Unfolding Simulation of Ubiquitin with Coarse-Grained Model

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Folding is a major event of forming a structure of protein which can function as it is designed. However, misfolding of protein leads to malfunction and becomes disease (e.g. Alzheimer's disease). Unfolding experiments and simulations have shown kinetics of bond rupture and free energy landscape of chemical bond and protein folding. BLN (Hydrophobic-Hydrophilic-Neutral) model is a coarse-grained model developed to simulate folding event of protein considering hydrophobicity. In this work, we have studied how ubiquitin is pulled with coarse-grained simulation with BLN model. Pulling order of ubiquitin and force curve is shown and compared with experiments and simulation with Gō-model. BLN model showed unfolding mechanism of ubiquitin very well. Hydrophobicity of protein structure is well imparted in unfolding simulation and it describes unfolding behavior of protein well.

Keywords: BLN model, coarse-grained model, coarse-grained simulation, unfolding simulation