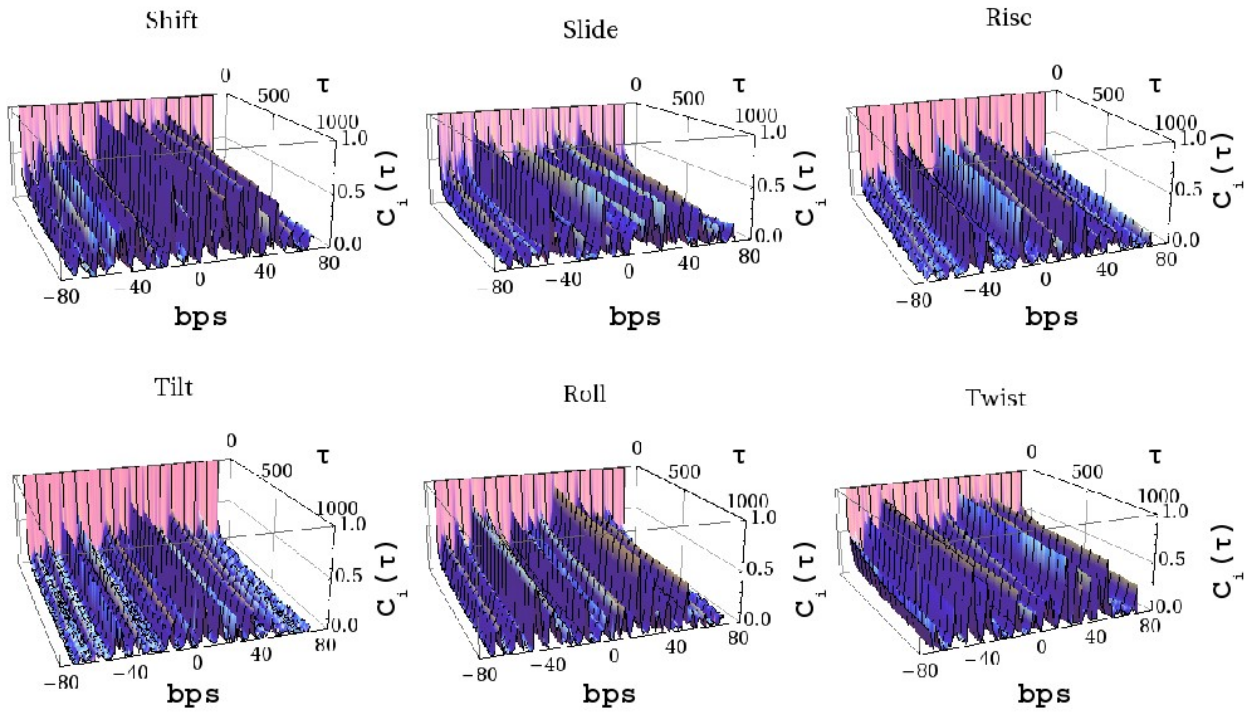
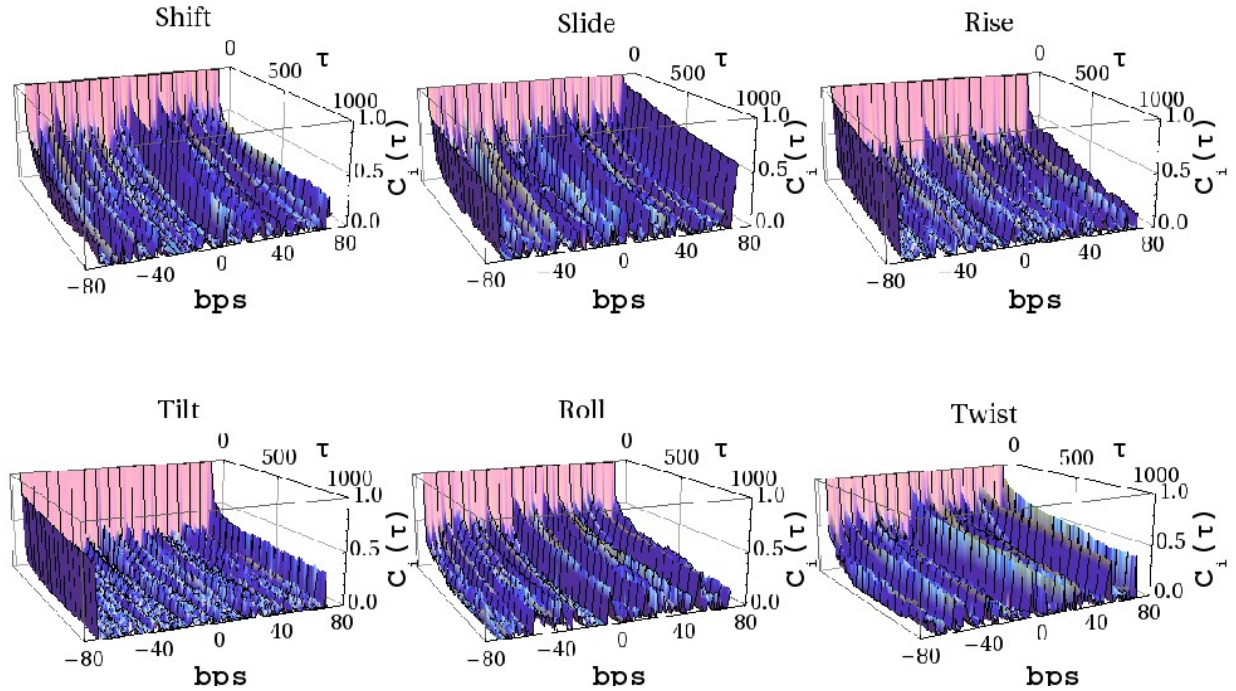
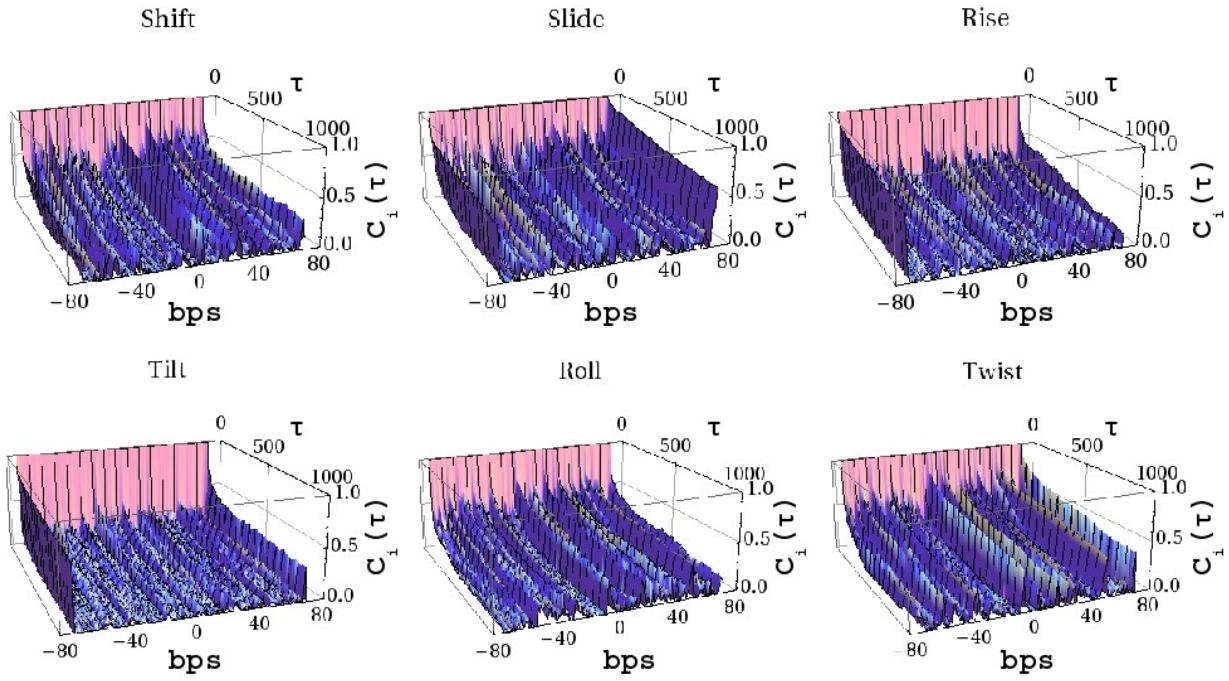
