

Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Computational modeling of the side chain dihedral angle distributions of methionine using hard-sphere repulsive and short-range attractive interactions¹ ALEJANDRO VIRRUETA, COREY O'HERN, LYNNE REGAN, Yale University — Methionine (Met) is a versatile amino acid found frequently both in protein cores and at protein-protein interfaces. Thus, a complete description of the structure of Met is tantamount to a fundamental understanding of protein structure and design. In previous work, we showed that our hard-sphere dipeptide model is able to recapitulate the side chain dihedral angle distributions observed in high-resolution protein crystal structures for the 8 amino acids we have studied to date: Val, Thr, Ser, Leu, Ile, Cys, Tyr, and Phe. Using the same approach, we can predict the observed Met side chain dihedral angle distributions $P(\chi_1)$ and $P(\chi_2)$, but not $P(\chi_3)$. In this manuscript, we investigate the possible origins of the discrepancy and identify the minimal additions to the hard-sphere dipeptide model necessary to quantitatively predict $P(\chi_3)$ of Met. We find that applying a Lennard-Jones potential with weak attraction between hydrogen atoms is sufficient to achieve predictions that match the observed χ_3 side chain dihedral angle probability distributions for Met, Nle, and Mse without negatively affecting our results for the 8 previously studied amino acids.

¹A. V. is supported by an NSF Graduate Research Fellowship and a Ford Foundation Fellowship.

Alejandro Virrueta
Yale University

Date submitted: 06 Nov 2015

Electronic form version 1.4