

Abstract Submitted
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Rigidity effects and mechanical unfolding of proteins OLEG VOROV, DENNIS LIVESAY, DONALD JACOBS, University of North Carolina, Charlotte — We describe a new method that shows promise for evaluating the partition function for a protein under an applied external force within a Distance Constraint Model (DCM). This approach is based on an approximate account for the rigidity effects due to hydrogen bond crosslinking using Maxwell constraint counting. Within a mean-field treatment, the free energy is estimated accurately over an ensemble of accessible conformations conditional upon the breaking of various weakest-link distance constraints, as they successively break due to a series of mini structural transitions. These calculations are performed using an exact transfer matrix approach combined with a combinatorial partitioning of the structure into different parts based on separating lines of unfolding pathways. The various shortest paths over an ensemble of structures that “crack” open in different ways are used to obtain the appropriate Boltzmann weight, related to the work done by the external pulling force. For structures with beta-hairpin geometry, all permutations of unfolding pathways are enumerated exactly. For a simple minimal DCM, results for extension-force curves agree markedly well with experiment. Using computational methods, this approach can be used to describe single-molecule experiments on mechanical protein unfolding under different settings, such as fixed extension, or constant force conditions. This work is supported by NIH R01 GM073082.

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