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Supporting Material

The Fip35 WW Domain Folds with Structural and Mechanistic Heterogeneity in Molecular Dynamics Simulations

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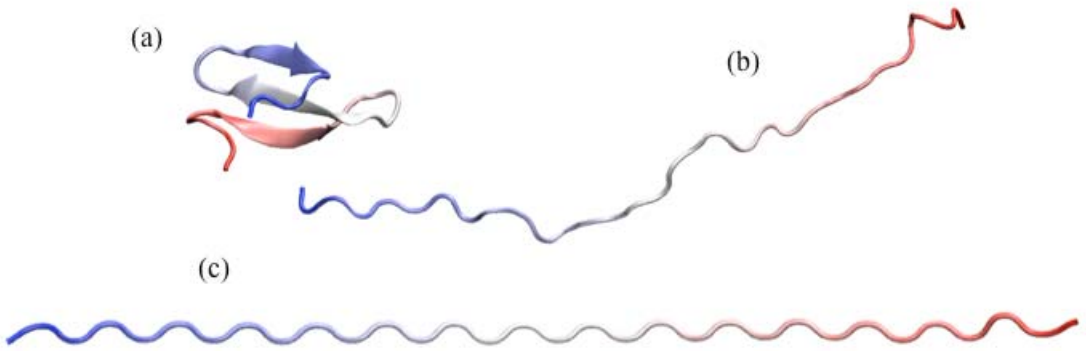
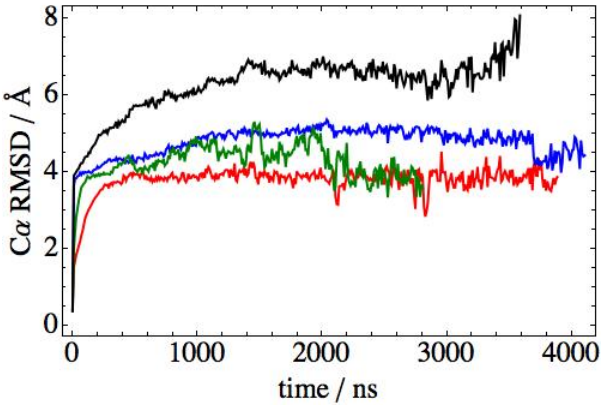
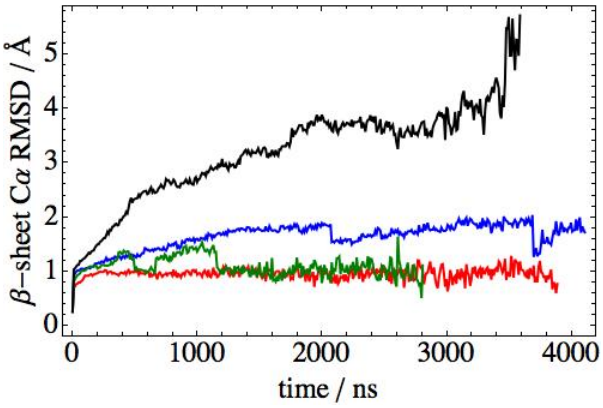
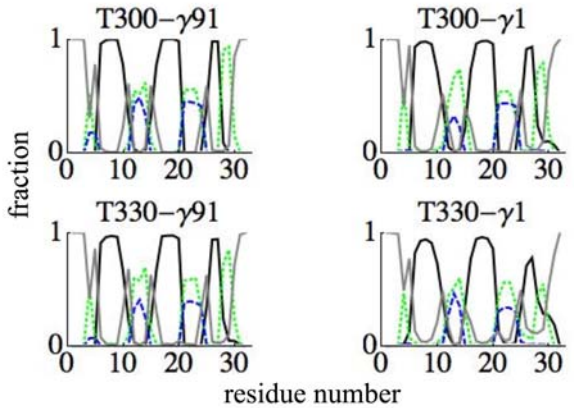
Supplementary Figure 1. Starting structures of Fip35 mutant of the Hpin1 WW domain for molecular dynamics simulations. (a) folded, (b) extended then equilibrated, (c) fully extended. Graphics were generated using VMD.[1]



Supplementary Figure S2. Structural characteristics of Fip35 WW domain in simulations started in the folded state. (a) Average Cα RMSD as a function of time for T300-γ91 (red), T300-γ1 (blue), T330-γ91 (green), T330-γ1 (black). (b) Average Cα RMSD for β-sheet residues as a function of time, with the same color scheme as part (a). (c) Average secondary structure by DSSP, with β-sheet "E" (black), coil "S" (green, dotted), turn "T" (blue, dashed), and no assignment (gray). The beta sheet is readily apparent.







1. Humphrey, W.; Dalke, A.; Schulten, K. Journal of Molecular Graphics 1996, 14(1), 33-&.