

Supplementary figure legends

Figure S1: Secondary structure of CTCF (PDB:2CT1) DNA binding domain.

Figure S2: Lowest energy structures of the docked C-allele:CTCF complex.

Figure S3: Lowest energy structures of the docked T-allele:CTCF complex.

Figure S4: Lowest energy structures of the docked me-C-allele:CTCF complex.

Figure S5: Conformational changes of DNA:Protein complexes over simulation time of 50 ns. Time 0 ns represent the start of reaction and 50 ns represent end of reaction. (A) C-allele:CTCF complex, (B) T-allele:CTCF complex, (C) me-C-allele:CTCF complex.

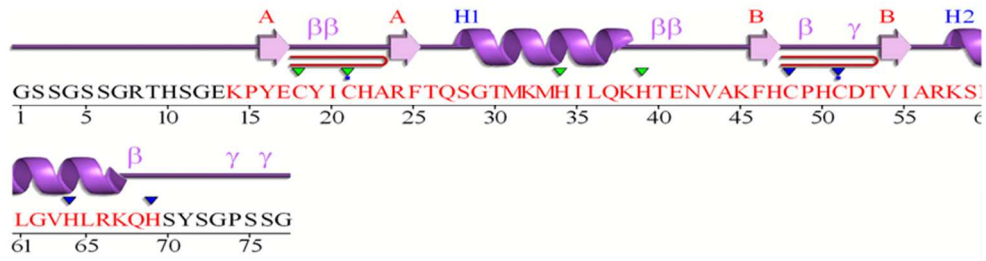
Figure S6: 2D graph showing the residue contacts of the docked complexes. (A) C-allele:CTCF complex, (B) T-allele:CTCF complex, (C) me-C-allele:CTCF complex.




Movie

Supplementary Video 1: Simulation movie of C-allele:CTCF complex.

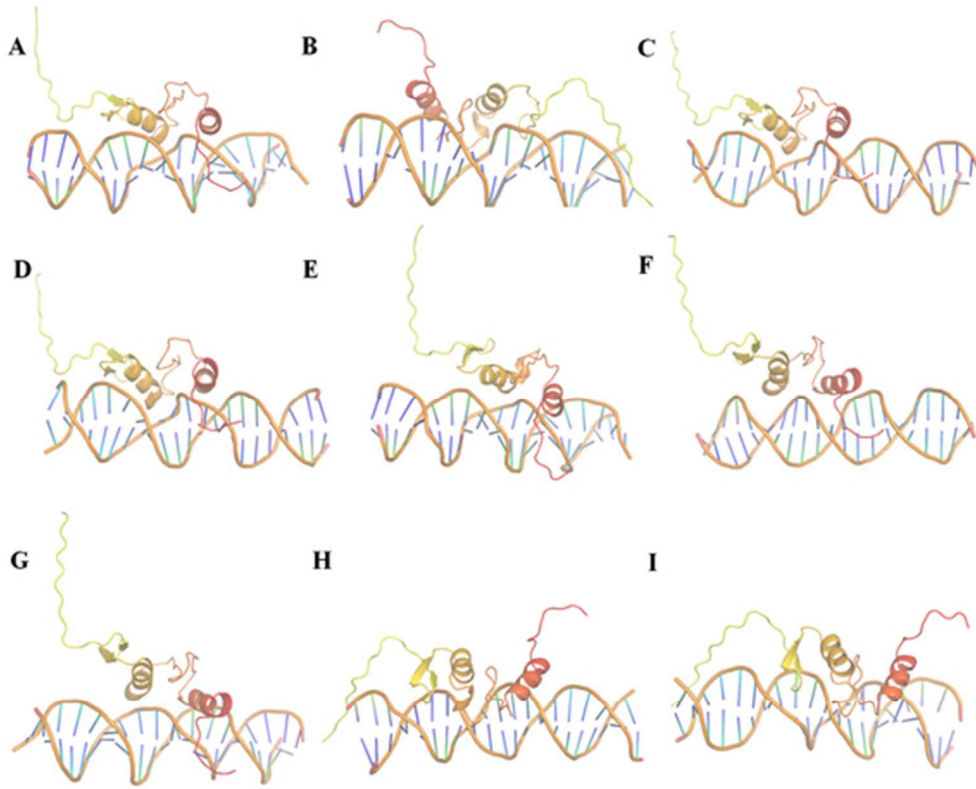
Supplementary Video 2: Simulation movie of T-allele:CTCF complex.

