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Thermal response of alpha-synuclein structure with knowledge-based residue-residue interactions[1] PETER MIRAU, BARRY FARMER, Air Force Research Laboratory, RAS PANDEY, University of Southern Mississippi — Structure and dynamics of alpha-synuclein (140 residues) are studied via a coarse-grained Monte Carlo simulation as a function of temperature. Knowledge-based residue-residue [1] interactions are used as input to a generalized LJ potential. We analyze a number of local and global physical quantities such as residue mobility profiles, contact map, radius of gyration, structure factor, etc. We find that the radius of gyration (R_g) of the protein increases on increasing the temperature within a range. Although the thermal response of the gyration radius shifts with the type of knowledge-based interaction potential, general feature of linear response is retained. These findings are consistent with the NMR measurements [2] on the variation of the gyration radius with the temperature. Detailed analysis of structure factor reveals the thermal response of multi-scale segmental conformations.

[1] S. Miyazawa and R.L. Jernigan, Macromolecules 18,534 (1985); M.R. Betancourt and D. Thirumalai, Protein Sci. 2,361 (1999).
[2] J.R. Allison et al. JACS 131, 18314 (2009).

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