

Abstract Submitted
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Protein structure, stability and folding in the cell – *in silico* biophysical approaches¹ MARGARET CHEUNG, University of Houston — How the crowded environment inside a cell affects the structural conformation of a protein with aspherical shape is a vital question because the geometry of proteins and protein-protein complexes are far from globules *in vivo*. Here we address this question by combining computational and experimental studies of a spherical protein (i.e. apoflavodoxin), a football-shaped protein (i.e., *Borrelia burgdorferi* VlsE) and a dumbbell-shaped protein (i.e. calmodulin) under crowded, cell-like conditions. The results show that macromolecular crowding affects protein folding dynamics as well as an overall protein shape associated with changes in secondary structures. Our work demonstrates the malleability of “native” proteins and implies that crowding-induced shape changes may be important for protein function and malfunction *in vivo*.

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