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Localized single-stranded bubble mechanism for cyclization of short DNAs

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Recent experiments (T.E. Cloutier, J. Widom, Mol. Cell 14, 355-62 2004) indicate that double-stranded DNA molecules of approximately 100 base pairs in length have a probability of cyclization which is up to 10^5 times larger than that expected based on the known bending modulus of the double helix. We argue that for short molecules, formation of small (few base pair) regions of single-stranded DNA can provide 'flexible hinges' that facilitate loop formation. A statistical-mechanical calculation using a transfer-matrix approach, which treats disordered double helix regions as thermally excited, highly flexible joints, indicates that this mechanism can explain the experimental data. Applications of this type of model and calculation to other situations where localized double helix structural defects may play a important role in DNA higher-order structure will also be discussed. This research was supported by NSF Grant DMR-0203963.

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