Supporting Information for "Molecular Simulations Indicate Marked Differences in Structure of Amylin Mutants, Correlated with known Aggregation Propensity"

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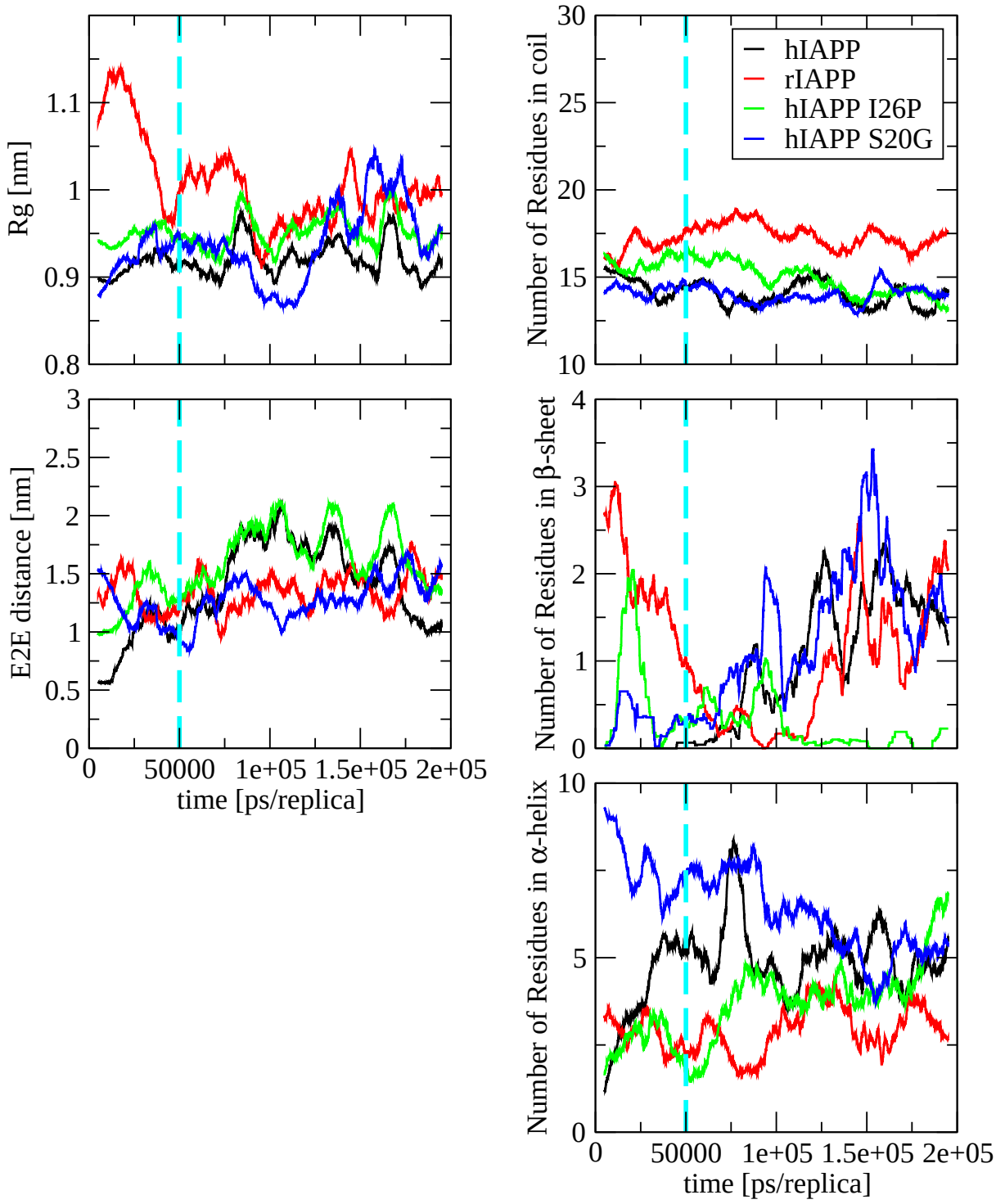

Figure S1: Equilibration IAPP trajectories at 300 K measured by (Left): Distances: R_g (Top), End-to-end distance (Middle), and (Rigth): Secondary structure formation: Coil (Top), β-sheet (Middle), α-helix (Bottom), illustrated by moving averages of 10 ns/replica. Data up to dashed cyan line has discarded for equilibration.