Supplementary Material



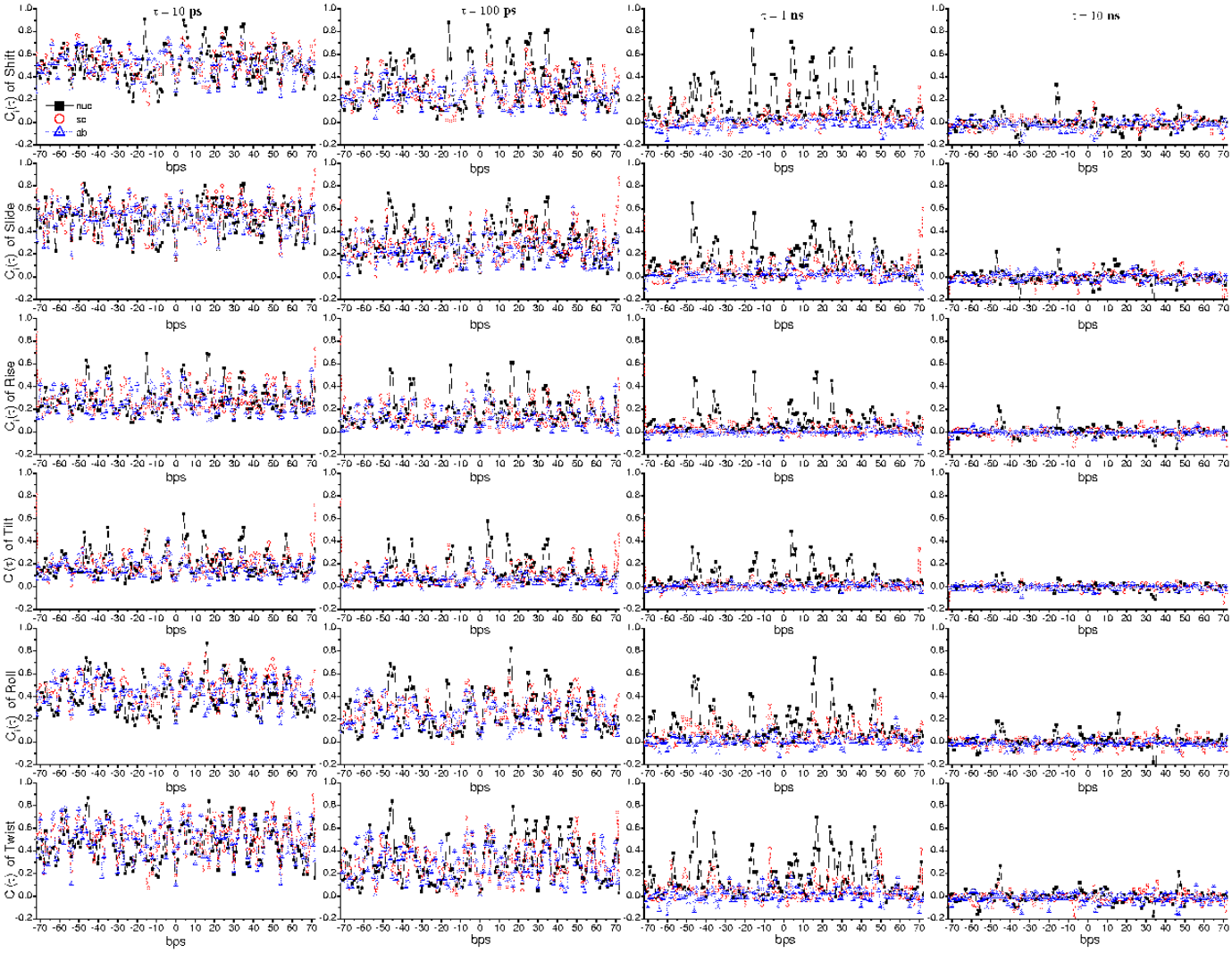
S1. 3D autocorrelation functions *C(τ)* of helix parameters for nuc-1id3, where *τ* is lag time, ps, and bps is DNA base pair number.



