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Towards multistage algorithm to model intrinsically unstructured proteins ANTTI NIEMI, Uppsala Univ, JIAOJIAO LIU, JIN DAI, JIANFENG HE, Beijing Institute of Technology, NEVENA ILIEVA, Bulgarian Academy of Sciences — We combine Landau mean field theory with all atom molecular dynamics into a multistage algorithm that can model protein folding and dynamics over very long time periods yet with atomic level precision. We propose that the approach is particularly suited to characterise the conformational states of intrinsically unstructured proteins. As an example we investigate an isolated monomeric Myc oncoprotein that has been implicated in many cancers. Under physiological conditions Myc is presumed to be an intrinsically disordered protein. Here we propose that room temperature Myc may have a stable folded conformation which we identify. For this we first use a Landau model investigation to confirm that as a monomer Myc is unstable, and uncover a highly degenerate structural landscape. We analyse its thermal stability properties using all atom molecular dynamics and observe a cluster of structures, with the two helical segments of the original leucine zipper aligned in parallel to each other. The cluster appears stable under room temperature all atom molecular dynamics simulations. During its stabilisation we identify a quasiparticle oscillation which is akin Davydov's Amide-I soliton, that fades away by diffusion.

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