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Predicting side-chain conformations of methionine using a hard-sphere model with stereochemical constraints[1] A. VIRRUETA, J. GAINES, C. S. O'HERN, L. REGAN, Yale University — Current research in the O'Hern and Regan laboratories focuses on the development of hard-sphere models with stereochemical constraints for protein structure prediction as an alternative to molecular dynamics methods that utilize knowledge-based corrections in their force-fields. Beginning with simple hydrophobic dipeptides like valine, leucine, and isoleucine, we have shown that our model is able to reproduce the side-chain dihedral angle distributions derived from sets of high-resolution protein crystal structures. However, methionine remains an exception - our model yields a chi-3 side-chain dihedral angle distribution that is relatively uniform from 60 to 300 degrees, while the observed distribution displays peaks at 60, 180, and 300 degrees. Our goal is to resolve this discrepancy by considering clashes with neighboring residues, and averaging the reduced distribution of allowable methionine structures taken from a set of crystallized proteins. We will also re-evaluate the electron density maps from which these protein structures are derived to ensure that the methionines and their local environments are correctly modeled. This work will ultimately serve as a tool for computing side-chain entropy and protein stability.

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