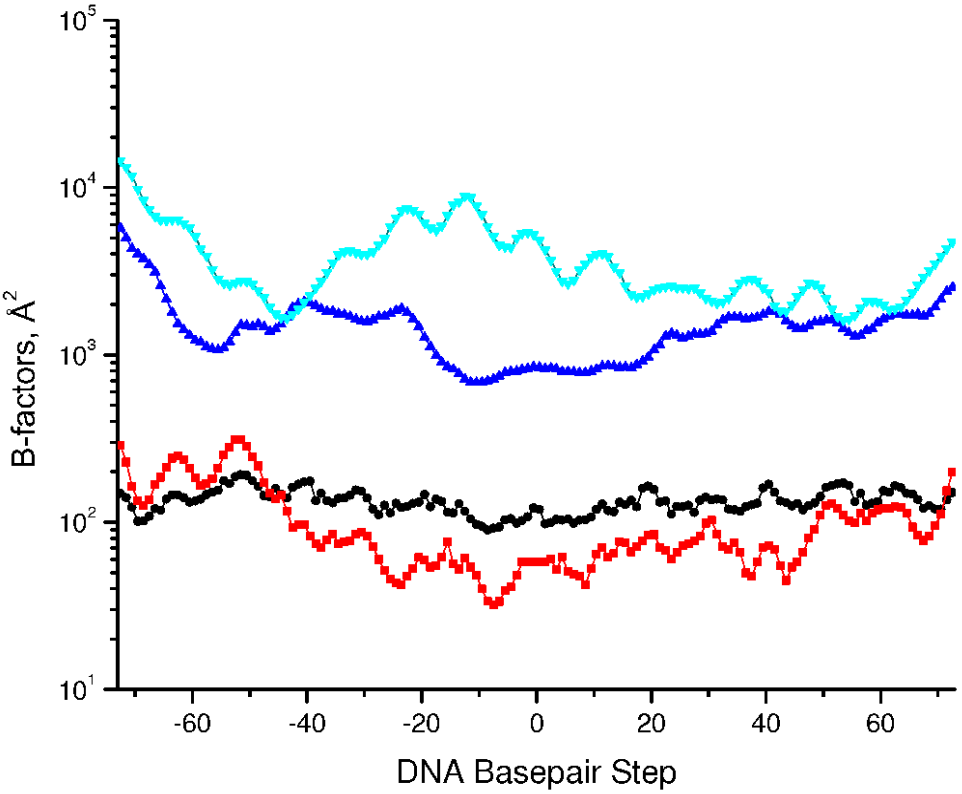
S2. 3D autocorrelation functions *C(τ)* of helix parameters for sc-DNA, where *τ* is lag time, ps, and bps is DNA base pair number.



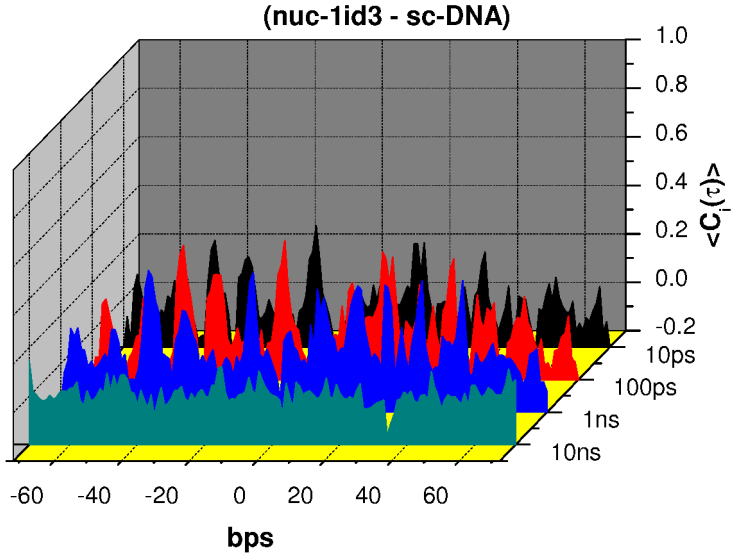
S3. 3D autocorrelation functions *C(τ)* of helix parameters for AB-DNA, where *τ* is lag time, ps, and bps is DNA base pair number.



