Supplemental Figures

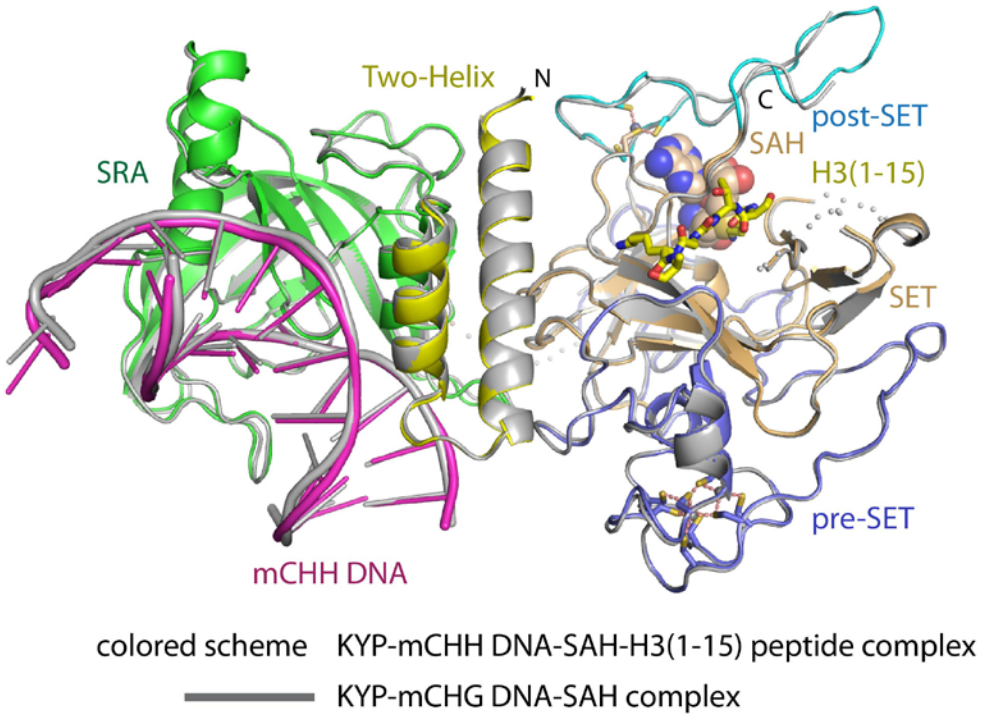

Figure S1 (related to Figure 1). The superposition of color-coded KYP-mCHH DNA-SAH-H3(1-15) peptide complex and gray-colored KYP-mCHG DNA-SAH complex.
The comparison indicates a common overall fold and DNA recognition mechanism.

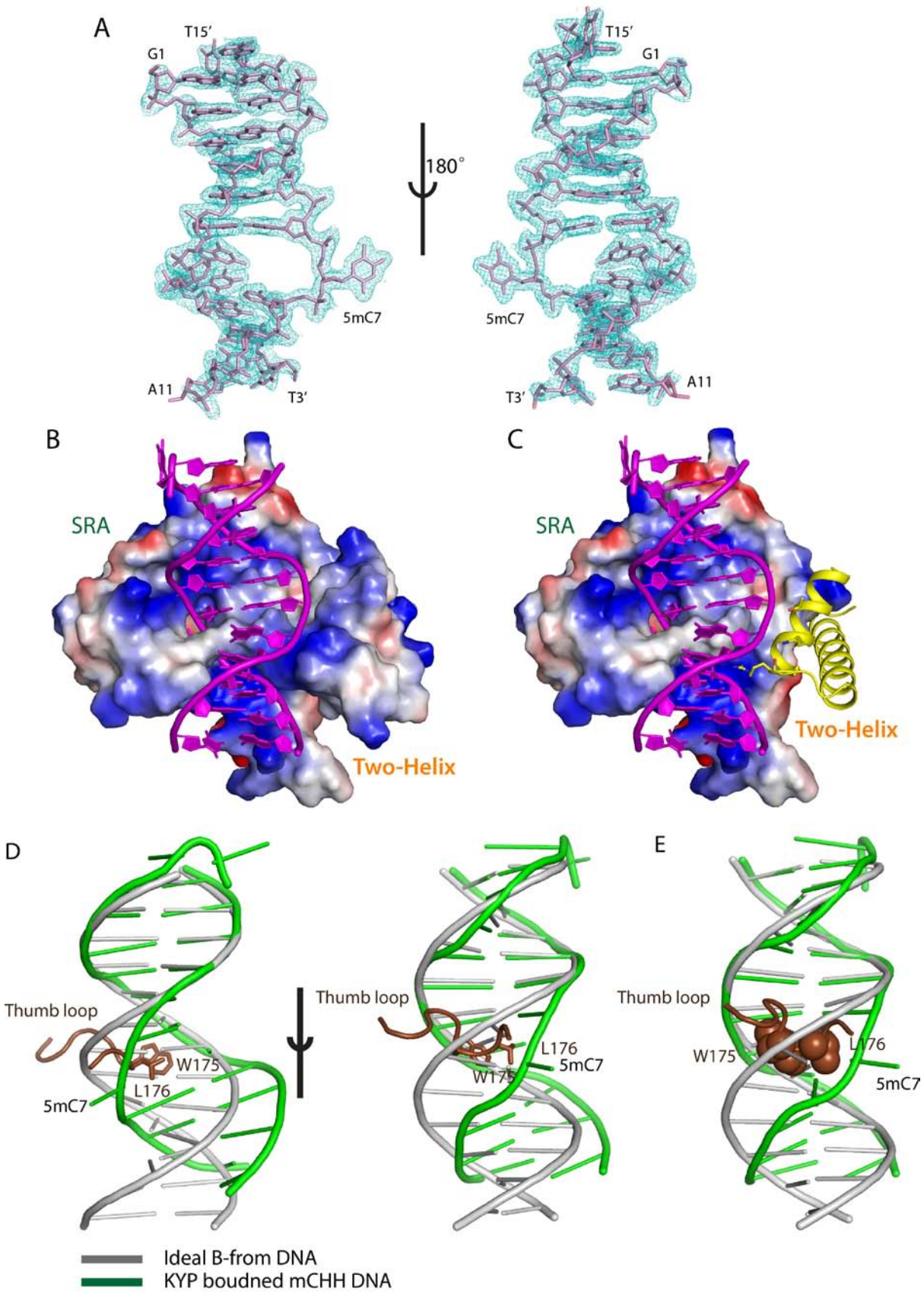
A
T15′
G1
5mC7
A11
T3′
180°
T15′
G1
5mC7
T3′
A11
B
SRA
Two-Helix
C
SRA
Two-Helix
D
Thumb loop
W175
L176
5mC7
Thumb loop
L176
5mC7
W175
E
Thumb loop
W175
L176
5mC7
Ideal B-from DNA
KYP boudned mCHH DNA

