Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Investigation of Dynamical flexibility of D5SIC-DNAM inside DNA duplex in Aqueous Solution: A Systematic Classical MD Approach

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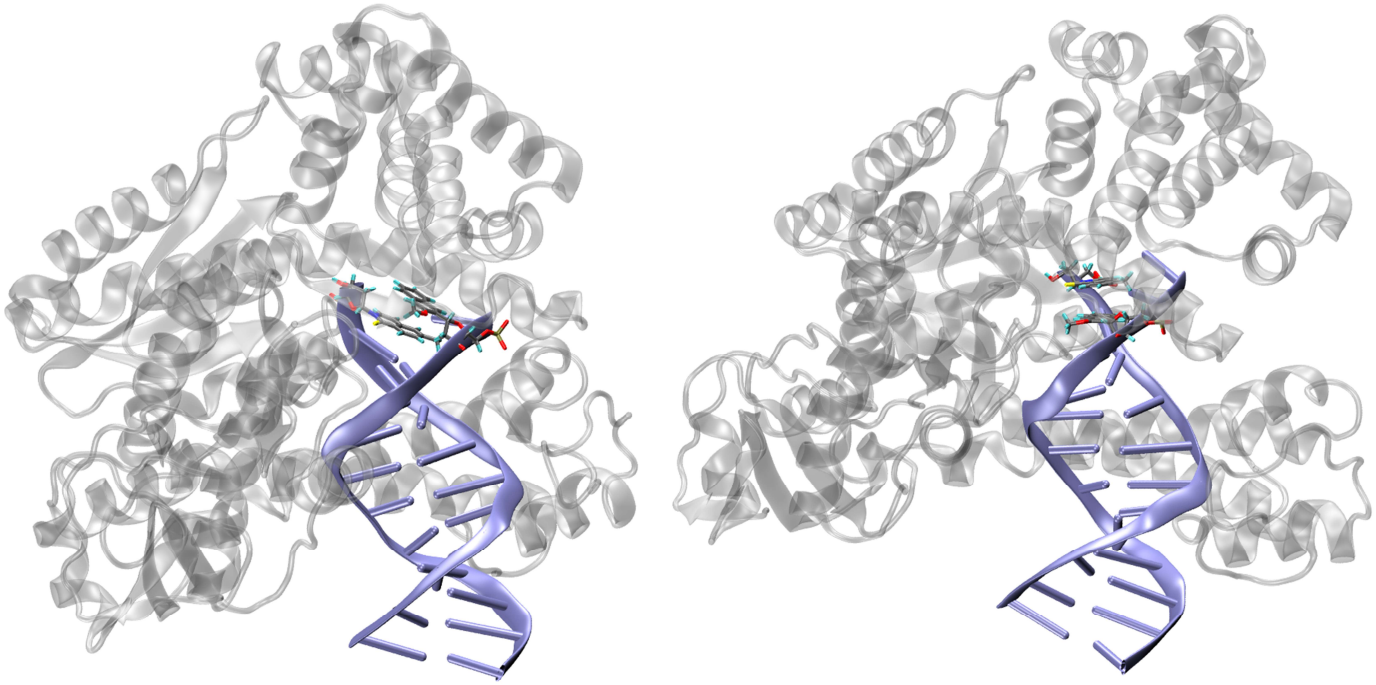

Figure S1*. 3D representation of the crystal structures of DS-DN incorporated DNA in Taq polymerase in the post-insertion site.*

