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Base-pair elasticity of free and complexed DNA NILS B. BECKER, Laboratoire de Physique, ENS Lyon and MPI-PKS Dresden, RALF EVERAERS, Laboratoire de Physique, ENS Lyon — The elastic properties of the DNA molecule are important for its function. On a base-pair scale, they modulate protein binding strength, while over hundreds of base–pairs, they govern the statistics of DNA loops. We have used the rigid base–pair (RBP) model to link experiments on DNA elasticity across these scales. In a study of the indirect readout mechanism in protein–DNA binding, we compare calculated DNA elastic free energy differences to experimental affinities. While quantitative predictions are beyond the precision of current parameter sets, qualitative predictions are meaningful; we propose a statistical marker for indirect readout sub-sites in a given co-crystal complex structure. Furthermore, we relate the RBP model to the worm–like chain (WLC) by a systematic coarse-graining procedure, reducing a total of 270 parameters to 6, which agree remarkably well with direct experimental results. Introducing sequence randomness adds fluctuations and renormalizes WLC stiffness. On short scales, sequence variability and bending anisotropy have a large effect, exhibiting the limits of applicability of the WLC model.

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