

Abstract Submitted
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A Physics-based Approach of Coarse-graining the cytoplasm of E. coli¹ QIAN WANG, MARGARET CHEUNG, University of Houston — We have investigated protein stability in an environment of E. coli cytoplasm using coarse-grained computer simulations. To coarse-grain a small slide of E. coli's cytoplasm consisting of over 16 million atoms, we developed a self-assembled clustering algorithm (CGCYTO). CGCYTO uses a tunable resolution parameter (λ , ranging from 0 to 1) to justify the resolution of a cytoplasm, depending on the size of a test protein for the computation of covolumes and the volume of a macromolecule in the cytoplasm. We compared the results from a polydisperse cytoplasm model (PD model) from CGCYTO with two other coarse-grained hard-sphere cytoplasm models: (1) F70 model, macromolecules in the cytoplasm were modeled by homogeneous hard spheres with a radius of 55Å and (2) HS model, each macromolecule in the cytoplasm is modeled by hard spheres of various sizes. It was found that the folding temperature T_f of a test protein (apoazurin) is ~ 5 degrees higher in a PD model than that in a F70 model. In addition, there is a deviation of 1.7 degrees on T_f when an apoazurin is randomly placed at different voids formed by particle fluctuations in a PD model, 0.7 degrees higher than that in a HS model.

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