

Structures of the E46K Mutant-Type α -Synuclein Protein and Impact of E46K Mutation on the Structures of the Wild- Type α -Synuclein Protein

Olivia Wise-Scira¹, Aquila Dunn,¹ Ahmet Aloglu,¹ Isin Sakallioglu,² Orkid Cosuner^{1,3}*

¹Department of Chemistry, The University of Texas at San Antonio, One UTSA Circle, San Antonio, Texas 78249, ²Department of Chemistry, Bilkent University, Ankara, Turkey 06800 and ³Neurosciences Institute, The University of Texas at San Antonio, One UTSA Circle, San Antonio, Texas 78249

Email: orkid.coskuner@utsa.edu

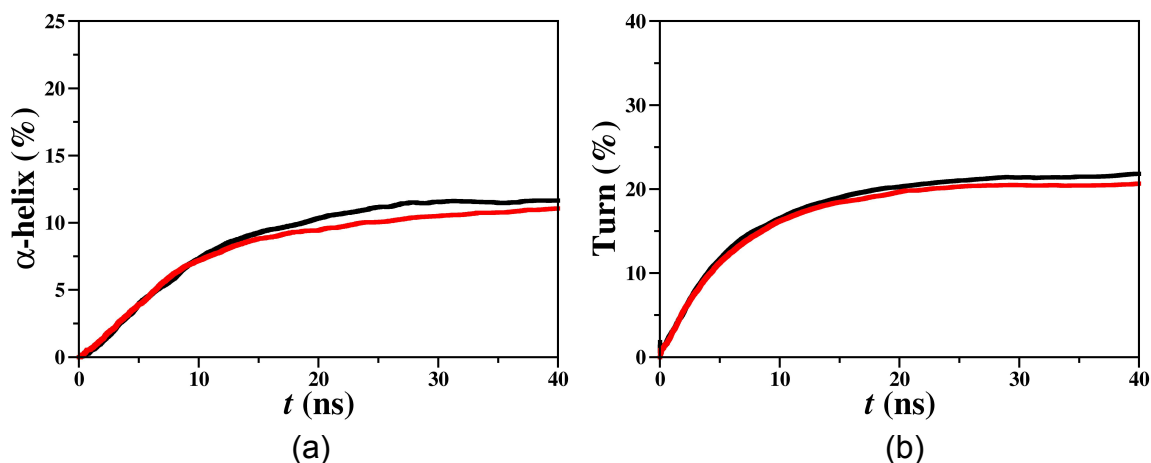


Figure S1. The cumulative average (a) α -helix and (b) turn contents of the wild-type (black) and E46K mutant-type (red) α -synuclein throughout the time course of our simulations for the replica closest to physiological temperature (~ 310 K).

