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

Supporting Information

Investigation of stability of D5SIC-DNAM-Incorporated DNA duplex in Taq Polymerase Binary system: A Systematic Classical MD Approach

Tanay Debnath[1], G. Andres Cisneros[1,2]

[1]Department of Physics, University of Texas at Dallas, Richardson, TX, USA

[2]Department of Chemistry and Biochemistry, University of Texas at Dallas, Richardson, TX, USA

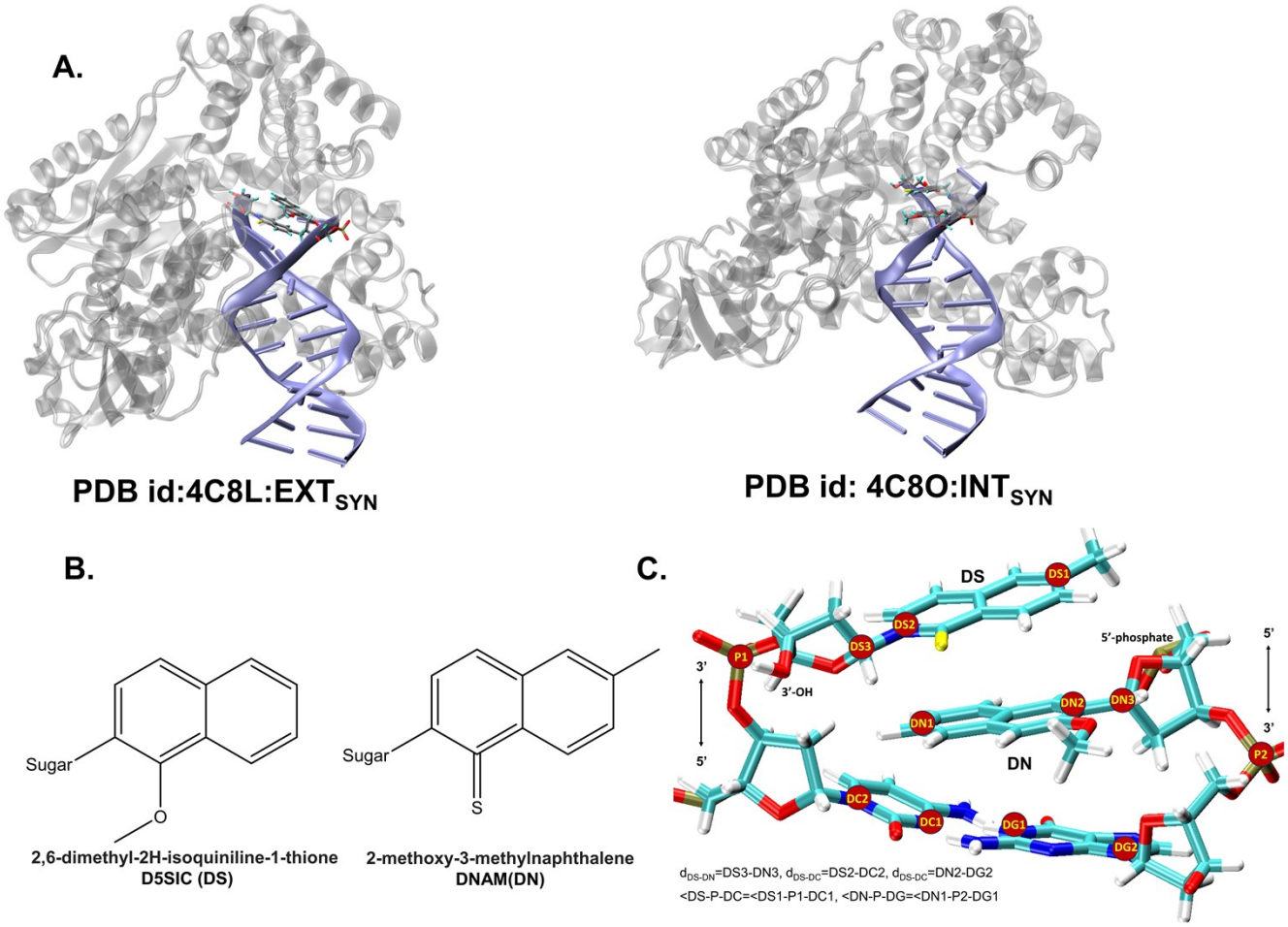

Figure S1. A. Crystal structure of EXT_{SYN} and INT_{SYN} , B. 2D representations of DS and DN, C. Schematic representation of distance and angles associated with UB and adjacent NB.

