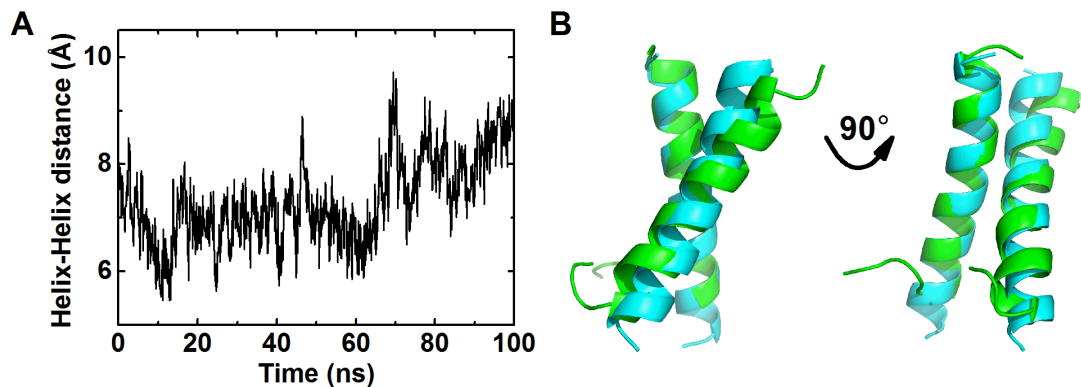


Figure S8. The GpA conformation during simulation. (A) The helix-helix distance shows that the helices do not dissociate. (B) Comparison of the last snapshot (green) to the crystal structure (cyan) shows about 10° change in the crossing angle.

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}

^aThe 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. ^bEnergy calculated using GROMACS 4.5.5.¹ ^cRelative change of the NAMD energy compared to the GROMACS energy, i.e., Difference = $(E_{\text{NAMD}} - E_{\text{GROMACS}}) / E_{\text{NAMD}}$.

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.