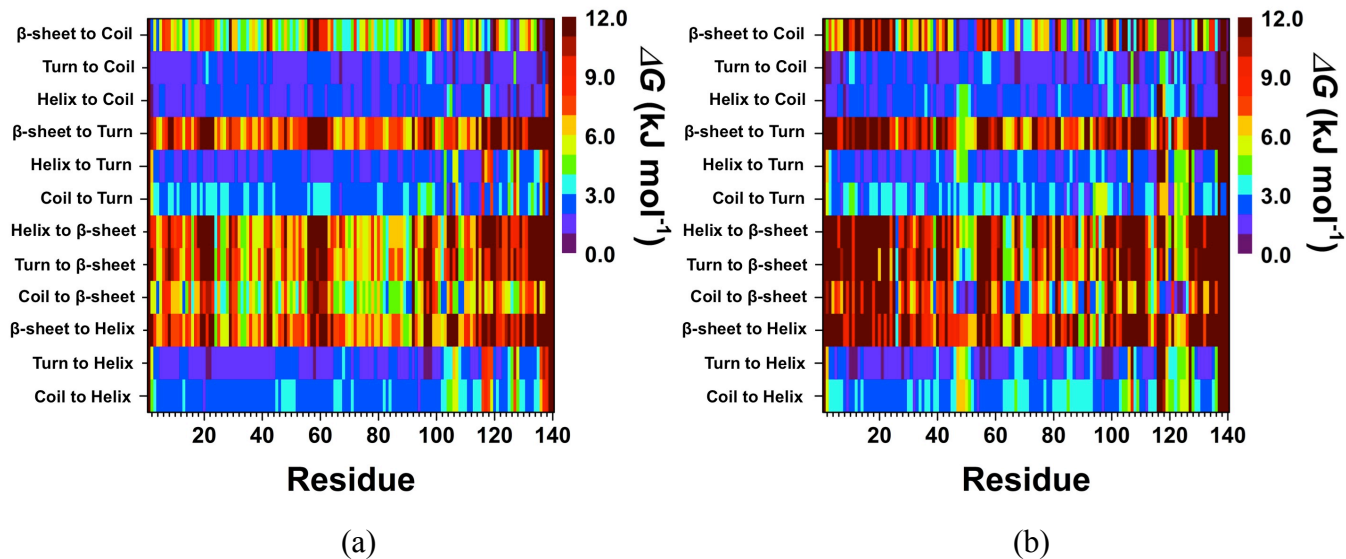


Figure S2. The stability of secondary structure transitions between two specific secondary structure components per residue for the wild-type α -synuclein protein in aqueous solution from the first (a) 36 ns and (b) 38 ns of our simulation. The color scale corresponds to the free energy value associated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

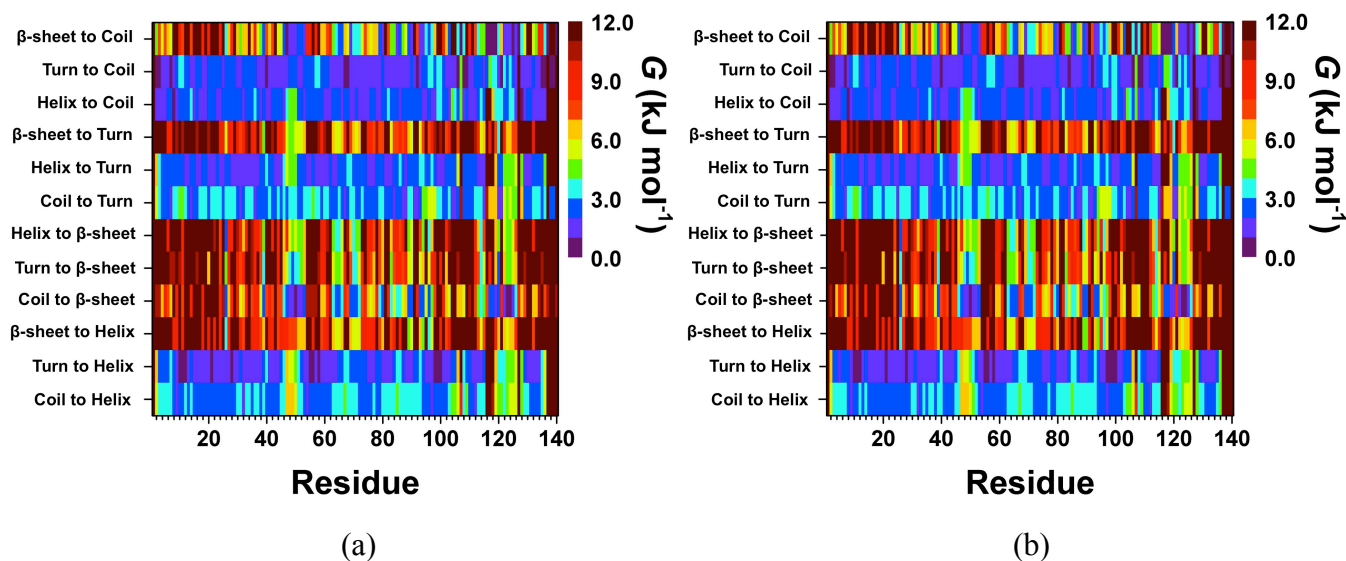


Figure S2. The stability of secondary structure transitions between two specific secondary structure components per residue for the E46K mutant-type α -synuclein protein in aqueous solution from the first (a) 36 ns and (b) 38 ns of our simulation. The color scale corresponds to the free energy value associated with specific transitions between two secondary structure components for a specific residue.

