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The Folding Mechanism and Key Metastable State Identification of the PrP127-147 Monomer Studied by Molecular Dynamics Simulation and Markov State Model Analysis

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Figure caption

Fig. S1. The representative structures of macrostates S(16), S(8) and S(2) with β-sheet formed at the N-terminus and the hydrophobic residues are shown as sphere.

Fig. S2. The ensemble-averaged intrapeptide backbone H-bond map of the synthetic MSM trajectory. The contacts (i, i), (i, i+1) and (i, i+2) are not included.

Fig. S3. The superposition of structures in S(28). (a) the guanidyl of Arg136 was paralleled with the imidazole plane of His140, and (b) H-bond was formed between guanidyl of Arg136 and the N_{δ} of imidazole of His140.

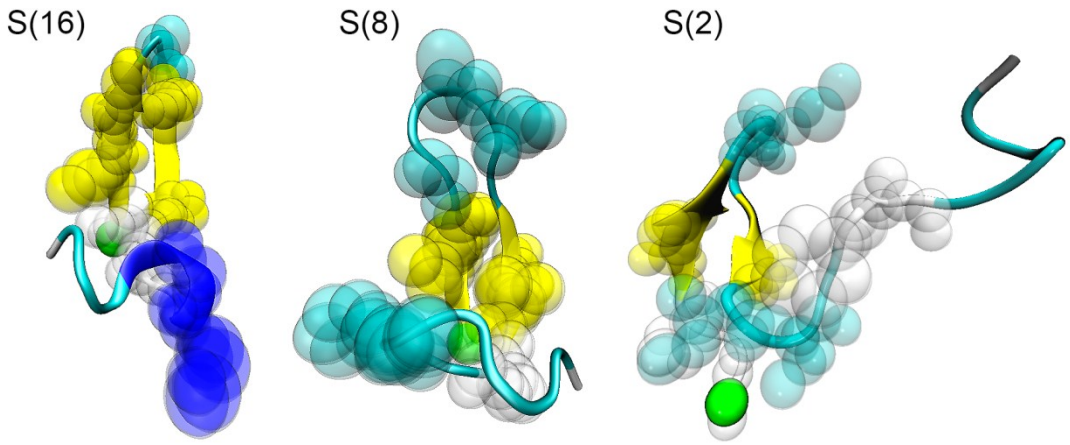

Figure S1

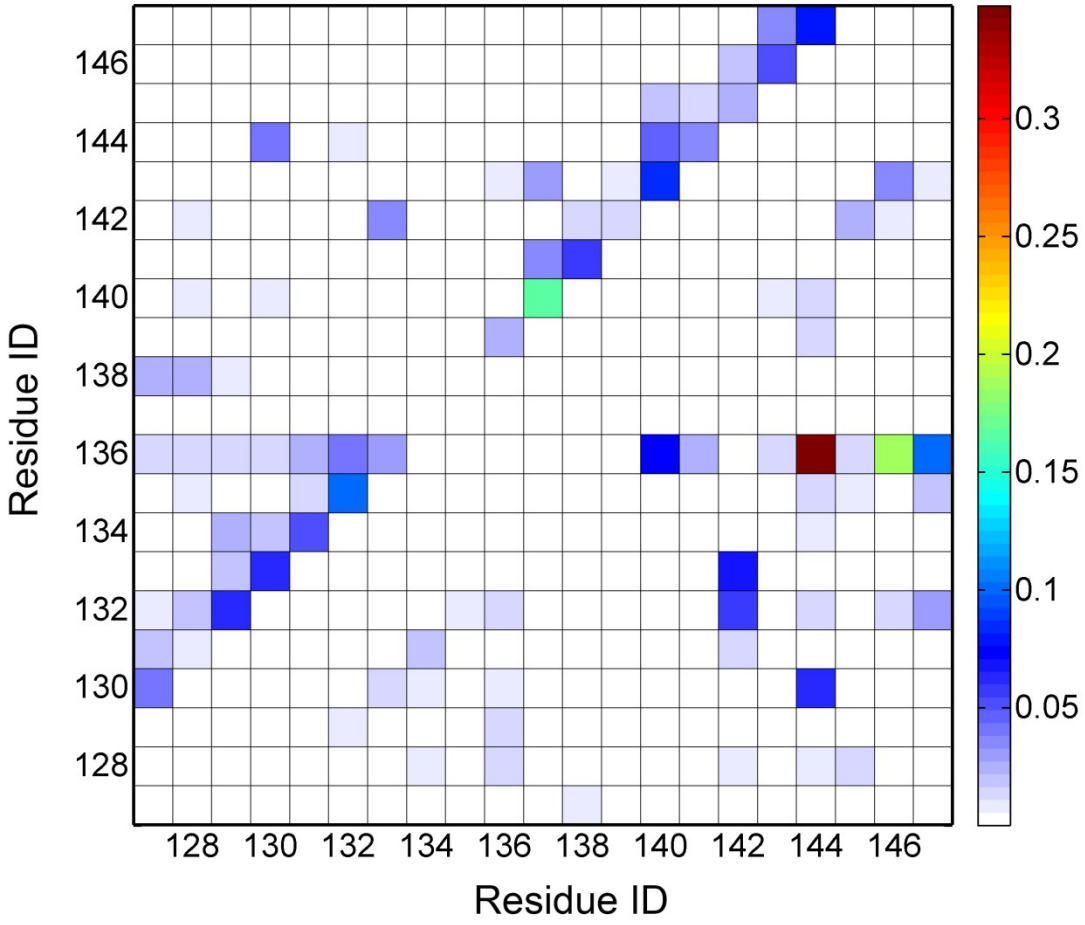
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Figure S2

