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The folding of an "average" beta trefoil protein. SHACHI GOSAVI, PAT JENNINGS, JOSE ONUCHIC, UCSD — The beta-trefoil fold is characterized by twelve beta strands folded into three similar beta-beta-beta-loop-beta (trefoil) units. The overall fold has pseudo-threefold symmetry and consists of a six stranded-barrel, capped by a triangular hairpin triplet. The loops connecting the beta-strands vary in length and structure. It is these loops that give the fold its varied binding capability and the binding sites lie in different parts of the fold. The beta-trefoil proteins have little sequence similarity (sometimes less than 17%) and bind a range of molecules, including other proteins, DNA, membranes and carbohydrates. Protein folding experiments have been performed on four of the beta trefoils, namely, interleukin-1 (IL1B), acidic and basic fibroblast growth factors (FGF-1 and FGF-2) and hisactophilin (HIS). These experiments indicate that the proteins fold by different routes. Folding simulations of the proteins identify the possible folding routes and also show that the shapes of the barriers are different for the different proteins. In this work, we design a model protein which contains only the core fold elements of the beta-trefoil fold. We compare the folding of this "average" protein to the folding of His, FGF and IL1B and make some connections with function.

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