STRETCHING OF MOLECULES OF PROTEINS — COMPARISON OF THEIR MECHANICAL PROPERTIES

Summary

Mechanical stretching of single proteins has been studied experimentally for about 55 proteins yielding a variety of force patterns and peak forces.

Here, we perform a theoretical survey of proteins of known native structure and map out the landscape of possible dynamical behaviors under stretching at a constant speed. We consider 7510 proteins each comprising not more than 150 amino acids. The model used is constructed based on the native geometry. It is solved by methods of molecular dynamics and validated by comparing the theoretical predictions to experimental results. We characterize the distribution of peak forces and correlations with the system size and with the structure classification as characterized by the hierarchical classification of protein domain structures (CATH). Despite the presence of such correlations, proteins with the same CATH index may belong to different classes of the dynamical behavior. We identify proteins with the biggest forces and show that they belong to few topology classes. We determine which protein segments act as mechanical clamps and show that, in most cases, they correspond to long stretches of parallel β-strands, but other mechanisms are also possible.