Supplementary Material

The Talin Dimer Structure Orientation is Mechanically Regulated

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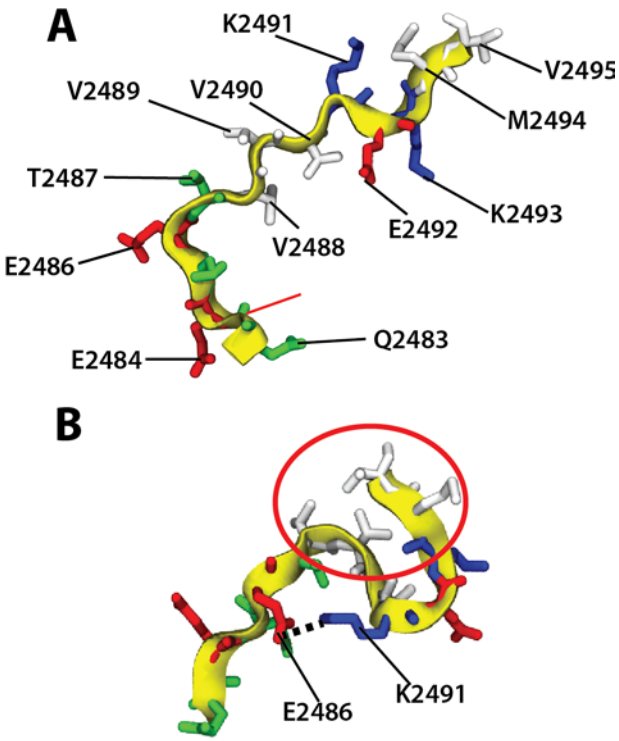
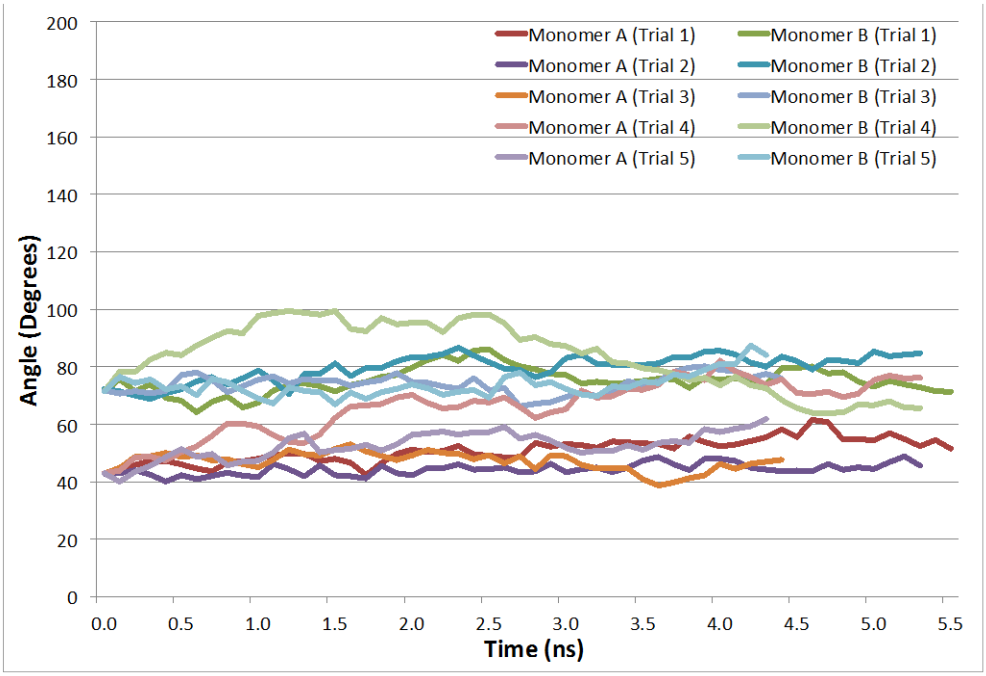


Figure S1. (A) The modeled linker region has no intrinsic structure. There are two nonpolar patches made up of residues V2488, V2489, and V2490, and M2494 to V2495. There are 5 charged residues: K2493, E2492, K2491, E2486, and E2484. The linker is modeled using homology modeling essentially as a random coil. **(B)** The linker region adopted different conformation in each of the 5 trials. Furthermore, each of the two linkers in a single talin dimer adopted a unique conformation after equilibration. An example conformation is shown stabilized by formation of a hydrophobic patch between the two nonpolar regions, and a single salt-bridge between E2486 and K2491.

