

## Supplementary Information

### 5-Formylcytosine Weakens the G-C Pair and Imparts Local Conformational Fluctuations to DNA Duplexes

Manjula Jaisal,<sup>†</sup> Rajesh Kumar Reddy Sannapureddi,<sup>†</sup> Arjun Rana, Bharathwaj Sathyamoorthy<sup>\*</sup>

Department of Chemistry, Indian Institute of Science Education and Research, Bhopal 462066, India

<sup>\*</sup>To whom correspondence should be addressed. Tel: +91-755-269-1323; Fax: +91-755-269-2392;  
Email: [bharathwaj@iiserb.ac.in](mailto:bharathwaj@iiserb.ac.in)

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## 1. Details of sparse sampling method optimization

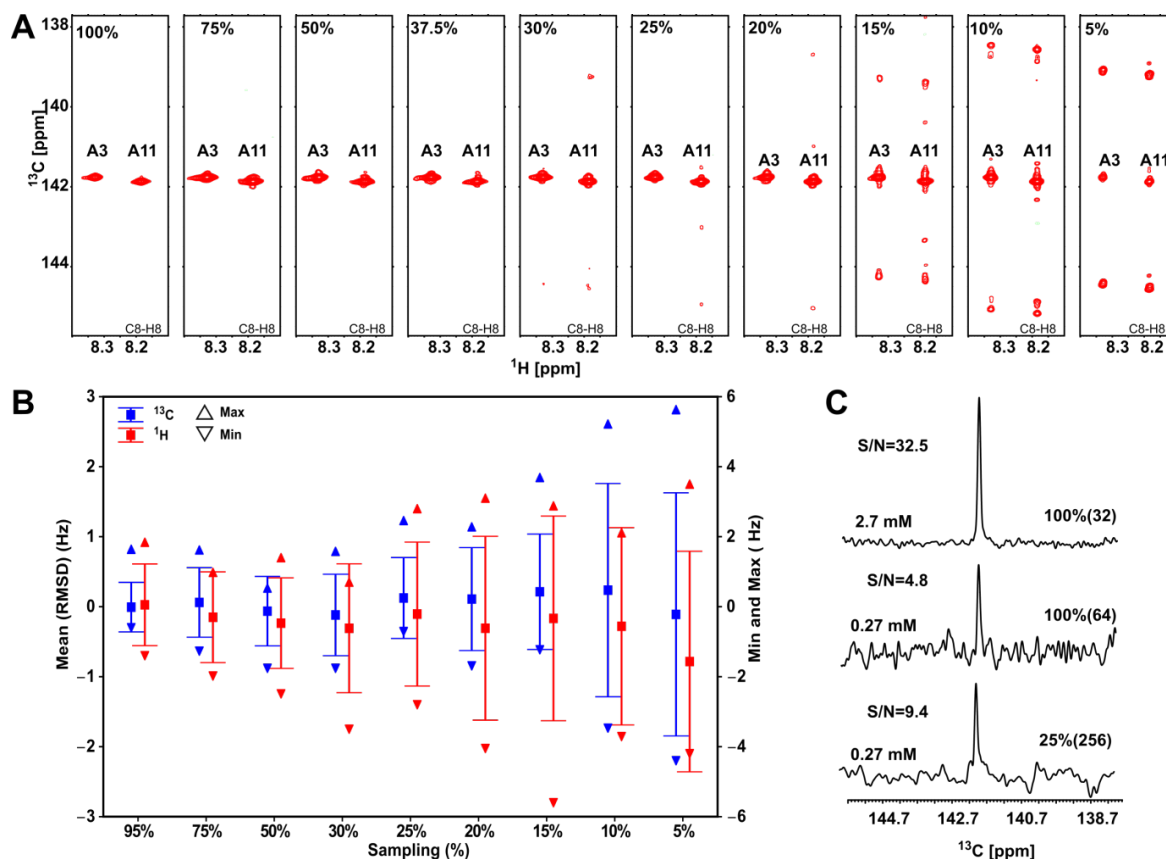
Acquisition of  $^{13}\text{C}/^{15}\text{N}$  data requires isotope enrichment or natural isotopic abundance samples at high concentration ( $> 1$  mM). Preparation of isotopically enriched DNA is expensive due to the inherent cost of  $^{13}\text{C}/^{15}\text{N}$  labeled nucleotide triphosphates and phosphoramidites. In particular, the precursors for modified nucleotides are seldom prepared with  $^{13}\text{C}/^{15}\text{N}$  isotope labeling restricting NMR to natural abundance samples.<sup>1</sup> Additionally, modified DNA samples are often limited in concentration due to poor yields limiting NMR to proton-based studies. For instance, DNA<sup>F3</sup> samples prepared in this study, following HPLC purification, provided an overall sample concentration of 90  $\mu\text{M}$  at natural abundance (i.e., 0.9  $\mu\text{M}$   $^{13}\text{C}$  and 0.4  $\mu\text{M}$   $^{15}\text{N}$ ).

