

Supplementary Information for:

Retinal Conformation Changes Rhodopsin's

Dynamic Ensemble

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Supplementary Material

S1 Supplementary Videos

Supplementary Video 1 This movie shows the average displacement of simulations along the first three principal components (also called right singular vectors). All 24 simulations are shown colored according to the starting structure. The movie shows the time progression of each simulation. Dark opsin simulations in green, opsin simulations in orange, Meta-I simulations in blue, and Meta-II simulations in red.

S2 Supplementary Tables

System	PDB ID	Notes	Simulation Time (ns)
Dark opsin	1U19	retinal removed	3,904
			3,935
			3,941
			4,209
			4,228
			4,216
Opsin	3CAP		2,968
			4,366
			3,945
			3,889
			3,926
			4,212
Meta-I	"Meta-I"	(from ref. 1)	4,902
			4,732
			4,857
			4,784
			4,758
			4,790
Meta-II	3PXO		3,907
			3,544
			3,926
			4,202
			4,203
			4,209
Total			100,553 ns

Table Si: Full simulation details.

S3 Supplementary Figures

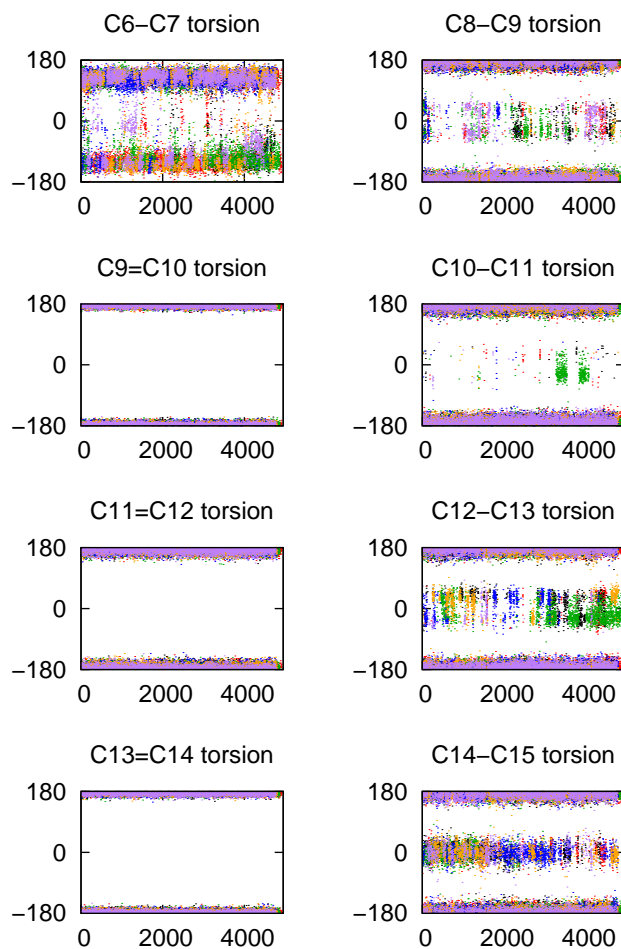


Figure S1: Retinal torsions in Meta-I simulations. Timeseries of retinal torsion angles for each of the six Meta-I trajectories. Torsions are labeled above each plot (part 1 of 2). X-axis is time in units of ns, y-axis is angle in degrees.

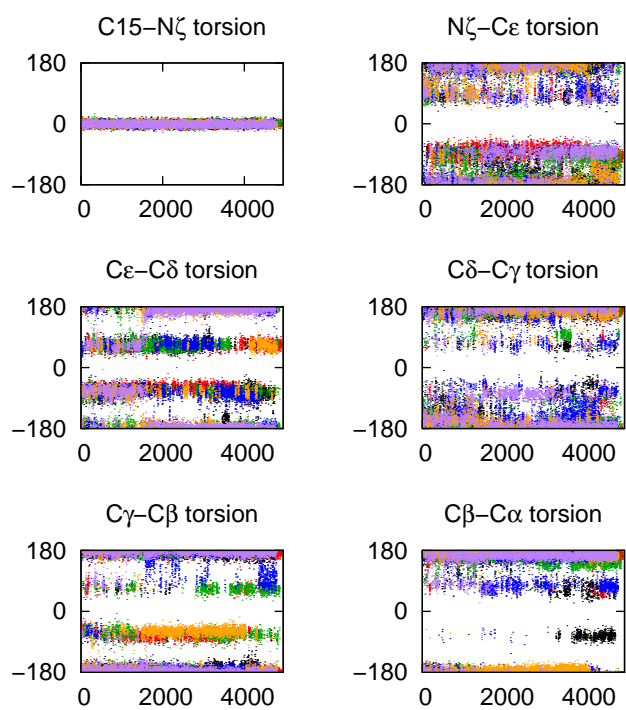


Figure S2: Retinal torsions in Meta-I simulations. Timeseries of retinal torsion angles for each of the six Meta-I trajectories. Torsions are labeled above each plot (part 2 of 2). X-axis is time in units of ns, y-axis is angle in degrees.