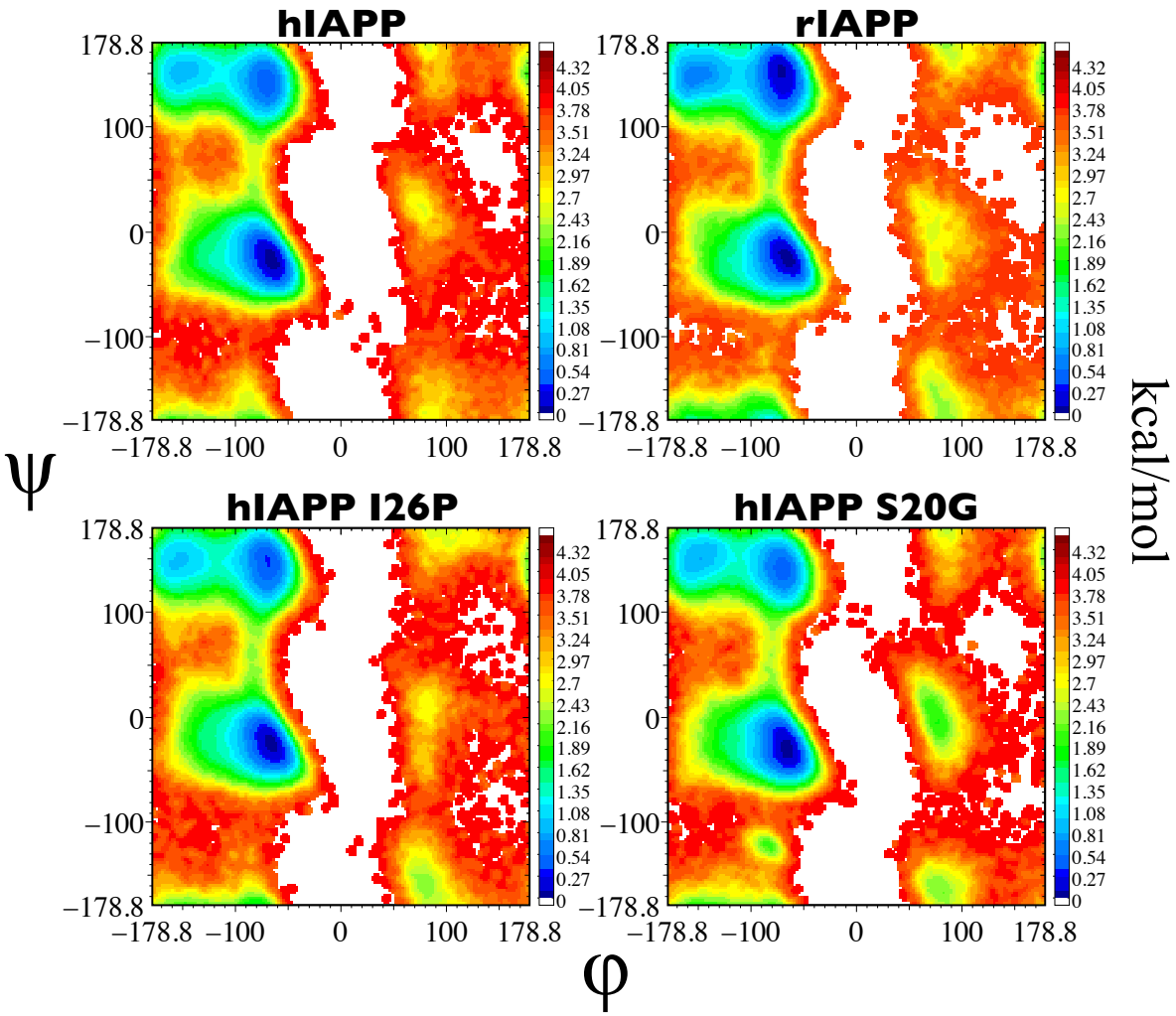

Figure S2: Ramachandran maps of IAPP equilibrated trajectories, free-energy contoured in kcal/mol.