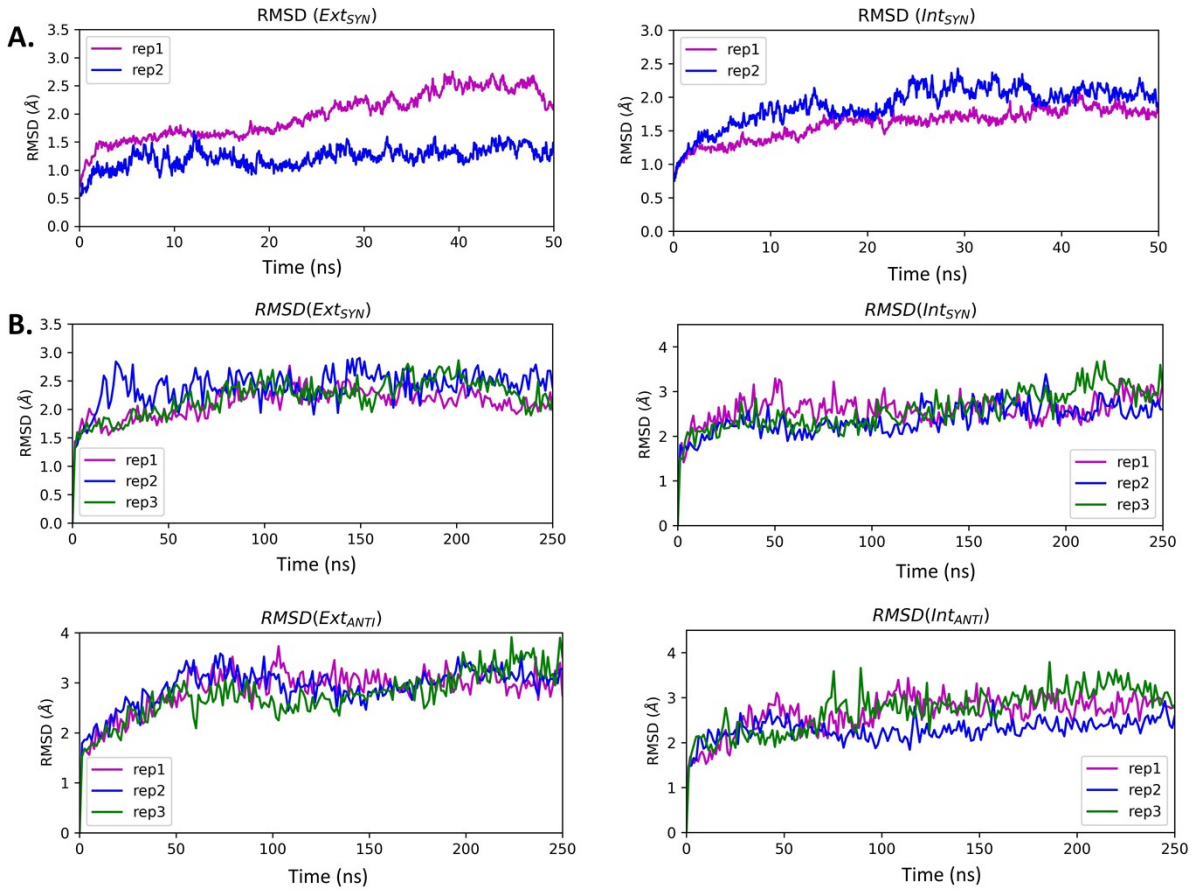

Figure S2. RMSD obtained from A. AMOEBA and B. AMBER force field mediated simulations for all the systems.

