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The Role of Entropic Effects on DNA Loop Formation DAVID WILSON, U of Michigan, ALEXEI TKACHENKO, University of Michigan, TODD LILLIAN, NOEL PERKINS, JENS CHRISTIAN MEINERS, University of Michigan
— The formation of protein mediated DNA loops often regulates gene expression. Typically, a protein is simultaneously bound to two DNA operator sites. An example is the lactose repressor which binds to the Lac operon of *E. coli*. We characterize the mechanics of this system by calculating the free energy cost of loop formation. We construct a Hamiltonian that describes the change in DNA bending energy due to linear perturbations about the looped and open states, starting from a non-linear mechanical rod model that determines the shape and bending energy of the inter-operator DNA loop while capturing the intrinsic curvature and sequence-dependent elasticity of the DNA. The crystal structure of the LacI protein provides the boundary conditions for the DNA. We then calculate normal modes of the open and closed loops to account for the thermal fluctuations. The ratio of determinants of the two Hamiltonians yields the partition function, and the enthalphic and entropic cost of looping. This calculation goes beyond standard elastic energy models because it fully accounts for the substantial entropic differences between the two states. It also includes effects of sequence dependent curvature and stiffness and allows anisotropic variations in persistence length. From the free energy we then calculate the J-factor and ratio of loop lifetimes.

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