Exploration of the Misfolding Mechanism of Transthyretin Monomer: Insights from Hybrid-Resolution Simulations and Markov Model Model Analysis

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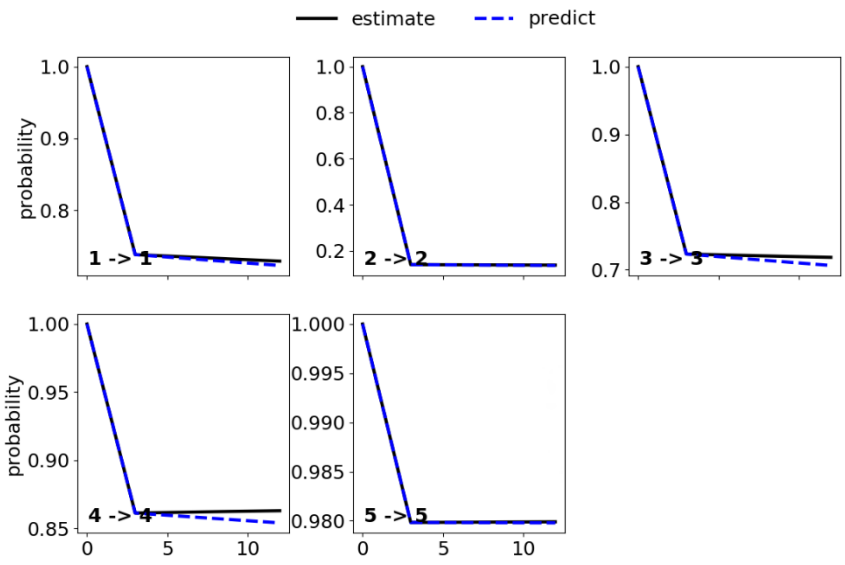

Figure S1. Chapman-Kolmogorov tests of the MSM constructed at lag time of 3 ns with 5 macrostates.

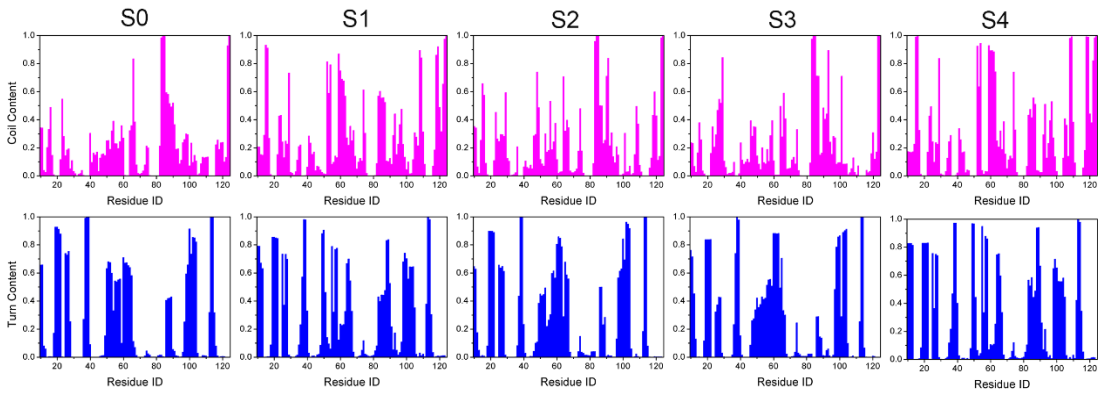

Figure S2. Probabilities of residues in TTR monomer adopting coil and turn structure for each macrostate.

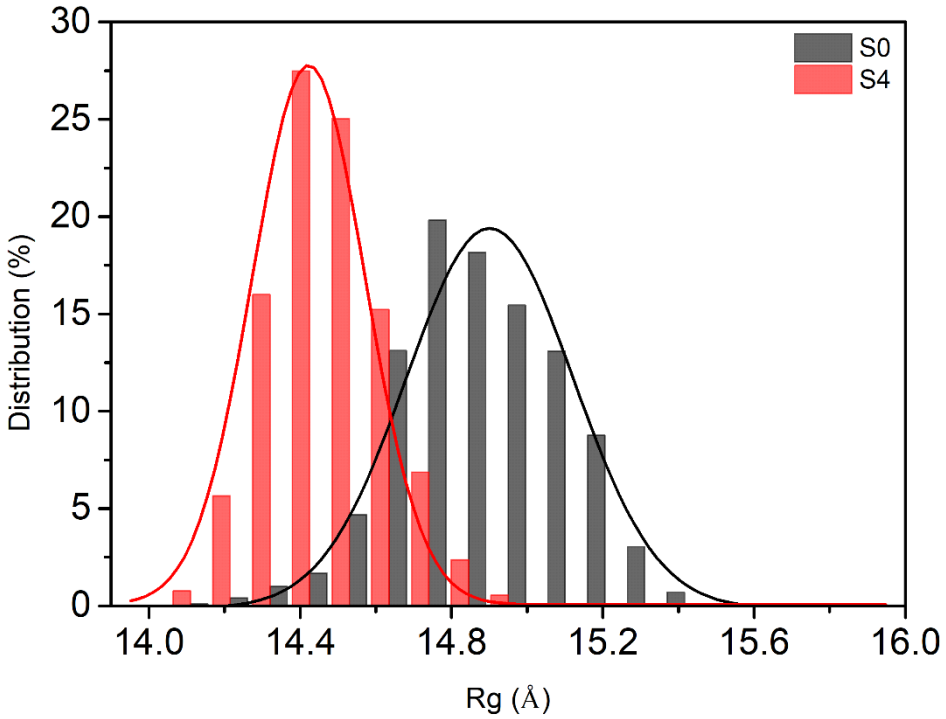

Figure S3. Distribution of radius of gyration (Rg) of macrostates S0 and S4.

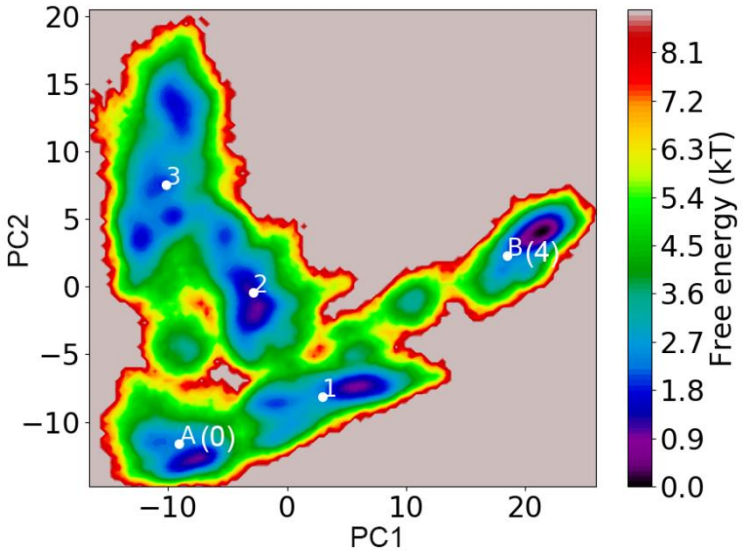

Figure S4. Free energy space of TTR monomer with average location of corresponding macrostates labeled. A and B representing the initial and final states in the transition pathways, respectively.