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Mechanism of folding/unfolding of Rd-apocyt b_{562}: a molecular dynamics simulation study HARIANTO TJONG, HUAN-XIANG ZHOU, Institute of Molecular Biophysics and Department of Physics, Florida State University, Tallahassee, FL 32306 — The four-helix bundle protein Rd-apocyt b_{562}, a redesigned stable variant of apocytochromeb_{562}, has been shown to exhibit two-state folding kinetics. Its transition-state ensemble has been characterized by Φ-value analysis and native-state hydrogen exchange. To elucidate the molecular basis of the transition-state ensemble, we have carried out high-temperature molecular dynamics simulations of the unfolding process. In agreement with experiment, helix one was found to melt first, followed by helix four, and then by helices three and two. This ordering among the four helices could be rationalized by differences in helix propensities and by the presence of tertiary contacts.

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