

SUPPORTING INFORMATION

Table S1. RMSDs between observed and calculated values of the dipolar coupling (DC), chemical shift anisotropy (CSA), and combined DC and CSA (TOT), obtained for each of the 24 test assignments of F24, F43, F115, F125. Assignments for F90, F107, F148 are taken from the lowest RMSD result in Table 2 (test assignment "A"). The peak numbers are as shown in Figure 1C. Data for the lowest RMSD assignment (A.20) are in bold face.

test assignment	assignments by peak numbers							RMSD*	RMSD*	RMSD
	F24	F43	F90	F107	F115	F125	F148	DC	CSA ‡	TOT
A.1	3	5	1	7	6	2	4	0.197	0.120	0.159
A.2	3	5	1	7	2	6	4	0.219	0.138	0.179
A.3	3	6	1	7	5	2	4	0.212	0.134	0.173
A.4	3	6	1	7	2	5	4	0.230	0.147	0.189
A.5	3	2	1	7	5	6	4	0.088	0.050	0.069
A.6	3	2	1	7	6	5	4	0.081	0.041	0.061
A.7	5	3	1	7	6	2	4	0.221	0.127	0.174
A.8	5	3	1	7	2	6	4	0.241	0.145	0.193
A.9	5	6	1	7	3	2	4	0.282	0.175	0.228
A.10	5	6	1	7	2	3	4	0.287	0.178	0.233
A.11	5	2	1	7	3	6	4	0.206	0.123	0.165
A.12	5	2	1	7	6	3	4	0.191	0.109	0.150
A.13	6	3	1	7	5	2	4	0.240	0.142	0.191
A.14	6	3	1	7	2	5	4	0.256	0.155	0.205
A.15	6	5	1	7	3	2	4	0.286	0.176	0.231
A.16	6	5	1	7	2	3	4	0.292	0.180	0.236
A.17	6	2	1	7	3	5	4	0.223	0.135	0.179
A.18	6	2	1	7	5	3	4	0.212	0.126	0.169
A.19	2	3	1	7	5	6	4	0.039	0.040	0.039
A.20	2	3	1	7	6	5	4	0.018	0.028	0.023
A.21	2	5	1	7	3	6	4	0.162	0.112	0.137
A.22	2	5	1	7	6	3	4	0.142	0.096	0.119
A.23	2	6	1	7	3	5	4	0.176	0.123	0.149
A.24	2	6	1	7	5	3	4	0.162	0.112	0.137

* RMSDs are scaled by the frequency range of 20 kHz.

† RMSDs are scaled by the frequency range of 150 ppm.

‡ $CSA = \hat{\delta}_{\text{bicelle}} - 125$

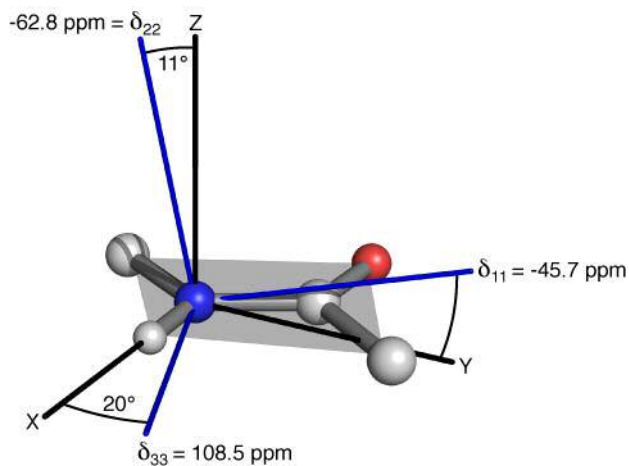


Figure S1. Magnitudes and orientations of the traceless components of the ^{15}N chemical shift tensor used in the data analysis. The δ_{33} component is in the plane of the peptide bond and makes an angle of 20° with the NH bond; δ_{11} and δ_{22} are rotated off the peptide plane by 11° ; $\delta_{11} = -45.8$ ppm, $\delta_{22} = -62.8$ ppm, $\delta_{33} = 108.5$ ppm. The X, Y, Z molecular axes are defined with X parallel to the NH bond, Z perpendicular to the peptide plane, and Y orthogonal to X and Z.

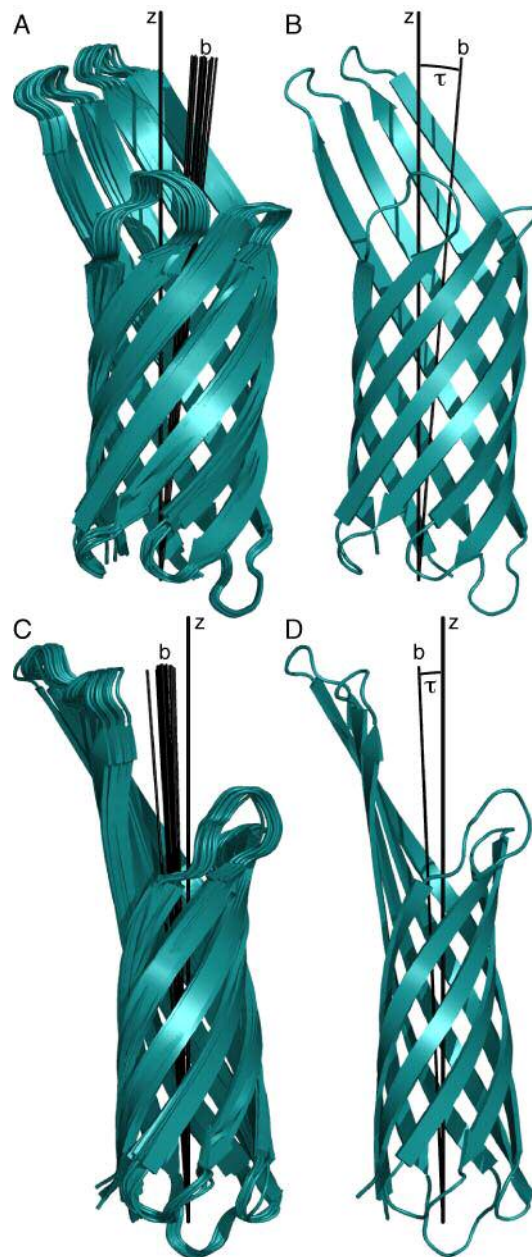


Figure S2. Front and side views of the membrane orientation of OmpX obtained from the experimental dipolar couplings. **(A, C)** Overlay of the 20 calculated structures and corresponding barrel axes. **(B, D)** Average of 20 calculated structures showing all the barrel axes. The average tilt angle (τ) between the barrel axes (b) and the membrane normal (Z) is $7.3^\circ (\pm 1.6^\circ)$.