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Looping and Clustering model for the organization of protein-DNA complexes on the bacterial genome

The bacterial genome is organized by a variety of associated proteins inside a structure called the nucleoid. These proteins can form complexes on DNA that play a central role in various biological processes, including chromosome segregation. A prominent example is the large ParB-DNA complex, which forms an essential component of the segregation machinery in many bacteria. ChIP-Seq experiments show that ParB proteins localize around centromere-like parS sites on the DNA to which ParB binds specifically, and spreads from there over large sections of the chromosome. Recent theoretical and experimental studies suggest that DNA-bound ParB proteins can interact with each other to condense into a coherent 3D complex on the DNA. However, the structural organization of this protein-DNA complex remains unclear, and a predictive quantitative theory for the distribution of ParB proteins on DNA is lacking.

Here, we propose the Looping and Clustering (LC) model, which employs a statistical physics approach to describe protein-DNA complexes. The LC model accounts for the extrusion of DNA loops from a cluster of interacting DNA-bound proteins that is organized around a single high-affinity binding site. Conceptually, the structure of the protein-DNA complex is determined by a competition between attractive protein interactions and the configurational and loop entropy of this protein-DNA cluster. Indeed, we show that the protein interaction strength determines the "tightness" of the loopy protein-DNA complex. Thus, our model provides a theoretical framework to quantitatively compute the binding profiles of ParB-like proteins around a cognate parS binding site.

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