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Diffusion-limited formation of internal loops in polymer chains[1]
DANA DOUCET, ADRIAN ROITBERG, STEPHEN HAGEN, University of Florida — The speed of diffusional motion of a polypeptide places an upper limit on the speed of protein folding: folding often requires two distant portions of the polypeptide chain to diffuse into contact. Although several studies have investigated the speed at which external (i.e. end-to-end) loops form in polypeptide chains, the more realistic case of internal loops (i.e. connecting two interior points) involves additional excluded volume and potentially slower dynamics. We have used a simple statistical approach to estimate this effect. We generate model chains in continuous, three-dimensional space, where the hard-sphere, excluded volume interaction represents the only deviation from ideal chain behavior. This yields the probability distribution for the distance between particular sites in the chain. We then use a first-passage-time approach (Szabo, Schulten, and Schulten 1980) to estimate the rate of contact formation under various combinations of loop lengths, "tail" lengths, and excluded volume. We find that the addition of just a few extra links to an end-to-end loop significantly reduces the speed of loop formation.

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