A.



B.

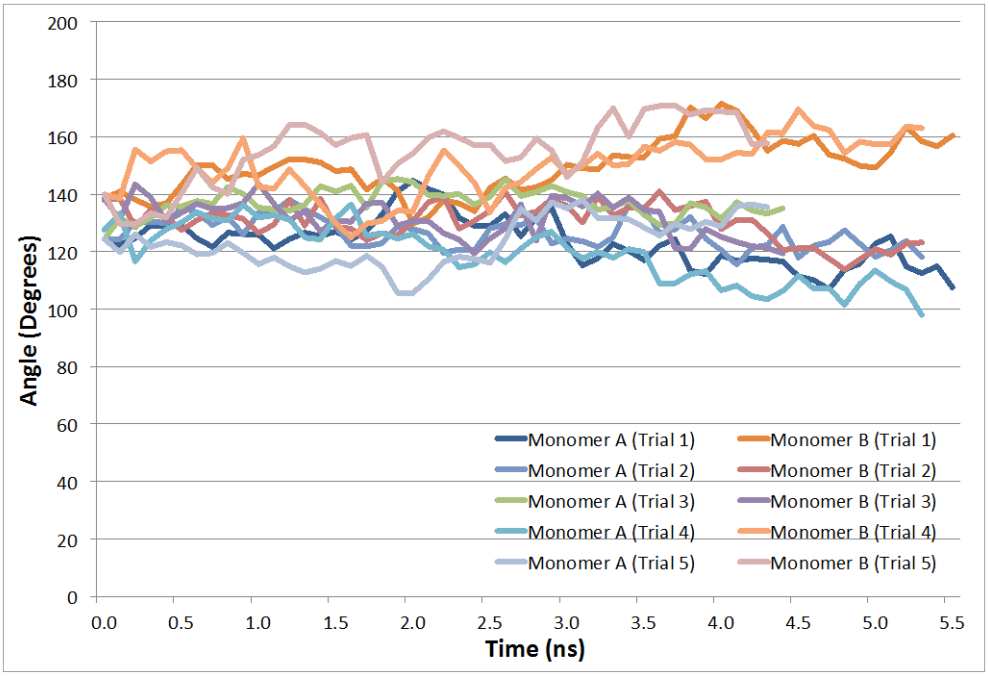
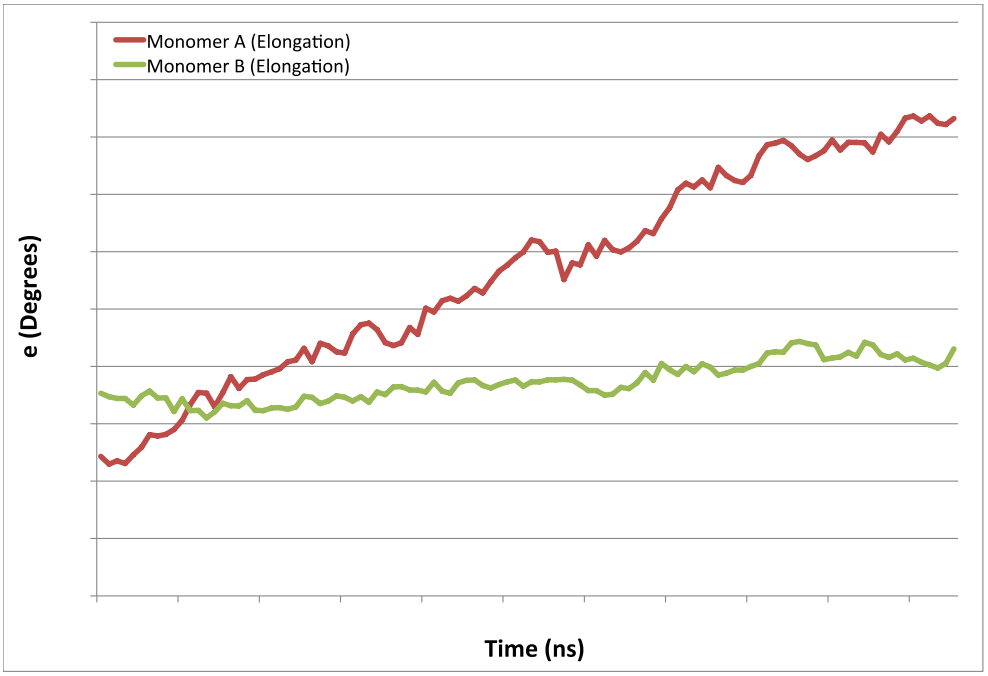


