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Generic Coarse-Grained Model for Protein Folding and Aggregation TRISTAN BEREAU, MARKUS DESERNO, Dept. of Physics, Carnegie Mellon University, Pittsburgh, PA 15213 — The complexity involved in protein structure is not only due to the rich variety of amino acids, but also the inherent weak interactions, comparable to thermal energy, and important cooperative phenomena. This presents a challenge in atomistic simulations, as it is associated with high-dimensionality and ruggedness of the energy landscape as well as long equilibration times. We have recently developed a coarse-grained (CG) implicit solvent peptide model which has been designed to reproduce key consequences of the above-mentioned weak interactions. Its intermediate level of resolution, four beads per amino acid, allows for accurate sampling of local conformations by designing a force field that relies on simple interactions. A realistic ratio of α-helix to β-sheet content is achieved by mimicking a nearest-neighbor dipole interaction. We tune the model in order to fold helical proteins while systematically comparing the structure with NMR data. Very good agreement is achieved for proteins that have simple tertiary structures. We further probe the effects of cooperativity between amino acids by looking at peptide aggregation, where hydrophobic peptide fragments cooperatively form large-scale β-sheet structures. The model is able to reproduce features from atomistic simulations on a qualitative basis.

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