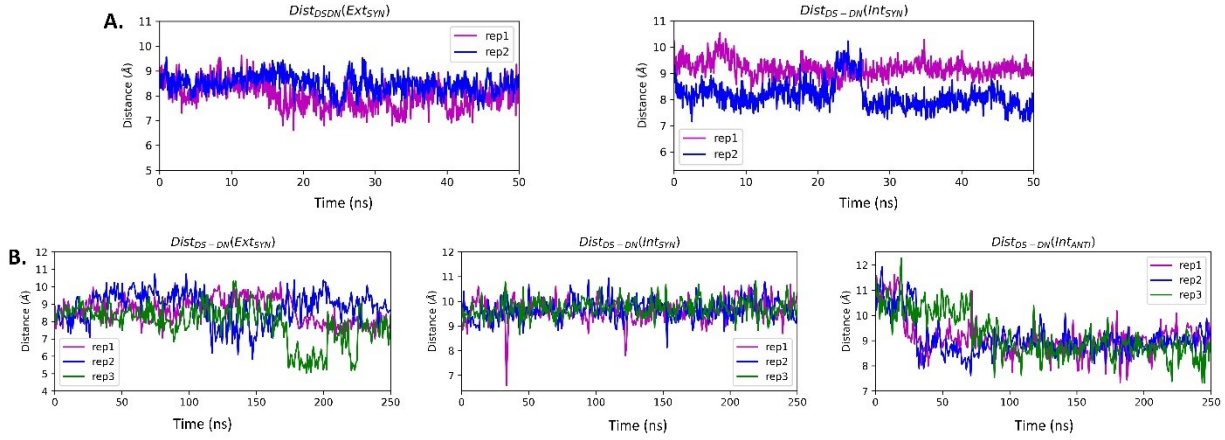

Figure S3. DS-DN distances obtained from A. AMOEBA and B. AMBER force field mediated simulations for all the systems.

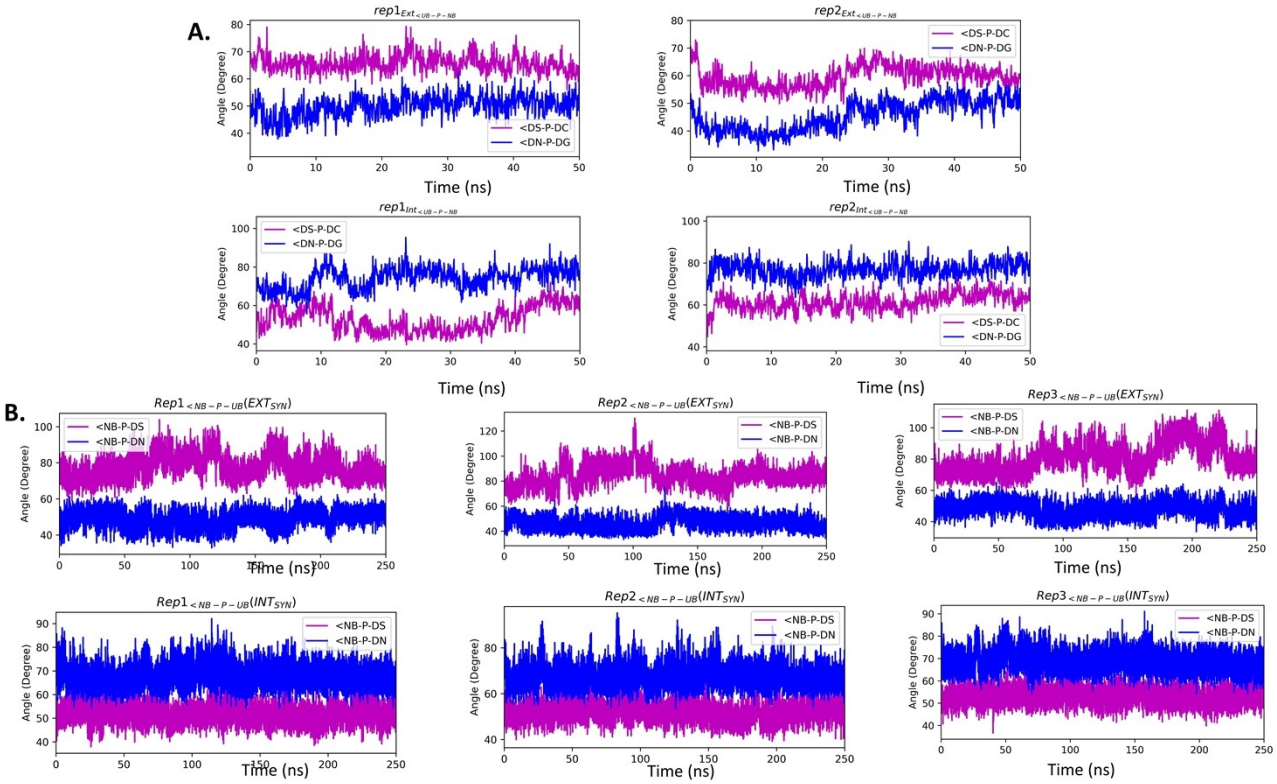

Figure S4. <UB-P-NB obtained from A. AMOEBA and B. AMBER force field mediated simulations for all the systems. In the crystal structure, <DS-P-DC and <DN-P-DG are 69.1 degree and 51.1 degree respectively for EXT_{SYN} and 51 degree and 68 degree respectively for INT_{SYN}.

