Supporting Information for:

Stability of the N-terminal Helix and its Role in Amyloid Formation of Serum Amyloid A

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Contents

Results

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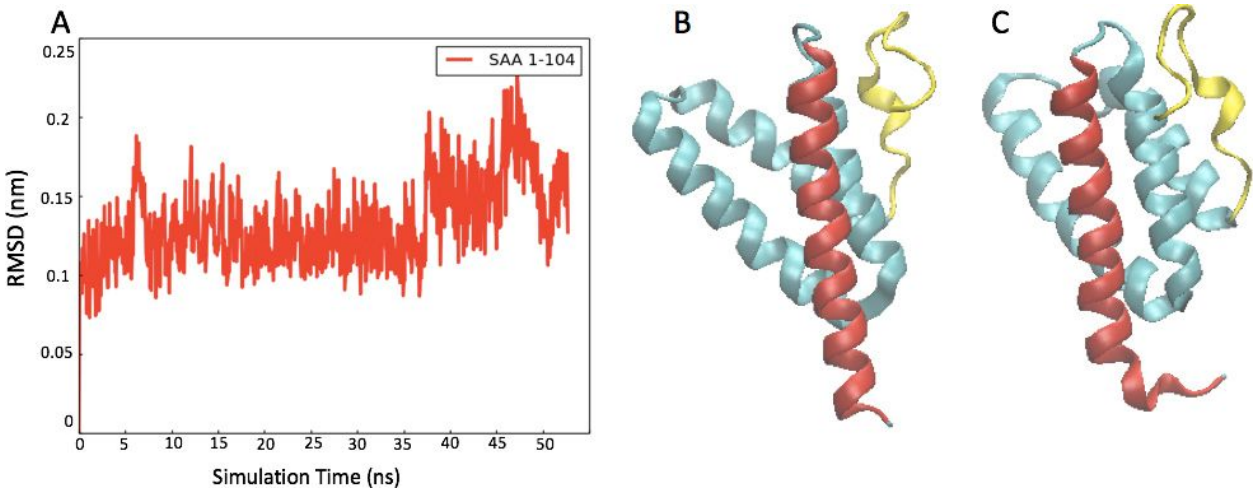

Figure S1. Root-mean-square-deviation (RMSD) to the crystal structure for the full-sized SAA protein as function of time (A). The initial configuration is shown in (B) and the final one in (C), where helix I is marked in red, helix II-IV in cyan, and the C terminal tail in yellow. Data are from a 40ns molecular dynamic simulation at 310 K, using the set-up described in the manuscript.