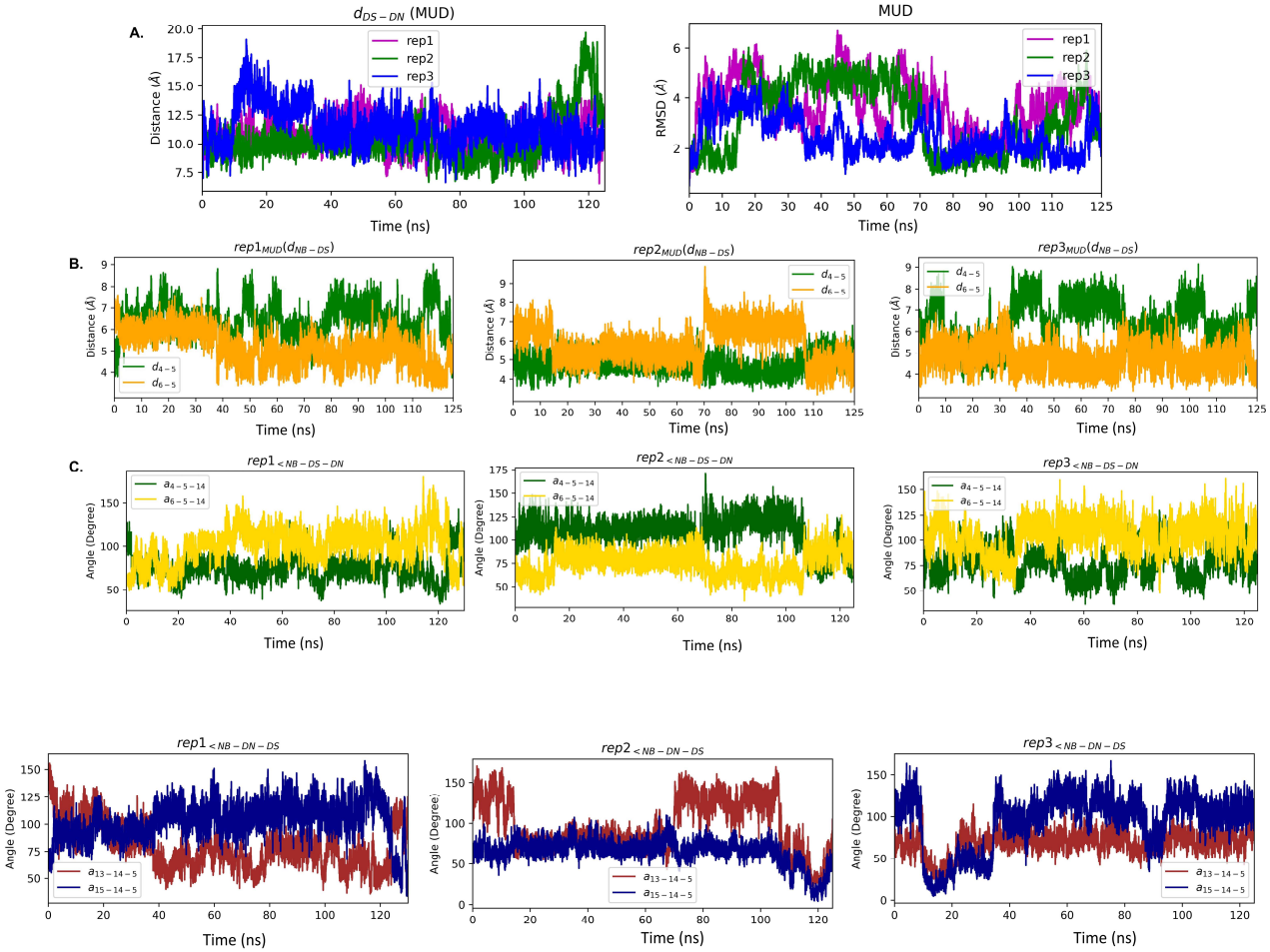

Figure S2. *A. DS-NB (left), RMSD (right) B. NB-DS, C. <UB-NB-NB values obtained from AMOEBA force fields.*

