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Thermodynamics of helix-coil transitions of polyalanine in open carbon nanotubes. DYLAN SUVLU, SENEVIRATNE SAMARATUNGA, Univ of Maine, DAVE THIRUMALAI, Univ of Texas at Austin, JAYENDRAN RASAIAH, Univ of Maine — Understanding structure formation of polypeptide chains and synthetic polymers encapsulated in pores is important in biology and nanotechnology. The stability of ordered structures in confined spaces is determined by the interplay between hydration and confinement. Using replica exchange molecular dynamics simulations of a capped twenty three residue alanine peptide in open nanotubes (NTs) of varying diameters (D) and NT hydrophobicity we show that an alpha-helix forms only over a narrow range of diameters (D $\approx$ 13-15). Helix stability decreases sharply outside this range. Increasing the hydrophobicity of the NT leads to an enhancement in helix content for all diameters, which we show is due to an anti-correlation between water density inside the nanotube and structure formation. We find that helix formation is driven by a negative enthalpy and positive entropy at 300 K whereas the corresponding entropy of formation in bulk water is strongly negative resulting in helix destabilization. Our findings provide insights into alpha-helix formation within the folding zones of the ribosome tunnel, which has an average diameter remarkably close to that found for optimal helix formation in open NTs.

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