Supplemental Data

Kinking Occurs during Molecular Dynamics Simulations of Small DNA Minicircles
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We made five simulations in total starting from two sets of $Lk = 9$ initial data, rough and smooth or $L9r$ and $L9s$, and two sets of $Lk = 8$ initial data, rough and smooth, with the smooth simulation being branched after 43 ns, for $L8r$, $L8sa$ and $L8sb$. In Figures S1-S4 of the Supplemental Data we provide for simulations $L9r$, $L8r$ and $L8sb$ the analogues of Figures 1-3 and 5 of the main text but for simulations $L9s$ and $L8sa$. We also provide PDB files and movies of the final structures of all five simulations.
Figure S1. (cf. Fig. 1) Final Conformations of Minicircles

L9r at 80ns exhibits a swiss roll structure with two kinks similar to L9s. L8r at 85 ns exhibits a single kink teardrop structure similar to that of L8sa, while L8sb has no kink and remains close to circular. Starting structures are in the inserts.
Figure S2. Time Evolution of the Average Twist of L9r (Red), L8sb (Green) and L8r (Blue)

Note the decrease of average twist of the L9r minicircle signaling the development of a highly writhed structure.
Figure S3a. Time Evolution of Roll and Propeller for L9r (Left) and L8r (Right)

The L9r minicircle develops three kinks (at steps 1, 4 and 45), although two of them are located very close to each other, and can be regarded as a single compound kink. L8r exhibits one kink at step 24. Within the last 20 ns of the simulation, a series of conformational changes occurs around base pair 85 in L8r which at several occasions resemble a Type II kink and eventually end up with the two bases of pair 85 stacked on top of each other. No breaking of neighboring base pairs was observed.
**Figure S3b.** Time Evolution of Roll and Propeller for L8sb, the Branch of the L8s Simulation which Develops No Kink

Note the large fluctuations in the roll distribution over time, which indicates that the register of the minicircle changes substantially during the simulation.
**Figure S4a.** Profiles of Helical Parameters along the Minicircles

Simulation L9r (left) and L8r (right). Top diagrams: tilt (green), roll (blue), twist (red). Bottom: shift (green), slide (blue), rise (red). The kinks are characterized by high negative roll, high rise, and high negative or positive tilt. Note the two kinks very close to each other in L9r, are treated as one compound kink in our analysis. The second peak in rise of L8r (around bp 85) is the structural anomaly described in the text (bases of the same pair stacked on top of each other).
Figure S4b. Same Data as in S4a, but for the Unkinked Branch of the L8s Simulation