Numerous NMR methods have been developed in the past decade to address acquiring multidimensional data for sensitivity-limited samples.<sup>2,3</sup> Under-sampling in the indirect dimension relative to conventionally Nyquist methods presents itself as an attractive alternative immensely reducing measurement times.<sup>2,3</sup> We investigated the effectiveness of sparse sampling methodology by adopting the Poisson-Gap sampling (along  $^{13}\text{C}$  dimension) that has been proved effective for measuring two-dimensional (2D) heteronuclear correlation data.<sup>4</sup> To assess the optimum under-sampling rate,  $^{13}\text{C}$ - $^1\text{H}$  data spectra were acquired at 5-95% of the conventional experiment for the natural abundance DNA<sup>control</sup> sample (2.7 mM), with otherwise identical experimental parameters (number of scans, spectral width, recycle delay, acquisition times, etc.). The data were processed with a compressed sensing methodology<sup>5</sup> that provides high fidelity with frequency and intensity measurement. The spectra were benchmarked on their ability to measure  $^{13}\text{C}$  and  $^1\text{H}$  chemical shifts reliably compared to the conventional 2D experiment.

Reduction of sampling rate is accompanied with loss of precision in the measurement of  $^{13}\text{C}$  and  $^1\text{H}$  shifts (Figure S1A and S1B). Reduction of sampling rate to 25% in the indirect dimension produces a root-mean-square-deviation (RMSD) of 4 (0.7 Hz) and 2 (1.7 Hz) ppb for  $^{13}\text{C}$  and  $^1\text{H}$  shifts, respectively, for cross-peaks across the aromatic (C2, C6/C8) and sugar (C1' and C2') moieties with mean absolute deviations of  $< 0.2$  Hz. Subsequent reduction of the sampling rate (i.e.,  $< 25\%$ ) increases the RMSD to 0.8-3.0 and 2.0-4.0 Hz for  $^{13}\text{C}$  and  $^1\text{H}$  chemical shifts, respectively, and introduces spectral artifacts (Figure S1A) reducing overall resolution in the severely aliased spectrum. Thus, 25% sampling provided the optimum time reduction and the necessary precision required for heteronuclear correlation.

