Supporting Information

Koga et al. 10.1073/pnas.0904756106

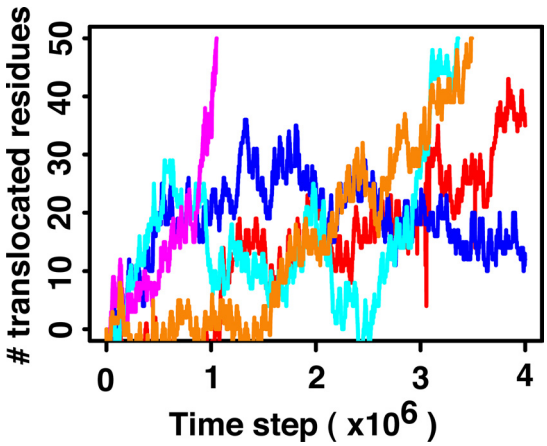


Fig. S1. CG simulations of substrate translocation. Five trajectories of the simulations where the substrate was translocated by HslU are shown. The hexameric HslU was spatially fixed at its interface to HslV, whereas the substrate threaded into the HslU pore was free to move. The number of the substrate residues that exited from the HslU pore is plotted on the vertical axis along the time.

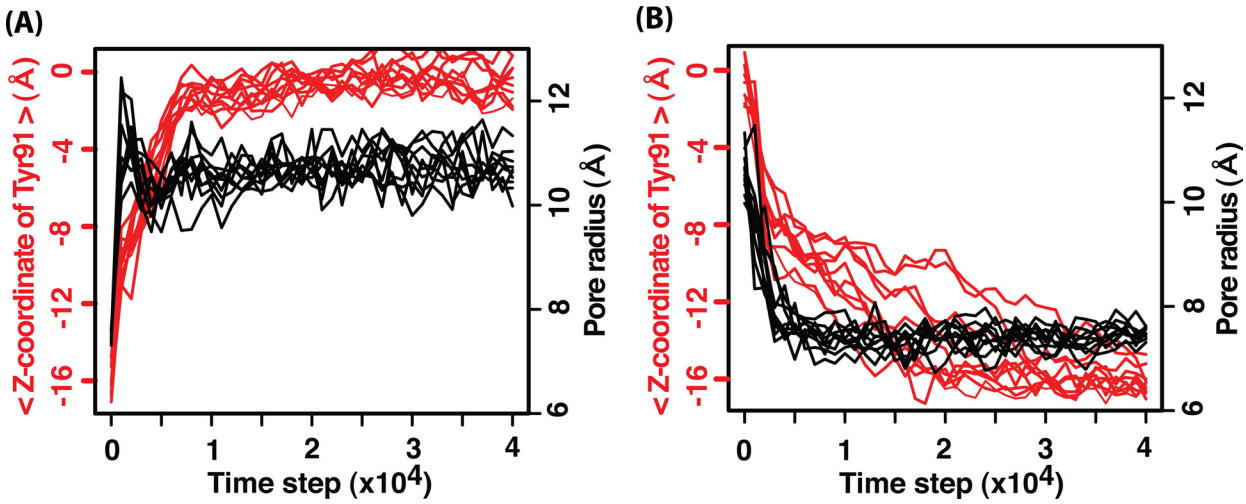
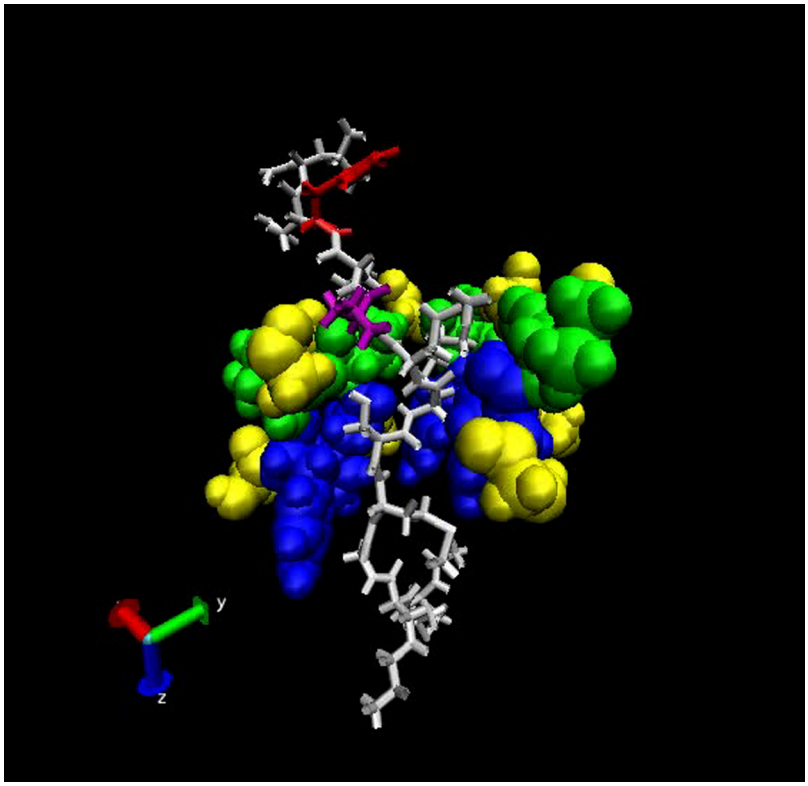
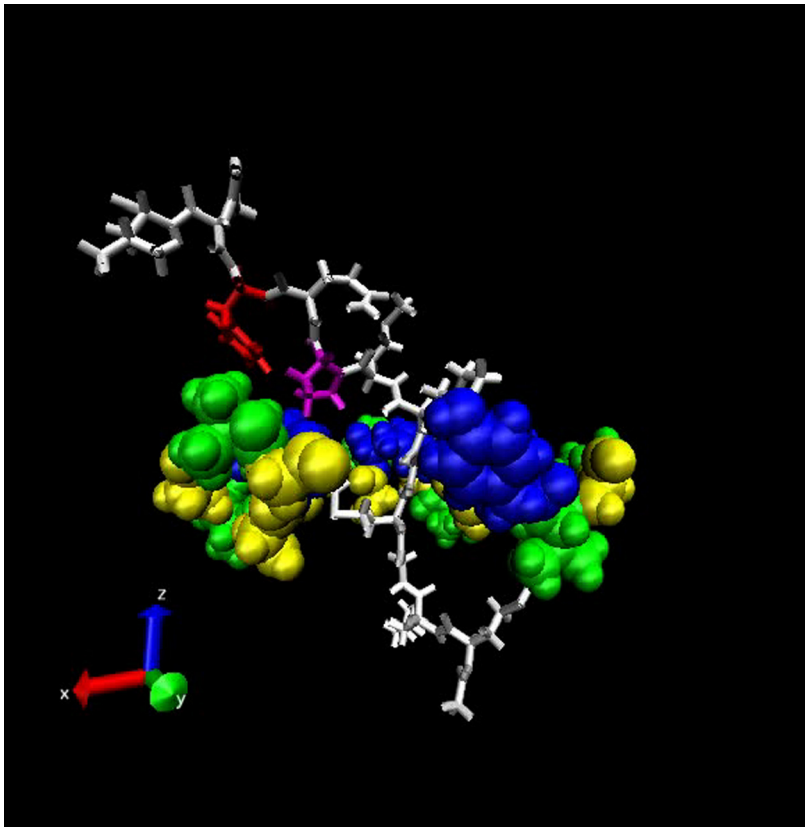


Fig. S2. Time scales of up-down motions and pore-radius changes. Relaxation of the average of *z*-coordinates of Tyr-91s (red) and the pore radius (black) when the switchings of ΔV_{bias} were conducted to induce the conformational changes of HslU, CD → OU (*A*) and OU → CD (*B*). The plotted trajectories are from a single simulation run that was performed in Fig. 5*B*, and the trajectory was split into $\Delta V_{\mathrm{bias}} = \Delta V_{\mathrm{OU\text{-}biased}}$ (*A*) and $\Delta V_{\mathrm{bias}} = \Delta V_{\mathrm{CD\text{-}biased}}$ (*B*). The *z* coordinates of Tyr-91s (labeled on the left axis) and the pore radius (labeled on the right axis) are plotted as a function of duration time after the switching.



