Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Folding Kinetics and Thermodynamics of a Model Alpha Helical Hairpin Peptide PREM CHAPAGAIN, BERNARD GERSTMAN, Department of Physics, Florida International University, Miami, FL 33199 — Using MC simulations, we study the folding kinetics and thermodynamics of a specially designed alpha-turn-alpha helix that forms a two-helix bundle. This protein structure contains the hierarchy of secondary and tertiary structural elements. The model protein resembles the de novo design of alpha-turn-alpha helical hairpin peptide of Fezoui et al [PNAS (91), 1994]. Because of its size and simplicity, the two-helix bundle model protein is especially valuable from the protein design and engineering point of view. We systematically study how the folding kinetics depend on variations in the helix size and the inter-helical interactions. We find that strategic placement of non-hydrophobic residues in the helical interface leads to faster protein folding and reduces the chance of misfolding due to off-set of the helices. Depending on the nature of the inter-helical side chain packing, the helix bundle can be made to behave as a two-state system, or be made to follow more complicated kinetics.

Prem Chapagain
Department of Physics, Florida International University, Miami, FL 33199

Date submitted: 18 Nov 2004 Electronic form version 1.4