

Monte Carlo simulation on the conformational statistics of worm-like DNA chains: effect of DNA juxtaposition and topoisomerase action

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Efficient Monte Carlo moves are developed to sample the conformations of wormlike DNA chains. The knot properties of DNA chains under various juxtaposition constraints are investigated to show how the local juxtaposed geometry can be utilized by the type II DNA topoisomerases to unknot entangled DNA molecules when the size of a topoisomerase is substantially smaller than the DNA molecule.