Supporting Materials

Solid-State NMR Observable-based Ensemble Dynamics Simulations of Membrane Protein in Explicit Membranes

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TABLE S1. Structural statistics

	MD1	ED1	ED2	ED4	ED8	ED16	ED32
Number of experimental solid-state NMR restraints							
^{15}N CSA[a]	0	38	38	38	38	38	38
^{1}H-^{15}N DC[b]	0	38	38	38	38	38	38
RMSD from solid-state NMR restraints[c]							
^{15}N CSA (ppm)	26.7 ± 5.7	5.6 ± 0.6	4.2 ± 0.6	3.2 ± 0.3	2.9 ± 0.2	2.7 ± 0.2	2.6 ± 0.2
^{1}H-^{15}N DC (kHz)	5.7 ± 1.2	0.8 ± 0.1	0.6 ± 0.1	0.5 ± 0.0	0.5 ± 0.0	0.4 ± 0.0	0.4 ± 0.0
RMSD from PDB structure (Å)[d]							
Residues 1-50	4.5 ± 0.6	4.5 ± 0.6	4.8 ± 0.7	4.7 ± 0.7	4.5 ± 0.7	4.7 ± 0.7	4.8 ± 0.7
Residues 8-18 (PP[e])	0.5 ± 0.1	0.4 ± 0.1	0.5 ± 0.1	0.5 ± 0.1	0.5 ± 0.1	0.5 ± 0.1	0.5 ± 0.2
Residues 21-45 (TM[f])	2.5 ± 0.2	2.3 ± 0.2	2.2 ± 0.2	2.2 ± 0.2	2.2 ± 0.2	2.3 ± 0.2	2.3 ± 0.2
Residue 8-18 and 21-45	3.0 ± 0.4	2.4 ± 0.2	2.6 ± 0.5	2.6 ± 0.5	2.5 ± 0.5	2.7 ± 0.5	2.7 ± 0.5
Residue 21-35	1.2 ± 0.1	1.2 ± 0.1	1.2 ± 0.2	1.2 ± 0.1	1.2 ± 0.1	1.2 ± 0.1	1.2 ± 0.1
Residue 38-45	0.9 ± 0.1	0.5 ± 0.1	0.7 ± 0.3	0.7 ± 0.3	0.7 ± 0.3	0.8 ± 0.4	0.8 ± 0.4

[a]11 CSA for the transmembrane domain, 25 CSA for the periplasmic domain, and 2 for the loop linking the transmembrane and periplasmic domains.
[b]11 DC for the transmembrane domain, 25 DC for the periplasmic domain, and 2 for the loop linking transmembrane and periplasmic domains.
[c]Evaluated as RMSD.
[d]Evaluated as RMSD for backbone atoms (CA, C, N and O).
[e]PP for the periplasmic domain.
[f]TM for the transmembrane domain.