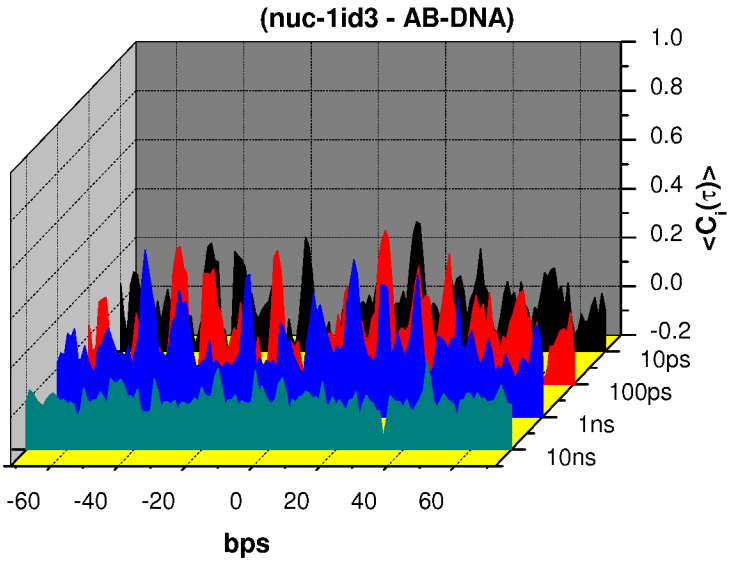
S4. 2D cross sections of 3D autocorrelation data of shift, slide, rise, tilt, roll and twist for nuc-1id3, sc-DNA and AB-DNA at times τ = 10 ps, 100 ps, 1 ns, 10 ns.



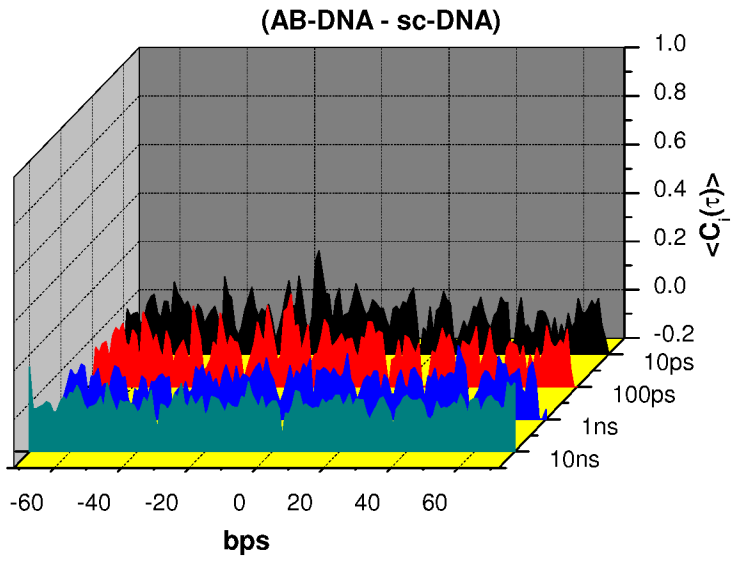
S5. B-factors from 1id3 x-ray structure (black circles) and simulations of nuc-1id3 (red squares), sc-DNA (blue triangles) and AB-DNA (cyan down triangles) as a function of DNA basepair.



