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

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Highlights

- Tensile stiffness of a single G-actin was investigated in both axial and lateral directions.
- The effects of nucleotide binding pocket 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 obtained results 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.

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