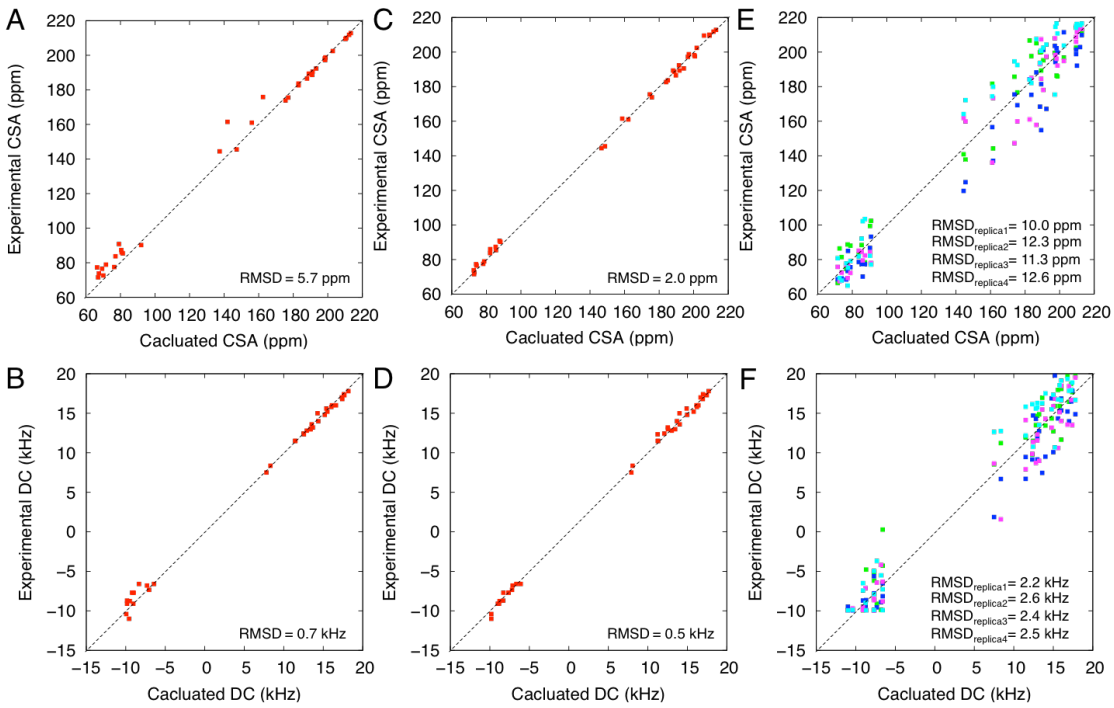

FIGURE S1. Comparison between the experimental and back-calculated CSA and DC for the fd coat protein in (A, B) PDB:1MZT, and (C-F) a representative snapshot of ED4 system at 20 ns. In (C, D), CSA and DC for each residue are averaged over the ensemble structures from the four replicas. In (E, F), CSA and DC for each residue are calculated for each structure in the four replicas (represented in four different colors: replica1 in green, replica2 in blue, replica3 in cyan, replica4 in magenta). Note that by definition each structure in the restrained ensemble simulations (with more than one replica) may not satisfy the experimental restraints, but the ensemble structures from individual replicas collectively satisfy the experimental restraints.

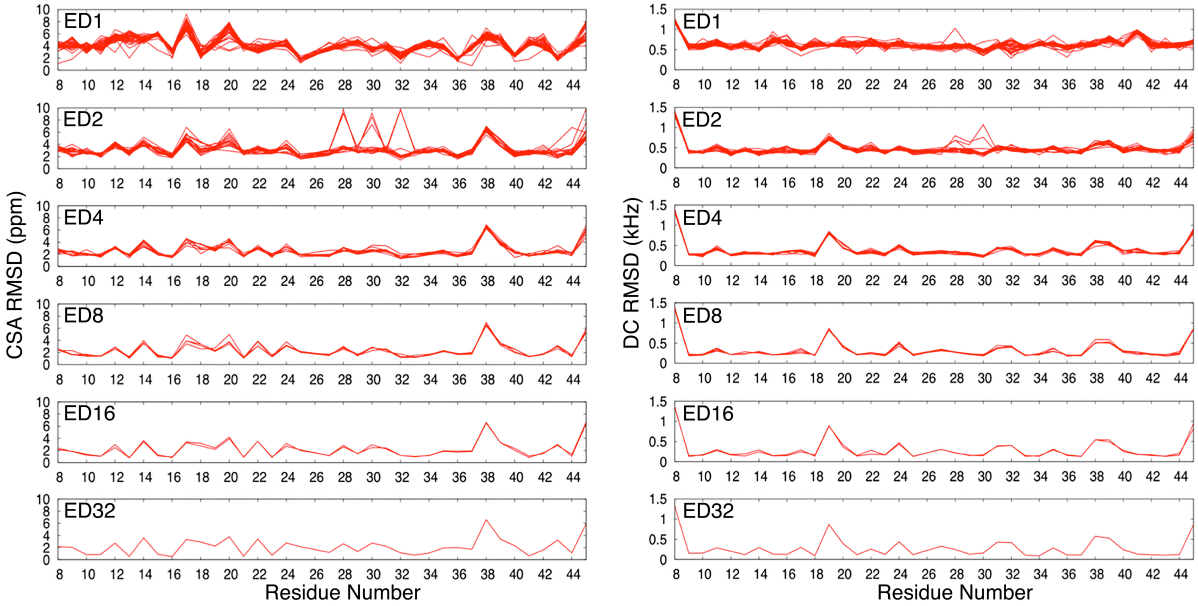

FIGURE S2. Average CSA and DC RMSD from the experimental values for each residue in the replicas in each ED system.

