

Abstract Submitted
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Multi-scale structure of a protein (histone H3.1) via a knowledge-based potential¹ RAS PANDEY, University of Southern Mississippi, BARRY FARMER, Air Force Research Laboratory — A coarse-grained computer simulation model is used to investigate the multi-scale structures of a histone H3.1, a protein with 136 residues in an effective solvent medium. The protein chain consisting of residues (nodes) tethered together by fluctuating bonds on a cubic lattice where empty lattice sites constitute the effective solvent matrix. Each residue interacts with surrounding solvent sites and other residues via Lennard-Jones (LJ) potential. A knowledge-based interaction matrix is used for the residue-residue interaction coefficient of the LJ potential. Interaction between the residue and solvent sites, a measure of the solvent quality, is varied. Each residue executes its stochastic motion with the Metropolis algorithm. We examine a number of local and global physical quantities some of which include mobility and energy profiles of each residue and their local structural histogram, radius of gyration (R_g), radial distribution function, and structure factor of the protein for a range of the solvent interactions. Variation of R_g with the solvent quality of solvent exhibits a maximum.

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