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Multiple-scale polymer model of bacterial chromosomes

Supercoiled DNA often adopts tree-like double-folded branching configurations. In this context, we proposed a framework to generate expected bacterial chromosome structures at multiple scales. We built a coarse-grained model of bacterial DNA, which is known to adopt tree-like plectonemic structures due to negative DNA supercoiling. To this end, we extended our previous model of elastic polymer chains on an FCC lattice for tightly double-folded ring polymers [1] to include the possibility of generating long branches, with the average length becoming the parameter of the model. Considering DNA concentration and cylindrical confinement similar to the in vivo situation, we adjusted this average length parameter to reproduce as well as possible contact properties between chromosomal loci as obtained from high- throughput chromosome conformation capture methods (Hi-C). Finally, we obtained various coarse-grained models that are consistent with each other and that allow capturing contact properties of various bacteria, from 2 kb to 1 Mb scale. In other words, we are able to rationalize from first principles contact properties between bacterial chromosomal loci as measured from Hi-C methods.

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