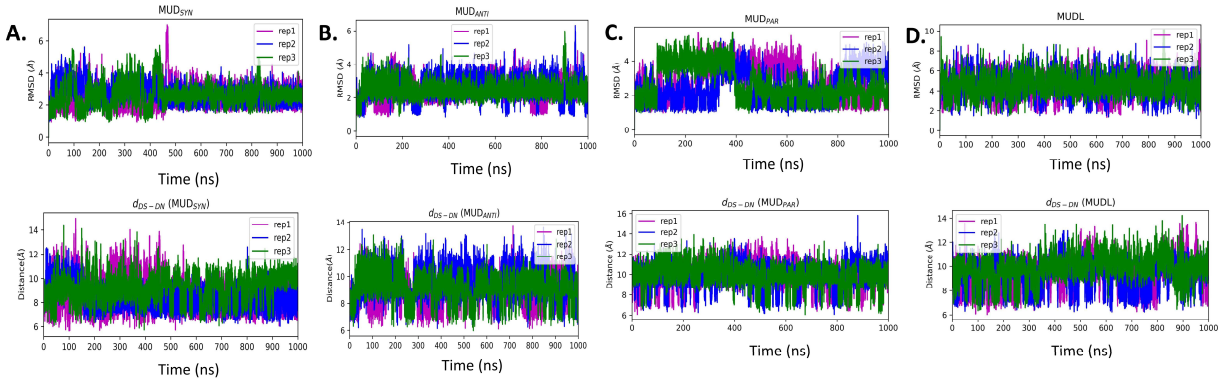

Figure S3*. DS-DN distance and RMSD values for A. MUD_{SYN}, B. MUD_{ANTI},* C. *MUD_{PAR} and D. MUDL structures obtained from 1μs simulation employing AMBER force fields.*

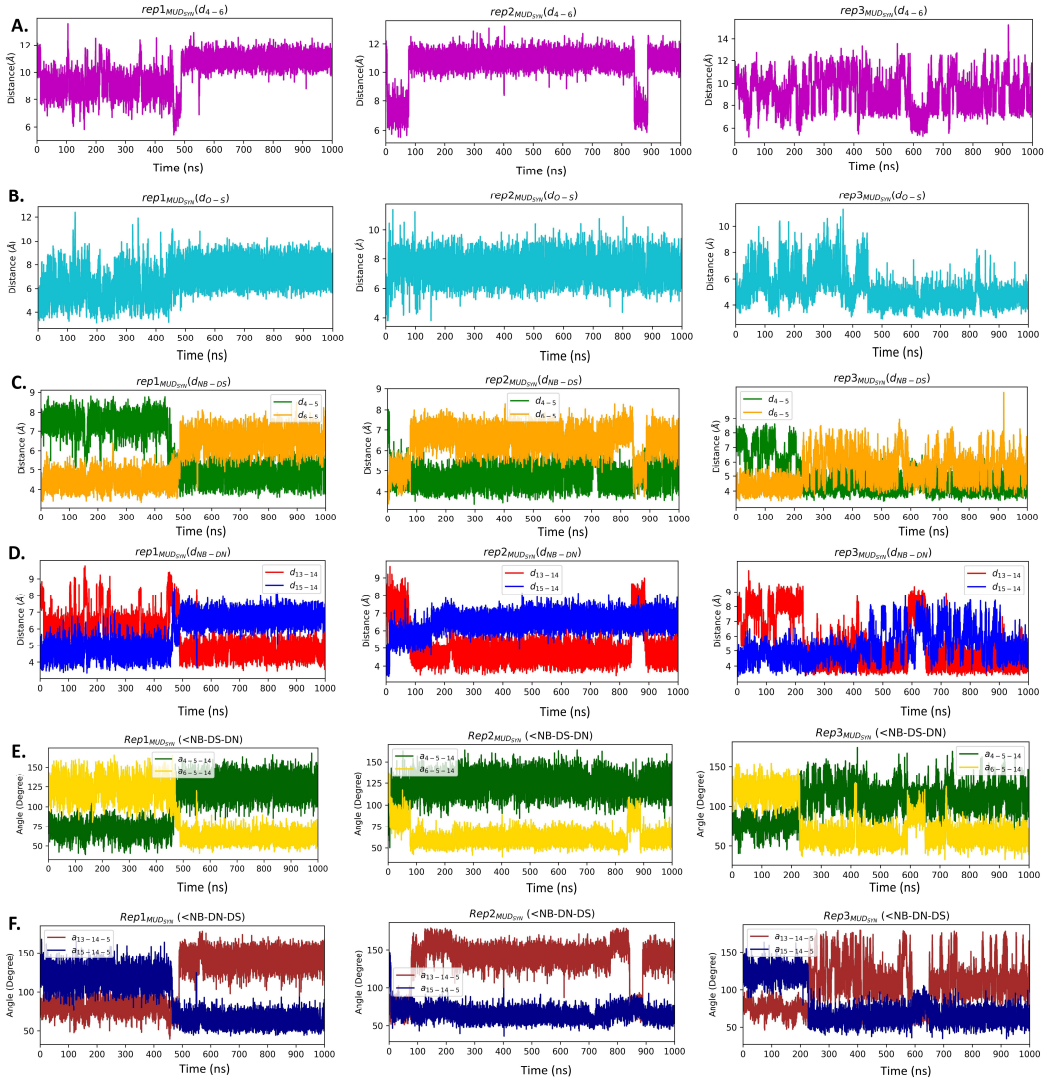

Figure S4. *A) $d_{4\text{-}6}$, B) O-S, C) DS-NB, D) DN-NB, E) <NB-DS-DN, F) <NB-DN-DS values for MUD_{SYN} obtained from AMBER force fields.*

