

Supplementary Materials

Effects of the A117V mutation on the Folding and Aggregation of Palindromic Sequences (PrP113-120) in Prion: Insights from Replica Exchange Molecular Dynamics Simulations

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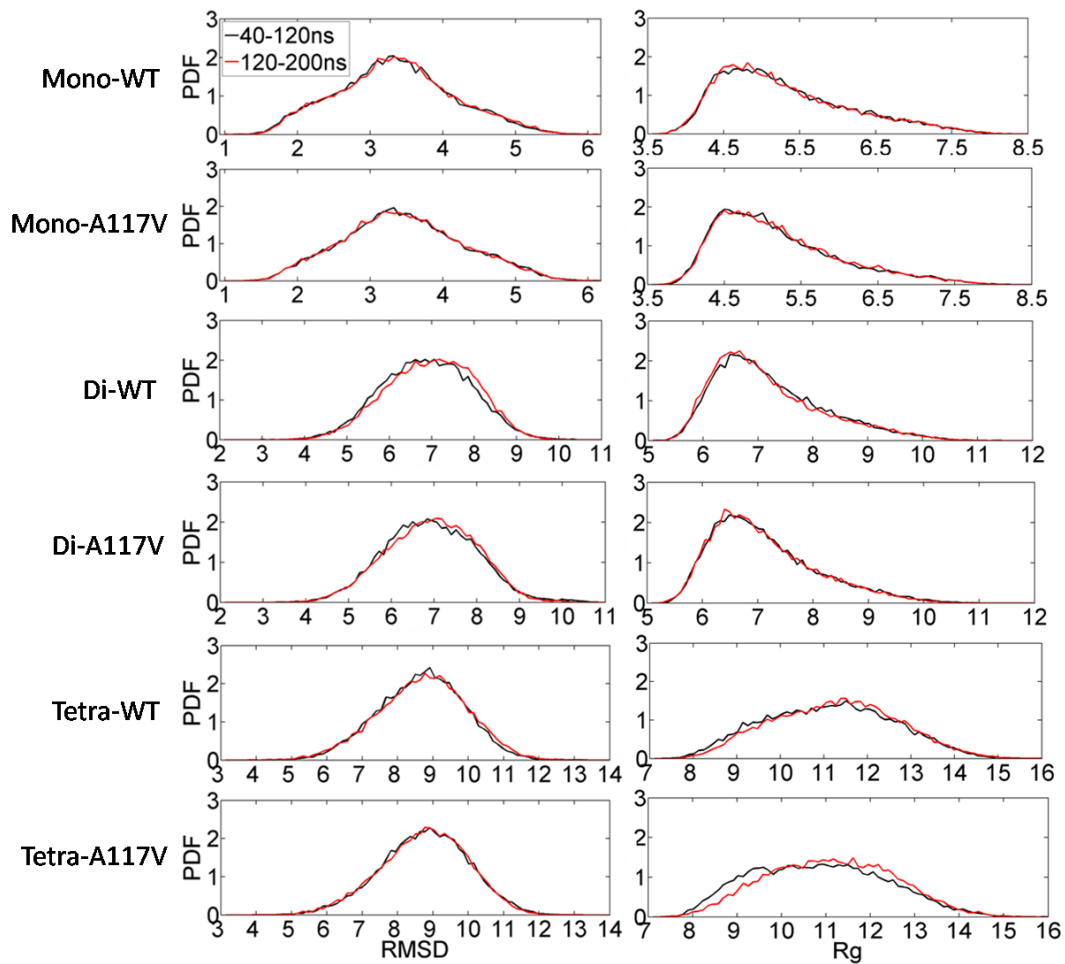


Figure S1: The convergence evaluation of REMD simulations for 1-, 2-, 4-peptide systems of the WT and A117V peptides. The respective convergence of the REMD simulations was rigorously checked by calculating the probability distribution functions (PDF) of backbone RMSD and backbone radius of gyration (Rg) within the two time intervals, 40-120 ns and 120-200 ns.

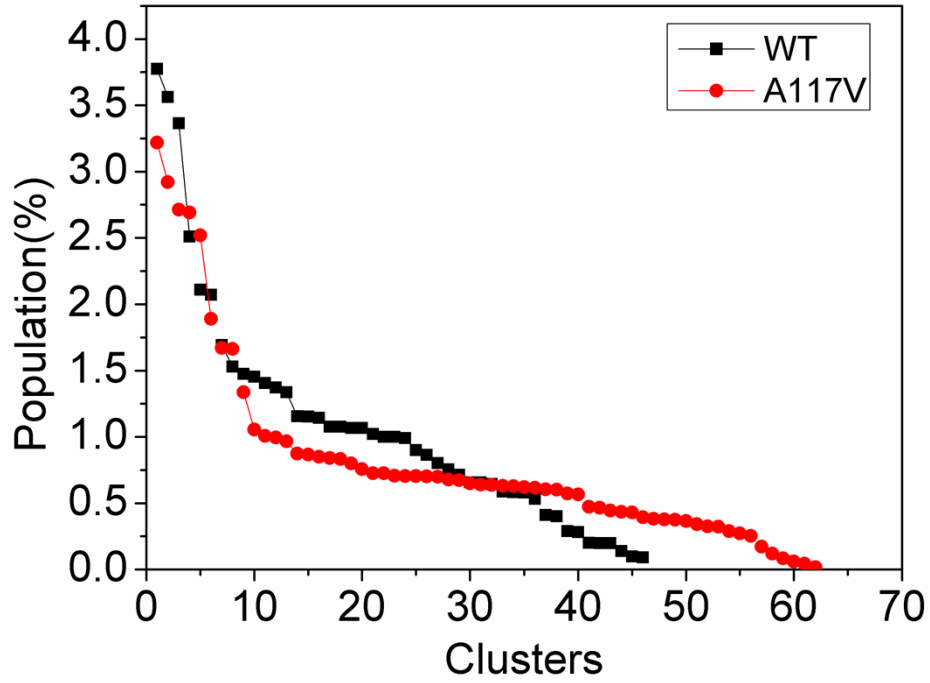


Figure S2: The populations of all clusters of the wild type (black) PrP113-120 and the A117V mutant (red).