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Protein structure, stability and folding in the cell – *in silico* biophysical approaches[1]

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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 several aspherical proteins (calmodulin, VlsE, and phosphoglycerate kinase) under crowded, cell-like conditions. The results show that macromolecular crowding affects protein folding dynamics, structures and functions. 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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