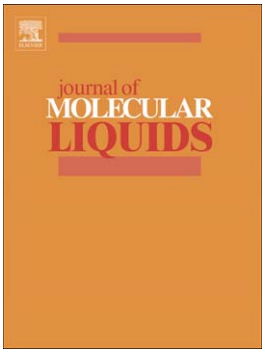

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How the stability of a folded protein depends on interfacial water properties and residue-residue interactions

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Abstract

Proteins tend to adopt a single or a reduced ensemble of configurations at natural conditions [1], but changes in temperature T and pressure P induce their unfolding. Therefore for each protein there is a stability region (SR) in the T–P thermodynamic plane outside which the biomolecule is denaturated. It is known that the extension and shape of the SR depend on i) the specific protein residue-residue interactions in the native state of the amino acids sequence and ii) the water properties at the hydration interface. Here we analyze by Monte Carlo simulations of different coarse-grained protein models in explicit water how changes in i) and ii) affect the SR. We show that the solvent properties ii) are essential to rationalize the SR shape at low T and high P and that our findings are robust with respect to parameter changes and with respect to different protein models, representative of the ordered and disordered proteins. These results can help in developing new strategies for the design of novel synthetic biopolymers.

Keywords: Protein folding; Cold denaturation; Pressure denaturation;

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