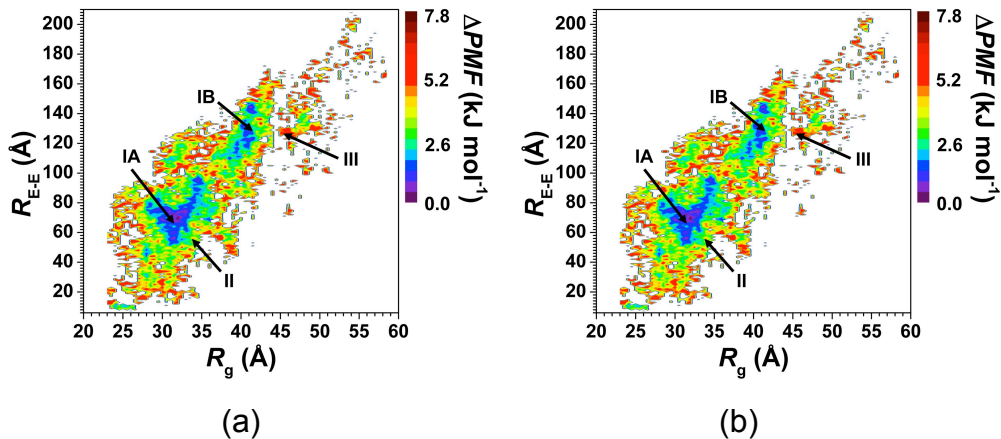


Figure S4. PMF surfaces based on R_{E-E} and R_g values of the wild-type α -synuclein using the converged structures from the first (a) 36 ns and (b) 38 ns of our simulation.

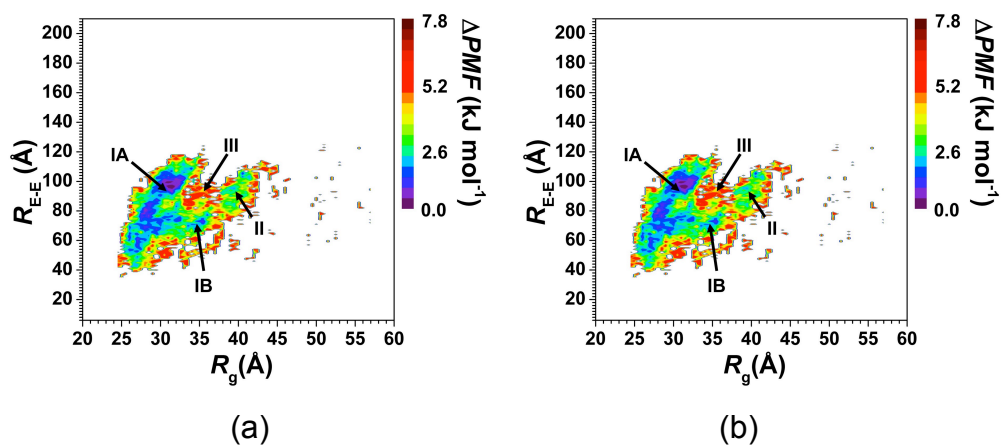


Figure S5. PMF surfaces based on R_{E-E} and R_g values of the E46K mutant-type α -synuclein using the converged structures from the first (a) 36 ns and (b) 38 ns of our simulation.