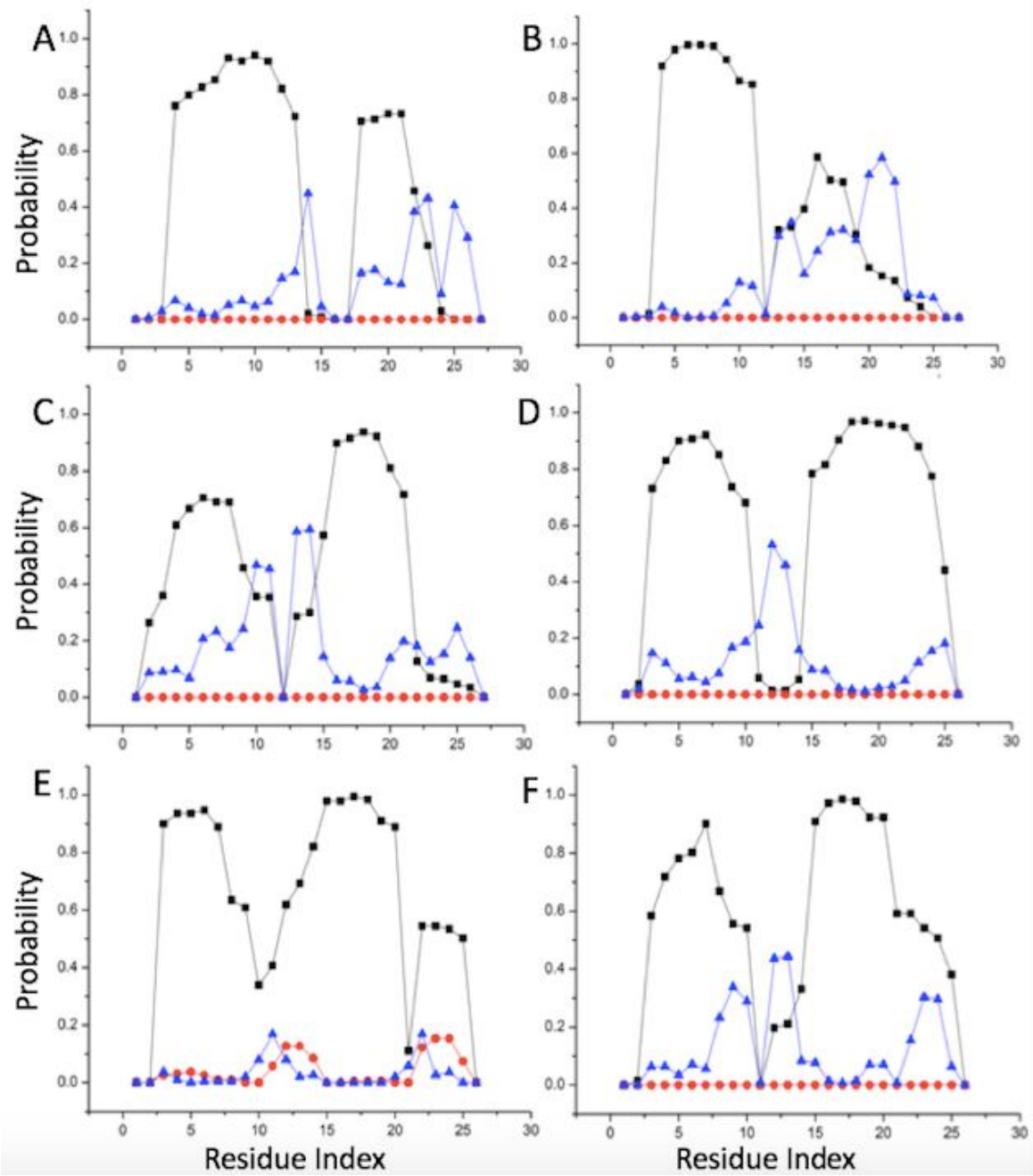

Figure S2. A and B, Secondary structure probability for the box size of 4.8 nm. C and D, Secondary structure probability for the box size of 5.4 nm. E and F, Secondary structure probability for the box size of 5.6 nm. The frequency of α-helices is drawn in black, that of turns in blue, and of β-strands in red.

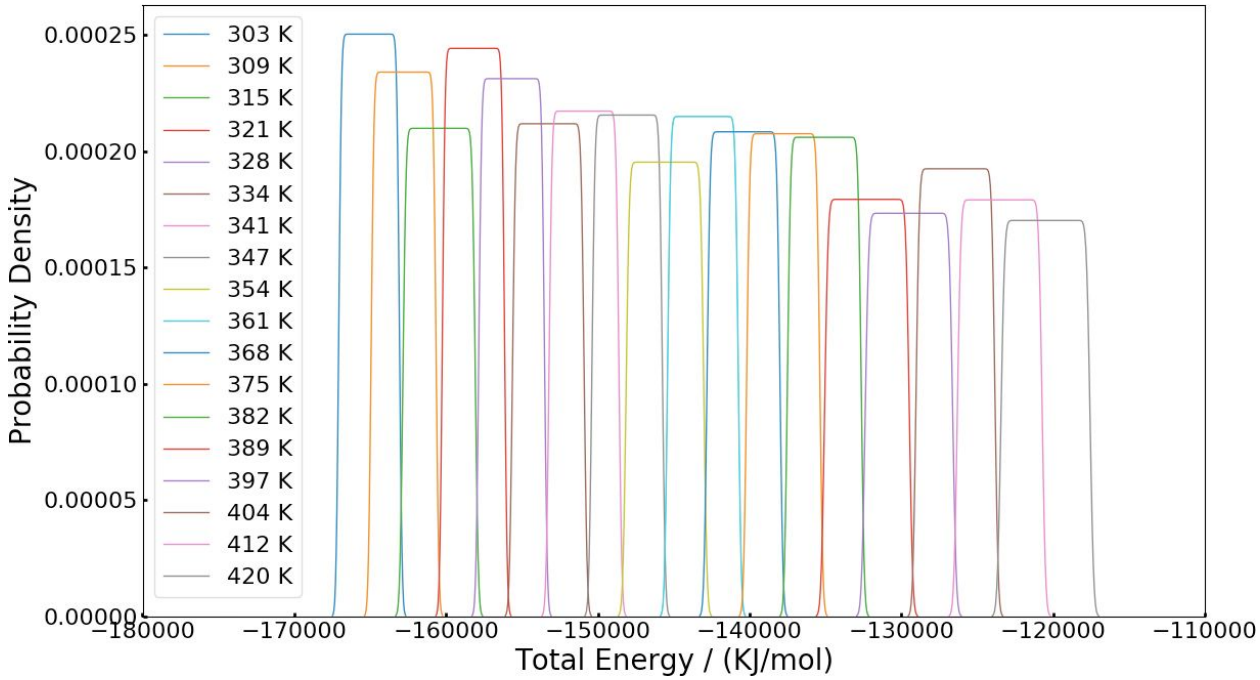

Figure S3. Distribution of potential energies for the 36 replicas distributed in a temperature interval between 300K and 420 K. Only every second replica is shown.

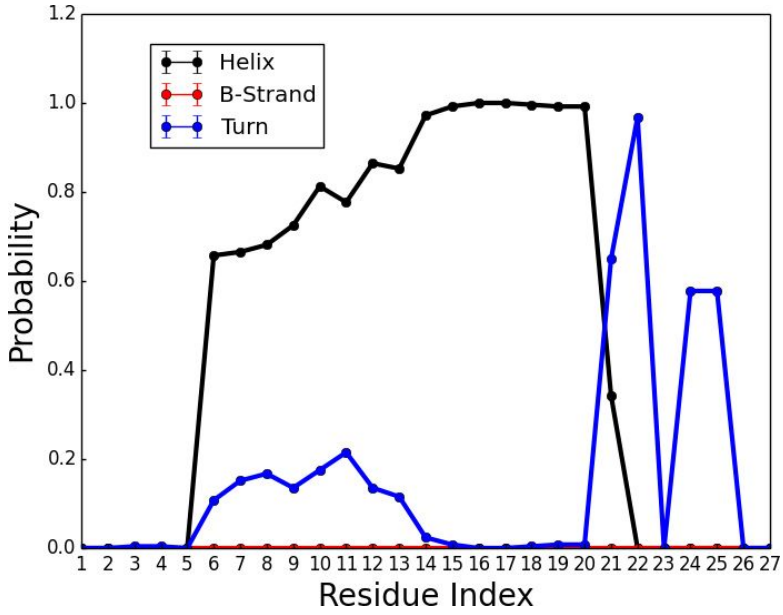

Figure S4. Secondary structure probability analysis for molecular dynamics simulation of the mutation E9A based on the straight structure from wild type.