Supplementary Video 3: Simulation movie of me-C-allele:CTCF complex.

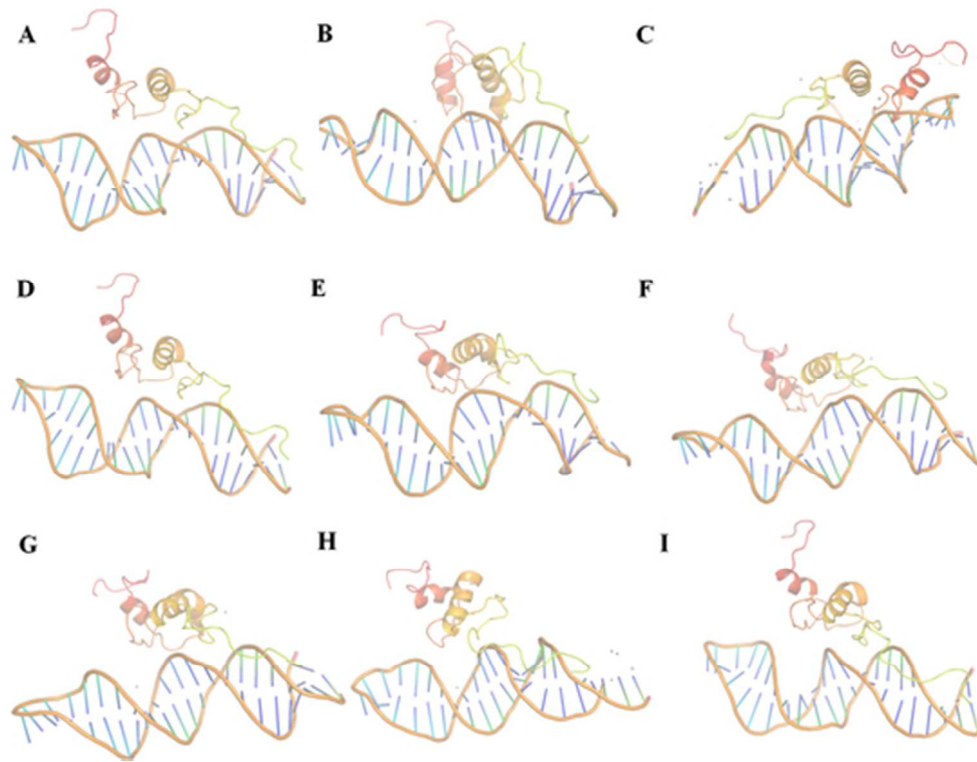


Motifs: β beta turn γ gamma turn  beta hairpin
 Residue contacts:  to metal
 PDB SITE records:  AC1  AC2

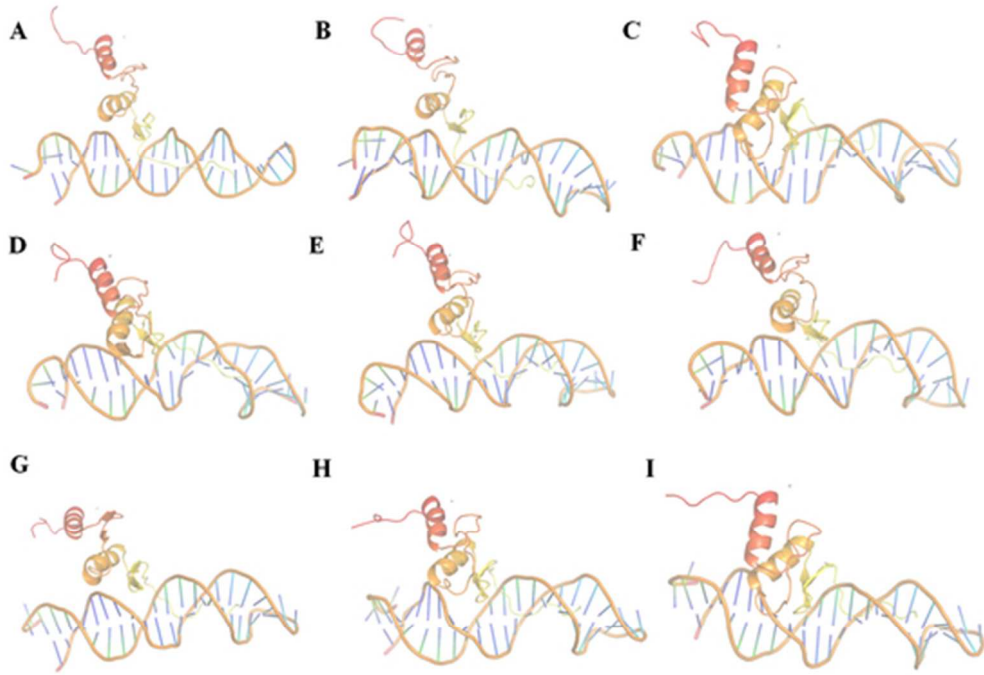
Secondary structure of CTCF (PDB:2CT1) DNA binding domain.



