

Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

How Single-site Mutation Affects HP Lattice Proteins¹

GUANGJIE SHI, DAVID P LANDAU, Center for Simulational Physics, The University of Georgia, THOMAS VOGEL, Theoretical Division, Los Alamos National Laboratory, THOMAS WÜST, Swiss Federal Research Institute WSL, YING WAI LI, Oak Ridge National Laboratory — We developed a heuristic method based on Wang-Landau² and multicanonical sampling for determining the ground-state degeneracy of HP lattice proteins³. Our algorithm allowed the most precise estimations of the (sometimes substantial) ground-state degeneracies of some widely studied HP sequences. We investigated the effects of single-site mutation on specific long HP lattice proteins comprehensively, including structural changes in ground-states, changes of ground-state degeneracy and thermodynamic properties of the systems. Both extremely sensitive and insensitive cases have been observed; consequently, properties such as specific heat, tortuosities etc. may be either largely unaffected or may change significantly due to mutation. More interestingly, mutation can even induce a lower ground-state energy in a few cases.

¹Supported by NSF

²T. Wüst and D. P. Landau, *J. Chem. Phys.* **137**, 064903 (2012).

³K. A. Dill, *Biochemistry* 24, 1501 (1985); K. F. Lau and K. A. Dill, *Macromolecules* 22, 3986 (1989).

Guangjie Shi
Center for Simulational Physics, The University of Georgia

Date submitted: 15 Nov 2013

Electronic form version 1.4