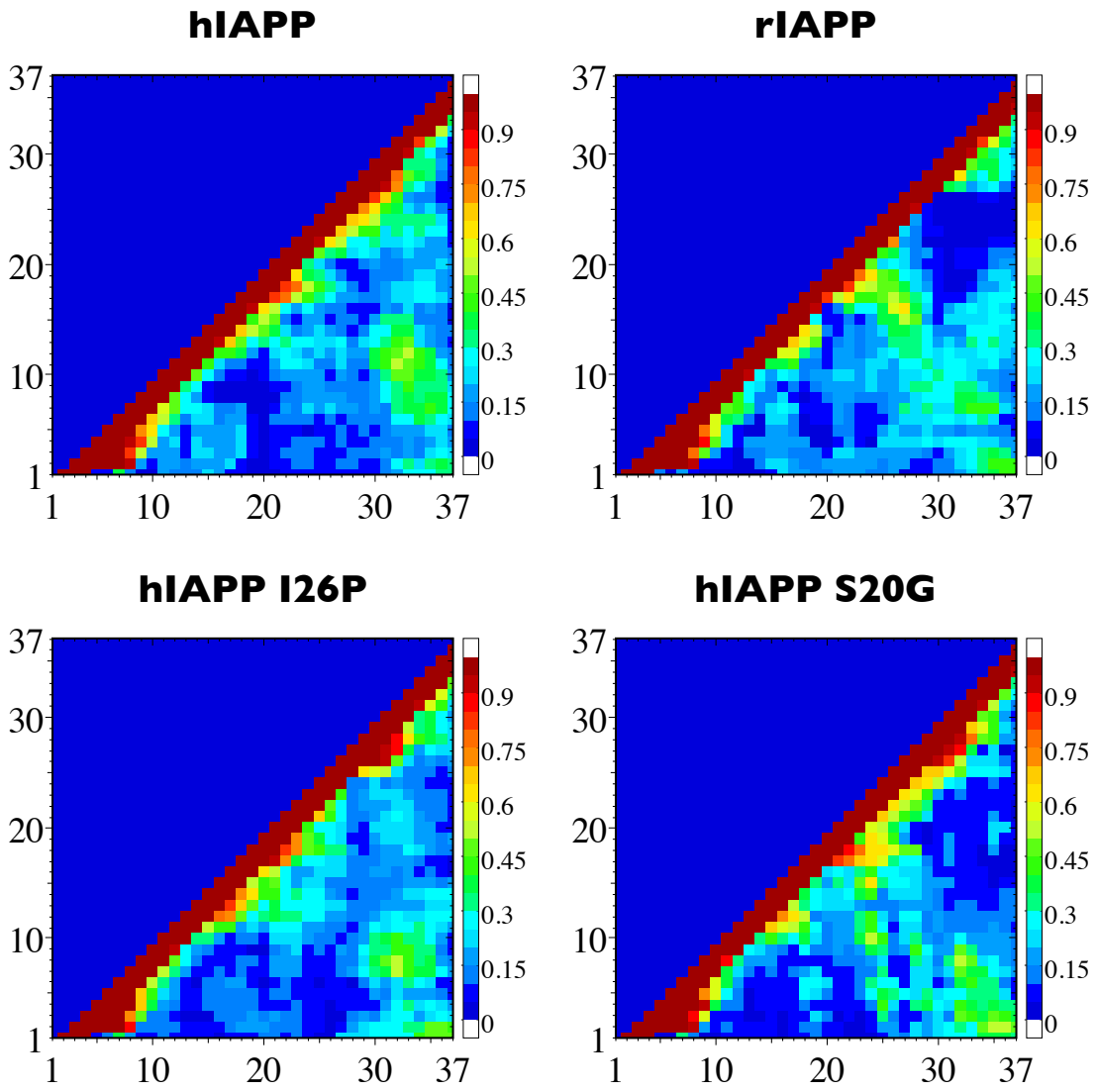

Figure S3: Contact maps of equilibrated IAPP trajectories calculated based on backbone where cutoff distance is 0.8 nm.