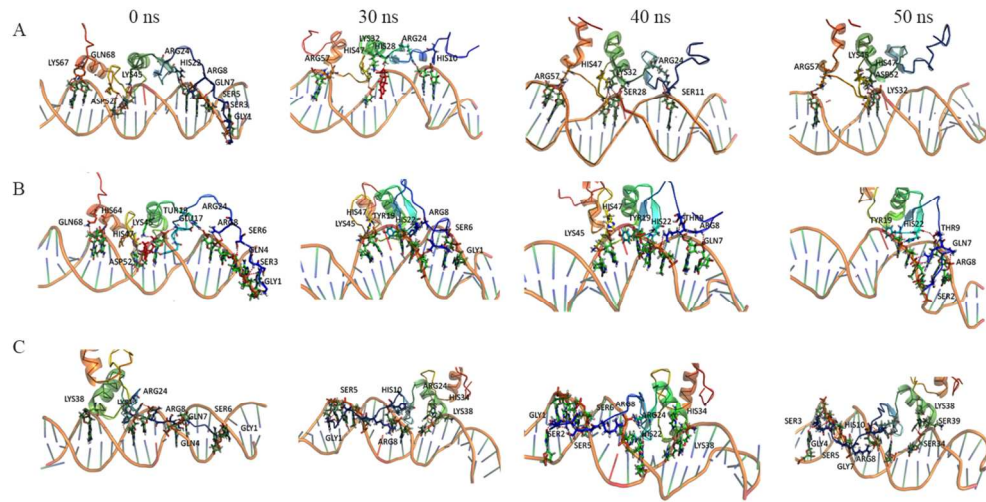
Lowest energy structures of the docked C-allele:CTCF complex.



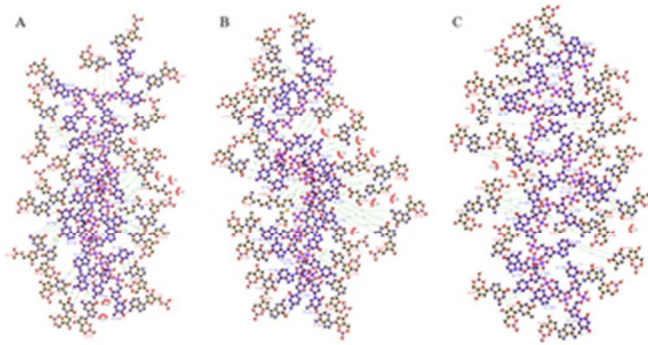
Lowest energy structures of the docked T-allele:CTCF complex.



Lowest energy structures of the docked me-C-allele:CTCF complex.



Conformational changes of DNA:Protein complexes over simulation time of 50 ns. Time 0 ns represent the start of reaction and 50 ns represent end of reaction. (A) C-allele:CTCF complex, (B) T-allele:CTCF complex, (C) me-C-allele:CTCF complex.



2D graph showing the residue contacts of the docked complexes. (A) C-allele:CTCF complex, (B) T-allele:CTCF complex, (C) me-C-allele:CTCF complex.