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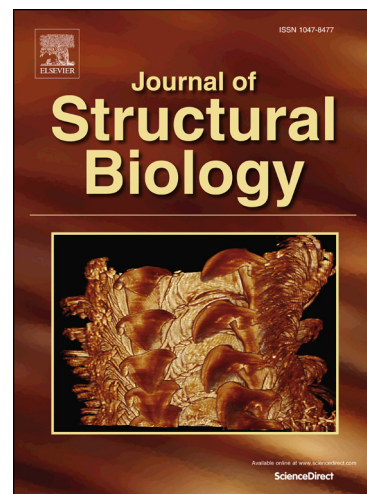
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Mechanical variations in proteins with large-scale motions highlight the formation of structural locks

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A preliminary version of this work, <https://doi.org/10.1101/221077>, was deposited in bioRxiv.

Abstract: Protein function depends just as much on flexibility as on structure, and in numerous cases, a protein's biological activity involves transitions that will impact both its conformation and its mechanical properties. Here, we use a coarse-grain approach to investigate the impact of structural changes on protein flexibility. More particularly, we focus our study on proteins presenting large-scale motions. We show how calculating directional force constants within residue pairs, and investigating their variation upon protein closure, can lead to the detection of a limited set of residues that form a *structural lock* in the protein's closed conformation. This lock, which is composed of residues whose side-chains are tightly interacting, highlights a new class of residues that are important for protein function by stabilizing the closed structure, and that cannot be detected

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