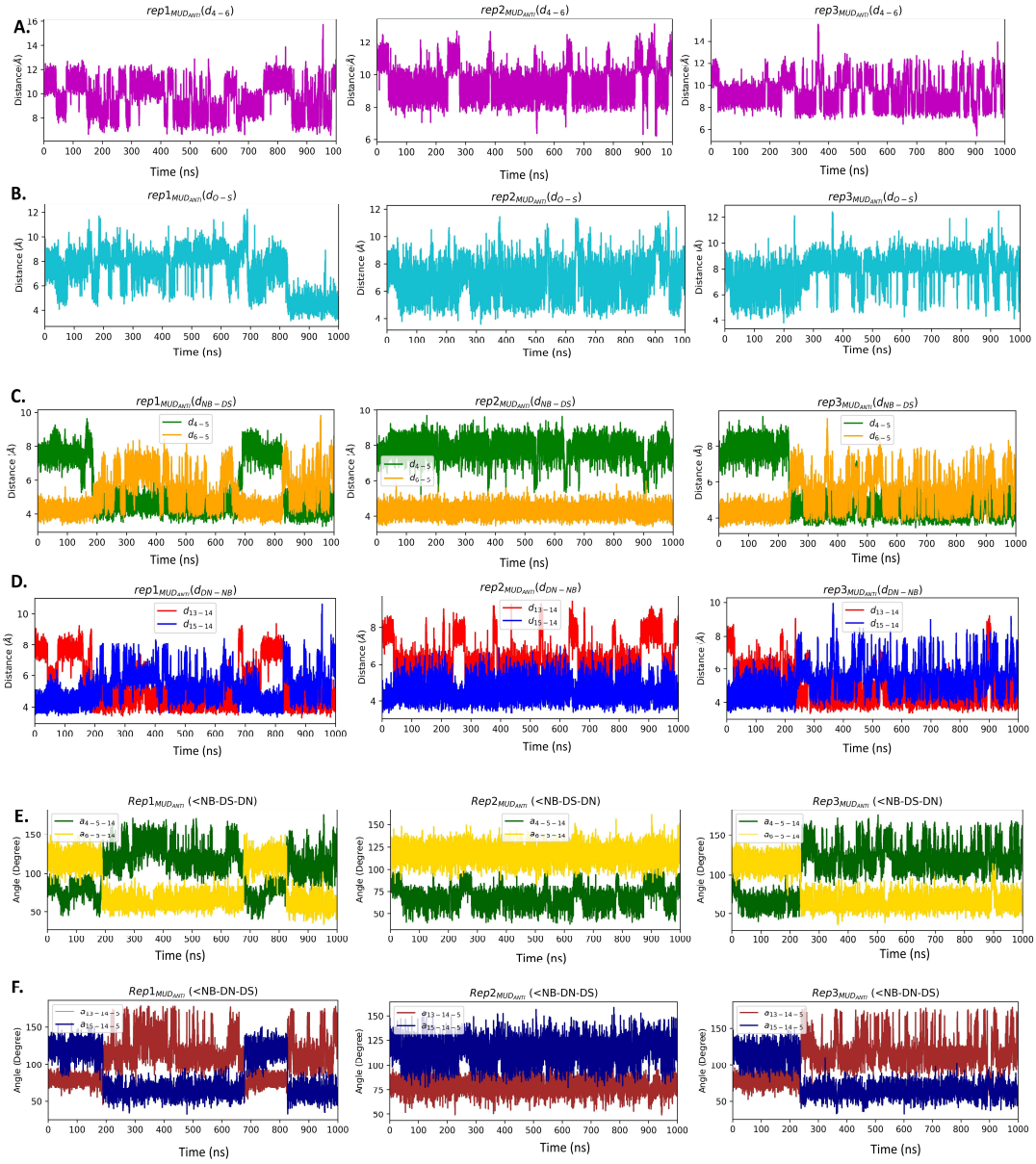

***Figure S5**. A) $d_{4\text{-}6}$, B) O-S, C) DS-NB, D) DN-NB, E) <NB-DS-DN, F) <NB-DN-DS values for MUD_{ANTI} obtained from AMBER force fields.*

