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A multi-grain approach to protein (H3.1) structure in effective solvent with knowledge-based residue-residue interactions[1] RAS PANDEY, University of Southern Mississippi, BARRY FARMER, Air Force Research Laboratory — Using a coarse-grained Monte Carlo simulation we examine the structure and dynamics of a histone (H3.1) in effective solvent at a range of temperature [1]. Knowledge-based residue-residue and hydropathy index based residue-solvent interactions are used as input to a generalized LJ potential. Large scale simulations are performed to analyze the structure of protein for a range of residue-solvent interaction strength (f) and temperature. We find that the radius of gyration (R_g) of the protein responds non-monotonically to solvent interaction strength with a maximum at a characteristic interaction. Broadening of peak occurs on raising the temperature. Fine-grain representation of protein enhances the structural resolution while retaining the fundamental characteristics of the structural response.

[1] R.B. Pandey and B.L. Farmer, PLoS One 8, e76069 (2013).

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