

Supplementary Animations

Video animations illustrating interesting conformational transitions over the course of the μ s-long trajectory are available at the following URLs (animations utilize the same coloring conventions and graphical representation schemes as in the main Figures and other Supporting Information):

- a) <http://mccammon.ucsd.edu/~cmura/DNA/XStrandStacking.mpg> – A video illustration of the cross-strand intercalative stacking (“XSIS”) that first appears in the $\approx 0.8 \mu$ s region of the trajectory (Figs. 3–6, S5, S6). This transition is characterized by severe disruption of the (A·T)₁₂ Watson-Crick base pair, such that the constituent bases (Ade_{1,12} and Thy_{2,9}) shear apart and assume a coaxial rather than coplanar arrangement – *i.e.*, they become stacked upon one another, with Ade_{1,12} staggered towards the 5’ direction and the cross-strand partner Thy_{2,9} translated towards the 3’ direction (with respect to the 5’→3’ path of the parent strand along the global helical axis). This large-scale structural transition is closely coupled to the base flipping of thymine at the adjacent (A·T)₁₃ base pair.
- b) <http://mccammon.ucsd.edu/~cmura/DNA/BaseFlipping.mpg> – This animation visualizes the spontaneous Thy_{2,8} base flipping event that arises near the end of the μ s-long trajectory (Figs. 3, 4, 7, S5, S6). Occurring well beyond 0.9 μ s and immediately adjacent to the sheared/XSIS (A·T)₁₂ base pair, the thymine base that is the focal point of this transition can be seen to swivel entirely out of the double helical stack, thereby eliminating the (A·T)₁₃ base pair and forming an abasic (apyrimidinic) lesion. Notably, the extruded Thy_{2,8} (together with Ade_{1,13}) forms the junction between the AGAA and TTCC κ B half sites which together comprise the nonameric ⁵AGAANTTCC³ DNA recognition element for (c-Rel)₂ and related members of this subfamily of NF- κ B transcription factors.
- c) <http://mccammon.ucsd.edu/~cmura/DNA/BarbedTerminus.mpg> – This illustration shows the formation of a “barbed” structure at the 5’ terminus of the GGGT… sequence (sense) strand (Figs. 4, 8, S7). This peculiar structure is characterized by a “peeling”-away of the cytosine base from the terminal (G·C)₁ guanine, followed by stable positioning of the Cyt pyrimidyl moiety into the proximal minor groove of its parent strand (antisense strand in Fig. S1c). This barbed terminus (*i*) is distinct from the documented base pair “fraying” events observed in ns-scale MD simulations of helical nucleic acids, (*ii*) recurs at long times ($>0.7 \mu$ s) in the trajectory, and (*iii*) stably persists for lengths of time on the order of 100 ns (as seen in Figs. 8, S7, and as evidenced by persistence of the barbed conformation in structures averaged over 100 ns-wide windows; Fig. 4c-f).
- d) <http://mccammon.ucsd.edu/~cmura/DNA/Overview.mpg> – Providing an overview of the entire trajectory, this animation depicts the dynamics of the κ B DNA from two views (transverse and axial) over the course of 1,021 ns. The animation is rather lengthy (3.5 min); viewers are encouraged to advance to at least the half-way point ($\approx 0.5 \mu$ s), as that is nearer to the onset of the interesting barbing, XSIS, and base flipping transitions.