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Protein Crit-Structural **Fluctuations** \mathbf{at} icality in the Temperature-pressure-crowding Folding Phase Diagram¹ ANDREI GASIC, MARGARET CHEUNG, University of Houston, Department of Physics; Center for Theoretical Biological Physics, Rice University — In the cell, proteins perform complex biological functions through large-scale motion, which are induced by slight environmental perturbations. This characteristic of having high susceptibility is similar to a physical system near a critical point. Indeed, experimental and computational findings demonstrate that protein folding transitions in the temperature (T), pressure (P), and crowding volume-fraction (ϕ) phase diagram point toward signatures of criticality, where distinct folding phases merge. Here, using coarse-grained molecular dynamics simulations, we theoretically show that at the critical regime, fluctuations exhibit high susceptibility and long-range correlations up to the size of the protein. Meaning that near criticality, the dynamics of each residue is influenced by each other residue even across the entire protein. We investigate the structural origin and the effect of macromolecular crowding on this critical behavior. Furthermore, this study leads us one step closer to developing universal principles of protein folding and function in vivo.

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