

Abstract Submitted
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Using Go-Model Simulation to Capture the Complexity of the α -Spectrin¹ DANIEL GAVAZZI, JOHN PORTMAN, Kent State University — The protein α -spectrin is composed of a repeating helical structure that can be separated into three domains named R15, R16, and R17. Although each domain is highly homologous, the folding mechanism and kinetics are distinct. Most strikingly, the folding time of R15 is three orders of magnitude larger than R16, with R17 being the slowest. The origin of this wide range of rates has been attributed to roughness in energy landscapes and internal friction. We show that a simple analytic model is able to capture the subtleties of folding each domain, despite their structural similarities. In particular, our model predicts the increasing complexity from R15 to the R16 and R17 domains which explains the kinetic trends seen in experiments.

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