Fig. 10. Time variation plot of the solvent-accessible surface area difference of the MD structures of ETS–GGAA (black) and ETS–GGAG (red). The difference in SASA was calculated as: $SASA_{\text{difference}} = (SASA_{\text{Ets-1}} + SASA_{\text{DNA}}) - SASA_{(\text{Ets-1+DNA})}$
Fig. 11. Time variation plot of separation involving the crystal waters: Wat1 oxygen and indole nitrogen of Trp375 of Ets-1 (a), Wat1 and phosphate unesterified oxygen O2P of T₄' nucleotide (b), Wat19 and O2P of T₅' nucleotide (c), and Wat32 and O2P of T₅' (d) of ETS–GGAA (black) and ETS–GGAG (red) MD structures.
Supporting Figure 12

Fig. 12. Mapping of the correlated motions of the secondary structure of the MD averaged complexes: ETS–GGAA (a) and ETS–GGAG (b). The binding region of the protein, helix-3 is shown as cylinder and the DNA contact residues Arg391, Arg394, and Tyr395 by tubes. The positive correlated residues are designated by the same colored stars. Residues with no significant anti-correlated motions are in gray. The anti-correlated motions among Ets-1 residues are represented by the same color. As multiple anti-correlated motions are observed among various residue regions, representation of color is truncated for clarity.
Fig. 13. Order parameter, $S^2$, for the $\psi$ torsion of Ets-1 residues of the MD averaged structures: ETS–GGAA (black) and ETS–GGAG (red). The secondary structural elements of Ets-1 are indicated.
Fig. 14. Ramachandran plot representing the protein \( \phi \) and \( \psi \) conformations visited by residues Asn380 (a and b) and Gly423 (c and d) of the MD structures of ETS–GGAA and ETS–GGAG, respectively. The dashed lines indicate the corresponding values of the crystal structure.