Supplementary Materials

Transmembrane Helix Orientation and Dynamics: Insights from Ensemble Dynamics with Solid-State NMR Observables

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Table S1. System parameters for each standard molecular dynamics simulation system

System	Number of				Total Atoms	Initial Size (Å)
	PC	PG	Water	K^+/Cl^-		
DOPC/DOPG	126	14	6,823	25 / 11	40,218	$69.8 \times 69.8 \times 79.6$
DMPC/DMPG	126	14	6,798	23 / 9	37,340	$66.4 \times 66.4 \times 79.6$
DLPC/DLPG	126	14	7,017	22 / 8	36,316	$64.5 \times 64.5 \times 79.6$

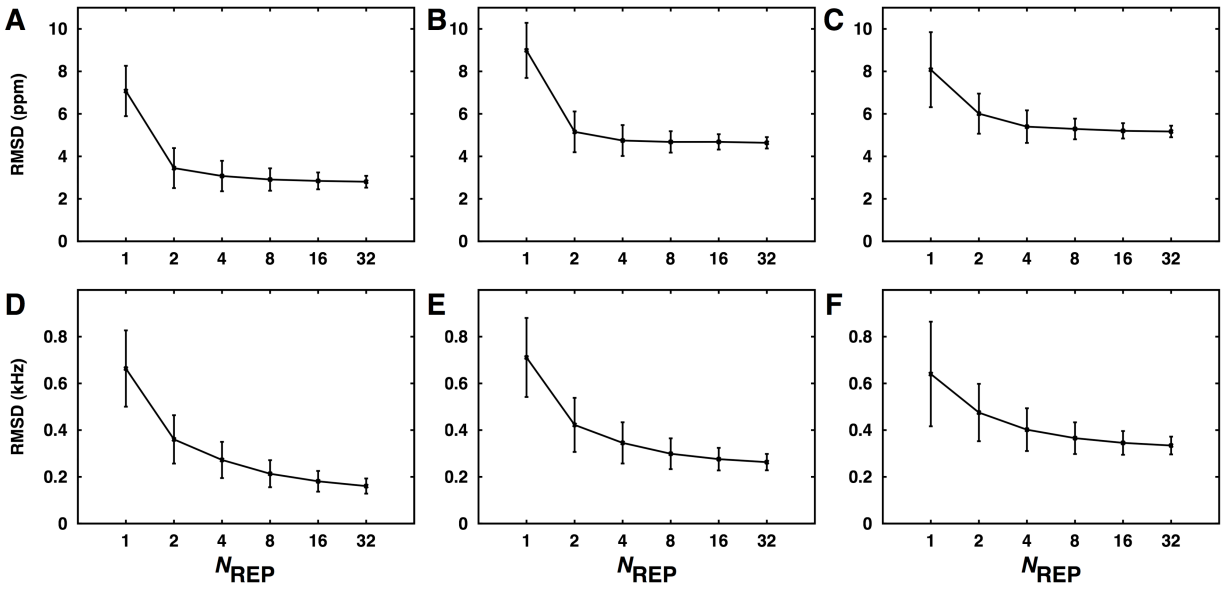

Figure S1. CSA and DC RMSD of structure ensemble determined by SSNMR-ED. (*A*, *B*, and *C*) CSA RMSD in DOPC, DMPC, and DLPC, respectively. (*D*, *E*, and *F*) DC RMSD in DOPC, DMPC, and DLPC, respectively.

