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Excluded volume entropic effects on protein unfolding times and intermediary stability PREM CHAPAGAIN, BERNARD GERSTMAN, Department of Physics, Florida International University, Miami FL 33199, THEORETICAL BIOPHYSICS TEAM — The dynamics of protein folding result from both enthalpic and entropic contributions to the free energy. In this paper we focus on entropic volume exclusion effects. We carry out computer simulations using a model that allows us to independently change the size or biochemical properties of amino acid residues. To determine the importance of excluded volume effects, we investigate the effects of changing the size of side chains on the unfolding dynamics of a model four-helix bundle protein. In addition, we also investigate the effects of changing the thickness of the chain's backbone. This has relevance to the behaviour of synthetic polymers where the size of the constituent units can be varied. We find that entropic excluded volume effects are crucially important for stabilizing the organized native state relative to the molten globule.

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