

Structures and Free Energy Landscapes of the Wild-Type and A30P Mutant-Type α -Synuclein Proteins with Dynamics

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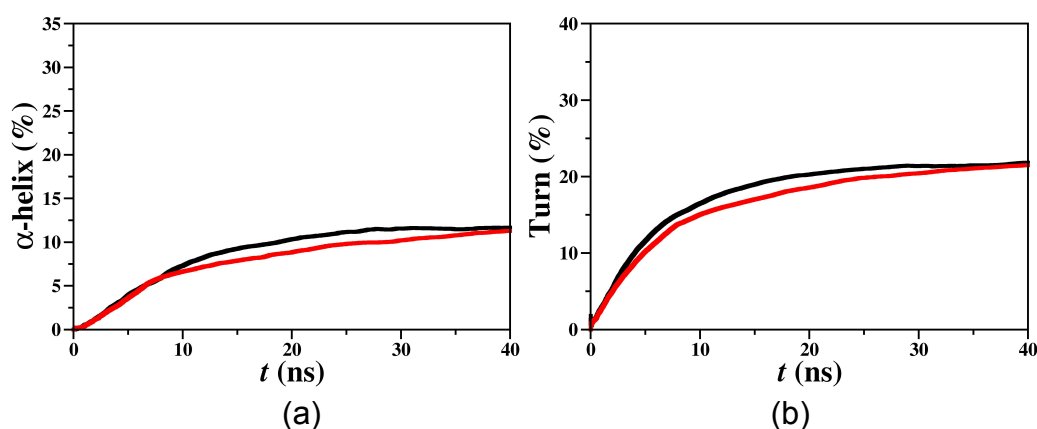
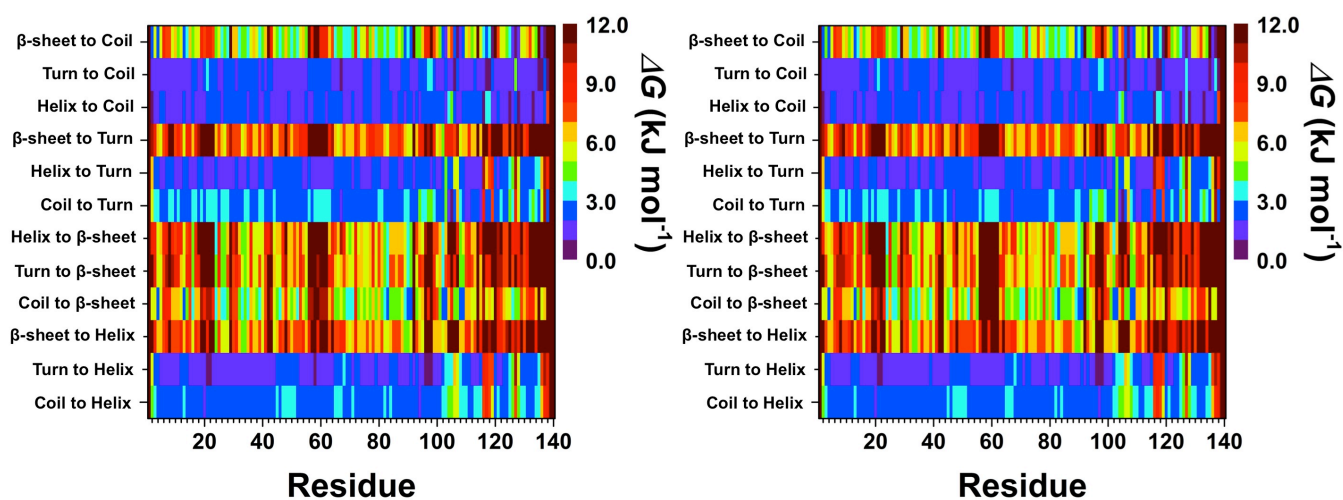


Figure S1. The cumulative average (a) α -helix and (b) turn contents of the wild-type (black) and A30P mutant-type (red) α -synuclein.



(a)

(b)

Figure S2. The stability of secondary structure transitions between two specific secondary structure components per residue for the wild-type α -synuclein protein in aqueous solution from the first (a) 36 ns and (b) 38 ns of our simulation. The color scale corresponds to the free energy value associated with specific transitions between two secondary structure components for a specific residue.

