Supporting Material of the article

"A Coarse-Grained DNA Model Parameterized from Atomistic Simulations by Inverse Monte Carlo"

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Figure S1. Radial distribution (RDF, green solid curves) and force potential in kJ·mol^{-1} (blue dashed curves) functions for the internal bonds (**A–C**) and angles (**D–F**) of the coarse-grained model of DNA. Types of bonds and angles are indicated at the top of the graphs (see Figure 1B). RDFs were calculated from the data of all-atom MD simulations; potential functions were determined using the inverse Monte Carlo method [1]. In calculations of RDFs and potentials, a 22-bp DNA fragment was coarse-grained on two types (D and P) of particles while the particles at the ends of the DNA were treated together with the particles from the middle of the DNA. This mixing of central and more flexible terminal base pairs resulted in appearance of additional maxima on the D–D (**A**) and D–P (**B**) RDFs and is reflected in the two-minimum shape of the respective potential functions. Separate treatment of the DNA termini gives RDFs and potential with a single extreme (see Figure 2 of the main text).

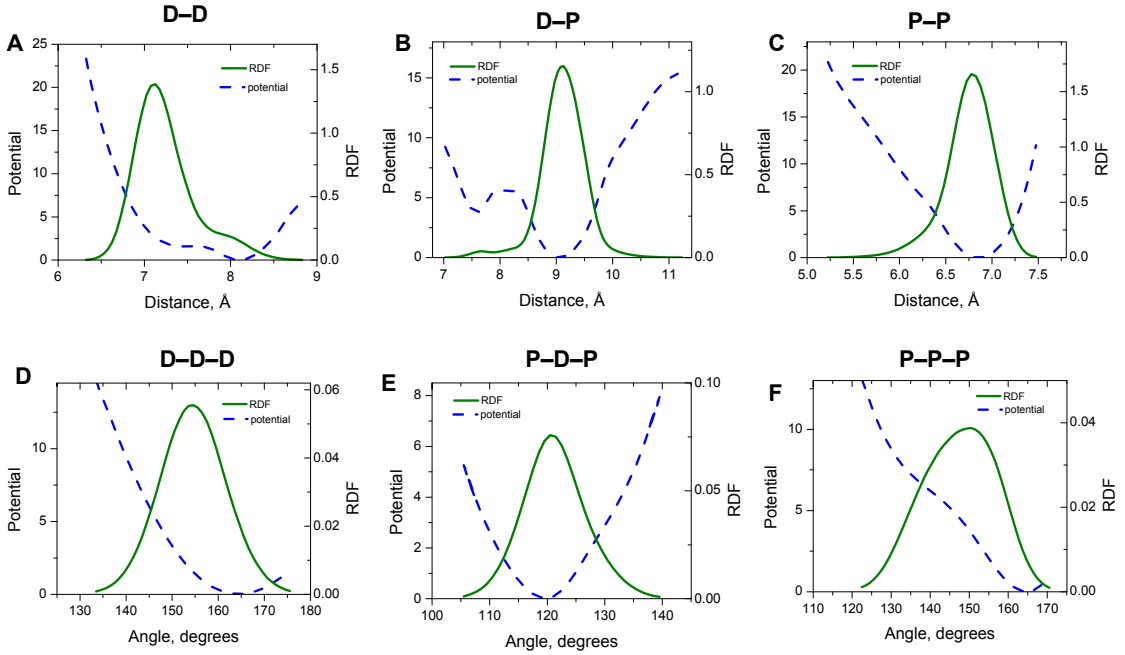


Figure S2. Radial distribution (RDF, green solid curves) and force potential in kJ·mol^{-1} (blue dashed curves) functions for intermolecular interactions of the coarse-grained DNA and counterions. Interactions between three types of particles (D and P of the CG-DNA, K is for K^+ ion) are shown as indicated at the top of the graphs. RDFs were calculated from the data of all-atom MD simulations; potential functions were determined using the inverse Inverse Monte Carlo method [1].