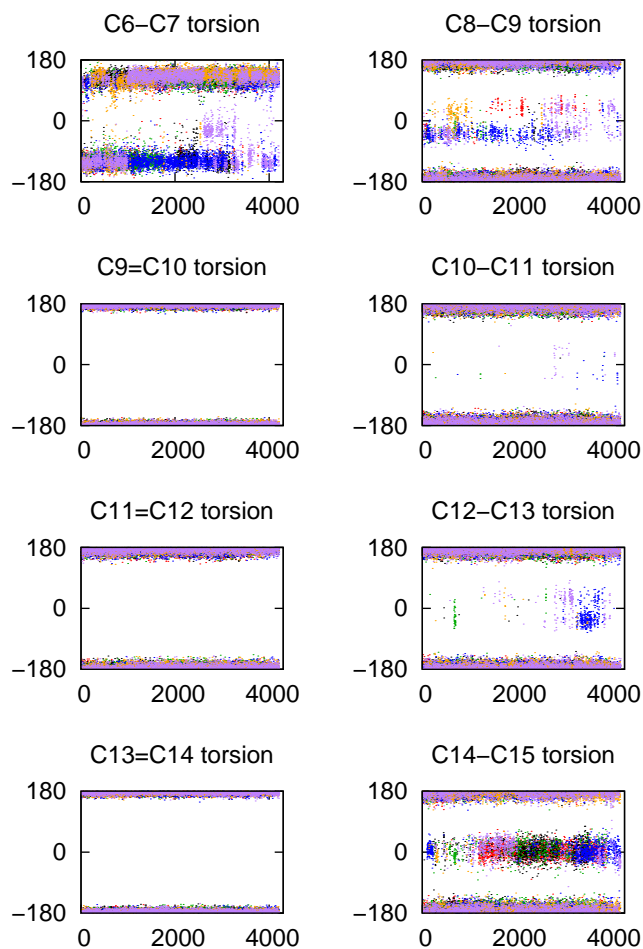


Figure S3: Retinal torsions in Meta-II simulations. Timeseries of retinal torsion angles for each of the six Meta-II trajectories. Torsions are labeled above each plot (part 1 of 2). X-axis is time in units of ns, y-axis is angle in degrees.

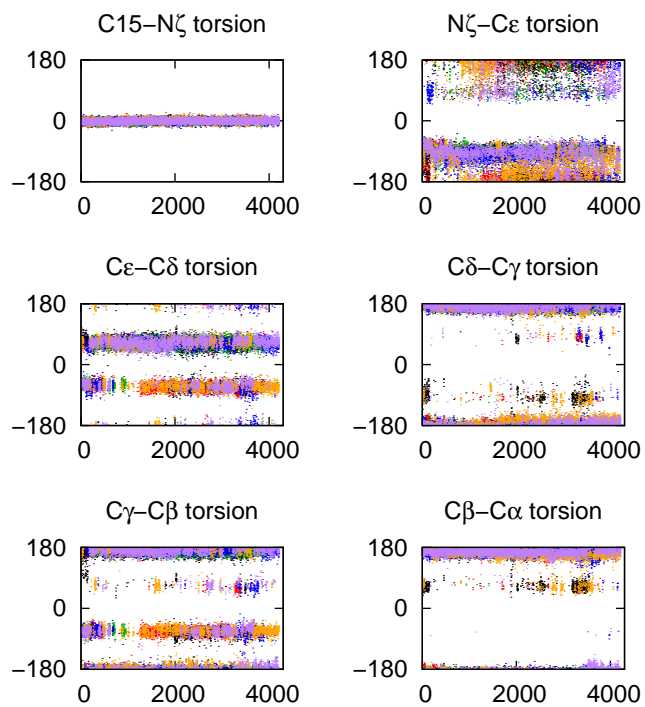


Figure S4: Retinal torsions in Meta-II simulations. Timeseries of retinal torsion angles for each of the six Meta-II trajectories. Torsions are labeled above each plot (part 2 of 2). X-axis is time in units of ns, y-axis is angle in degrees.