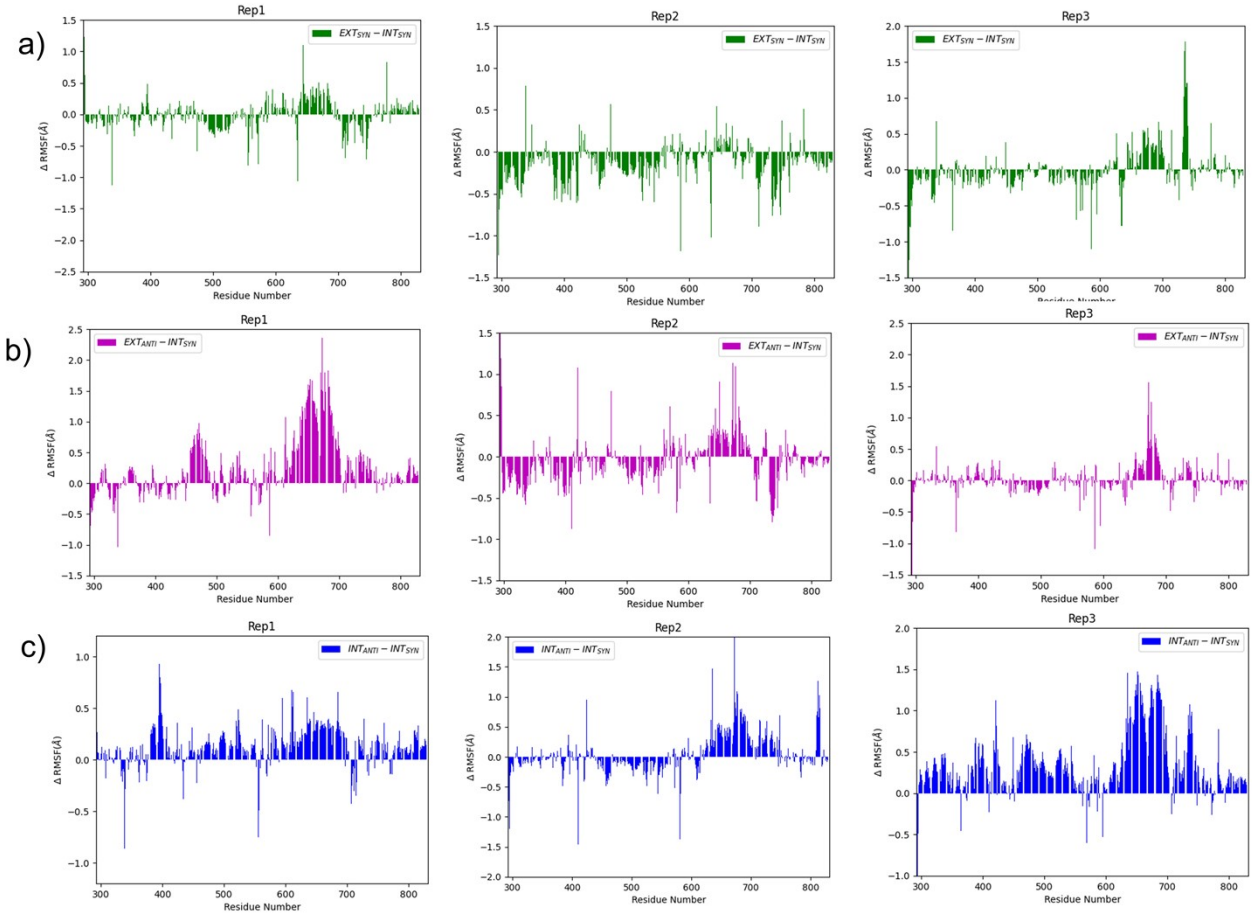

Figure S5. Δ RMSF of all three replicates (rep1: left, rep2: middle, rep3: right) with respect to INT_{SYN} conformers obtained from AMBER force field mediated simulations.

