Supporting Information for Structure-Mechanics Statistical Learning Uncovers Mechanical Relay in Proteins

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Supporting Information Available

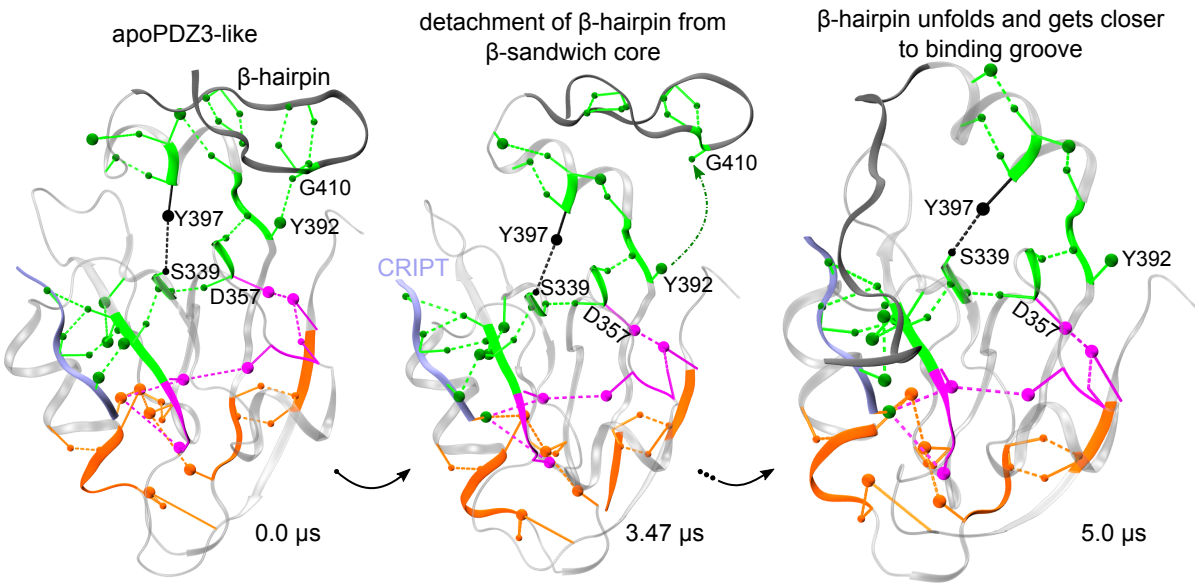

Figure S1: The inter-domain conformational change in PDZ3 upon CRIPT binding. Left: the initial structure of apoPDZ3. Center: the β-hairpin detachment ($\Delta k_{\text{G410-Y392}}$ off) from the β-sandwich core. Right: the unfolding of the β_7-β_8 hairpin that comes close to the peptide binding groove. The β_7-β_8 hairpin is colored in gray, while the other secondary structures displayed in transparent silver. The three mechanical relay systems are also shown following the coloring scheme in Fig. 4 and Fig. 6(b). The CRIPT peptide is colored in ice-blue. The important Y397-S339 interaction persisting throughout the conformational change is shown in black.

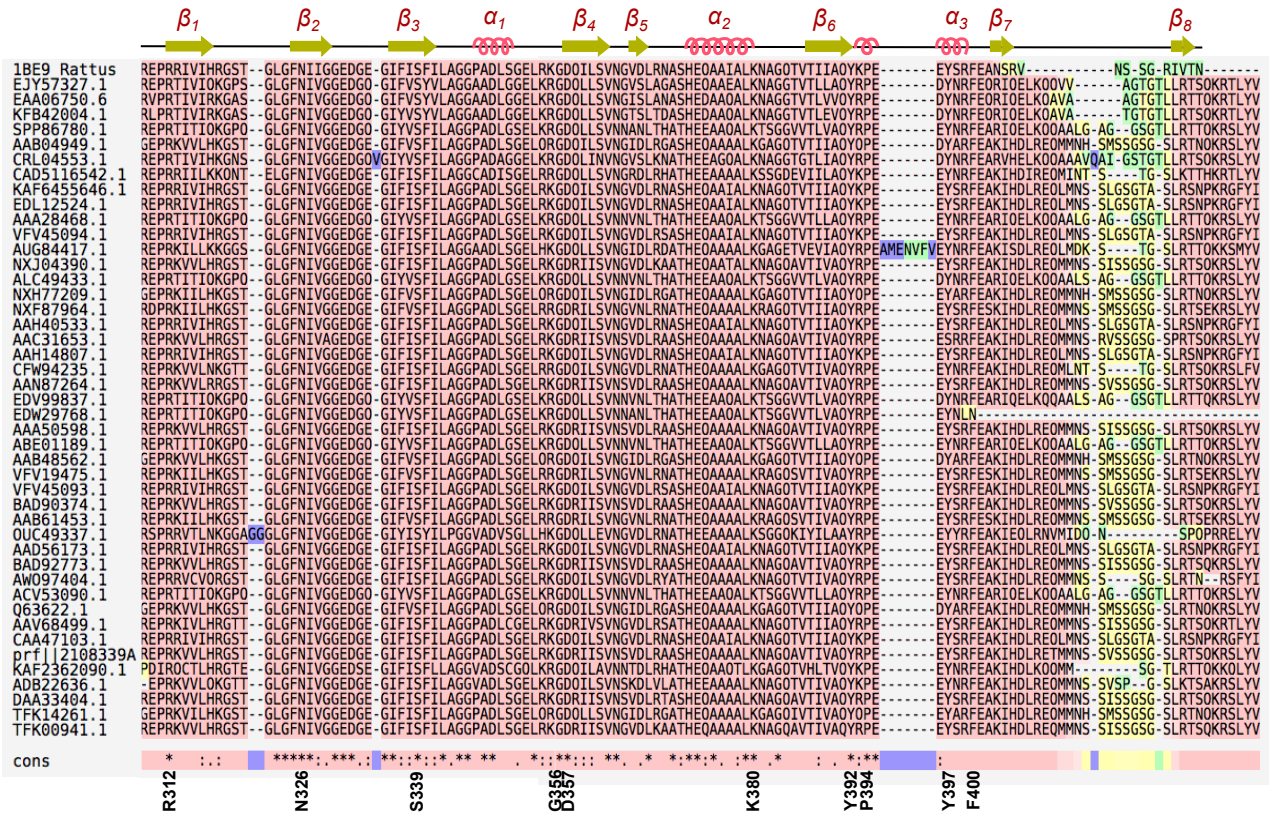

Figure S2: Multiple sequence alignment for the PDZ3 sequences containing the CT-extension $\alpha 3$. The prominent rigidity modes that contain residues involved in the mechanical communication with $\alpha 3$, i.e., inter-domain allostery, are highlighted to illustrate their very high levels of conservation. The asterisk label at bottom indicates the fully conserved residues in the MSA.