**Slow motions in A•T rich DNA sequence**

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**Figures:**



**Tables:**

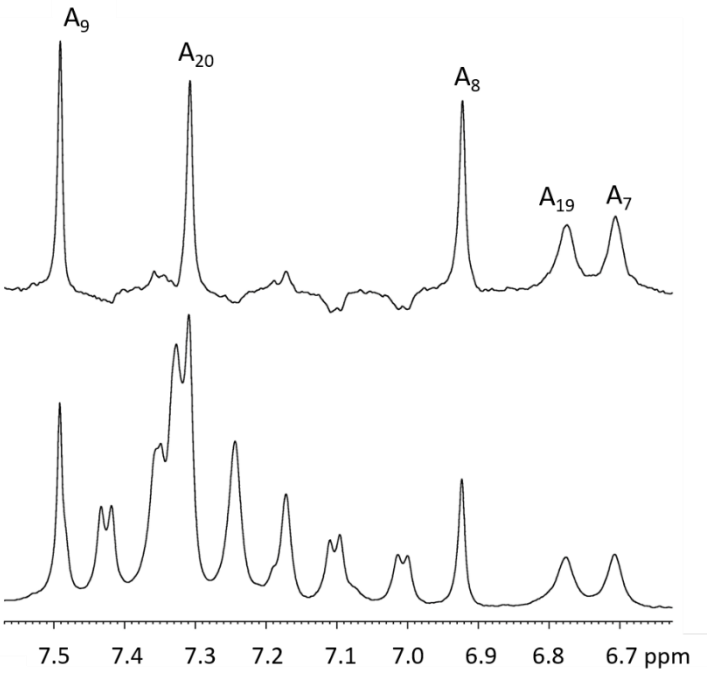


**Figure S1:** 1D and 1D-T1 inversion recovery spectra of the DNA aromatic region.

A: 1D (bottom) and 1D-T1 inversion recovery (top) spectra of the aromatic region of the unlabeled oligomer at 25°C in $^{2}H_2O$. The inversion recovery delay was optimized to selectively visualize the H2 resonances of adenines, which showed large differences in T1 values. The adenine numbering is recall on the top of the Figure.

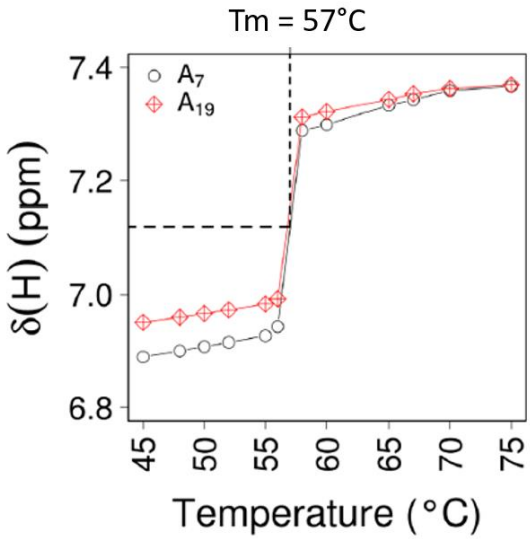


**Figure S2.** Chemical shift variations of H2 adenine protons as a function of temperature.

The variations of the H2 chemical shifts (δH) of $A_7$ and $A_{19}$ located at the dodecamer center, were plotted as a function of temperature; accordingly, the Tm of the studied dodecamer is 57°C.