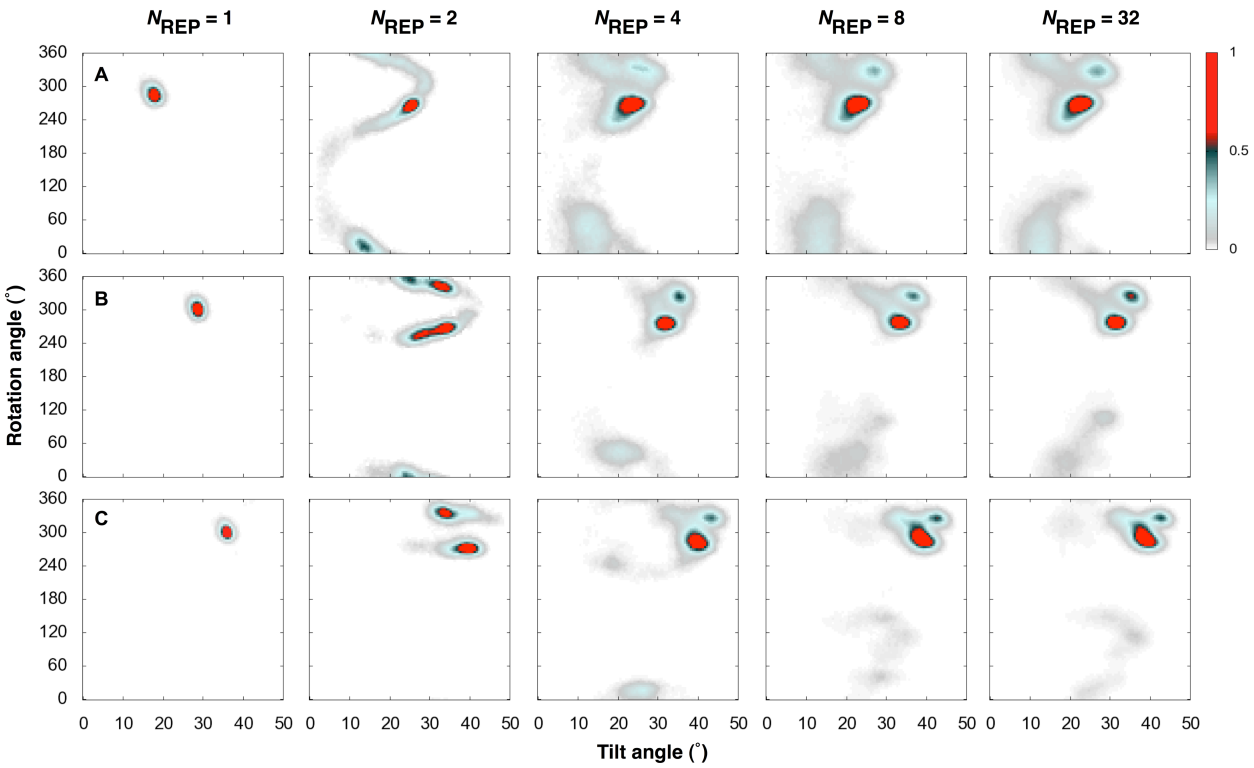

Figure S2. Orientational distributions of VpuTM structure ensembles in different bilayer environments: (*A*) DOPC, (*B*) DMPC, and (*C*) DLPC. Populations are normalized for easy comparison.

