MAR16-2015-000440

Abstract for an Invited Paper for the MAR16 Meeting of the American Physical Society

Random close packing in protein cores¹ COREY OHERN, Yale University

Shortly after the determination of the first protein x-ray crystal structures, researchers analyzed their cores and reported packing fractions $\phi \approx 0.75$, a value that is similar to close packing equal-sized spheres. A limitation of these analyses was the use of 'extended atom' models, rather than the more physically accurate 'explicit hydrogen' model. The validity of using the explicit hydrogen model is proved by its ability to predict the side chain dihedral angle distributions observed in proteins. We employ the explicit hydrogen model to calculate the packing fraction of the cores of over 200 high resolution protein structures. We find that these protein cores have $\phi \approx 0.55$, which is comparable to random close-packing of non-spherical particles. This result provides a deeper understanding of the physical basis of protein structure that will enable predictions of the effects of amino acid mutations and design of new functional proteins.

 1 We gratefully acknowledge the support of the Raymond and Beverly Sackler Institute for Biological, Physical, and Engineering Sciences, National Library of Medicine training grant T15LM00705628 (J.C.G.), and National Science Foundation DMR-1307712 (L.R.).