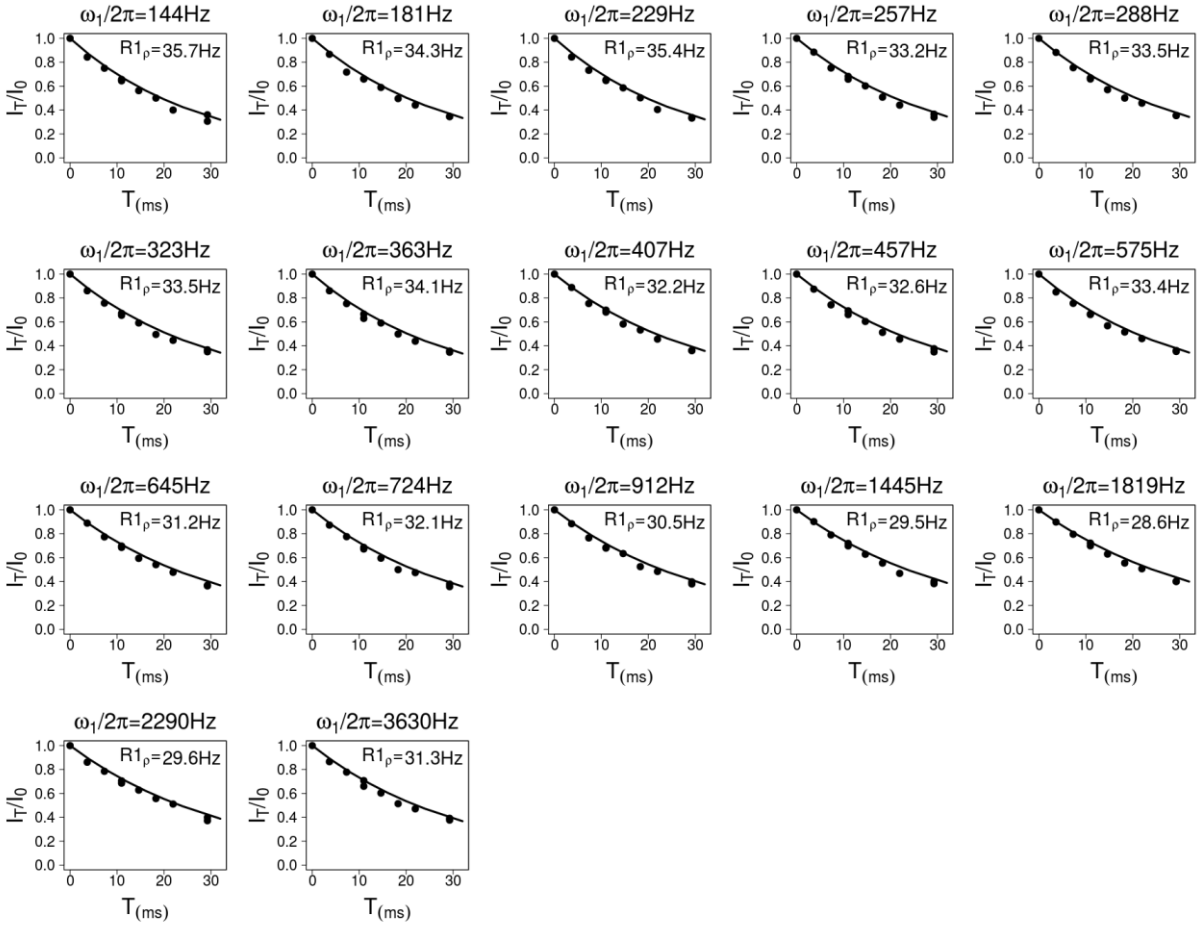


**Figure S3:** Examples of mono-exponential decays of relative peak intensities.

The mono-exponential decays of relative peak intensities presented here were measured on the C2 atom of the adenine $A_{19}$. $I_T$ is the peak intensity of the C2 atom of $A_{19}$ at each measured relaxation time T in millisecond (ms); $I_0$ is the intensity at T=0. The $I_T/I_0$ ratio is plotted as a function of T, from experiments performed with various spinlock powers ($\omega_1/2\pi$) specified above each panel. The R1ρ values given within the panels were obtained by fitting the decay curves with the equation $I_T = I_0 \exp(-RT)$, R being the time constant of the exponential.

