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Understanding ensemble protein folding at atomic detail.[1]

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Here we present a new all-atom model and development of simple potential functions (inspired by discoveries of general principles of protein folding) that allow to fold small proteins from sequence to near native structure at an atomic level of detail. Availability of numerous successful all-atom folding trajectories and their novel graph theoretical analysis, makes it possible to gain a detailed atomic level understanding of folding pathways/intermediates/transition states for engrailed homeodomain - a small alpha-helical protein that has been recently studied experimentally.

[1]In collaboration with Isaac Hubner, Eric Deeds, and Jae Shick Yang, Harvard University.