

SUPPLEMENTARY INFORMATION

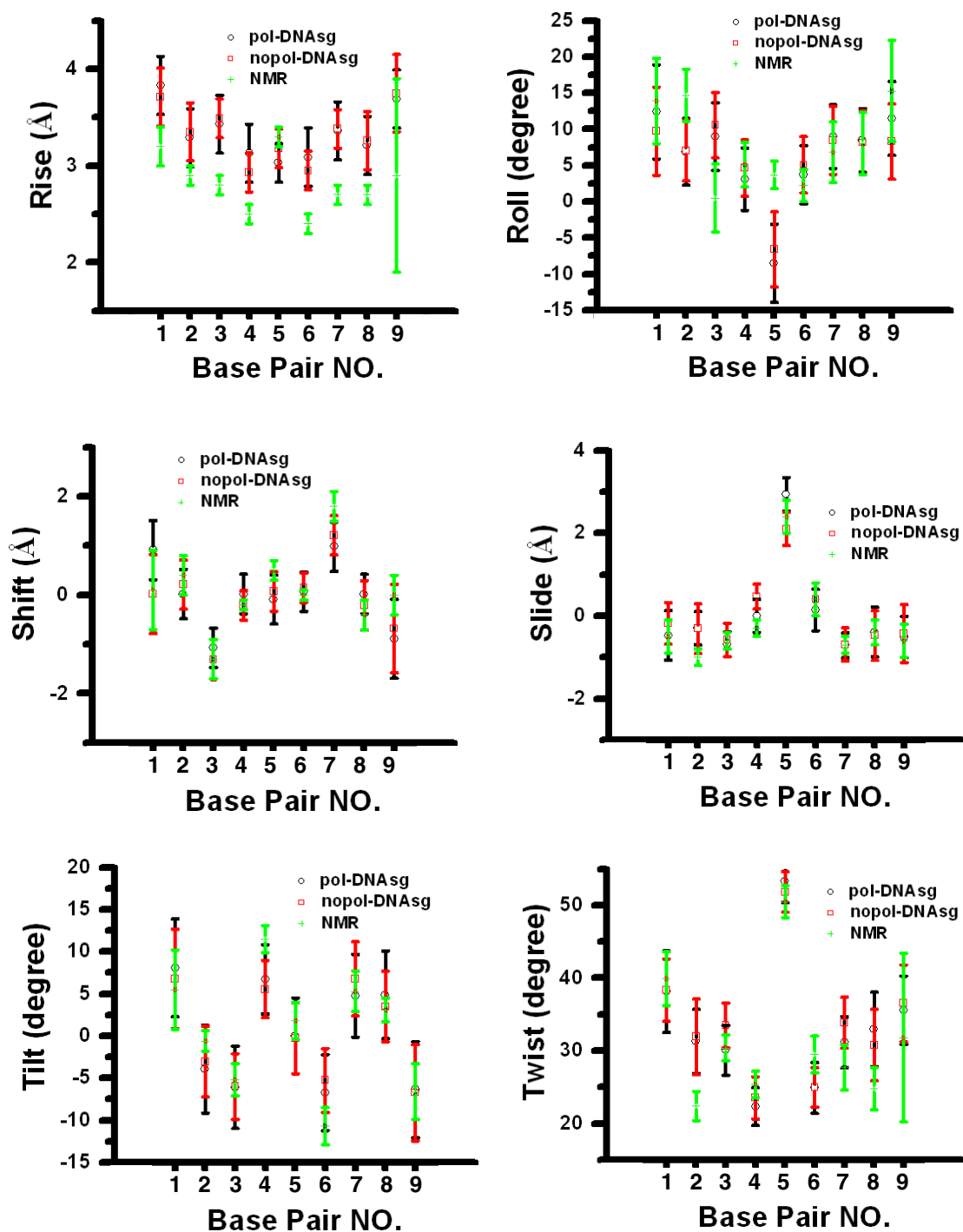


Figure S1. Comparison of the step parameters for DNA in the complex with thiazotropsin A between the NMR (green) and simulated structures based on the polarizable (black) and non-polarizable (red) force fields for the last ns of the complex trajectory. The first and the last base pair parameters were not taken into account because these termini were added for the purposes of the MD simulations.

