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Computational Studies of Protein Core Mutations[1] JENNIFER GAINES, LYNNE REGAN, COREY O'HERN, Yale University — Predicting the effects of protein core mutations is a necessary first step in developing methods for computational protein design. Current computational methods have found limited success in predicting the changes in stability arising from protein core mutations. We implement a stereochemical plus hard-sphere (SHS) model for amino acid structure, which allows us to investigate in detail the physical mechanisms that give rise to differences in stability between natural and mutated protein cores. Here, we show that the SHS model can recapitulate the side chain dihedral angle distributions for amino acids in natural protein cores. In addition, we show that in many cases the SHS model can predict the experimentally measured changes in free energy due to mutations. In other cases, we find that add a term that favors packing fractions near those of natural protein cores, we are able to predict the stability of the mutated cores. These methods will be applicable to studying protein-protein interfaces and developing new protein-protein binding partners.

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