Sequence determines the structure and microsecond-scale dynamics of B-DNA and its bound cations.

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DNA-binding proteins specifically recognise their genomic target sites both by "reading" the base sequence and by probing the mechanical deformability of DNA. Specific protein-DNA interactions are fundamental in many important cellular processes, such as DNA replication, genome organisation and transcription regulation. The mechanical properties of DNA at the basis of these indirect recognition processes are highly sequence dependent, and as such can be regarded as a second genetic code. Understanding how the two layers of genetic information interact requires extensive structural and dynamical knowledge of B-DNA, currently unavailable from experiment. Using molecular dynamics (MD) simulations, an international consortium of laboratories combined efforts to obtain a large database of microsecond-scale MD simulations of a set of B-DNA oligomers with sequences designed to allow the comprehensive study of base-sequence effects. Our analysis of the MD trajectories elucidates in atomic detail how sequence affects the structure and dynamics of DNA, modulating the relative stability of its conformational substates and shaping the distributions of its tightly bound couterions. We expect these results will be instrumental in the study of how base sequence influences the interactions of DNA with proteins and other molecules.