



Figure 14. Structures of methylcytosine-binding proteins bound to fully methylated 5mCpG DNA. (A) NMR solution structure of MBD1 protein bound to fully methylated 5mCpG-containing DNA duplex (PDB: 1IG4). Two loops L1 and L2 are colored in yellow. The methyl groups of 5mC's are marked by magenta dotted circles. (B) Schematic of intermolecular contacts centered about the 5mCpG/5mCpG site involving loops L1 and L2, and the amino-terminal α -helix adjacent to L2. Methyl group of 5mC is represented by the magenta circle. Hydrophobic interactions between the 5mC residues and side chains of MBD1 are indicated by magenta colored arrows. (C) 2.5-Å crystal structure of MeCP2 protein bound to fully methylated 5mCpG-containing DNA duplex (PDB: 3C2I). The methyl groups of 5mCs are marked by magenta dotted circles. (D) Intermolecular contacts between hydrophilic amino acids of MeCP2 (green stick representation) and the 5mC groups (magenta dotted circles) in the major groove of the duplex, including C—H••O hydrogen bonds to tightly bound water molecules.