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Effect of Mutations on HP Lattice Proteins[1] GUANGJIE SHI, THOMAS VOGEL, DAVID P. LANDAU, The University of Georgia, YING WAI LI, Oak Ridge National Laboratory, THOMAS WÜST, Swiss Federal Research Institute WSL — Using Wang-Landau sampling with approriate trial moves[2], we investigate the effect of different types of mutations on lattice proteins in the HP model. While exact studies have been carried out for short HP proteins[3], the systems we investigate are of much larger size and hence not accessible for exact enumerations. Based on the estimated density of states, we systematically analyse the changes in structure and degeneracy of ground states of particular proteins and measure thermodynamic quantities like the stability of ground states and the specific heat, for example. Both, neutral mutations, which do not change the structure and stability of ground states, as well as critical mutations, which do change the thermodynamic behavior qualitatively, have been observed.

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[2]T. Wüst and D. P. Landau, J. Chem. Phys. **137**, 064903 (2012).
[3]C. Holzgräfe, A. Irbäck and C. Troein, J. Chem. Phys. **135**, 195101 (2011).

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