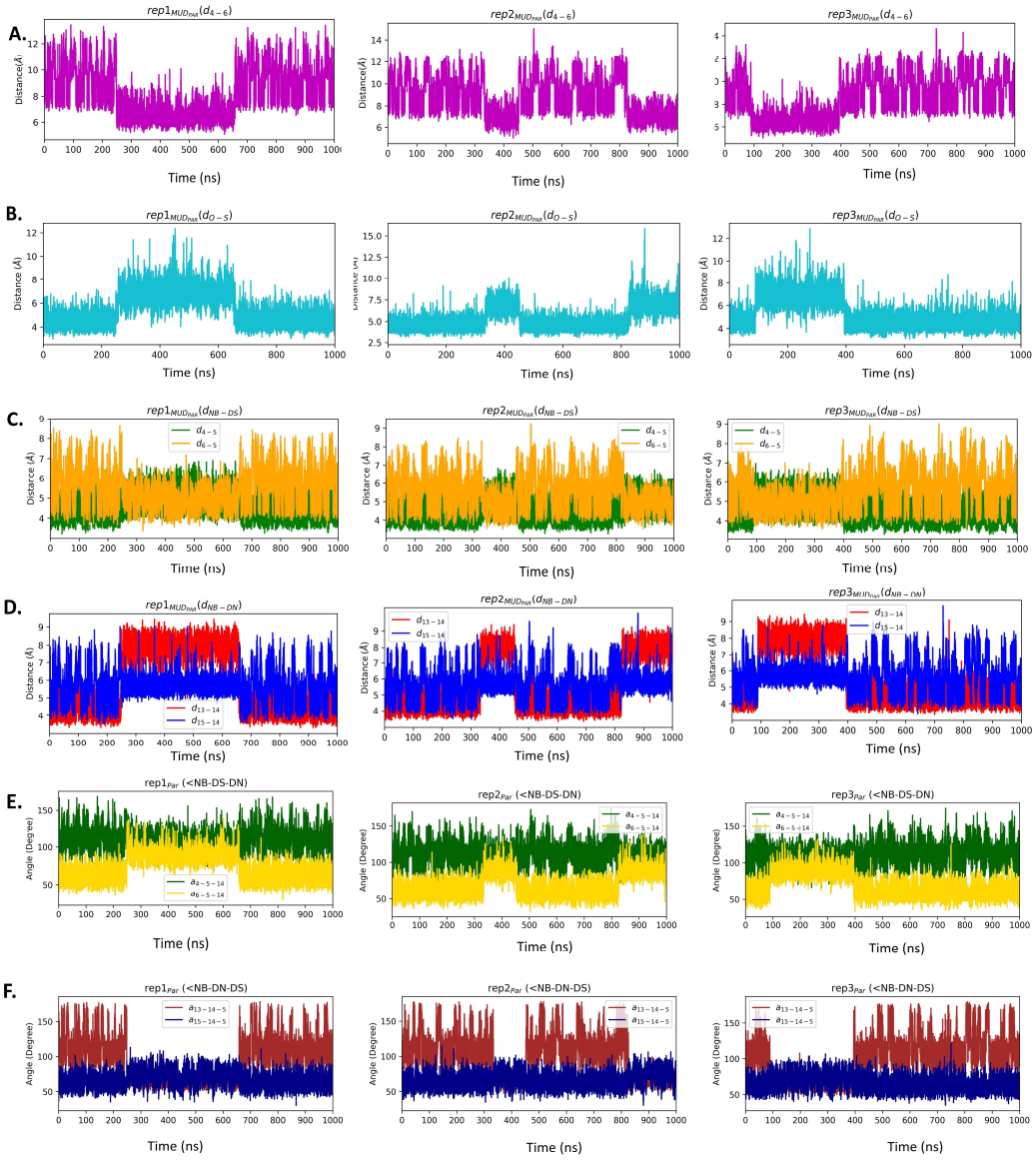

Figure S6. A) $d_{4\text{-}6}$, B) O-S, C) DS-NB, D) DN-NB, E) <NB-DS-DN, F) <NB-DN-DS values for MUD_{PAR} obtained from AMBER force fields

