Protein mechanical unfolding: importance of non-native interactions

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ABSTRACT

Mechanical unfolding of the fourth domain of *Distyostelium discoideum* filamin (DDFLN4) was studied by all-atom molecular dynamics simulations, using the GROMOS96 force field 43a1 and the SPC explicit water solvent. Our study reveals an important role of non-native interactions in the unfolding process. Namely, the existence of a peak centered at the end-to-end extension $\Delta R \sim 22$ nm in the force-extension curve, is associated with breaking of non-native hydrogen bonds. Such a peak has been observed in experiments but not in Go models, where non-native interactions are neglected. We predict that an additional peak occurs at $\Delta R \sim 2$ nm using not only GROMOS96 force field 43a1 but also Amber 94 and OPLS force fields. This result would stimulate further experimental studies on elastic properties of DDFLN4.