Electronic Supplementary Information

Conformational features of Aβ_{42} peptide monomer and its interaction with surrounding solvent

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Table SI-1 Simulation cell type, cell dimensions at the beginning and after the equilibration runs, and the number of water molecules for different Aβ peptide monomers

system	cell type	initial dimension ($Å^3$)	dimension after equilibration ($Å^3$)	no of water molecules
S1	cubic	80 x 80 x 80	78.47 x 78.47 x 78.47	16098
S2	cubic	70 x 70 x 70	68.48 x 68.48 x 68.48	10643
S3	orthorhombic	90 x 75 x 75	88.02 x 73.51 x 73.51	15886
S4	cubic	60 x 60 x 60	58.70 x 58.70 x 58.70	6586
S5	cubic	64 x 64 x 64	62.65 x 62.65 x 62.65	8075
S6	cubic	60 x 60 x 60	58.64 x 58.64 x 58.64	6580
S7	orthorhombic	85 x 55 x 60	82.50 x 53.72 x 58.52	8614
S8	orthorhombic	85 x 65 x 65	83.02 x 63.71 x 63.71	11160

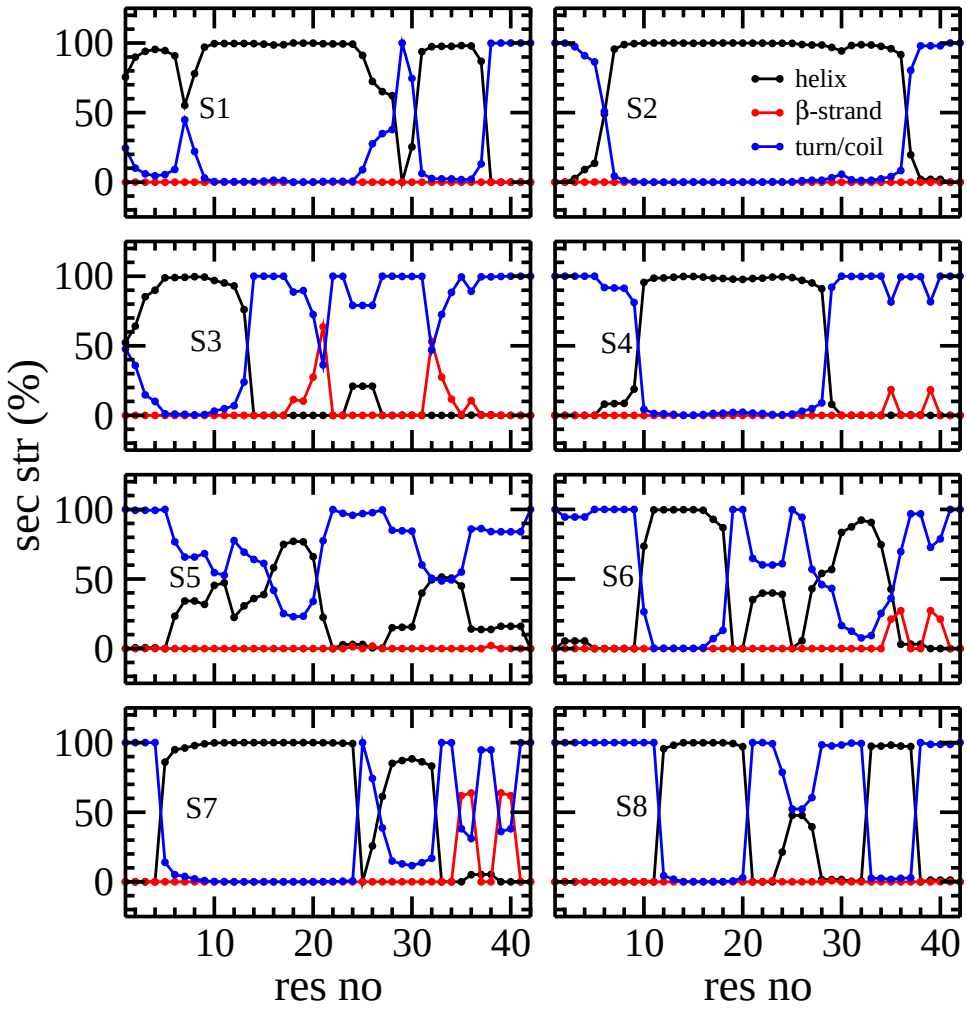

Fig. SI-1 Residue-wise secondary structural propensity (in %) of the Aβ peptide monomers as obtained from simulations S1 to S8.