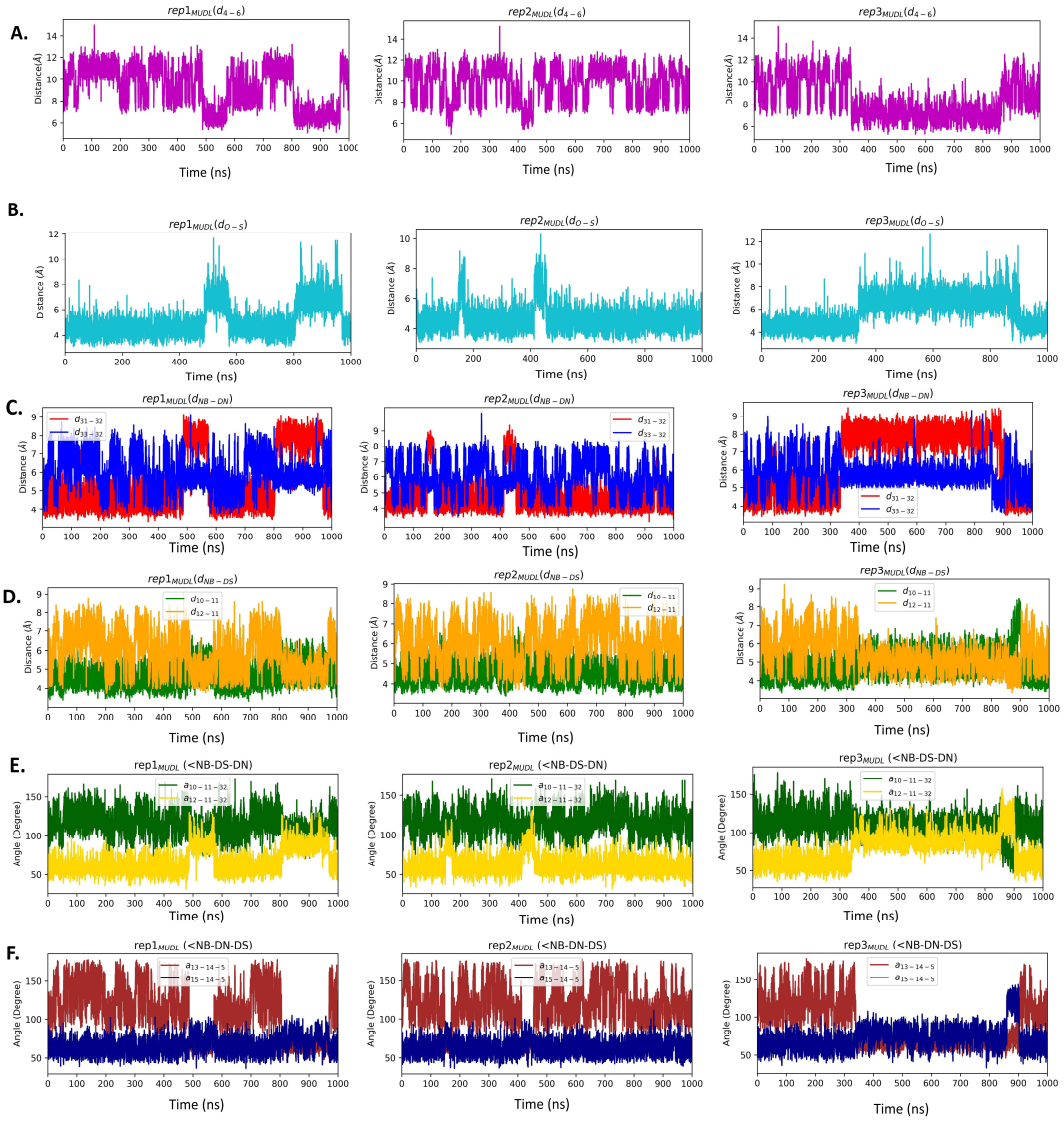

***Figure S7**. A) d_{4-6} , B) O-S, C) DS-NB, D) DN-NB, E) <NB-DS-DN, F) <NB-DN-DS values for MUDL obtained from AMBER force fields.*