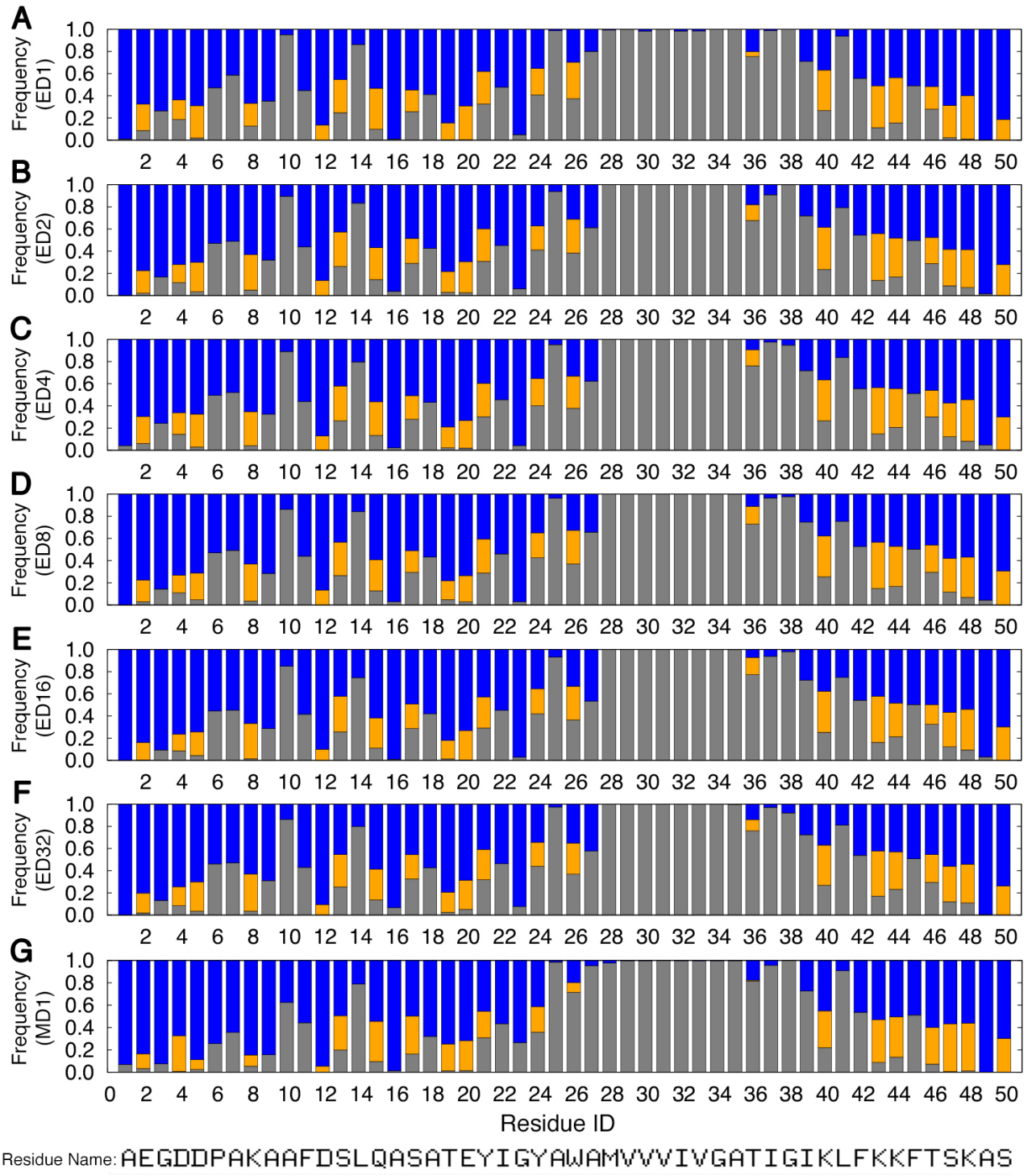

FIGURE S3. Interactions between each residue and solvent components. The graph shows the frequency with which each one or more atoms of a specific residue is found within 4 Å of a lipid hydrocarbon site (gray), lipid headgroup site (orange), or water molecule (blue), in system (A) ED1, (B) ED2, (C) ED4, (D) ED8, (E) ED16, (F) ED32, and (G) MD1.