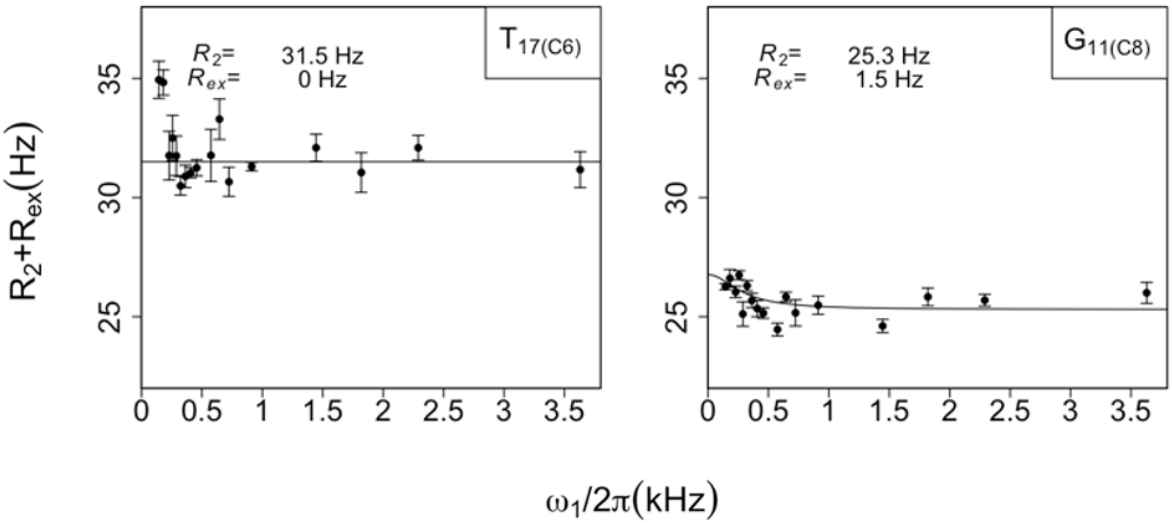


**Figure S4:** Examples of on-resonance $^{13}$C6/8 $R_{1\rho}$ relaxation dispersion profiles for nucleotides not submitted to conformational exchange.

$R_{1\rho}$ (= $R_2$ + $R_{ex}$) rates of the $T_{17}$-C6 and $G_{11}$-C8 atoms were plotted as a function of the effective spin lock field strength (ω1/2Π). The experiments were performed twice at 25°C. The two-state model fits (solid lines) were obtained using the protocol described in Materials and Methods. ($R_2$ + $R_{ex}$) standard deviations were calculated from the 500 runs carried out for each fit. The averaged $R_2$ and $R_{ex}$ values are specified in each panel.

