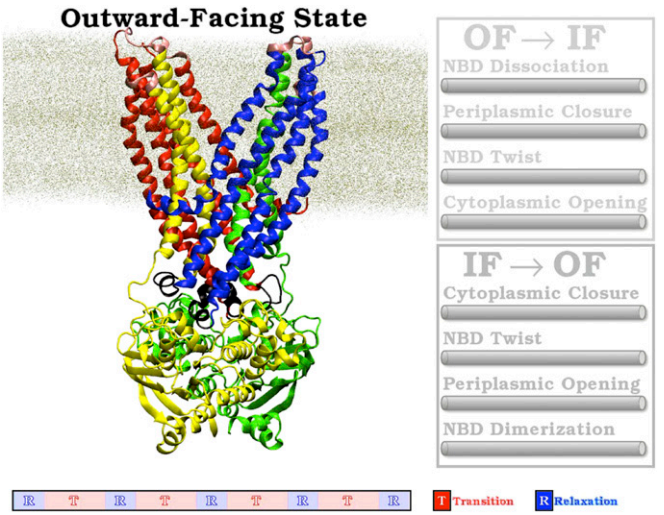
Supporting Information

Moradi and Tajkhorshid 10.1073/pnas.1313202110



Movie S1. IF ↔ OF conformational transition of *apo* MsbA. The OF → IF transition was induced using the optimized protocol ($d_{NBD} \rightarrow \gamma \rightarrow \alpha$). The backward process was not simulated (although shown here by reversing the movie). The total simulation time was 220 ns including four 40-ns "transition" stages (using nonequilibrium-driven MD) and three 20-ns interstage "relaxation" simulations (using RMD). The NBD/TMD conformational changes associated with each transition stage are given.

Movie S1

Other Supporting Information Files

SI Appendix (PDF)