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Effects of solvent (effective medium versus explicit) on the structure of a protein (H3.1) RAS PANDEY, University of Southern Mississippi, BARRY FARMER, Air Force Research Laboratory — Structure and dynamics of a histone (H3.1) are studied in the presence of effective medium and explicit solvent over a range of temperatures with coarse-grained Monte Carlo simulations. The protein is represented by a coarse-grained chain of residues whose interactions are described by knowledge-based residue-residue and hydrophathy-index-based residue-solvent interactions. Each empty lattice site acts as a solvent in effective medium while a fraction of sites are occupied by mobile solvent constituents in explicit solvent medium. The presence of fluctuations with explicit solvent may affect the structure and dynamics of protein differently than that in effective solvent medium. Large scale simulations are performed to analyze the structure of the protein for a range of residue-solvent interactions and temperature, and a number of local and global physical quantities are analyzed. Differences due to type of solvent on the response of some of these quantities as a function of temperature will be presented.

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