Supporting Information

The Impact of Retinal Configuration on the Protein-Chromophore Interactions in Bistable Jumping Spider Rhodopsin-1

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Equilibration and Production

As mentioned in the main text the crystal structure of JSR1 (PDB ID: 6I9K) with the all-*trans*, 9-*cis* and 11-*cis* isomers of retinal were embedded in a membrane using the CHARMM-GUI website. These systems were minimized, heated and then long time-scale dynamics were performed for 380 ns using the AMBER ff14SB and lipid14 forcefields along with our derived retinal chromophore parameters.[15] The restraints used in each step are outline in Table S1. Each structure was first minimized using the classical force field for 100,000 steps. During the minimization step a restraint weight of 10 kcal/mol·Å^2 was placed on all heavy and light atoms. A thermal equilibration step was then performed by heating the models from 0 to 300 K stepwise over 50 ps using a timestep of 1 fs, followed by constant temperature and volume for the remaining 450 ps. Next, six separate steps of equilibration were performed for 250 ps each at a constant pressure of 1 atm and temperature of 300 K and slowly releasing the constraints on the heavy and light atoms. Following the release of the constraints, a long time-scale classical step was performed for 300 ns at constant pressure and temperature with a 2 fs timestep. Finally, SHAKE was removed from the protein and an additional 80 ns equilibration step was performed with a timestep of 1 fs.

Table S1. Constraints (kcal/mol·Å^2) used during each step of dynamics with Amber.

Equilibration step	Protein	Lipid	Ions
NVT (500 ps)	10.0	5.0	10.0
NPT 1 (250 ps)	10.0	5.0	10.0
NPT 2 (250 ps)	5.0	2.5	0.0
NPT 3 (250 ps)	2.5	1.0	0.0
NPT 4 (250 ps)	1.0	0.5	0.0
NPT 5 (250 ps)	0.5	0.1	0.0
NPT 6 (250 ps)	0.1	0.0	0.0
NPT 7 (300 ns)	0.0	0.0	0.0
NPT without SHAKE (80 ns)	0.0	0.0	0.0

The trajectories were then continued as outlined in the main text to determine the absorption maxima of the three isomers.