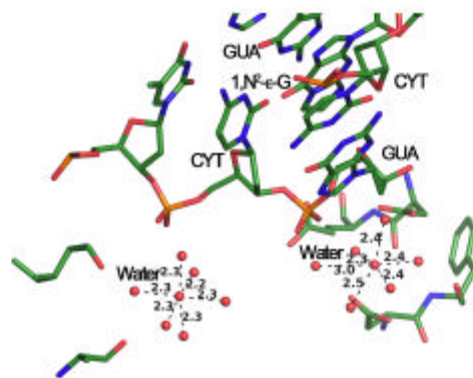


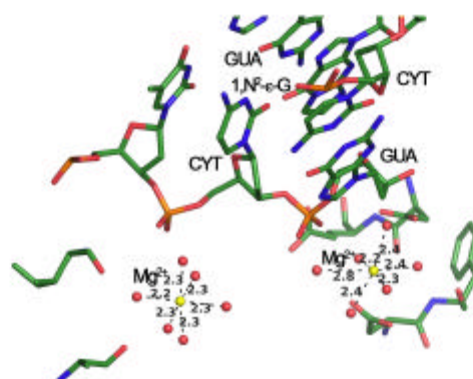
Supplementary Material

FIGURE S1. Various interpretations regarding the nature of electron density peaks in the vicinity of the active site in the binary Dpo4-Mg²⁺ complex. (A) Treating all peaks in the region typically occupied by metal ions A and B (right-hand side of panel) and near the site occupied by the primer phosphate following translocation (left-hand side of panel) as water molecules. Interactions between the central assigned water molecules and the surrounding waters are highlighted with dashed lines and distances are in Å. (B) Assignment of Mg²⁺ ions (yellow spheres) to the central solvent peaks in the two above regions. (C) Assignment of Na⁺ ions (blue spheres) to the central solvent peaks in the two above regions.

A



B



C

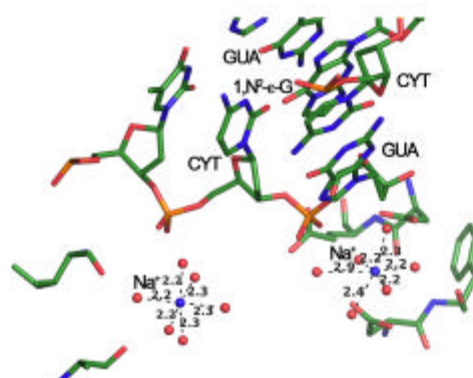


FIGURE S2. Superimpositions of the structures of Mg^{2+} - (green) and Ca^{2+} -form Dpo4-DNA complexes. Comparisons of the overall structures, the conformations of the template-primer duplexes and the active site geometries for the (A-C) binary complexes, (D-F) ternary dGTP complexes, and (G-I) ternary dCTP complexes. Divalent metal ions are depicted as solid spheres.