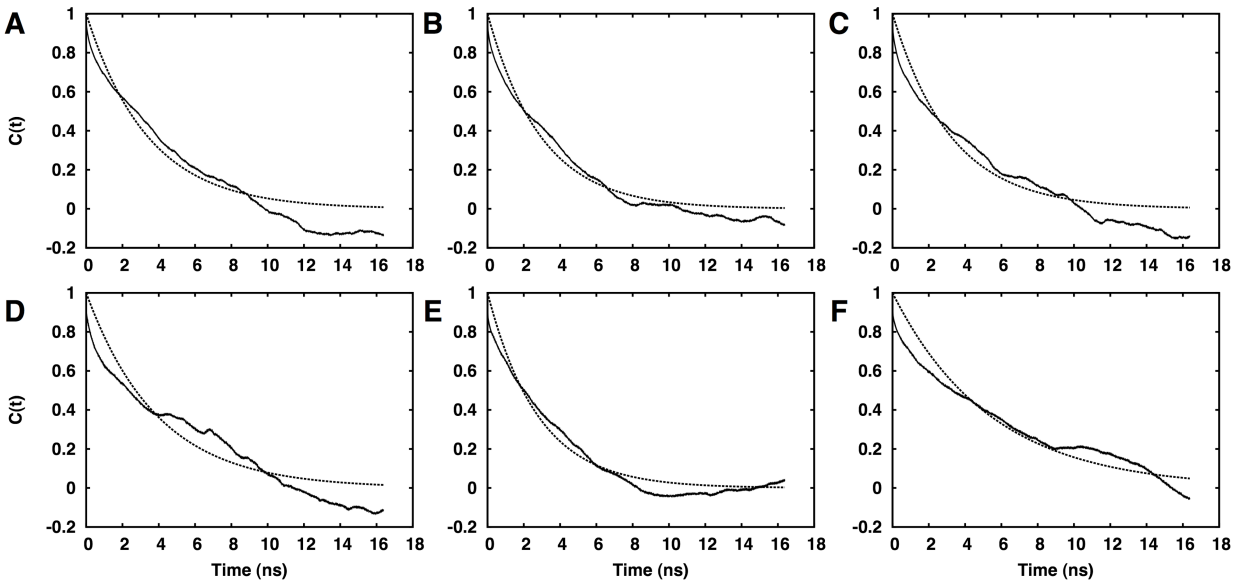

Figure S3. Correlation functions of VpuTM tilt and rotation in different bilayer environments. (*A*, *B*, and *C*) Tilt angles in DOPC, DMPC, and DLPC, respectively. (*D*, *E*, and *F*) Rotation angles in DOPC, DMPC, and DLPC, respectively. The solid line is the average correlation function over five independent simulation trajectories. The dotted line is a least-square fit to a single exponential decay, $C(t) \approx e^{-t/\omega}$. The tilt relaxation times (ω) are 3.4 ± 0.8 ns (DOPC), 3.0 ± 0.8 ns (DMPC), and 3.3 ± 0.5 ns (DLPC). The rotation relaxation times (ω) are 4.0 ± 1.8 ns (DOPC), 2.8 ± 0.4 ns (DMPC), and 5.4 ± 1.3 ns (DLPC).

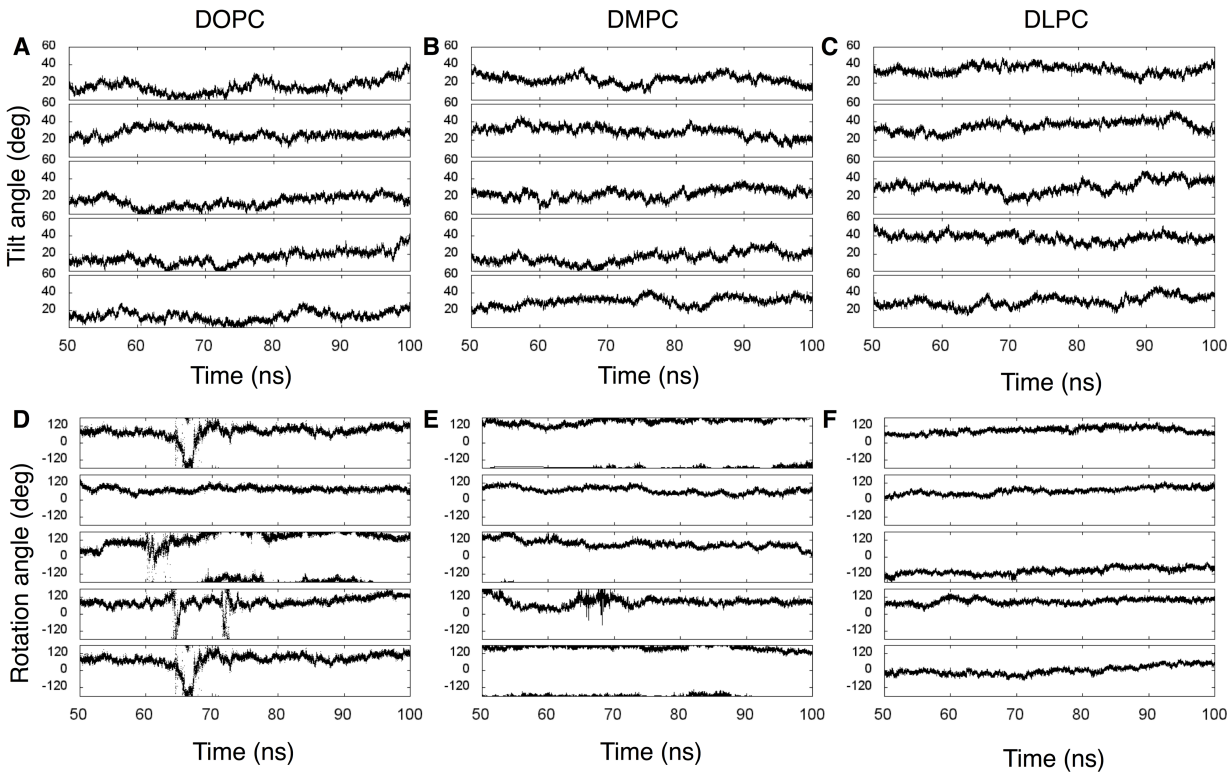

Figure S4. Time series of VpuTM tilt and rotation angles in different bilayer environments. (*A*, *B*, and *C*) Tilt angles in DOPC, DMPC, and DLPC, respectively. (*D*, *E*, and *F*) Rotation angles in DOPC, DMPC, and DLPC, respectively. Note that, by definition, the rotation angle is not well defined when the tilt angle is very small.