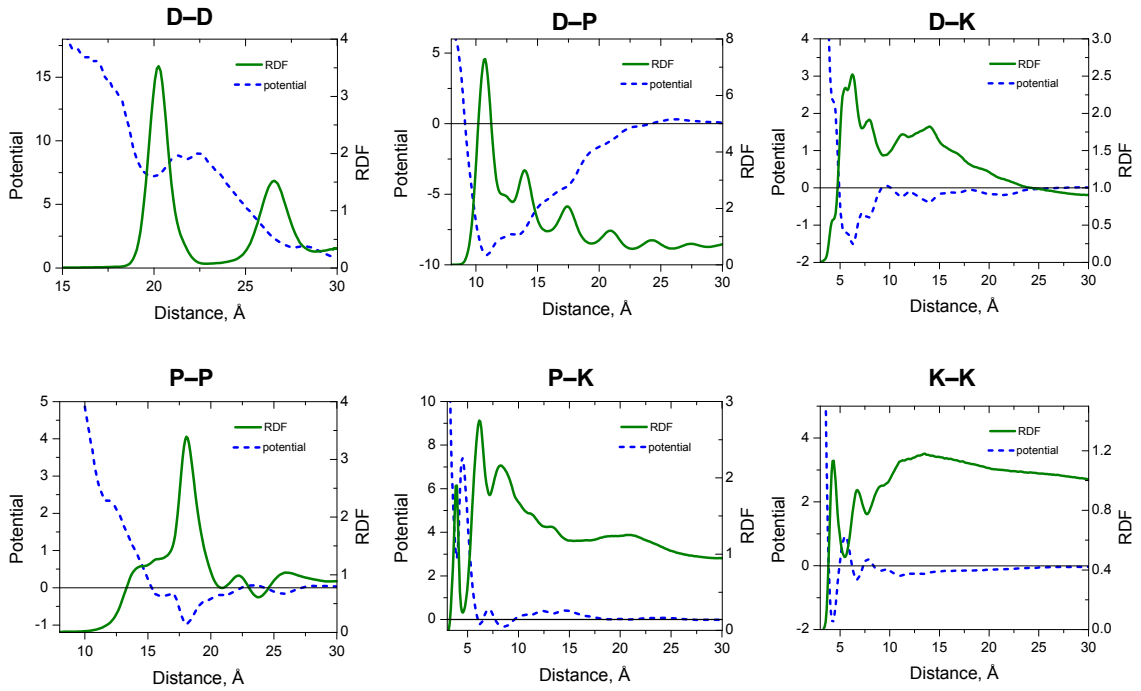
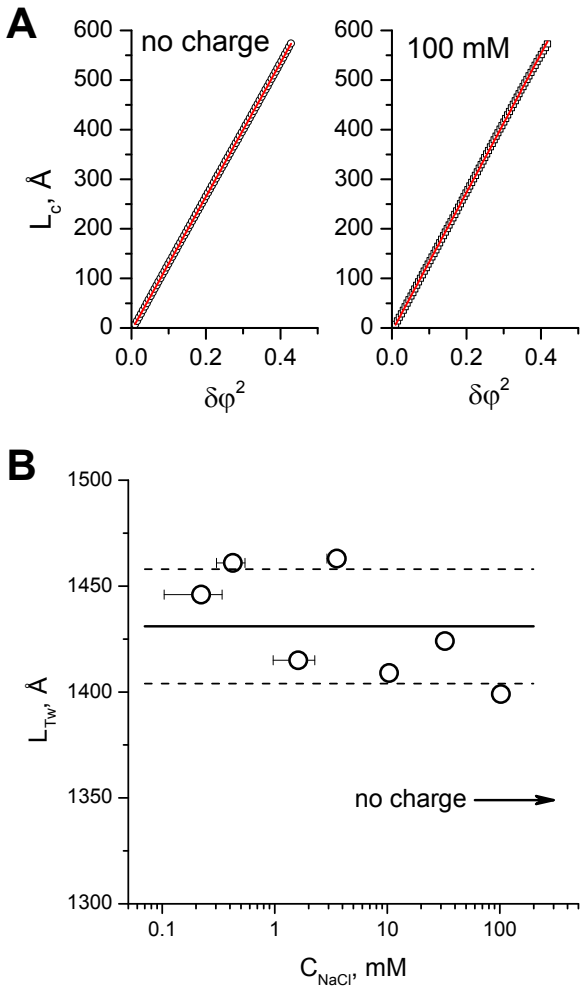


Figure S3. (**A**). Determination of the torsional persistence length, L_T, from the slope of the dependence of DNA contour length, L_C, on the variation of the torsional angle, $\delta\phi^2$. Examples of data calculated for the uncharged and charged model of DNA in 100 mM NaCl are given. Thin red lines show linear fitting of the data. (**B**). Salt dependence of L_T for calculated for the CG model of DNA. The arrow indicates the value determined for the uncharged DNA. Solid horizontal line is an average of the data (value for the uncharged DNA is not included) with standard deviation shown as dashed lines.



Supporting Reference

1. Mirzoev, A.; Lyubartsev, A.P. MagiC: Software package for multiscale modeling. *J. Chem. Theory Comput.* **2013**, *9*, 1512–1520.