Effect of Initial Positions on the Interactions of Monovalent and Divalent Ions with a DNA Duplex as Revealed with Atomistic Molecular Dynamics Simulations

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Supplemental Figure Captions

Figure S1.

Sequence dependence of ion binding. The Y-axis is the percent of contacts defined as sum of occupied frames for contacts with the given residues over sum of all occupied frames for all observed contact pairs over the entire trajectory. O1/O2P contact refers to contacts made with only O1P/O2P and all contact refers to contacts made with all atoms except hydrogen atoms. One strand is represented by residues 1-12, the second strand by residues 13-24 with residues 1 and 24 paired. (a) 31Na_A system; (b) for 31Na_B system.

Figure S2.

Dependence of percent of contacts on residue number for Mg^{2+} ions of type B simulations.

Supplemental Figures

S1

(a)

(b)

S2