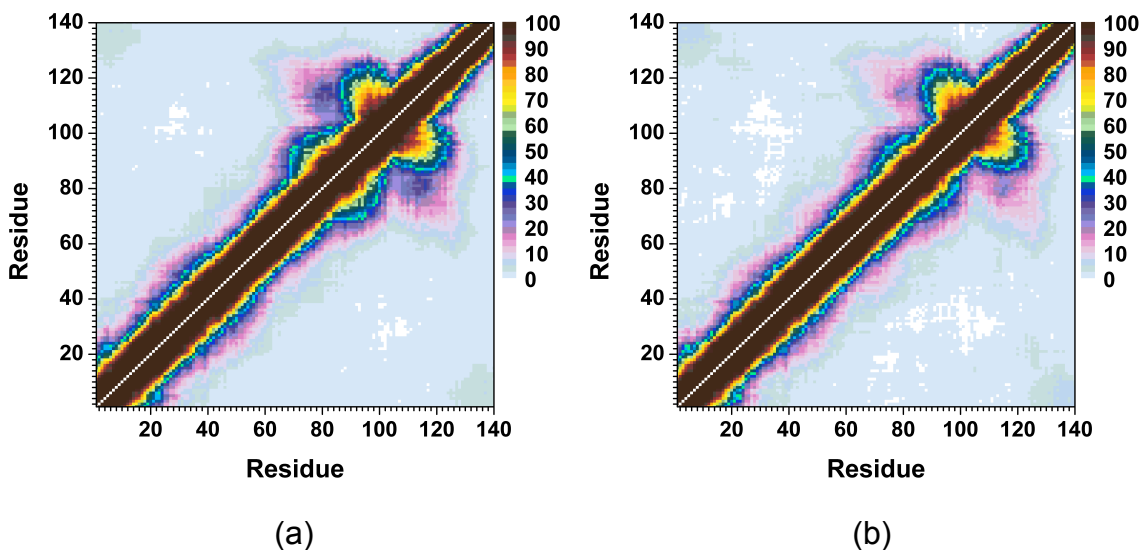


Figure S6. The intra-molecular peptide interactions for the wild-type α -synuclein structures located in (a) basin II and (b) basin III of the PMF surface (Figure 5). The color scale corresponds to the probability (P) of a heavy atom a residue being ≤ 20 Å from a heavy atom of any other residue.

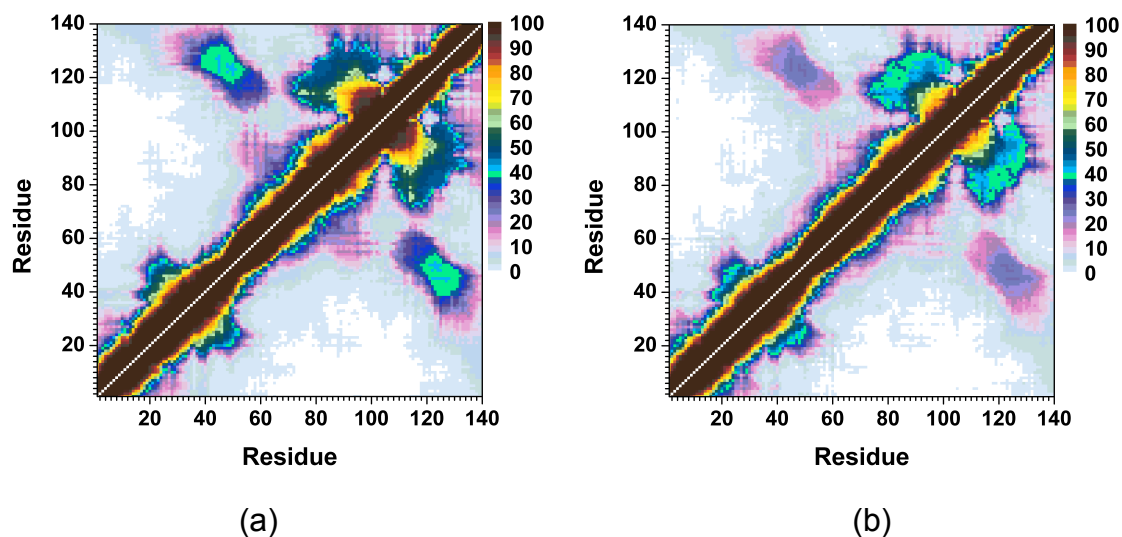


Figure S7. The intra-molecular peptide interactions for the E46K mutant-type α -synuclein structures located in (a) basin II and (b) basin III of the PMF surface (Figure 5). The color scale corresponds to the probability (P) of a heavy atom a residue being ≤ 20 Å from a heavy atom of any other residue.