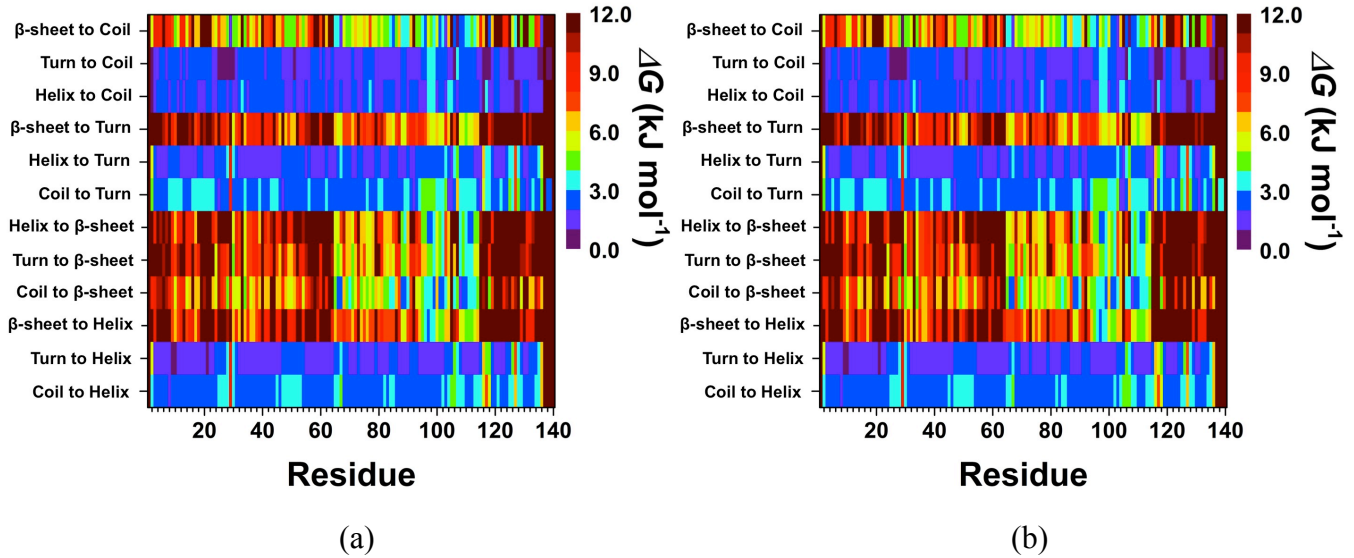


Figure S2. The stability of secondary structure transitions between two specific secondary structure components per residue for the A30P mutant-type α -synuclein protein in aqueous solution from the first (a) 36 ns and (b) 38 ns of our simulation. The color scale corresponds to the free energy value associated with specific transitions between two secondary structure components for a specific residue.

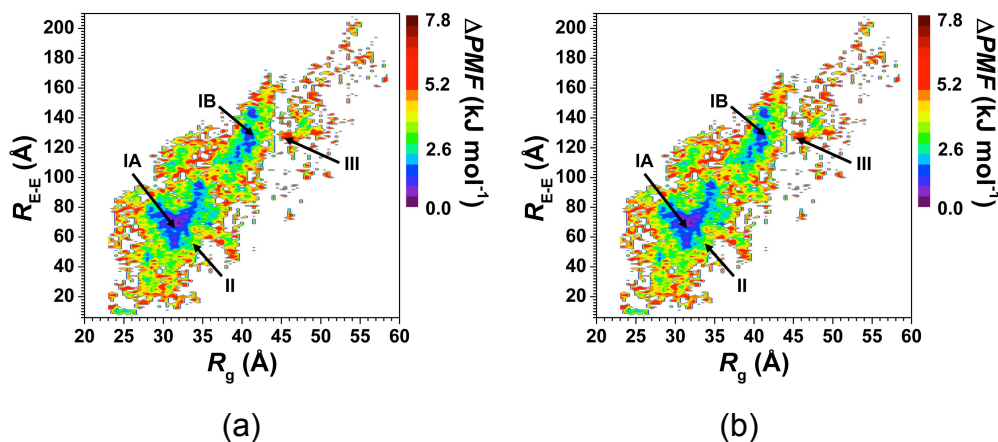


Figure S4. PMF surfaces based on R_{E-E} and R_g values of the wild-type α -synuclein using the converged structures from the first (a) 36 ns and (b) 38 ns of our simulation.

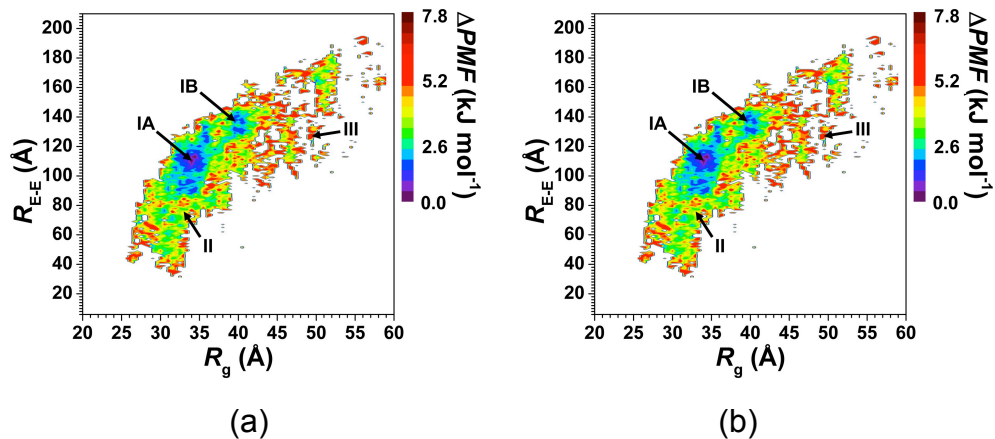


Figure S5. PMF surfaces based on R_{E-E} and R_g values of the A30P mutant-type α -synuclein using the converged structures from the first (a) 36 ns and (b) 38 ns of our simulation.

