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Protein folding and dynamics from simulations of coarse protein models.[1]

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The dynamics and folding transitions of proteins are studied by computer simulations of coarse-grained models. The simulations are related to experimental studies of the unfolding of proteins under mechanical force, and the effects of mutations on the folding rates using phi-value analysis. Coarse protein models have also been useful in studies of slow conformational transitions. Applications to the helix-to-sheet transition of an arc repressor mutant, and the open-to-closed transition of the calmodulin C-terminal domain indicate that local unfolding events can contribute significantly to the slow dynamics of these proteins.

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