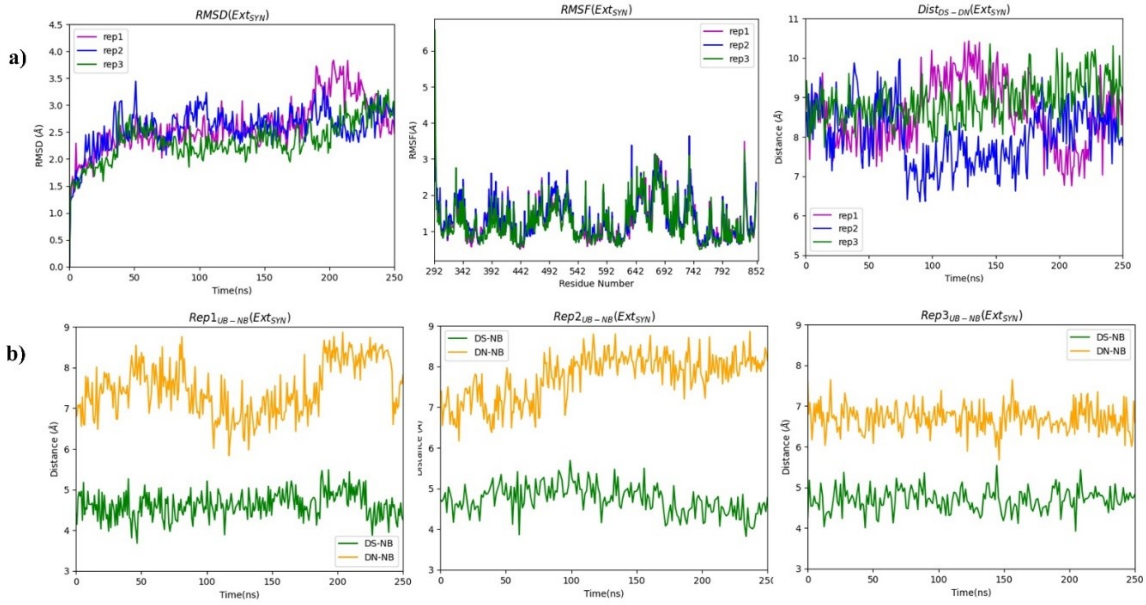

Figure S6. a) RMSD, b) RMSF, c) DS-DN distances of all three replicates. d) UB-NB distance of no-hang EXT_{SYN} systems obtained from AMBER force field mediated simulations.

