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Thermal response of a protein (H3.1) by a coarse-grained model with knowledge-based interactions[1] BARRY FARMER, Air Force Research Laboratory, RAS PANDEY, University of Southern Mississippi — The effect of temperature on the conformation of a histone (H3.1) is studied by a coarse-grained Monte Carlo simulation based on three knowledge-based contact potentials (MJ[1], BT[2], BFKV[3]). We find that the histone H3.1 undergoes a systematic (possibly continuous) structural transition from a random coil to a globular conformation on reducing the temperature, a general feature from each potential. The range over which such a systematic response in variation of the radius of gyration (R_g) with the temperature (T) occurs, however, depends on the potential. Multi-scale structures of the protein are examined by analyzing the scaling of the structure functions with the wave vector. Quantitative comparison of the structure emerging from three potentials will be presented.

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[2] M.R. Betancourt and D. Thirumalai, Protein Sci. 2, 361 (1999).
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