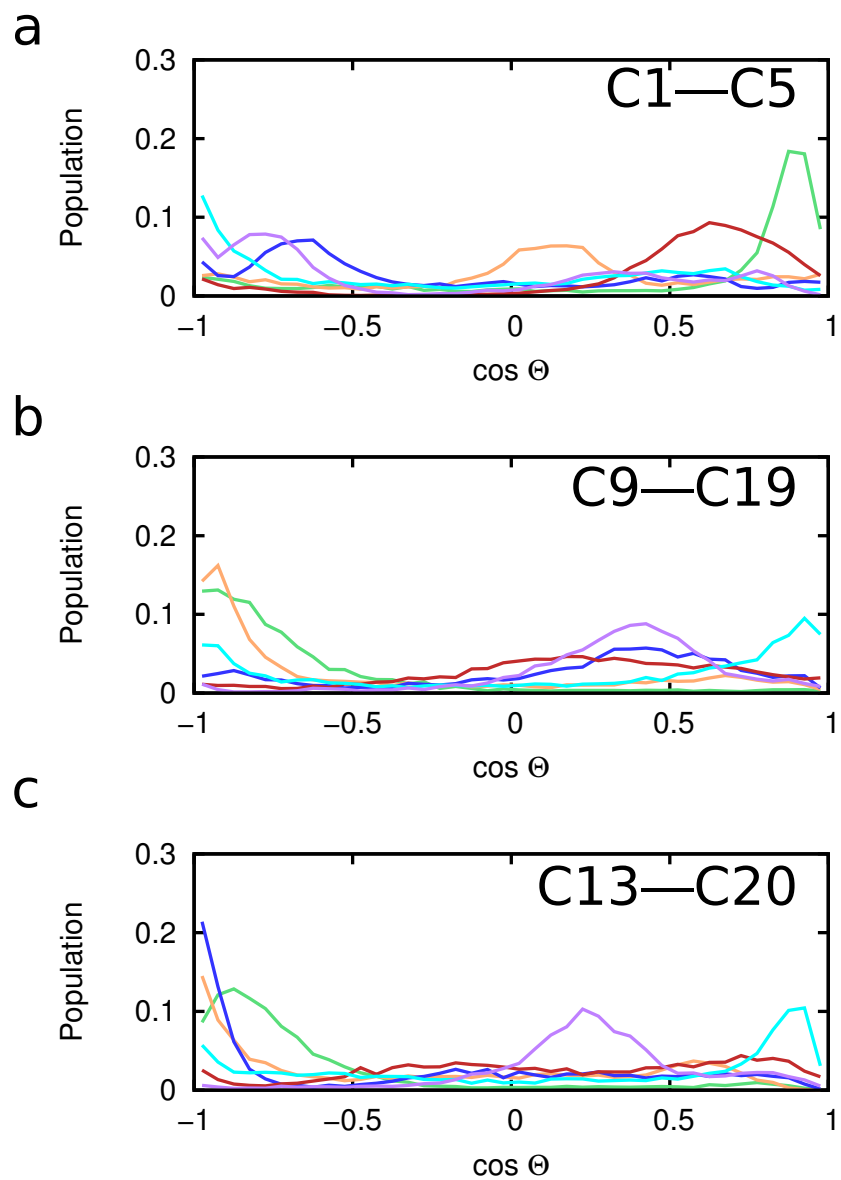


Figure S5: Retinal orientation in Meta-I simulations. Histograms of retinal orientations for each trajectory as described in Section 3.1.1. Histograms show population of (a) a vector drawn from the C1 atom to C5, (b) a vector drawn from the C9 atom to C19, or (c) a vector drawn from the C13 atom to C20, dotted against the membrane normal.

