

Abstract Submitted
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Steric clashes determine differences in side chain dihedral angle distributions: A study of Thr versus Val¹ ALICE ZHOU, COREY O'HERN, LYNNE REGAN, Yale University — With the long-term goal to improve the design of protein-protein interactions, we develop a simple hard sphere model for dipeptides that can predict the side-chain dihedral angle distributions of Val and Thr in both the α -helix and β -sheet backbone conformations. We find that it is essential to include the non-polar hydrogens in the model; indeed interatomic clashes involving the non-polar hydrogens largely determine the form of side-chain dihedral angle distributions. Further, we are able to explain key differences in the side-chain dihedral angle distributions for Val and Thr from intra-residue steric clashes rather than inter-residue steric clashes or hydrogen bonding. These results are the crucial first step in developing computational models that can predict the side chain conformations of residues at protein-peptide interfaces.

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Alice Zhou
Yale University

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