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Interplay between secondary and tertiary structure formation in a lattice model alpha helical hairpin peptide PREM CHAPAGAIN, Department of Physics, Florida International University, BERNARD GERSTMAN, Department of Physics, Florida International University, THEORETICAL BIOPHYSICS GROUP TEAM — We present results from Monte Carlo simulations of folding dynamics of a model alpha helical hairpin peptide. The dynamics shows that the peptide chain folds in a two step fashion that involves the formation of partial helical segments followed by the formation of a stable tertiary structure by joining these semi-stable helical segments. The interplay between the formation of secondary and tertiary structures during the folding process was investigated by calculating the heat capacity and other thermodynamic quantities at various simulation temperatures. In addition to a sharp peak in the heat capacity curve for the transition between unfolded state and folded native state, the helix-random coil transition in the unfolded state is also cooperative.

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