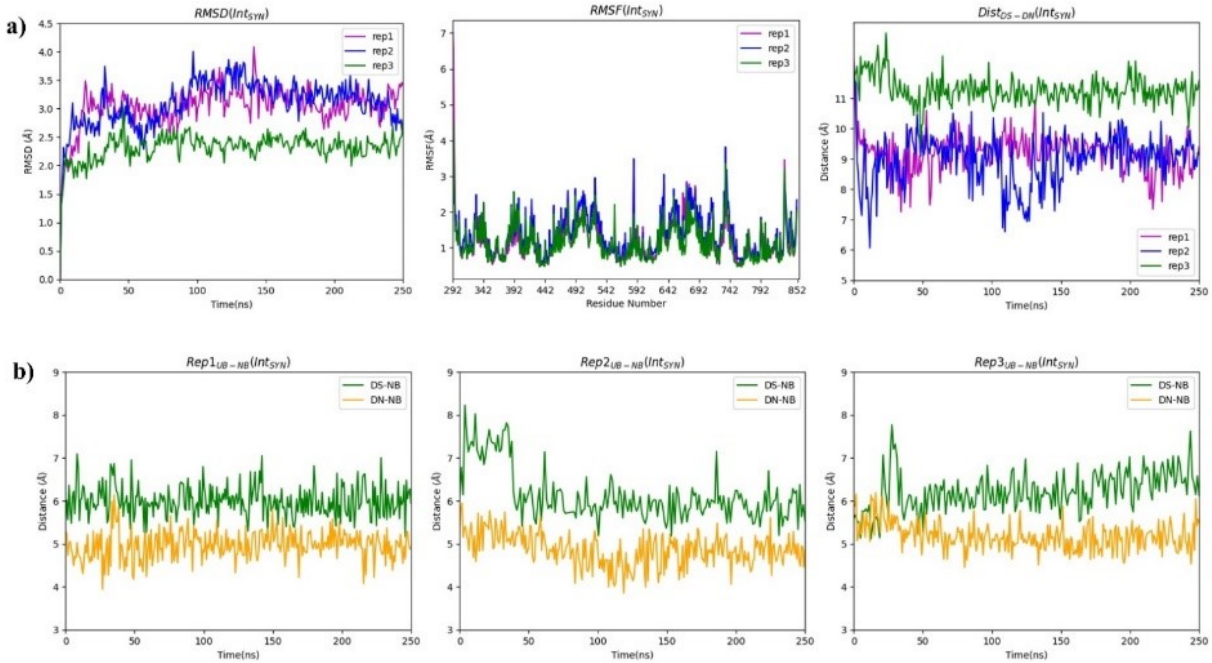

Figure S7. a) RMSD, b) RMSF, c) DS-DN distances of all three replicates. d) UB-NB distance of no-hang INT_{SYN} systems obtained from AMBER force field mediated simulations.

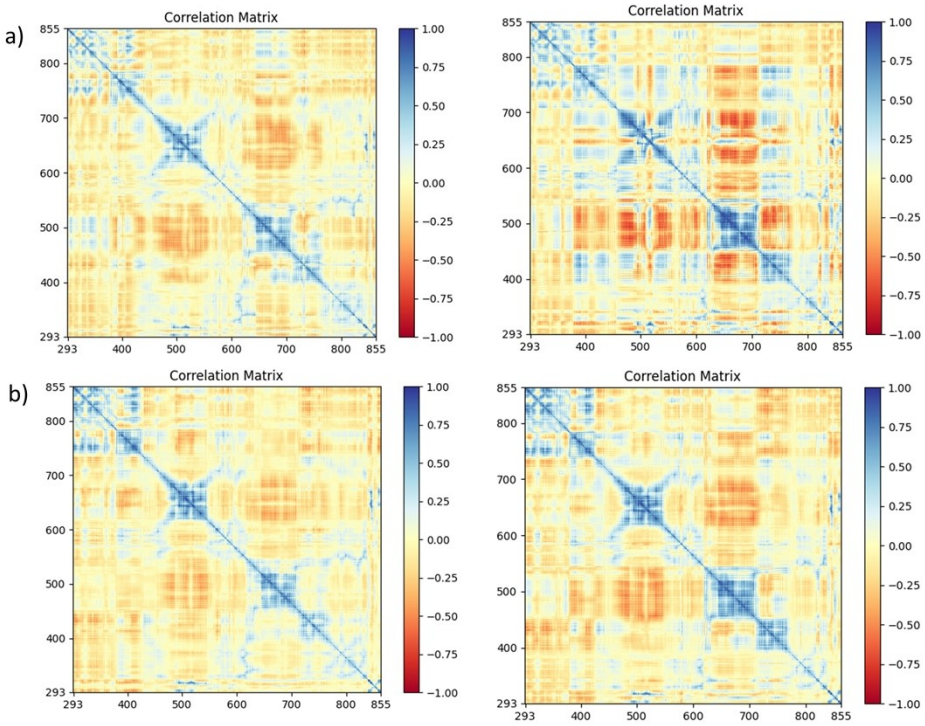

Figure S8. Cross correlation matrix for a) EXT and b) INT (SYN: left, ANTI: right) conformers.

