The intrinsic mechanics of B-DNA in solution characterized by NMR

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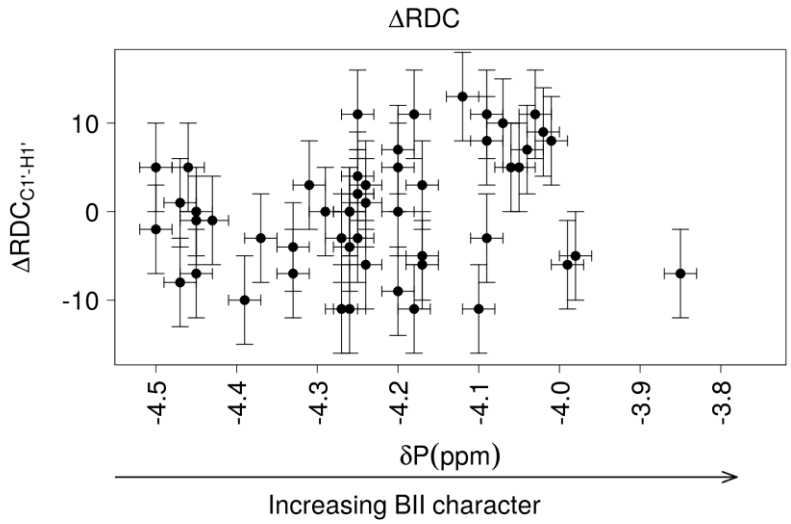
Figure S1: $\Delta RDC_{C1'\text{-}H1'}$ as a function of δP



The backbone conformation is represented by ^{31}P chemical shifts (δP). $\Delta RDC_{C1'\text{-}H1'}$ (Hz) are defined as the difference between the $RDC_{C1'\text{-}H1'}$ values of two consecutive vectors, measured on residues i and i+1: $\Delta RDC_{C1'\text{-}H1'} = RDC_{C1'\text{-}H1'(i+1)} - RDC_{C1'\text{-}H1'(i)}$. The data exclude the terminal steps. The vertical bars are the estimated experimental errors on ΔRDC. The experimental error on δPs (horizontal bars) is estimated to ±0.05 ppm. Clearly, δP and $\Delta RDC_{C1'\text{-}H1'}$ are not correlated; this is confirmed by the low correlation coefficient of 0.2.

Table S1 : Correlations between ΔRDCs and δPs for each of the four dodecamers

	$\Delta RDC_{C8\text{-}H8}/\delta P$		$\Delta RDC_{C3'\text{-}H3'}/\delta P$		$\Delta RDC_{C4'\text{-}H4'}/\delta P$	
	N	CC	N	CC	N	CC
Oligo 1	16	-0.83	12	0.76	7	-0.79
Oligo 2	18	-0.52	11	0.62	9	-0.84
Oligo 3	18	-0.61	11	0.95	11	-0.84
Oligo 4	8	-0.93	3	--	2	--

This table reports the characteristics of the correlations between ΔRDCs and δPs, obtained from the NMR measurements. These correlations are illustrated in Figure 4. The number of experimental data (N) and correlation coefficient (CC) for each dodecamer are given for each type of ΔRDCs.

Table S2 : Correlations between D_{inter} and δPs for each of the four dodecamers

	$D_{inter}(H6/8_i\text{-}H6/8_{i+1})/\delta P$		$D_{inter}(H2'_i\text{-}H6/8_{i+1})/\delta P$		$D_{inter}(H2''_i\text{-}H6/8_{i+1})/\delta P$	
	N	CC	N	CC	N	CC
Oligo 1	8	0.76	10	0.89	11	0.82
Oligo 2	7	0.71	7	0.83	8	0.63
Oligo 3	6	0.68	9	0.91	14	0.77
Oligo 4	9	0.73	7	0.53	9	0.72

This table reports the characteristics of the correlations between D_{inter} and δPs, obtained from the NMR measurements. These correlations are illustrated in Figure 4. The number of experimental data (N) and correlation coefficient (CC) for each dodecamers are given for each type of D_{inter}.

Table S3: NMR data collected on terminal nucleotides

		D_{intra}(H1'-H6/8)	I($TOCSY_{H1'-H4'}$)	$RDC_{C6/8-H6/8}$
Oligo1	T1	4.5	0	12
	T12	3.75	2.22e+07	Overlap
	A13	4.3	6.40e+06	5
	A24	4.22	7.22e+06	Overlap
Oligo2	G1	4.5	3.54e+05	12
	G12	4.02	1.39e+06	7
	C13	Overlap	6.90e+05	7
	C24	4.02	2.61e+06	3
Oligo3	C1	4.3	8.19e+07	9
	C12	3.9	8.70e+07	6
	G13	4.2	0	12
	G24	4.1	1.47e+08	8
Oligo4	C1	3.8	1.49e+08	6
	G12	3.9	1.68e+08	7
	C13	3.8	1.49e+08	6
	G24	3.9	1.68e+08	7

The D_{intra}(H1'-H6/8) values (Å) reported here are typical of the anti orientation of the glycosidic bond. The intensity of H1'-H4' TROSY cross-peaks, null and thus not observable for pure *South* sugars, indicates a population of *North* or *East* on most terminal sugars. The $RDC_{C6/8-H6/8}$ values (Hz) are similar to those obtained on internal nucleotides. Some of them are observable but not measurable because of overlaps. The data were collected at 20°C (D_{intra}(H1'-H6/8), $TOCSY_{H1'-H4'}$) and 25°C ($RDC_{C6/8-H6/8}$).

Table S4: Interdinucleotide distances collected on terminal dinucleotides

		D_{inter} ($H2'_i$-$H6/8_{i+1}$)	D_{inter} ($H2''_i$-$H6/8_{i+1}$)	D_{inter} ($H6/8_i$-$H6/8_{i+1}$)	D_{inter} ($H5_i$-$H6/8_{i+1}$) or ($H6/8_i$-$H5_{i+1}$)
Oligo 1	T1pC2	4.2	2.58	5.2	5.2
	C11pT12	3.2	Overlap	> 6	> 6
	A13pG14	3.2	2.5	4.9	na
	G23pA24	4.2	Overlap	> 6	na
Oligo 2	G1pC2	3.8	2.5	5.1	~5.5
	C11pG12	4.1	3.1	~5.5	~5.5
	C13pG14	3.4	3.2	~5.5	> 6
	G23pC24	Overlap	Overlap	4.16	4.16
Oligo 3	C1pC2	3.5	2.14	4.8	4.6
	G11pC12	Overlap	2.5	5.2	4.3
	G13pC14	3.09	Overlap	4.56	4.02
	G23pG24	Overlap	Overlap	> 6	na
Oligo 4	C1pG2	3.8	2.1	4.2	4.3
	C11pG12	3.52	2.8	~5.5	~5.5
	C13pG14	3.8	2.1	4.2	4.3
	C23pG24	3.52	2.8	~5.5	~5.5

$D_{inter}(H2'_i\text{-}H6/8_{i+1})$ and $D_{inter}(H2''_i\text{-}H6/8_{i+1})$ (Å) are observable on all the terminal dinucleotides. D_{inter} that are only observable in NOESY spectra recorded with a mixing time of 300ms were estimated to ~5.5Å. Some D_{inter} are observable but not measurable because of overlaps. D_{inter} involving the H5 atom of cytosine are not available (na) in ApG, GpA and GpG steps. The data were collected at 20°C.