Figure S2 (Related to Figure 2). Recognition of DNA in the KYP Complex.
(A) The SIGMAA weighted 2Fo-Fc map of bound mCHH DNA in the KYP-mCHH DNA-SAH-H3(1-15) peptide complex at 1σ level shown in two views rotated by 180°. The methylated strand can be traced from G1 to A11 with 5mC7 flipped out, while the unmethylated strand can be traced from T3' to T15'.
(B) An electrostatic surface view of the SRA domain and the two helix arrangement with the mCHH DNA shown in magenta representation. The 5mC is isolated from the duplex by the thumb loop and NKR finger loop, which form a continuous surface to penetrate the DNA duplex.
(C) A similar view as in (B) but with the two-helix arrangement highlighted in ribbon representation with residues involved in DNA recognition highlighted in stick representation.
(D) Superposition of KYP-bound mCHH DNA and an ideal B-form DNA in two views representing different orientations. The insertion of thumb loop residues Trp175 and Leu176 from the minor groove into the DNA duplex pushes the methylated strand, thereby moving it away from the ideal B-form.
(E) A space filling view of Trp175 and Leu176 residues shows the insertion has a large size.

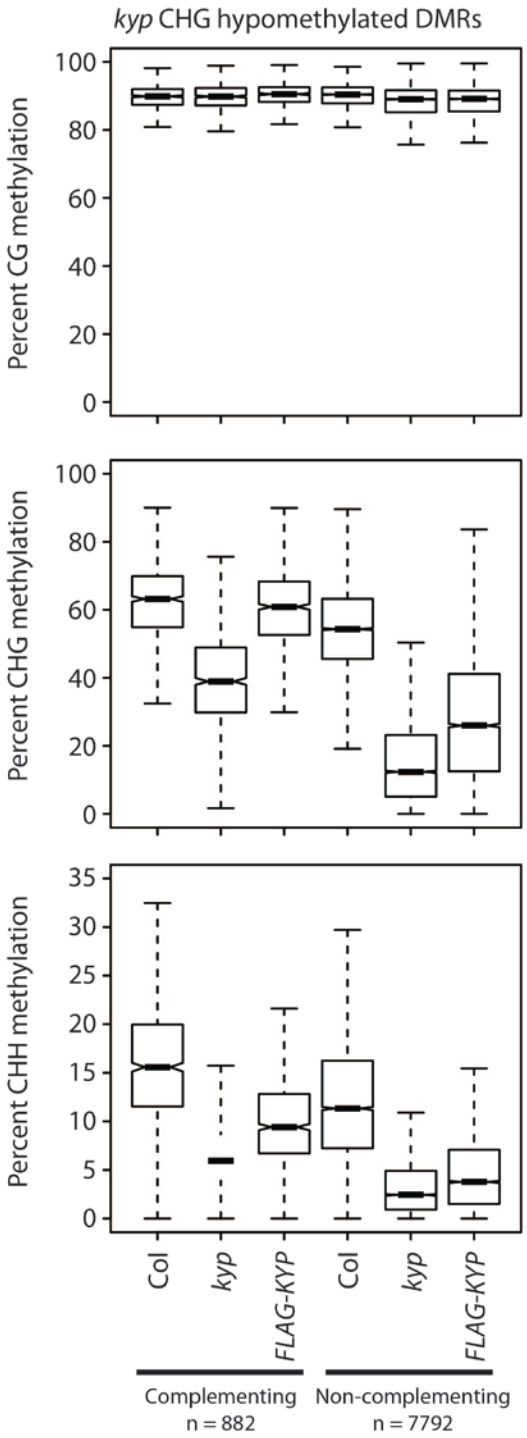

Figure S3 (related to Figure 2). Boxplots of CG, CHG and CHH context DNA methylation at kyp CHG hypomethylated DMRs.

These boxplots are classified as complementing or non-complementing in a kyp; FLAG-KYP transgenic line as compared to a Col line and a kyp mutant.