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**$\alpha$-Helical to $\beta$-Helical Conformation Change in the C-Terminal of the Mammalian Prion Protein** JESSE SINGH, UC Davis, PAUL WHITFORD, Los Alamos National Laboratory, NATHA HAYRE, DANIEL COX, UC Davis Physics, JOSÉ ONUCHIC, Center for Theoretical Biological Physics, UCSD — We employ all-atom structure-based models with mixed basis contact maps to explore whether there are any significant geometric or energetic constraints limiting conjectured conformational transitions between the alpha-helical ($\alpha$H) and the left handed beta helical (LHBH) conformations for the C-terminal (residues 166-226) of the mammalian prion protein. The LHBH structure has been proposed to describe infectious oligomers and one class of in vitro grown fibrils, as well as possibly self-templating the conversion of normal cellular prion protein to the infectious form. Our results confirm that the kinetics of the conformation change are not strongely limited by large scale geometry modification and there exists an overall preference for the LHBH conformation.

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