

Figure S1. Time evolution of the root-mean-square deviation (calculated for all heavy atoms) from the corresponding refined initial structure along the molecular dynamics trajectory for the covalent 3·(ET743)-d(GTGGCGGGCGGCC)₂ complex.

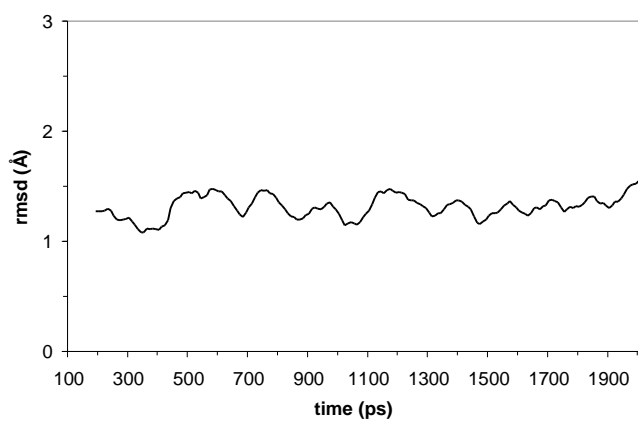


Figure S2. Time evolution of the root-mean-square deviation (rmsd) for the $d(\text{GTGGCGGCGGCC})_2$ oligonucleotide along the two molecular dynamics trajectories (blue, starting B-DNA conformation; pink, starting A-DNA conformation). The rmsd was calculated for all heavy atoms with respect to the energy-refined average structure obtained in the simulation of the B-DNA dodecamer.