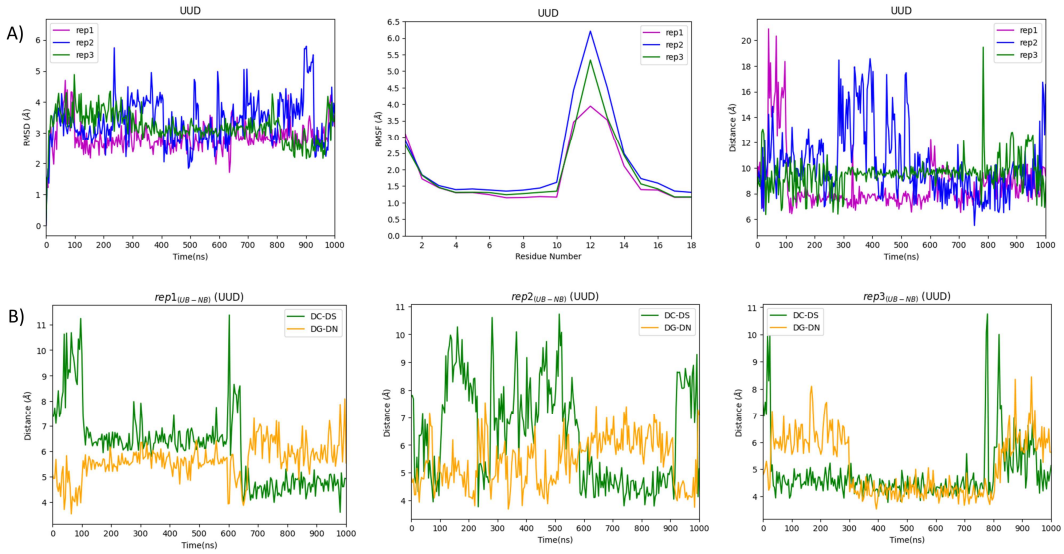

Figure S8. *A) RMSD (left), RMSF (middle), d_{DS-DN} and B) d_{DS-NB} values of UUD structures obtained from obtained from 1μs simulation employing AMBER force fields.*

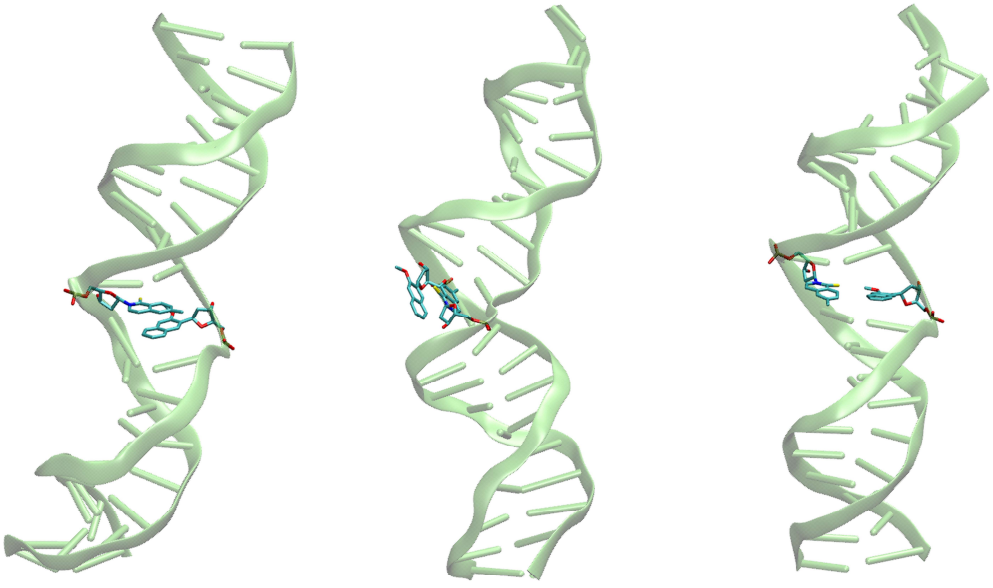

Figure S9. *Different conformers obtained from long UBP-incorporated DNA duplex.*

***Table S1**. Fragmentation of energies at ωB97xD/ 6-311++G(d,p) between DS and DN. Energy values are given in kcal/mol.*

UBP	Electrostatic	Dispersion	Induction	Exchange	Total
SYN	-8.8	-17.5	-3.3	18.9	-10.8
ANTI	-7.2	-15.3	-3.0	16.4	-9.1