Determination of the conformation of folding initiation sites in proteins by computer simulation.

Experimental evidence and theoretical models both suggest that protein folding begins by specific short regions of the primary sequence. We have constructed a program to determine the conformation of these regions by computer simulation. The program uses a Monte Carlo technique to sample the phase space of the protein. The results of simulations on several small proteins indicate that the program is capable of finding the most stable conformation in a reasonable amount of time. Extensions of the methods to the folding of larger portions of proteins are suggested.