

Table S2. Comparison of the RMSD values for each of the six UNC119 chains and their associated ligands.

Structures were overlapped on the UNC119 protein carbon- α atoms only. Ligand atoms were not included in the overlap calculation. RMSD values are given for the overlap of all protein atoms in each chain, all atoms related to residue 501 (glycine and the attached lauroyl group), and the carbon- α trace for the peptide attached to the lauroyl group in each ligand.

Chains Overlapped	RMSD for all protein atoms	RMSD for residue 501 ^a	RMSD of C α trace ^b
B on A	0.373	0.252	0.190 (501-507)
C on A	0.459	0.315	0.180 (501-504)
D on A	0.320	0.284	0.182 (501-504)
E on A	0.449	0.370	0.323 (501-503)
F on A	0.458	0.635	0.424 (501-507)

^aRMSD values calculated using all atoms on residue 501 with residue 501 defined as glycine plus the attached lauroyl group.

^bNumbers in parentheses refer to residues on the ligand from which the RMSD values were calculated.