Abstract Submitted
for the SES05 Meeting of
The American Physical Society

The Role of Backbone Desolvation in Helix Folding HUGH NYMEYER, Florida State University — Replica exchange molecular dynamics simulations are used to study the helix-coil transition in different peptides with the amino-acid sequence YKAAXAKAAXAKAAXAK, where X is a substitutable site. Although numerous studies have compared the average helical propensity of different force-fields, little attention has been given to the ability of force-fields to capture the relative helical propensity of different amino-acids. Comparisons are made using two commonly used force- fields (GROMOS and AMBER). Beta-branched amino-acids are found to be destabilizing to helical structure, but this destabilization is consistently overestimated. The temperature dependence of this destabilization is also used to determine the difference in the enthalpy of helix-formation for different amino-acid substitutions. Although the enthalpic component of this destabilization is too strong, it appears sensitive to the particular force-field, which suggests that it may be useful for force-field parameterization.

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Date submitted: 05 Aug 2005 Electronic form version 1.4