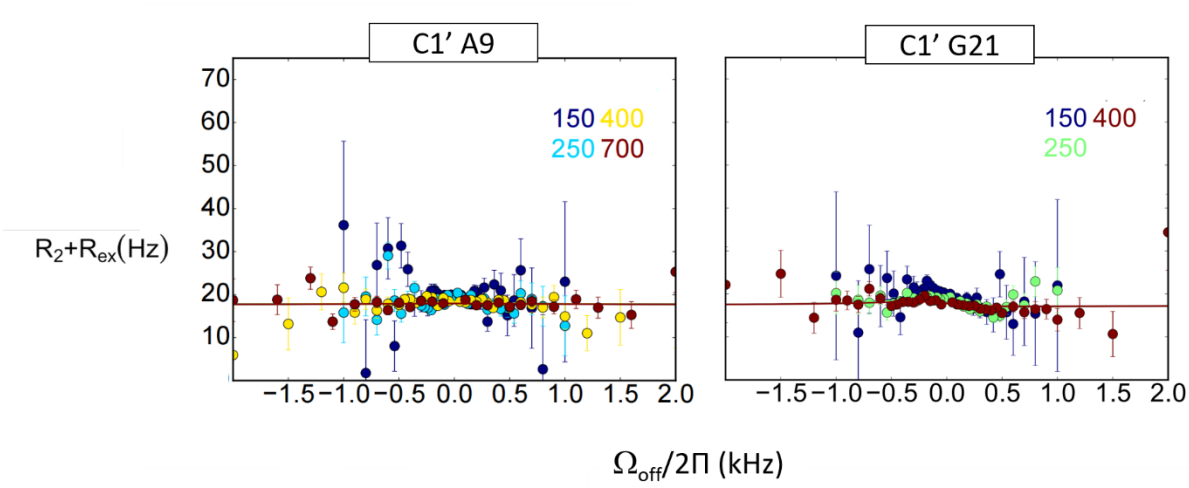


**Figure S5:** Off-resonance $^{13}C$ $R_{1\rho}$ relaxation dispersion profiles for C1' atoms of $A_9$ and $G_{21}$.

$R_2$ + Rex (= $R_{1\rho}$) values are given as a function of the resonance offset from the major state ($\Omega_{off}/2\Pi$). Error bars represent experimental uncertainties. The experiments were carried out at four different spin lock powers (from 150 to 700 Hz, color code in insets).

**Table S1 :** Parameters used for the R1ρ relaxation dispersion experiments.

**On resonance experiments**

*1-* ***Aromatic carbon probes (N: nucleotide, Cx: aromatic carbon) :***

$C_1$ C6, $C_2$ C6, $G_3$/$G_{15}$ C8, $C_4$ C6, $T_5$ C6, $T_6$/$T_{18}$ C6, $A_7$/$A_{19}$ C8, $A_7$ C2, $A_{19}$ C2, $A_8$ C8, $A_8$ C2, $A_9$/$A_{20}$ C8, $A_9$ C2, $A_{20}$ C2, $C_{10}$ C6, $G_{11}$ C8, $C_{12}$ C8, $G_{13}$ C8, $C_{14}$ C6, $G_{15}$/$G_3$ C8, $T_{16}$ C6, $T_{17}$ C6, $G_{21}$ C8, $C_{22}$ C6, $G_{23}$ C8; the slash symbol indicates overlapping signals in the HSQC spectra.

17 values of spin lock power (ω): 144, 181, 229, 257, 288, 323, 363, 407, 457, 575, 645, 724, 912, 1445, 1819, 2290, 3630 Hz

*2-* ***C1' probes :***

$C_1$ C1', $C_2$ C1', $G_3$/G11 C1', $C_4$ C1', $T_5$ C1', $T_6$ C1', $A_7$ C1', $A_8$ C1', $A_9$ C1', $C_{10}$ C1', $C_{12}$ C1', $G_{13}$ C1', $C_{14}$ C1', $G_{15}$ C1', $T_{16}$ C1', $T_{17}$ C1', $T_{18}$ C1', $A_{19}$ C1', $A_{20}$ C1', $G_{21}$ C1', $C_{22}$ C1', $G_{23}$ C1', $G_{24}$ C1'; the slash symbol indicates overlapping signals in the HSQC spectra.

15 values of spin lock power (ω): 229, 257, 288, 323, 363, 407, 457, 575, 645, 724, 912, 1445, 1819, 2290, 3630 Hz