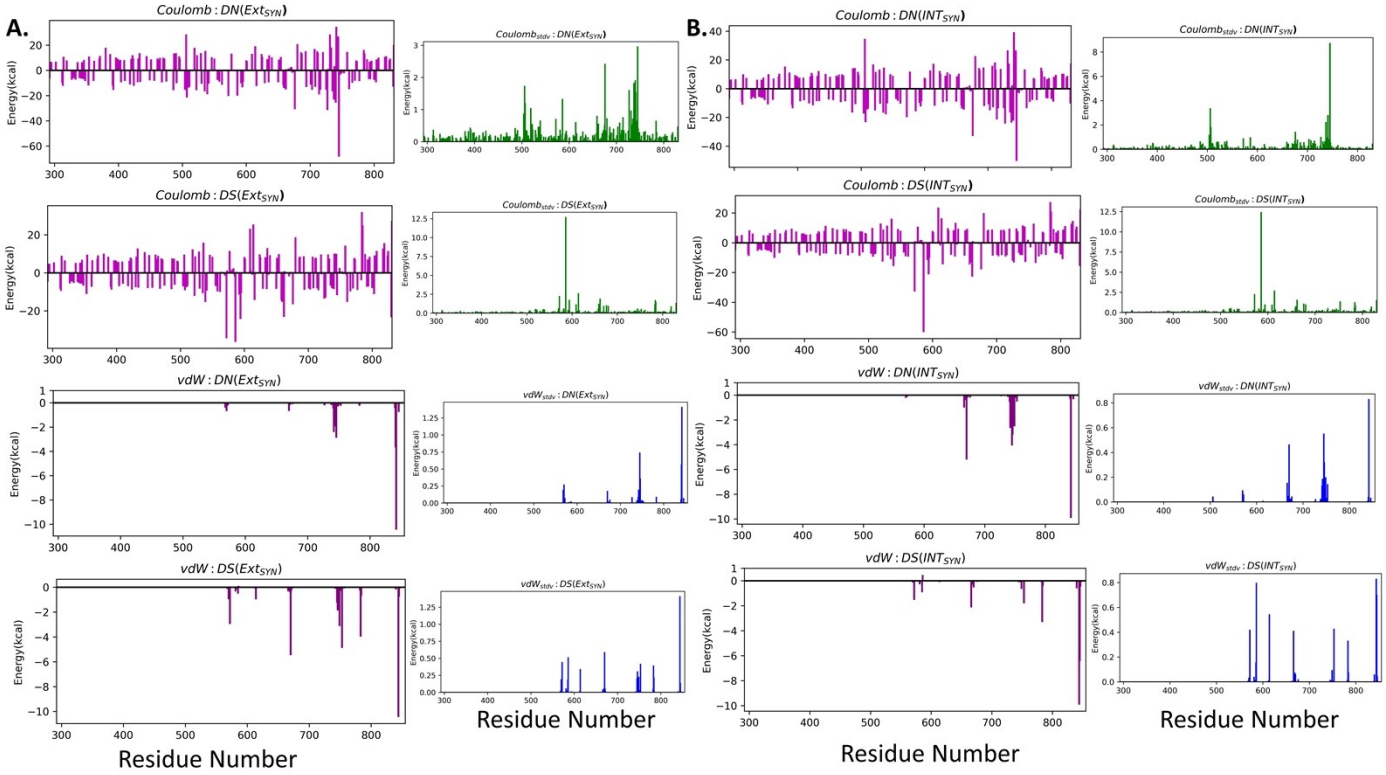

Figure S9. Coulomb (E_{Coul}) and vdW (E_{vdW}) interaction energies for DS and DN for A. EXT_{SYN} and B. INT_{SYN}.

