Abstract Submitted
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Investigations into the mechanical properties of fibrinogen using molecular simulations[1] AMIT DONGOL, RUXANDRA DIMA, University of Cincinnati — Fibrinogen, a hexameric molecule, is the main component of a blood clot [1]. The clots are under the action of large mechanical forces during blood flow or at the site of the wound. Hence it is crucial to study the mechanical properties of fibrinogen, which are likely to be responsible for the force response of the clots [2]. To understand the molecular origins of the mechanical properties of fibrinogen, we performed Langevin simulations of a minimalist polymer model of this molecule. Our model [3] enables us to simulate the force-induced unfolding of fibrinogen at experimental loading rates. Our simulations revealed critical unfolding forces in the range of 100 pN in accord with experimental results. By surveying the structures of the various metastable intermediates, we map features of the complex energy landscape of fibrinogen which are at the origin of clot elasticity.
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