**Off resonance experiments**

Off resonance spin lock power (ω) & ± {offset (Ω), 36 values}

***1- Adenine C1' probes :*** $A_7$ C1', $A_8$ C1', $A_9$ C1', $A_{19}$ C1', $A_{20}$ C1'

150 Hz & ±{30,60,90,120,150,180,210,240,270,300,360,420,480,540,600,700,800,1000}

250 Hz & ±{30,60,90,120,150,180,210,240,270,300,360,420,480,540,600,700,800,1000}

400 Hz & ±{50,100,150,200,250,300,350,400,450,500,600,700,800,900,1000,1200,1500,2000}

700 Hz & ±{100,200,300,400,500,600,700,900,1100,1300,1600,2000,2500,3000,3500,4000,5000,7500}

***2- Other C1' probes :*** $C_4$ C1', $G_{15}$ C1', $G_{21}$ C1'

150 Hz & ±{30,60,90,120,150,180,210,240,270,300,360,420,480,540,600,700,800,1000}

250 Hz & ±{30,60,90,120,150,180,210,240,270,300,360,420,480,540,600,700,800,1000}

400 Hz & ±{50,100,150,200,250,300,350,400,450,500,600,700,800,900,1000,1200,1500,2000}

**Table S2 :** $R_2$ and $R_{ex}$ values from fits of on-resonance $R_{1\rho}$ relaxation dispersion experiments

The $R_2$ and $R_{ex}$ values reported in these Tables were obtained from fits of on-resonance $^{13}C$ $R_{1\rho}$ relaxation dispersion data collected for three carbon types, C2, C6 or C8, and C1'. Standard deviations were estimated from duplicate data. Two nucleotides separated by a slash (N/N) indicate overlapping data. The data related to the five adenines of the dodecamer are stressed by a grey background.

***Table S2-1***

| atom | nucleotide | $R_2$ ($s^{-1}$) | $R_{ex}$ ($s^{-1}$) |
|---|---|---|---|
| C2 | $A_7$ | 30.2 ± 0.4 | 3.0 ± 1.4 |
| | $A_8$ | 30.3 ± 0.3 | 0.8 ± 0.4 |
| | $A_9$ | 30.2 ± 0.1 | 0 |
| | $A_{19}$ | 28.2 ± 0.7 | 6.2 ± 1.8 |
| | $A_{20}$ | 30.5 ± 0.2 | 0 |

***Table S2-2***

| atom | nucleotide | $R_2$ ($s^{-1}$) | $R_{ex}$ ($s^{-1}$) |
|---|---|---|---|
| C6 | $C_1$ | 28.7 ± 0.2 | 0 |
| C6 | $C_2$ | 31.8 ± 0.4 | 2.0 ± 1.2 |
| C6 | $C_4$ | 33.3 ± 0.1 | 0 |
| C6 | $T_5$ | 30.5 ± 0.5 | 0 |
| C8 | $A_8$ | 26.7 ± 0.2 | 7.4 ± 0.5 |
| C6 | $C_{10}$ | 33.5 ± 0.7 | 0 |
| C8 | $G_{11}$ | 25.3 ± 0.2 | 1.5 ± 0.5 |
| C6 | $C_{12}$ | 32.7 ± 0.2 | 0 |
| C6 | $C_{14}$ | 33.6 ± 0.2 | 2.3 ± 0.6 |
| C6 | $T_{16}$ | 31.8 ± 0.8 | 0 |
| C6 | $T_{17}$ | 31.5 ± 0.6 | 0 |
| C6 | $C_{22}$ | 32.9 ± 0.3 | 2.0 ± 0.8 |
| C8 | $G_{24}$ | 27.0 ± 0.1 | 0 |
| C8 | $G_3/G_{15}$ | 27.9 ± 0.5 | 0 |
| C6 | $T_6/T_{18}$ | 31.6 ± 0.2 | 3.9 ± 0.7 |
| C8 | $A_7/A_{19}$ | 26.9 ± 0.2 | 8.4 ± 0.7 |
| C8 | $A_9/A_{20}$ | 26.6 ± 0.2 | 6.7 ± 0.5 |