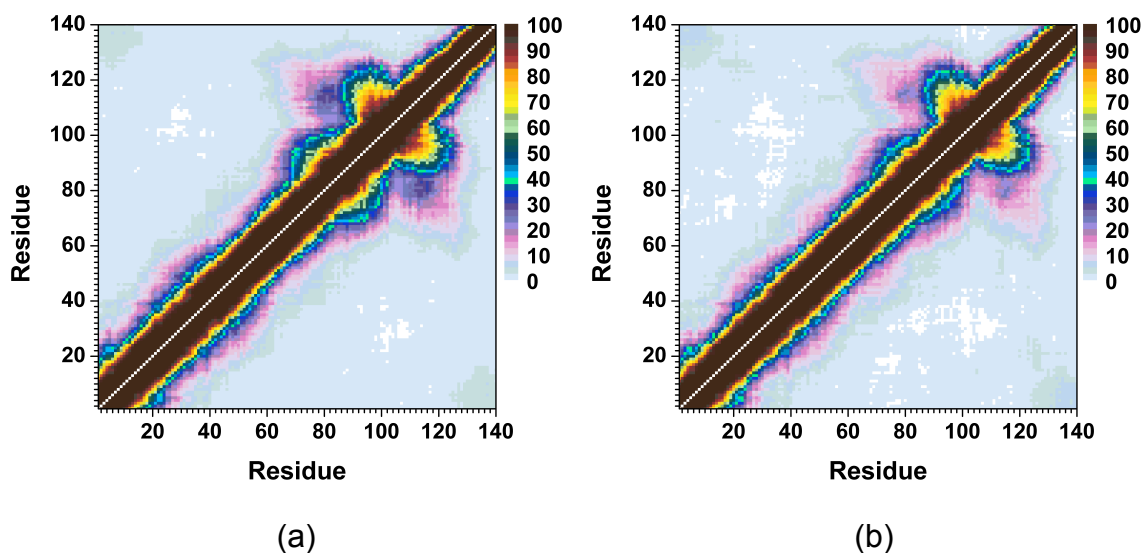
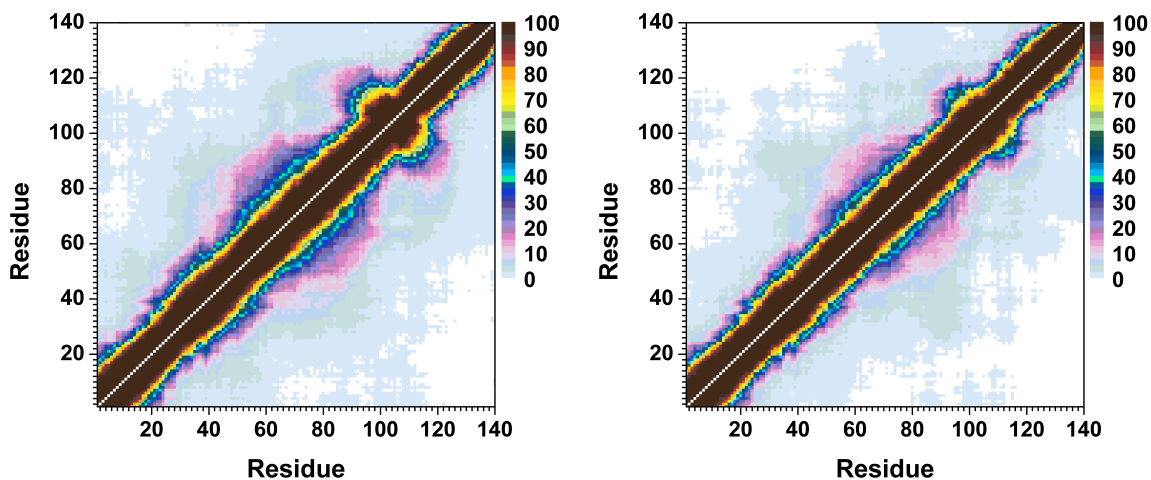


Figure S6. The intra-molecular peptide interactions for the wild-type α -synuclein structures located in (a) basin II and (b) basin III of the PMF surface (Figure 5). The color scale corresponds to the probability (P) of a heavy atom a residue being ≤ 20 Å from a heavy atom of any other residue.



(a)

(b)

Figure S7. The intra-molecular peptide interactions for the A30P mutant-type α -synuclein structures located in (a) basin II and (b) basin III of the PMF surface (Figure 5). The color scale corresponds to the probability (P) of a heavy atom a residue being ≤ 20 Å from a heavy atom of any other residue.