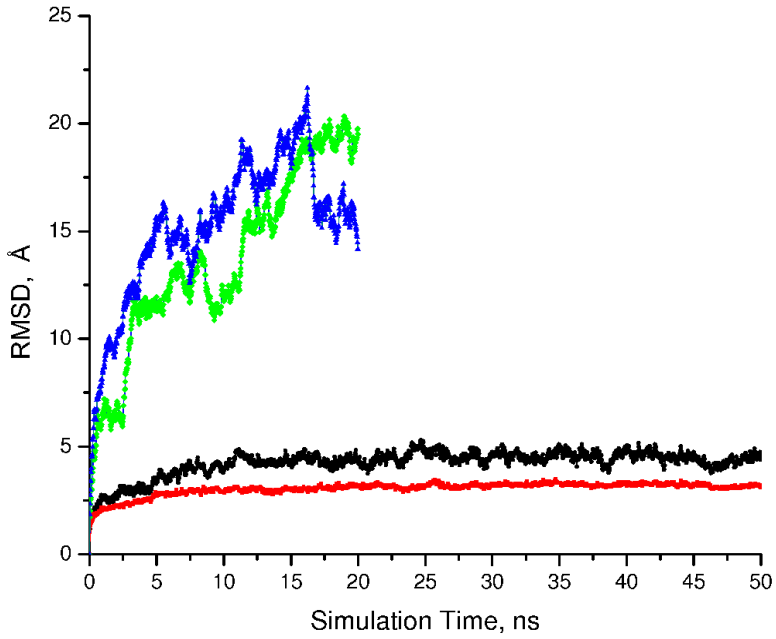
S6. Differential cross sections of 3D autocorrelation functions, $C_{nuc\text{-}1id3}(\tau)$-$C_{sc\text{-}DNA}(\tau)$, of helix parameters along the DNA length for nuc-1id3 at time instances τ = 10ps, 100ps, 1ns, 10ns. Original cross sections are provided in Figure 2.



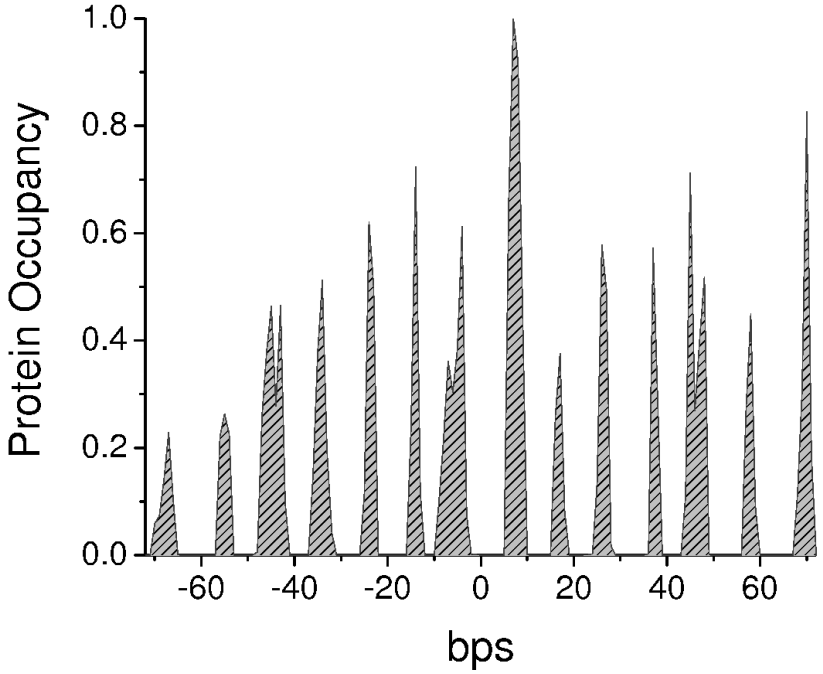
S7. Differential cross sections of 3D autocorrelation functions, $C_{nuc\text{-}1id3}(\tau)$-$C_{AB\text{-}DNA}(\tau)$, of helix parameters along the DNA length for nuc-1id3 at time instances τ = 10ps, 100ps, 1ns, 10ns. Original cross sections are provided in Figure 2.



S8. Differential cross sections of 3D autocorrelation functions, $C_{AB\text{-}DNA}(\tau)$-$C_{sc\text{-}DNA}(\tau)$, of helix parameters along the DNA length for AB-DNA at time instances τ = 10ps, 100ps, 1ns, 10ns. Original cross sections are provided in Figure 2.



S9. Root mean square deviations of nuc-1id3 (black circles - dna; red squares - protein), sc-DNA (green diamonds) and AB-DNA (blue triangles) with respect to their starting structures.



S10. Normalized protein occupancy as a function of DNA base pair step, bps, in nuc-1id3.