Figure S2. (A) The changes to the α-angle were measured throughout the equilibrium simulation of the talin C-terminus region. Two α-angles are recorded one for each monomer. The results plotted here show monomer B adopts a larger α-angle than monomer A. Although *in vivo* the two monomers are identical, *in silico* the linker between the dimerization domain and the actin-binding helical bundle are modeled and two slightly different models are build for each monomer. **(B)** Measurement of the β-angle shows no differentiation between monomers. In most of the trials the β-angle decreased after equilibration. In two trials the β-angle increased.

A.



B.

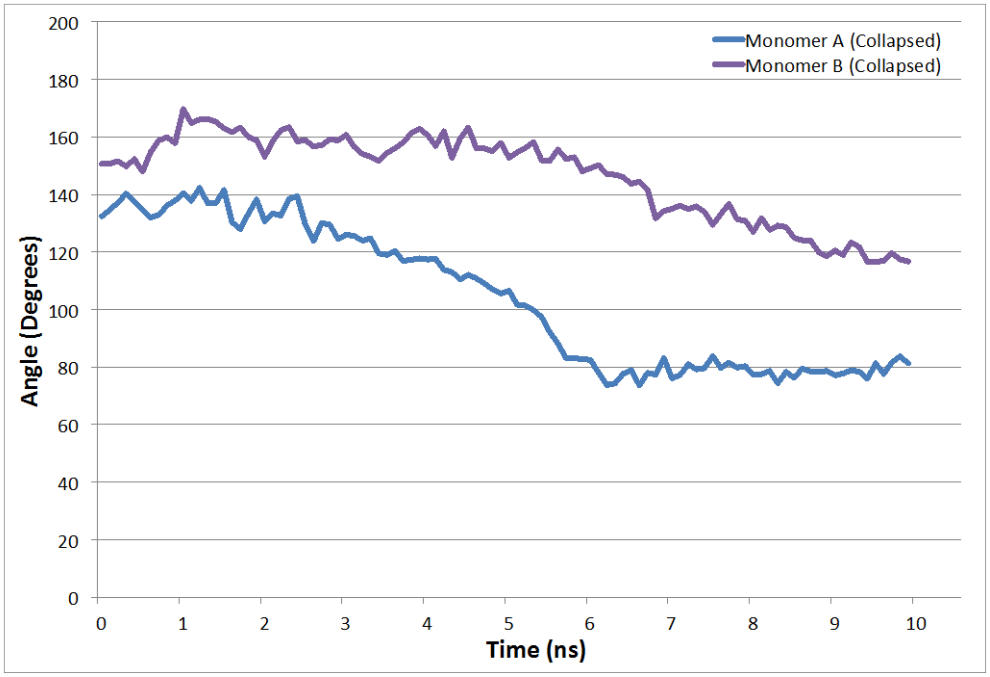


Figure S3. (A) Application of a force on the actin-binding helical bundle to simulate the movement of one ECM-bound integrin away from another resulted in formation of an elongated talin dimer conformation. During elongation the α-angle (shown here) of the monomer being pulled was increased drastically whereas the α-angle of the second monomer was less drastically increased. Perhaps pulling at a slower rate would result in elongation at both monomers. **(B)** Application of force on both actin-binding helical bundles to simulate the forced movement of two ECM-bound integrins towards each other resulted in formation of a collapsed talin dimer structure. Measurements of the β-angle (shown here) at both monomers during the simulated collapse shows significant decrease in the β-angles.

