Supplemental video legends

Supplemental video 1. Representative steered molecular dynamics simulation of unbinding of the N-terminal domain of WT GPIbα (grey) from the WT VWF A1 domain (mauve). The C_α atom of GPIbα C-terminal residue L267 was pulled via a spring (spring constant of ~700 pN/nm) that moved horizontally to the right at a constant speed (0.5 nm/ns) with the C_α atom of the A1 N-terminal residue H1268 harmonically constrained. Note the following sequential events: 1) Disruption of the salt bridge(s) between D1269 (red spheres) and R1306/R1450 (blue/green spheres). 2) Extension of the A1 N-terminal sequence and the counterclockwise rotation of A1. 3) Sliding of the GPIbα β-finger over A1. 4) Formation of a salt bridge between GPIbα E14 (red sticks) and A1 R1334 (blue sticks). 5) Dissociation of the GPIbα β-switch (blue β-strand) from the A1 central β-sheet (red β-strand). 6) Rupture of the E14:R1334 interaction. 7) Complete dissociation of GPIbα from A1.

Supplemental video 2. Representative steered molecular dynamics simulation of unbinding of the N-terminal domain of M239V GPIbα (grey) from the R1306Q VWF A1 domain (mauve). See Supplemental video 1 legend for detailed description. Note that the E14:R1334 salt bridge was formed at 0 ns before force was applied and that no new contact was formed during the simulation.