Supplemental material

Kiani et al., https://doi.org/10.1085/jgp.201812188

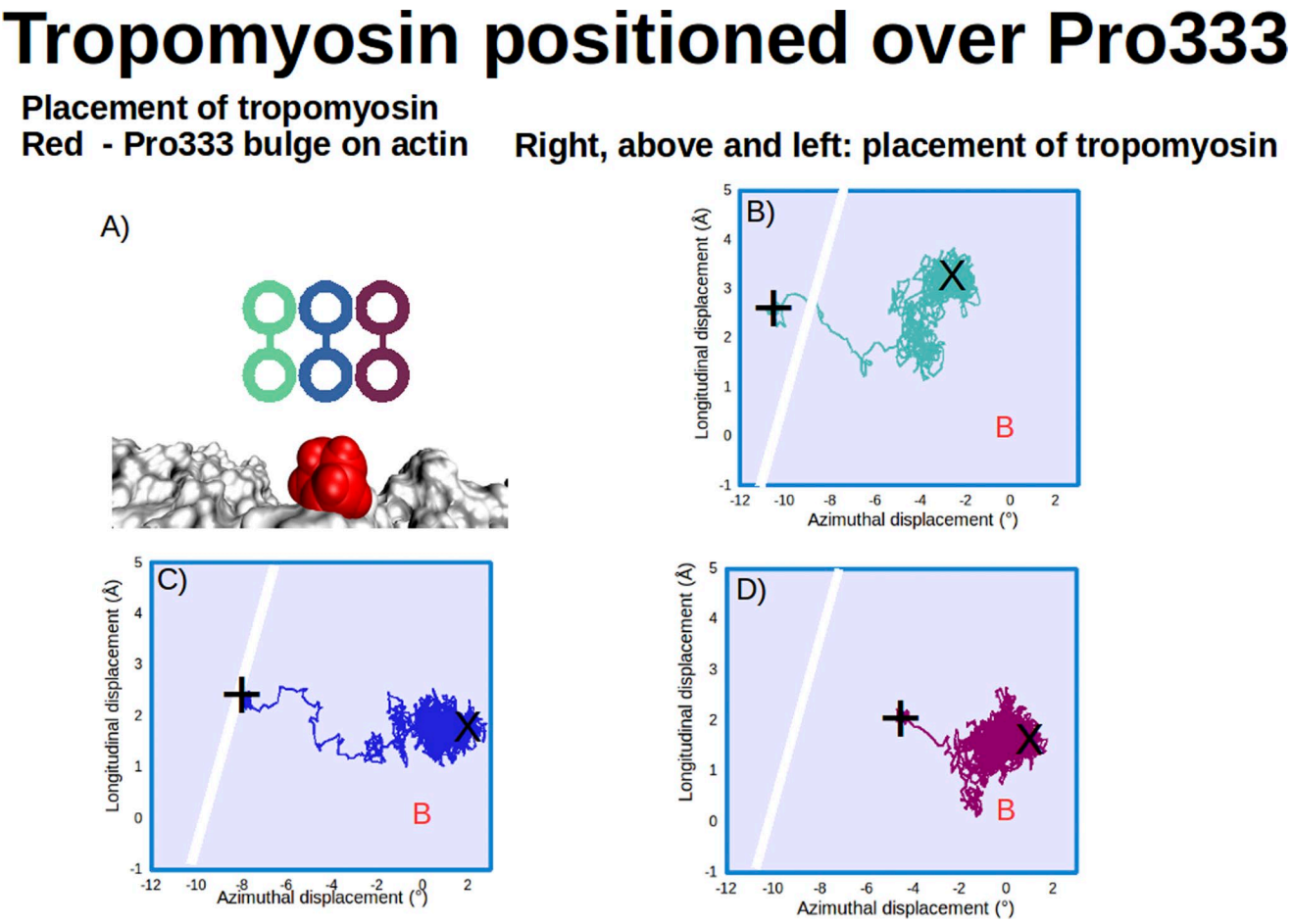


Figure S1. **Tropomyosin movement over actin when placed close to Pro333 is toward the B state. (A)** Tropomyosin was positioned at the start of MD simulations at three locations: just to the left (cyan) of, above (blue), and to the right (magenta) of Pro333 (red surface). The approximate starting position of the tropomyosin helices (represented by the connected circles) is shown relative to the actin surface, where Pro333 has been highlighted in red. **(B–D)** In all cases, when the position of tropomyosin during MD is plotted, tropomyosin movement from the starting position (indicated by +) is toward the B state, even translocating over Pro333 (represented by the white line) in (B) and (C). Last positions of tropomyosin are indicated by X in B–D. This shows that although Pro333 represents a good landmark for defining B-state versus C-state positions, it does not provide a large barrier to translocation.

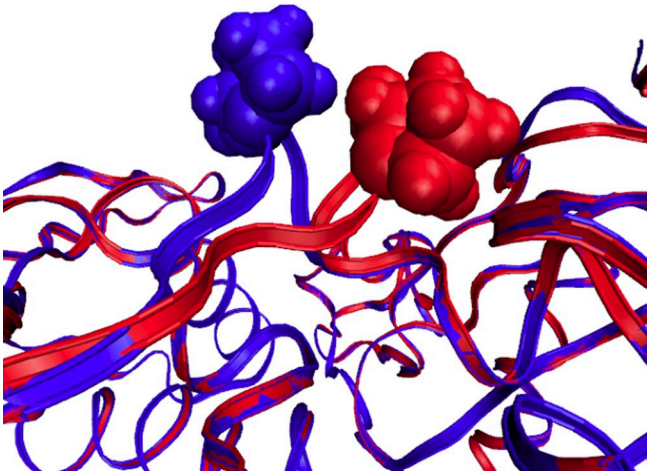
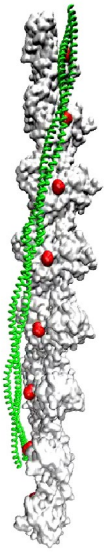
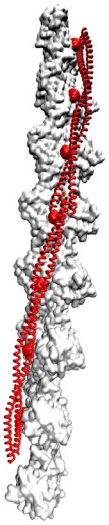


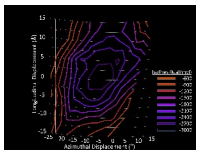
Figure S2. **Movement of actin residue Pro333 during MD simulations.** Shown is a ribbon diagram of a representative actin monomer with Pro333 highlighted in space-filling representation at the start of MD (blue) and a selected frame later in the simulation (red) oriented with the view looking down the filament axis toward the pointed end. Note that the proline position moves toward the