Mechanical differences between ATP and ADP actin states: A molecular dynamics study

Behzad Mehrafrooz, Amir Shamloo

PII: S0022-5193(18)30170-X
DOI: 10.1016/j.jtbi.2018.04.010
Reference: YJTBI 9425

To appear in: *Journal of Theoretical Biology*

Received date: 5 July 2017
Revised date: 31 March 2018
Accepted date: 6 April 2018

Please cite this article as: Behzad Mehrafrooz, Amir Shamloo, Mechanical differences between ATP and ADP actin states: A molecular dynamics study, *Journal of Theoretical Biology* (2018), doi: 10.1016/j.jtbi.2018.04.010

Highlights

- Tensile stiffnessof a single G-actin was investigated in both axial and lateral directions.
- The effects of nucleotide bindingpocket on the mechanical behavior of the actin monomer was studied.
- A simple structural model was proposed that describes actin filament as a hierarchical structure.
- This model can extend the obtainedresults for the monomeric G-actin scale to the actin filament.
- Using this model, the persistence length of actin filament was estimated to be 15.41 microns.