***Table S2-3***

| atom | nucleotide | $R_2$ ($s^{-1}$) | $R_{ex}$ ($s^{-1}$) |
|---|---|---|---|
| C1’ | $C_1$ | 10.5 ± 0.2 | 0 |
| | $C_2$ | 16.2 ± 0.3 | 0 |
| | $C_4$ | 17.4 ± 0.2 | 0 |
| | $T_5$ | 17.3 ± 0.2 | 4.9 ± 0.4 |
| | $T_6$ | 15.9 ± 0.1 | 2.7 ± 0.5 |
| | $A_7$ | 17.3 ± 0.4 | 15.1 ± 0.7 |
| | $A_8$ | 17.5 ± 0.3 | 7.5 ± 0.8 |
| | $A_9$ | 18.0 ± 0.1 | 6.0 ± 0.2 |
| | $C_{10}$ | 16.7 ± 0.2 | 3.6 ± 0.4 |
| | $C_{12}$ | 16.3 ± 0.2 | 0 |
| | $G_{13}$ | 12.2 ± 0.3 | 0 |
| | $C_{14}$ | 15.5 ± 0.2 | 0 |
| | $G_{15}$ | 18.5 ± 0.2 | 0 |
| | $T_{16}$ | 17.6 ± 0.3 | 3.5 ± 0.8 |
| | $T_{17}$ | 19.7 ± 0.2 | 0 |
| | $T_{18}$ | 18.6 ± 0.3 | 0 |
| | $A_{19}$ | 18.7 ± 0.2 | 15.9 ± 0.2 |
| | $A_{20}$ | 17.2 ± 0.1 | 2.5 ± 0.2 |
| | $G_{21}$ | 17.7 ± 0.1 | 0 |
| | $C_{22}$ | 17.2 ± 0.2 | 0 |
| | $G_{23}$ | 16.1 ± 0.1 | 0 |
| | $G_{24}$ | 14.4 ± 0.1 | 0 |

**Table S3:** $A_7$, $A_8$ and $A_{19}$ conformational exchange parameters from off-resonance $R_{1\rho}$ relaxation dispersion experiments.

The exchange parameters presented here complete those of the Table 2. $R_1$ and $R_2$ are the intrinsic longitudinal and transverse relaxation rates, respectively. These data were extracted using individual fits of experimental off-resonance relaxation dispersion data collected at 600 MHz, 25°C and pH 6.5.

| | | $R_1$ ($s^{-1}$) | | $R_2$ ($s^{-1}$) | |
|---|---|---|---|---|---|
| | | Method 1 | Method 2 | Method 1 | Method 2 |
| **C1'** | $A_7$ | 1.51 ± 0.29 | 1.44± 0.09 | 17.74 ± 1.39 | 17.13 ± 0.99 |
| | $A_8$ | 1.43 ± 0.31 | 1.26 ± 0.10 | 16.86 ± 1.24 | 16.36 ± 0.42 |
| | $A_{19}$ | 1.92 ± 0.18 | 1.76 ± 0.07 | 16.94 ± 1.31 | 19.0 ± 0.63 |

**Table S4:** Unusual α/γ backbone angles in X-ray B-DNA structures

The examined dataset is composed of 33 high resolution (R ≤ 2 Å) X-ray B-DNA structures, without mismatch, modified bases or phosphates, or non-paired bases. This Table reports the seven oligomers that contain unusual α/γ backbone angles (in bold and italic, underlined).

| PDB code | sequence | ***α/γ*** |
|---|---|---|
| 1IKK | CCTTTAAAGG | |
| | GGA***AA***TTTCC | ***g+/t*** |
| 1SK5 | CTTTT***AA***AAG | ***g+/t*** |
| | GAAAATTT***TC*** | ***g+/t*** |
| 1D49 | CGATTAATCG | |
| | GCT***AA***TTAGC | ***g+/t*** |
| 126D | CATGGCCATG | |
| | GTA***CC***GGTAC | ***g+/g-*** |
| 307D | C***AA***AGA***AAA***G | ***g+/g- * 3*** |
| | GTTTCTTTTC | |
| 307D | C***AA***AGA***AAA***G | ***g+/g- * 3*** |
| | GTTTCTTTTC | |
| 1ZFG | CCGAG***CT***CGG | ***g+/g-*** |
| | GGC***TC***GAG***CC*** | ***g+/g- * 2*** |