

Fig. S1a



Fig. S1b



Fig. S1c



Fig. S2



Fig. S3

LEGEND TO FIGURES IN SUPPLEMENTARY MATERIAL

Figure S1 : (a) View of the main ruthenium hexammine binding sites in the subtype-A DIS duplex localized between two stacked helices. The anomalous map is contoured at 10 σ above mean level. (b-c) Ruthenium hexammine binding sites in the subtype-B DIS duplex. The (2Fo-Fc) electron density map (1.7 σ above mean level) and the anomalous difference map (4.0 σ above mean level) are shown in blue and magenta, respectively. (b) Site 1 is localized in the major groove of the duplex and the cation is bound to four phosphates, as well as to a 2'-OH group and a phosphate of a symmetry-related molecule. Site 2, which is much weaker, involves binding to Hoogsteen sites of a guanine. (c) Site 3 in the major groove of a UGC/ACG sequence and to surrounding water molecules (represented as red spheres).

Figure S2 : Loose binding of Sr^{2+} ions. (2Fc-Fo) electron density map contoured at 1.4 σ above mean level is represented in blue around two delocalised strontium binding sites in the subtype-A DIS duplex.

Figure S3 : Potassium binding sites in the subtype-B DIS duplex. The (2Fo-Fc) electron density map contoured at 1.4 σ , and the anomalous difference maps contoured at 4.0 σ above mean level are shown in blue and red, respectively. Potassium ions and water molecules are represented as yellow and red spheres, respectively.