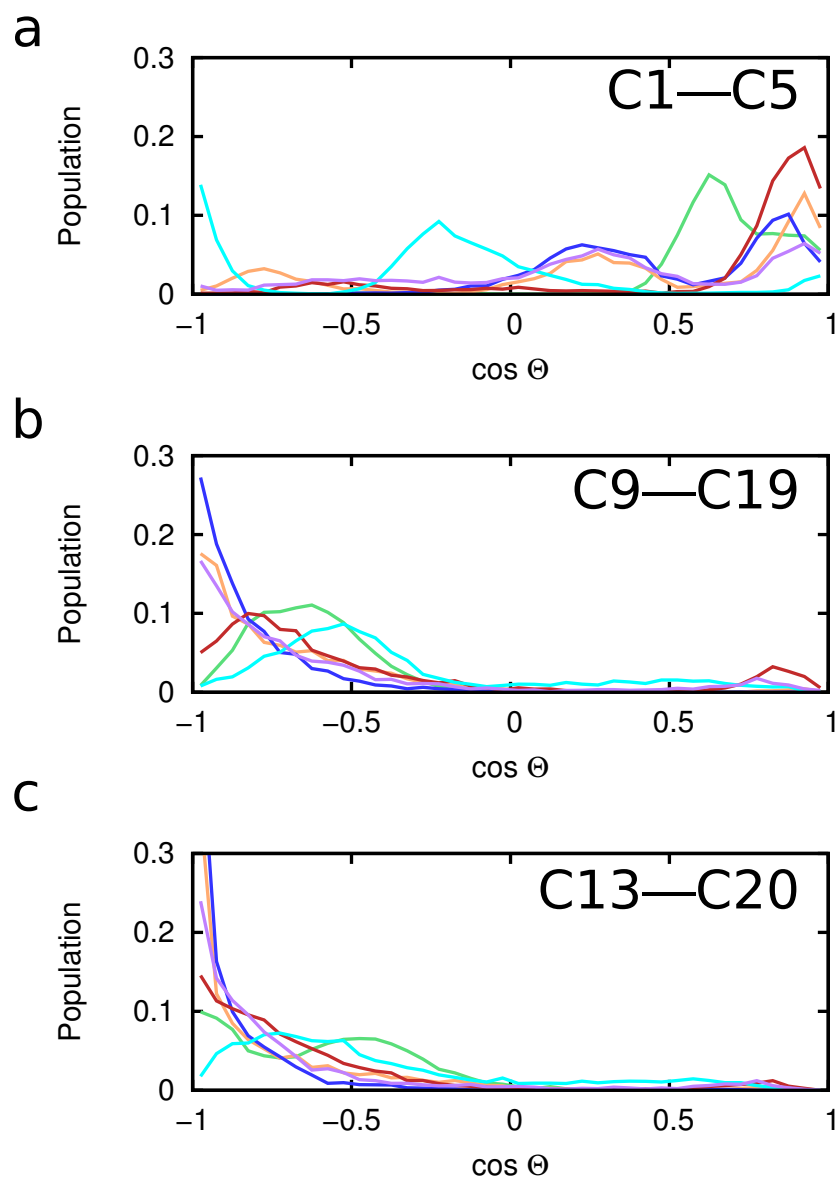


Figure S6: Retinal orientation in Meta-II simulations. Histograms of retinal orientations for each trajectory as described in Section 3.1.1. Histograms show population of (a) a vector drawn from the C1 atom to C5, (b) a vector drawn from the C9 atom to C19, or (c) a vector drawn from the C13 atom to C20, dotted against the membrane normal.

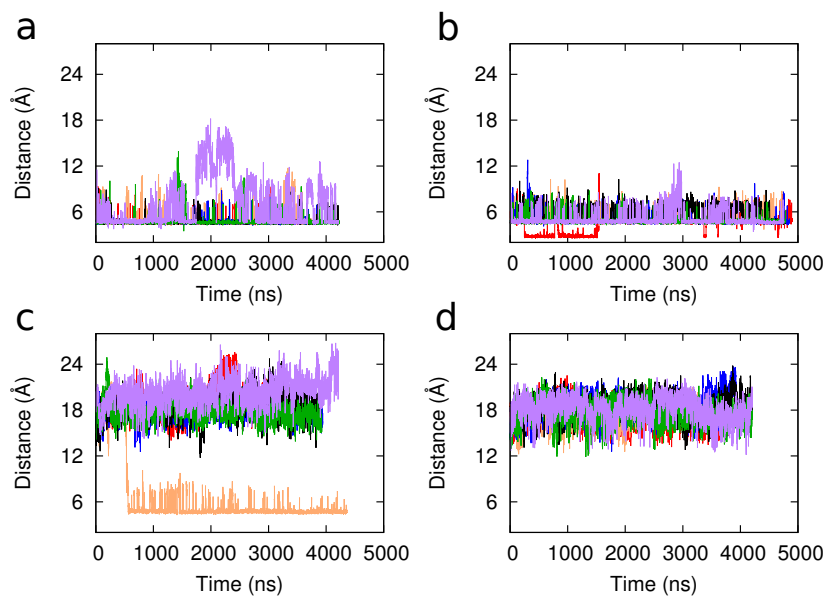


Figure S7: Ionic lock transitions. The minimum distance between Glu247^{6.30} oxygens and Arg135^{3.50} nitrogens is plotted as a function of simulation time. Data is shown for: (a) dark-opsin, (b) Meta-I, (c) opsin, and (d) Meta-II ensembles.