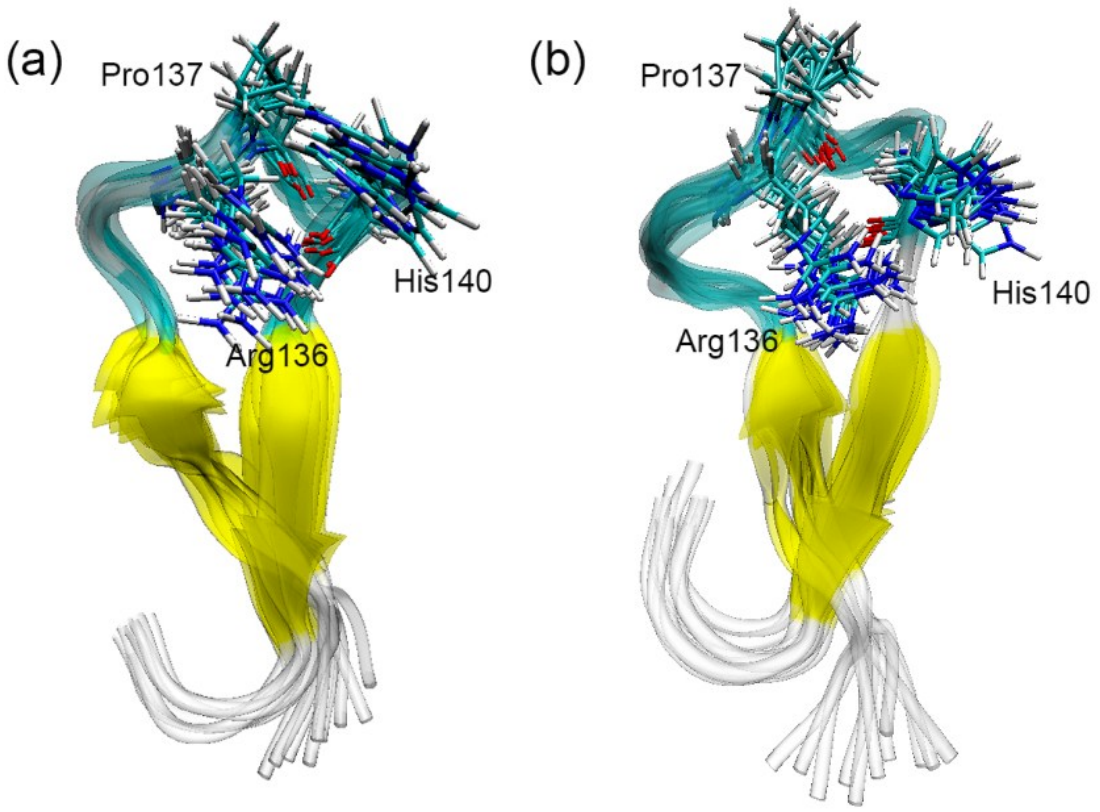

Figure S3