

Abstract Submitted
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Thermal response of proteins (histone H2AX, H3.1) by a coarse-grained Monte Carlo simulation with a knowledge-based phenomenological potential¹ MIRIAM FRITSCHÉ, DIETER HEERMANN, University of Heidelberg, Germany, RAS PANDEY, University of Southern Mississippi, BARRY FARMER, Air Force Research Laboratory — Using a coarse-grained bond fluctuating model, we investigate structure and dynamics of two histones, H2AX (143 residues) and H3.1 (136 residues) as a function of temperature (T). A knowledge based contact matrix is used as an input for a phenomenological residue-residue interaction in a generalized Lennard-Jones potential. Metropolis algorithm is used to execute stochastic movement of each residue. A number of local and global physical quantities are analyzed. Despite unique energy and mobility profiles of its residues in a specific sequence, the histone H3.1 appears to undergo a structural transformation from a random coil to a globular conformation on reducing the temperature. The radius of gyration of the histone H2AX, in contrast, exhibits a non-monotonic dependence on temperature with a maximum at a characteristic temperature (T_c) where crossover occurs from a positive (stretching below T_c) to negative (contraction above T_c) thermal response on increasing T . Multi-scale structures of the proteins are examined by a detailed analysis of their structure functions.

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