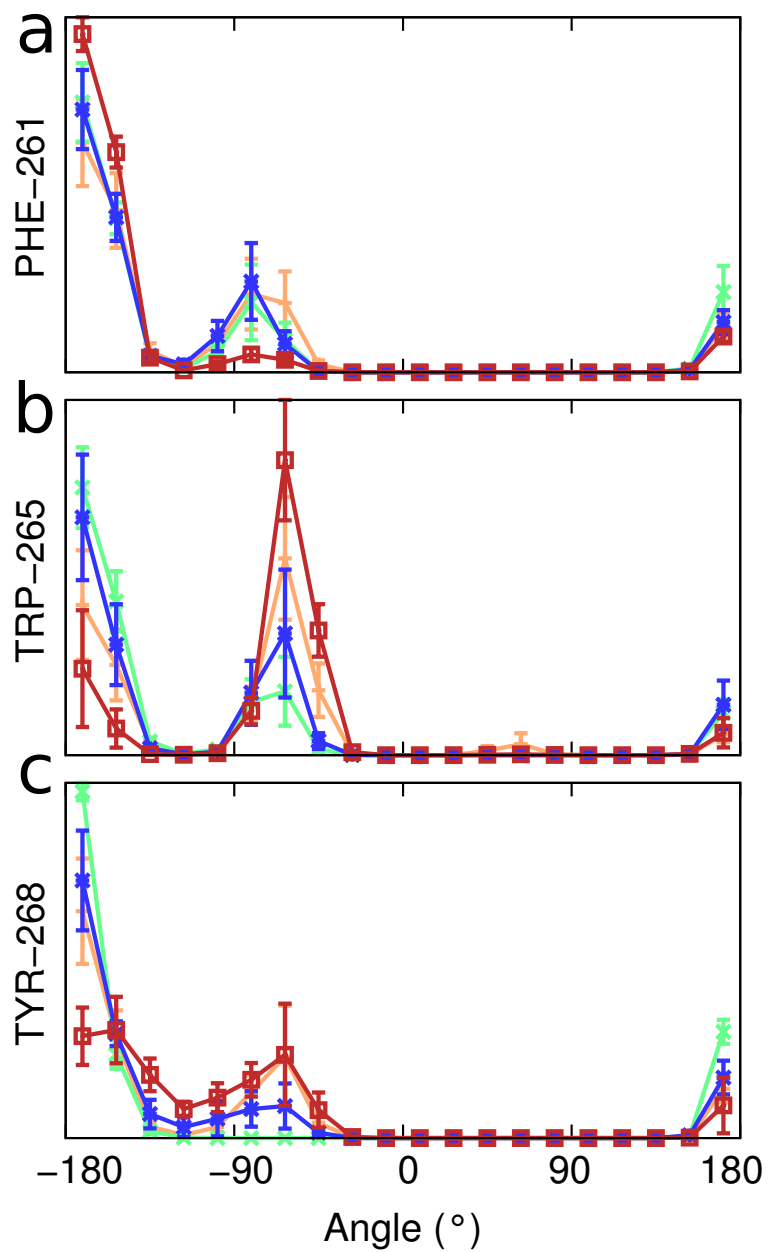


Figure S8: Toggle residue orientations. Histograms of the χ_1 torsion of the three rotamer toggle switch residues: Phe261^{6.44}, Trp265^{6.48}, and Tyr268^{6.51} are plotted as in Figure 3b. Here the only difference is the addition of error bars, indicating the standard error across each ensemble, treating each simulation as a single measurement.

References

1. Grossfield, A., M. C. Pitman, S. E. Feller, O. Soubias, and K. Gawrisch, 2008.

Internal hydration increases during activation of the G-protein-coupled receptor rhodopsin. *J Mol Biol* 381:478–486.

<http://dx.doi.org/10.1016/j.jmb.2008.05.036>.