

Abstract Submitted
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An Analytical Study of the Interplay between Geometrical and Energetic Effects in Protein Folding YOKO SUZUKI, Department of Physics, School of Sciences and Engineering, Meisei University, JEFF NOEL, JOSE ONUCHIC, Center for Theoretical Biological Physics, University of California at San Diego — We introduce a Gaussian filament with a C_α structure-based ($G\delta$) potential as a new theoretical scheme based on a Hamiltonian approach. This model takes into account geometrical information in a realistic fashion without the need of phenomenological descriptions. In order to make this model more appropriate for comparison with protein folding simulations and experiments, we introduce a many-body interaction into the potential term to enhance cooperativity. We apply our new analytical model to a β -hairpin type peptide and compare our results with a molecular dynamics simulation of a structure-based model. those comparisons successfully give the quantification of the interplay between geometrical and energetic effects.

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