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| Title: | Role of special cross-links in structure formation of bacterial DNA polymer |
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| Abstract: | Using data from contact maps of the DNA-polymer of Escherichia coli (E. Coli) (at kilobase pair resolution) as an input to our model, we introduce cross-links between monomers in a bead-spring model of a ring polymer at very specific points along the chain. Via suitable Monte Carlo simulations, we show that the presence of these cross-links leads to a particular organization of the chain at large (micron) length scales of the DNA. We also investigate the structure of a ring polymer with an equal number of cross-links at random positions along the chain. We find that though the polymer does get organized at the large length scales, the nature of the organization is quite different from the organization observed with cross-links at specific biologically determined positions. We used the contact map of E. Coli bacteria which has around 4.6 million base pairs in a single circular chromosome. In our coarse-grained flexible ring polymer model, we used 4642 monomer beads and observed that around 80 cross-links are enough to induce the large-scale organization of the molecule accounting for statistical fluctuations caused by thermal energy. The length of a DNA chain even of a simple bacterial cell such as E. Coli is much longer than typical proteins, hence we avoided methods used to tackle protein folding problems. We define new suitable quantities to identify the large scale structure of a polymer chain with a few cross-links |
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