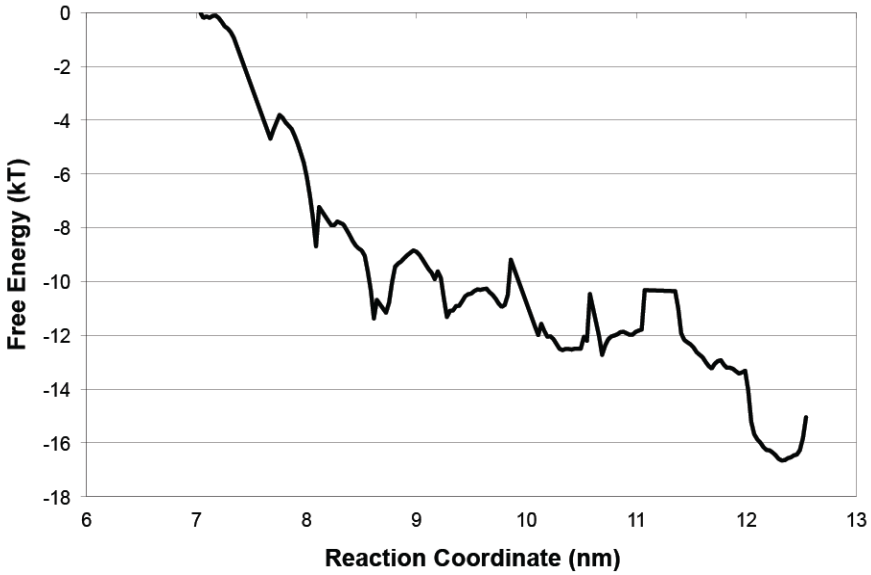


Figure S4. The potential of mean force for is calculated for the elongation of the talin dimer. The reaction coordinate is defined as the distance between the ends of each monomer's actin-binding helical bundle. The free energy difference is negative suggesting formation of an elongated conformation is favorable. It predicts that a talin C-terminus region will adopt a more elongated conformation and that forces will be needed to move the monomers towards each other.

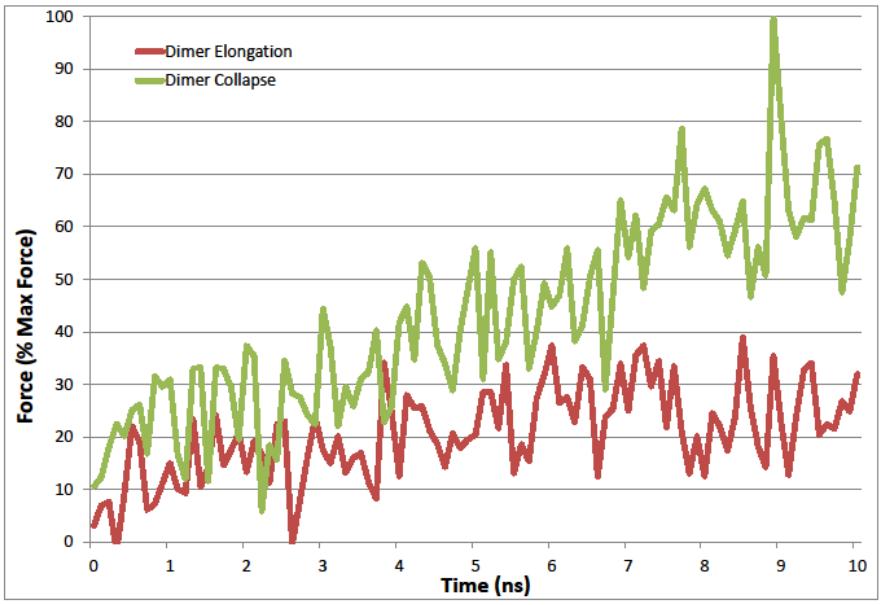


Figure S5. Constant velocity pulling forces were used to simulated both forced elongation of a talin dimer and forced collapse of a talin dimer. The resulting forces needed to induced both conformational changes within the 10ns simulation window are plotted here. Forces needed to elongate the talin dimer are shown in red, forces needed to collapse the talin dimer are shown in green.