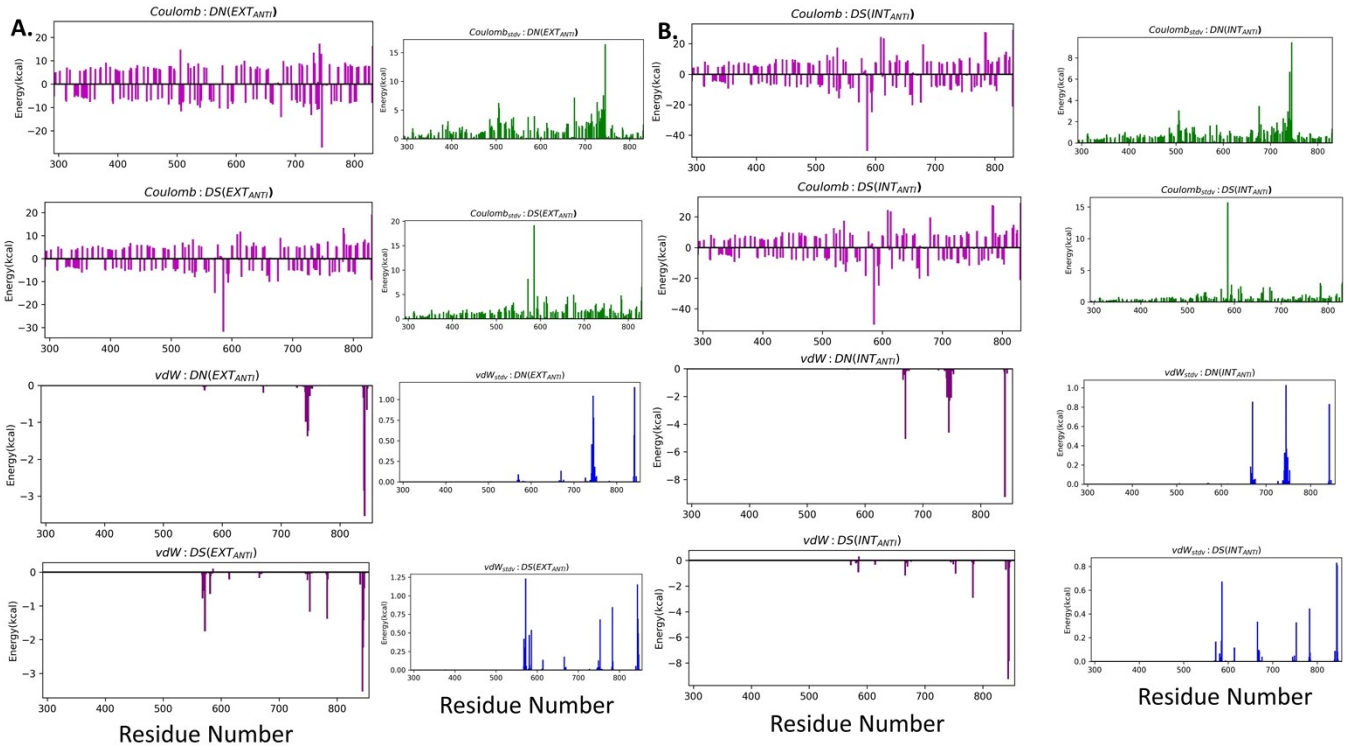

Figure S10. Coulomb (E_{Coul}) and vdW (E_{vdW}) interaction energies for DS and DN for A. EXT_{ANTI} and B. INT_{ANTI}.

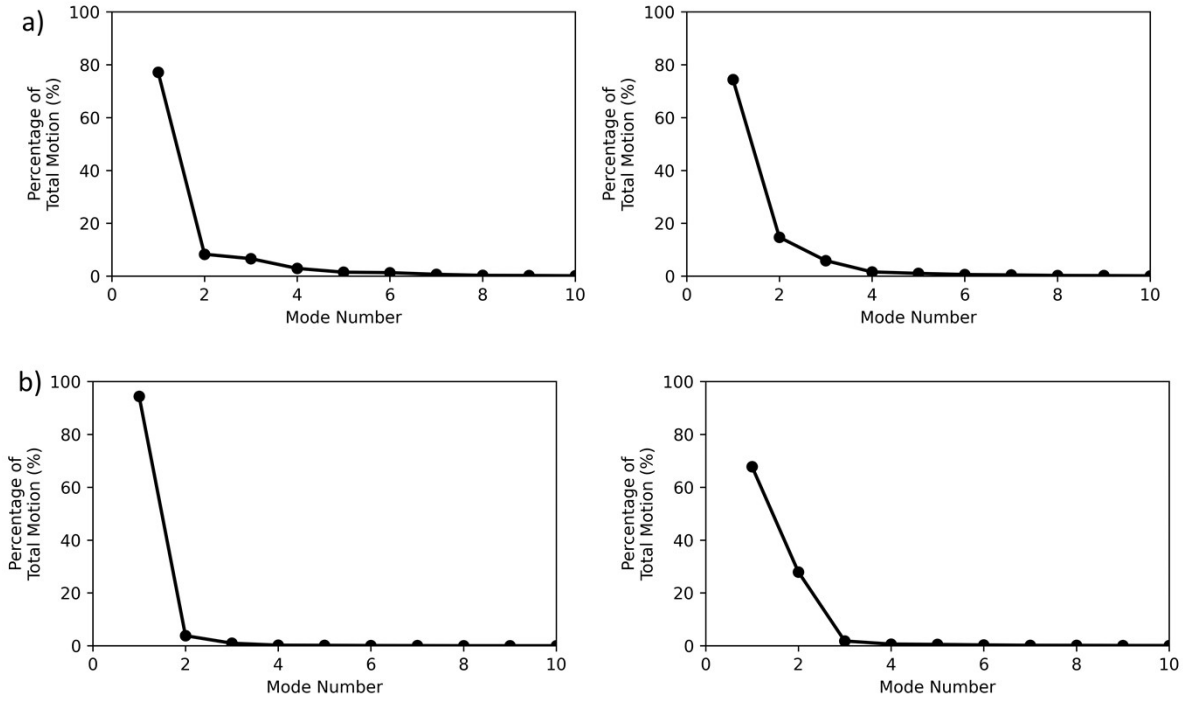

Figure S11. Percentage of Total motion (%) for a) EXT_{SYN} (left), INT_{SYN} (right), b) EXT_{ANTI} (left), INT_{ANTI} (right) conformers.