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Mechanisms of influence of divalent Mg cation on DNA–Dps complex revealed by molecular modeling methods

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In vitro experiments

DNA-Dps co-crystals were obtained under conditions that mimicked intracellular during stationary phase by the DNA:Dps mass ratio (1:6). Using the pBlueScript SK+/BaHI ring plasmid vector (2958 base pairs) as DNA.

Images of DNA-Dps crystals (Figures 1a,c) obtained on the analytical transmission electron microscope JEM-2100 (JEOL, Japan) and corresponding Fourier (Figures 1 b,d) transforms of the crystal images area performed with the Digital Micrograph program.

Molecular modeling

The simulations were performed in Gromacs software package using the AMBER99-PARMBSC1 all-atom force field. The Dps protein was modeled based on the structure of PDB ID:8OUC. Because the positions of the flexible amino acid residues from each N-terminus are missing in the PDB file, we have modelled separately each N-terminus using molecule editor. The double-stranded DNA 5’- GTACTATATTATGGGGTGATGGATA-3’ of 25 base pairs in B-form was modelled. Two systems with different contents of Mg^{2+} cations (1 and 251 per periodic box) were studied. In both systems, in addition to DNA, Dps, and Mg^{2+}, other ions were added in such a way as to maintain zero charge. The first system contained the following number of ions: 1 Mg^{2+}, 2 Ca^{2+}, 408 Na^{+}, 75 K^{+}, 393 Cl. In the second system: 250 Mg^{2+}, 3 Ca^{2+}, 279 Na^{+}, 90 K^{+}, 779 Cl^{-}. An increase in the concentration of chlorine ions imitated the addition of $MgCl_2$ dissociated in solution. Both type of systems were solvated by adding 145000 water molecules. The potential energy of the systems was minimized using the steepest descent method, after which the systems were successively relaxed in NVT and NPT for 100 ps. The trajectory lengths were 0.12 – 0.5 μs with an integration step of 2 fs. A constant temperature of 28°C (301 K) was maintained by a stochastic (Langevin) thermostat with a friction constant of 0.5 ps^{-1}. The simulations were carried out at a constant pressure maintained by a Parrinello-Raman thermostat with a time constant of 2 ps. Long-range electrostatic interactions were calculated using the PME method. The cutoff radii for all interaction types were set to 1.5 nm. The neighbor list was maintained using the Verlet cutoff scheme and updated every 10 fs. Fast degrees of freedom were constrained using the LINCS algorithm.

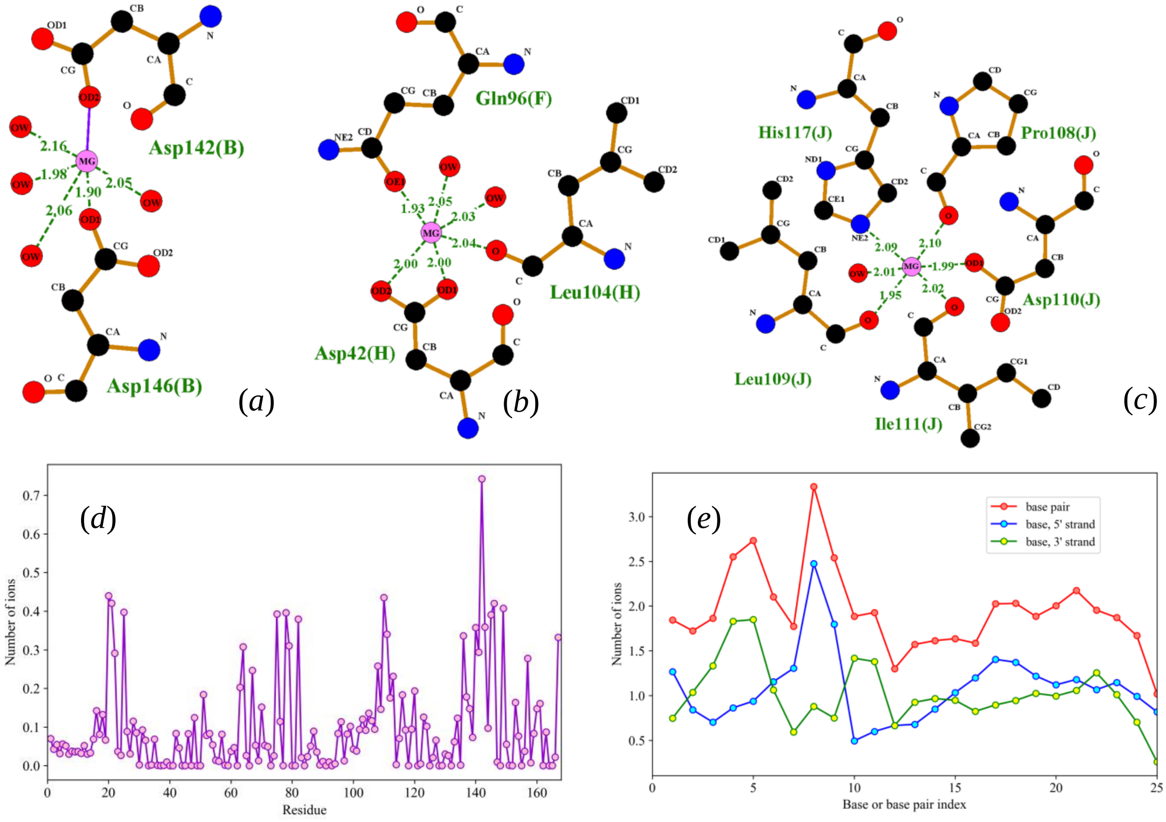

Figure S1. (*a*)-(*c*) Two-dimensional schemes of the interaction of magnesium ions with protein and water. Interaction of Mg^{2+} ions with oxygen atoms of two Asp residues (*a*); with oxygen atoms of the Asp side radical, oxygen atom of Gln and oxygen atoms of the Leu (main chain of the protein) (*b*); with oxygen atom of the Asp side radical, nitrogen atom of the His side radical and three oxygen atoms of the protein main chain (*c*). Red circles are oxygen atoms, blue ones are nitrogen, black ones are carbon, pink ones are magnesium, hydrogen atoms are not shown. Green letters indicate standard three-letter codes of amino acids, their ordinal numbers in subunits and chain names in the PDB file ID: 8OUC. Black letters indicate names of protein atoms according to the AMBER99-PARMBSC1 force field; OW letters indicate oxygen atoms of water, MG – magnesium ion. (*d*) The average number of Mg^{2+} in contact with the atoms of amino acid residues depending on residue ordinal number in the protein (per one protein subunit). (*e*) The average number of Mg^{2+} in contact with the atoms of DNA base pair (1), DNA bases of 5' strand (2) and 3'-strand (3).