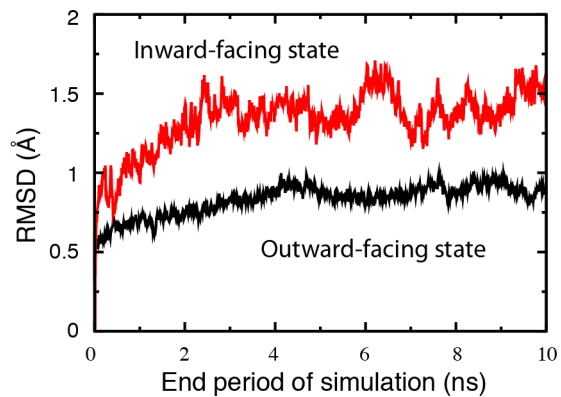


**Supplemental Fig. S1.** An outward-facing configuration retrieved from the last frame of the simulation (blue) is superimposed on the double-Trp crystal structure (cyan).



**Supplemental Fig. S2.** Root mean square deviations (RMSD) of the protein backbone in the final 10 ns of the simulations of the inward-facing (red) and outward-facing (black) states. The reference structure here is the first frame of the final 10 ns segment.