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All-or-none protein-like folding of a homopolymer chain[1] MARK TAYLOR, Hiram College, WOLFGANG PAUL, KURT BINDER, Johannes-Gutenberg-Universitat — Many small proteins fold via a first-order "all-or-none" transition directly from an expanded coil to a compact native state. Here we report an analogous direct freezing transition from an expanded coil to a compact crystallite for a simple flexible homopolymer. Wang-Landau sampling is used to construct the complete density of states for square-well chains up to length 256. Analysis within both the microcanonical and canonical ensembles shows that, for a chain with sufficiently short-range interactions, the usual polymer collapse transition is preempted by a direct freezing transition. Despite the non-unique homopolymer ground state, the thermodynamics of this direct freezing transition are identical to the thermodynamics of two-state protein folding. A free energy barrier separates a high entropy ensemble of unfolded states from a low entropy set of crystallite states and the transition proceeds via the formation of a transition-state folding nucleus. An Arrhenius analysis of the folding/unfolding free energy barrier yields a Chevron plot characteristic of proteins and the model chain satisfies the van't Hoff calorimetric criterion for two-state folding.

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