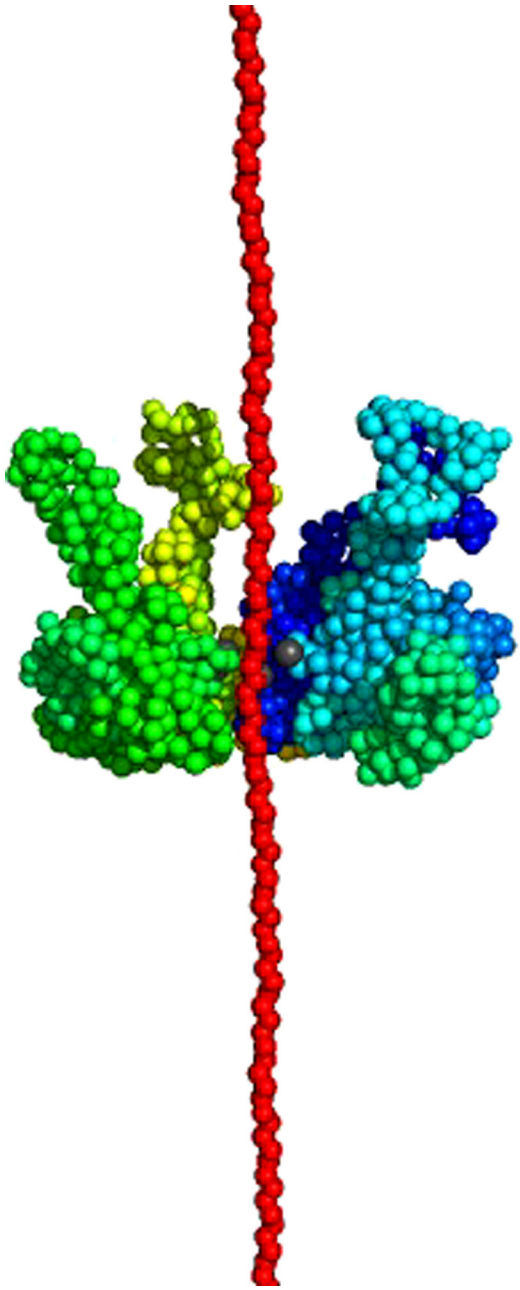
Movie S1. Fully atomistic simulation of substrate, the N-terminal 12 residues of Arc repressor, in the CD form of HslU. The N terminus of the substrate was weakly pulled from the HslV side. The representative trajectory is shown. In the HslU pore, Tyr-91s are in blue, Val-92s are in green, and Gly-90s and Gly-93s are in yellow. In the substrate, Pro-8 is in magenta and Phe-10 is in red. The bottom is the HslV side. For clarification, one subunit of HslU is omitted. Visualization was carried out by VMD (15).

Movie S1 (MPG)



Movie S2. Fully atomistic simulation of substrate, the N-terminal 12 residues of Arc repressor, in the OU form of HslU. N terminus of the substrate was weakly pulled from the HslV side. The representative trajectory is shown. In the HslU pore, Tyr-91s are in blue, Val-92s are in green, and Gly-90s and Gly-93s in yellow. In the substrate, Pro-8 is in magenta and Phe-10 is in red. The bottom is the HslV side. Visualization was carried out by VMD (15).

Movie S2 (MPG)



Movie S3. CG simulation of HslU translocation along substrate rail during multiple ATP cycles. The representative trajectory is shown. HslU is changing its conformation between the OU and CD forms during ATP cycles and moving along the substrate rail (red). To show the HslU pore, two subunits of HslU are omitted. The residues colored gray are Tyr-91s. Each snapshot was drawn by using PyMOL (DeLano Scientific).

Movie S3 (MPG)

Other Supporting Information Files

SI Appendix (PDF)