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DNA Structure within a Virus Particle

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Bacteriophage are viruses that attack bacteria. To successfully invade their host bacterium, a bacteriophage must succeed in packaging, transporting, and delivering its genome; these processes necessitate the precise manipulation of DNA throughout the virus life cycle. The exquisite control that a bacteriophage has over its DNA is desirable in many different biological and technological settings. Therefore, establishing a fundamental understanding of the underlying physical principles in DNA manipulation by a bacteriophage lends insight into the methods used by Nature to control DNA conformation and aids in determining how we can mimic such methods.

The bacteriophage phi29 assembles its protein capsid particle before the DNA is packaged. The phi29 genome is then forced into the empty capsid by an ATP-driven protein motor. As the capsid is filled with DNA, the packaging motor works against the increasing resistance associated with compacting the long polymer chain to near-crystalline density into the relatively small cavity. We study the evolving structure of the DNA within the phi29 capsid. Cryo EM reconstruction of the packaged bacteriophage exhibits a layered DNA structure, indicative of local order within the particle. Using Monte Carlo simulation, we predict the conformation of the DNA on the interior of the viral capsid and the forces required to achieve this structure. The resulting density plot from simulations show good agreement with the EM results, and the predicted forces are consistent with previous single-molecule measurements of the packaging forces. Conformations from the Monte Carlo simulations tend to exhibit local layer ordering with frequent defects associated with chain segments jumping across layers. We discuss the impact that such defects have on the overall order and the resistance to DNA packaging and ejection.

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