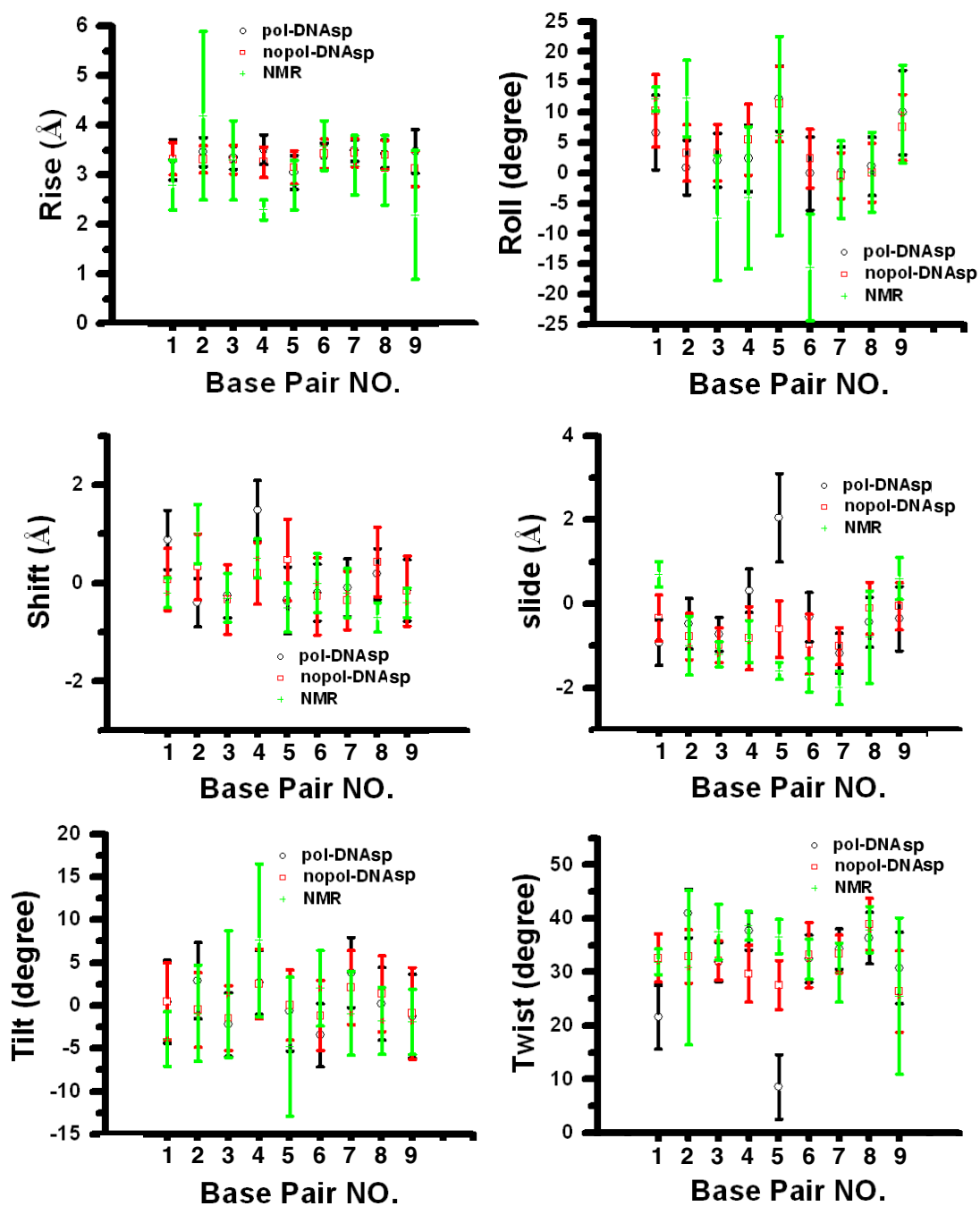


Figure S2. Comparison of the step parameters for the free form of DNA between the NMR (green) and simulated structures based on the polarizable (black) and non-polarizable (red) force fields for the last ns of the trajectory. The first and the last base pair parameters were not taken into account because these termini were added for the purposes of the MD simulation.