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Crowding Effects on the Unfolding of Ubiquitin[1] DAVID PINCUS, Institute For Physical Science and Technology, University of Maryland, DEVARAJAN THIRUMALAI, Director, Biophysics Program, University of Maryland — Using a coarse-grained representation of polypeptide chains, we probed the mechanical stability of Ubiquitin (Ub) monomers and trimers ($(Ub)_3$) in the presence of monodisperse spherical crowding agents. Our findings indicate that crowding increases the volume fraction (Φ_c)-dependent average force ($\langle f_u(\Phi_c)\rangle$), relative to the value at $\Phi_c = 0$, needed to unfold Ub and the polyprotein. Furthermore, we found that average unfolding forces increase with decreasing crowder diameter (σ_c). The average unfolding force $\langle f_u(\Phi_c)\rangle$ depends on the ratio $\frac{D}{R_g}$, where $D \approx \sigma_c(\frac{\pi}{6\Phi_c})^{\frac{1}{3}}$ with R_g being the radius of gyration of Ub (or $(Ub)_3$) in the unfolded state. Examination of the unfolding pathways shows that, relative to $\Phi_c = 0$, crowding promotes reassociation of ruptured secondary structural elements. Both the nature of the unfolding pathways and $\langle f_u(\Phi_c)\rangle$ for $(Ub)_3$ are altered in the presence of crowding particles with the effect being most dramatic for the subunit that unfolds last. We predict that $\langle f_u(\Phi_c)\rangle$ scales in a simple manner with Φ_c.

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David Pincus
Institute For Physical Science and Technology, University of Maryland

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