Title:	Unfolding Transitions of Peripheral Subunit Binding Domains Show Cooperative Behavior
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Abstract:	Characterization of native, intermediate, and denatured states is crucial for understanding the factors influencing the stability of proteins. We have carried out molecular dynamics simulations to study the unfolding of three peripheral subunit binding domains (PSBDs): E. coli BBL, Bacillus stearothermophilus E3BD, and human hbSBD, at three different temperatures: 300, 330, and 400 K, and in the presence of two solvents: water and 5 M guanidinium hydrochloride (GndCl) solution. These proteins share similar folds, with two parallel helices, maintained via a hydrophobic core comprising residues from their interconnecting loop. BBL is more sensitive to thermal and chemical denaturation in comparison to hbSBD, and E3BD is the most stable of all of the three proteins. The effect of temperature on the stability of these proteins is more pronounced in “water-only” simulations compared to that in the presence of guanidium hydrochloride in high concentrations. Our results show cooperative unfolding transitions of these proteins, which are triggered by an initial melting of the C-terminal helix H2. The consequent loss of interhelical interactions or native contacts, as observed, leads to the subsequent melting of the N-terminal helix H1.
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