



Figure 15. Structures of methylcytosine-binding zinc-finger proteins bound to fully methylated 5mCpG DNA. (A) 2.8-Å crystal structure of three zinc fingers of Kaiso protein bound to a pair of fully methylated 5mCpG-containing DNA duplex (PDB: 4F6N). The first, second, and third zinc fingers are colored in green, blue, and pink, respectively. Note that although the majority of the intermolecular contacts are with the major groove, involving zinc fingers 1 (green) and 2 (blue), there are also contacts with the minor groove, involving zinc finger 3 and the carboxy-terminal extension of Kaiso. Zinc ions are shown as silver balls. The methyl groups of 5mC are marked by magenta dotted circles. (B) Intermolecular contacts between amino acids of the first zinc finger (in green) of Kaiso and 5mC groups in the major groove of the duplex. (C) 0.99-Å crystal structure of two zinc fingers of Zfp57 protein bound to a fully methylated 5mCpG-containing DNA duplex (PDB: 4GZN). Zinc ions are shown as silver balls. The methyl groups of 5mC are marked by magenta dotted circles. (D) One of the 5mC groups in the Zfp57-DNA complex is involved in hydrophobic interactions through positioning between an Arg side chain and a neighboring guanine. (E) The second 5mC in the Zfp57-DNA complex interacts with a layer of ordered water molecules (red circles).