

Abstract Submitted
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Competition between chemical denaturation and macromolecular crowding effects on the folding dynamics of proteins¹ ANTONIOS SAMIOTAKIS, MARGARET CHEUNG, University of Houston — It is well known that proteins fold and function in the crowded environment of the cell's interior. In the recent years it has been established that the so-called “macromolecular crowding” effect can enhance the folding stability of proteins by destabilizing their unfolded states. On the other hand, chemical and thermal denaturation are often used in experiments as tools to destabilize protein structures when probing a protein's folding landscape. However, little is known about the combined effects of these competing phenomena on proteins. In this work, we use coarse-grained molecular simulations to study the thermodynamic and kinetic properties of the small peptide Trp-cage, in the combined presence of macromolecular crowders and chemical denaturant. With the use of an energy function derived by all-atomistic simulations in the presence of urea, we investigate the thermodynamics and kinetics of Trp-cage's folding mechanism at several concentrations of urea. The effects of the competition between stabilization by macromolecular crowding and destabilization by chemical denaturation will also be discussed.

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