B-state position (toward the outer domain of actin to the right in this orientation) during the simulation. This places the proline closer to the remaining surface residues of actin and may be important to allow tropomyosin to easily translocate across the proline during normal regulatory transitions.



Video 1. **The 27-ns MD simulation of tropomyosin starting in the M-state position.** Actin is rendered as a white surface with the position of Pro333 highlighted in red. Tropomyosin is shown as a green ribbon. Note that tropomyosin can be observed to move from the left side of Pro333 to the right side, thus translocating over the proline over the course of the simulation toward the outer (B-state) domain of actin. The video was made with the MovieMaker plugin in VMD (Humphrey et al., 1996).



Video 2. **The 22-ns MD simulations of tropomyosin starting in the B-state position, rendered similarly to Video 1.** Tropomyosin is shown as a red ribbon. Note that in this simulation, tropomyosin moves very little from its starting position.



Video 3. **The average azimuthal and longitudinal position of tropomyosin during the 27-ns MD shown in Fig. 1 is displayed over time on a cylindrical plot.** The isolines from the electrostatic interaction energy plot in Fig. 3 are shown for reference. Tropomyosin starting in the M state moves across the actin toward the basin in the electrostatic interaction energy plot, although it does not reach the minimum perfectly.

References

Humphrey, W., A. Dalke, and K. Schulten. 1996. VMD: Visual molecular dynamics. *J. Mol. Graph.* 14:33–38.