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DNA Packaging in Viral Capsids: A Computational Approach

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ABSTRACT

The packing of DNA inside bacteriophages arguably yields the simplest example of genome organisation in living organisms [1, 2]. An indirect indication of how DNA is packaged is provided by the detected spectrum of knots formed by DNA that is circularised inside the P4 viral capsid [3, 4].
The experimental results on the knot spectrum of the P4 DNA are here compared to results of coarse-grained simulation of DNA knotting in confined volumes. We start by considering a standard coarse-grained model for DNA which is known to be capable of reproducing the salient physical aspects of free, unconstrained DNA [5]. Specifically the model accounts for DNA bending rigidity and excluded volume interactions. By subjecting the model DNA molecules to spatial confinement it is found that confinement favours chiral knots over achiral ones, in agreement with P4 experiments. However, no significant bias of torus over twist knots is found, contrary to what found in P4 experiments [6, 7]. A good agreement with experiment is found, instead, upon introducing an additional interaction potential that accounts for tendency of contacting DNA portions to order as in cholesteric liquid crystals.
Accounting for this local potential allows us to reproduce the main experimental data on DNA organisation in phages, including the cryo-EM observations and detailed features of the spectrum of DNA knots formed inside viral capsids. The DNA knots we observe are strongly delocalized and, intriguingly, this is shown not to interfere with genome ejection out of the phage [8].

References

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