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Computational Studies of Protein-Protein Interface Designs JENNIFER GAINES, COREY O'HERN, LYNNE REGAN, Yale University — We implement a hard-sphere model for amino acid structure to study natural and designed protein-protein interfaces. Current computational methods have found limited success in designing novel interfaces and resorted to implementing several rounds of experimental mutation and selection to achieve successful designs. Here, we show that the hard-sphere model can recapitulate the side chain dihedral angle distributions for amino acids at natural protein-protein interfaces. In addition, we calculate the packing fraction in naturally occurring interfaces and find that it is comparable to dense random packing in protein cores. We then evaluate a number of successful and unsuccessful prior computational designs in terms of the number of allowed side chain dihedral angle conformations and the packing fraction of residues at the interface.

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