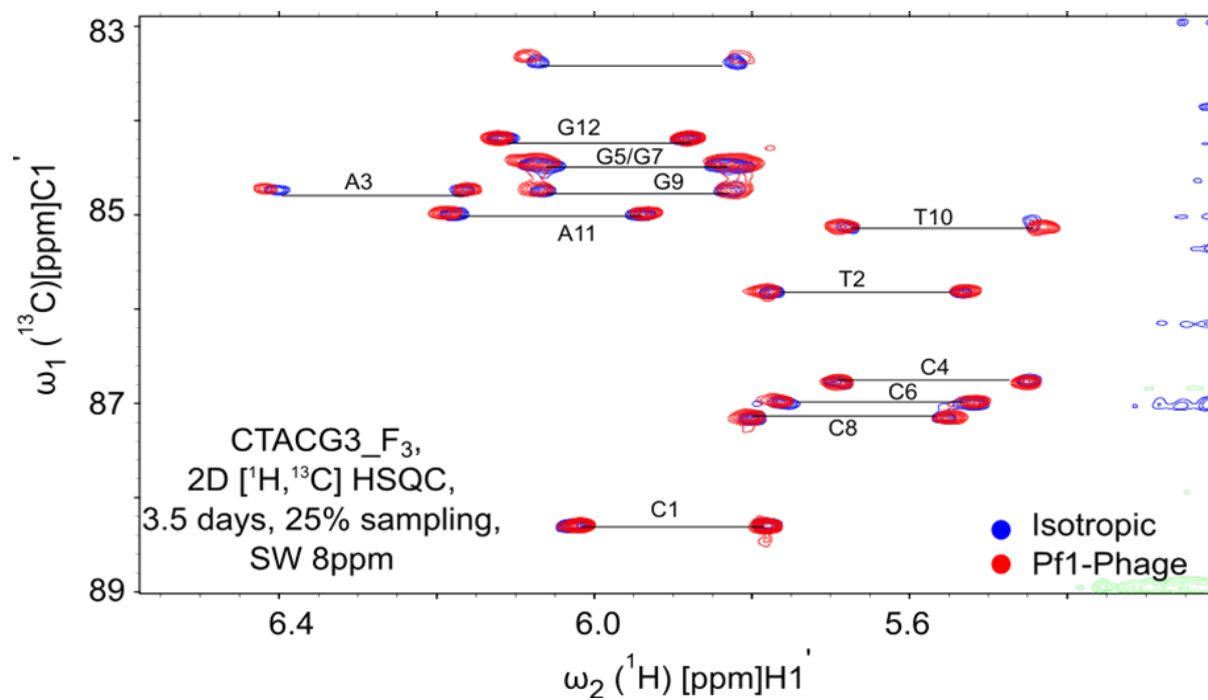
Robustness of the 25% sampling was tested with 2D  $^{13}\text{C}$ - $^1\text{H}$  spectra for DNA<sup>control</sup> sample at one-tenth concentration (270  $\mu\text{M}$ ) with conventional 100% (control) and sparse 25% sampling (total measurement time of 5.3 hours). The time saved for 25% sampling method was compensated by increasing the number of scans by four times. Increased scans achieve a better signal averaging and consequently a two-fold improvement in "apparent" signal-to-noise ratio<sup>6</sup> (Figures S1C) for the sparsely sampled data. Both 25% and 100% sampling datasets reproduced with  $^{13}\text{C}$  and  $^1\text{H}$  chemical shift RMSD of 1-2 Hz with mean absolute deviation of  $< 0.7$  Hz. These optimized sparse sampling parameters were employed in the subsequent data acquisition of all the modified samples and also for 2D  $^{15}\text{N}$ - $^1\text{H}$  SOFAST-HMQC data acquisition.

With frequencies reliably measured, we probed the ability of the experiment to measure one-bond  $^{13}\text{C}$ - $^1\text{H}$  scalar coupling ( $^1J_{\text{CH}}$ ). 2D HSQC spectrum was acquired without decoupling during acquisition providing  $^1J_{\text{CH}}$  the  $^1\text{H}$  dimension, while the  $^{13}\text{C}$  sparsely sampled dimension provided the necessary spectral resolution for the analysis. 25% sampling provides an overall  $^1J_{\text{CH}}$  RMSD of 1.2 Hz (for sugar C1'-H1' and nucleobase C2/5/6/8-H2/5/6/8 bonds) and mean deviation of -0.3 Hz, making these measurements amenable for scalar and residual dipolar coupling studies.



**Figure S1:** (A)  $^{13}\text{C}$ - $^1\text{H}$  spectra acquired with varied sampling % in  $^{13}\text{C}$  dimension for DNA<sup>control</sup> sample (2.7 mM), resonance peaks/contours are shown for **A3**-C8/H8 and **A11**-C8/H8. Both resonances are well represented even at 5% sampling. Spectral artifacts in the  $^{13}\text{C}$  dimension starts showing up below 25% sampling on upfield and downfield to actual chemical shifts, complicating the spectral analysis. (B) Chemical shift values of  $^{13}\text{C}$  and  $^1\text{H}$  (in Hz) for C6, C8, C1', C2' and H6, H8, H1', H2', H2'' were acquired at variable samplings % were compared with data acquired at 100% sampling (DNA<sup>control</sup>, 2.7 mM), mean absolute deviations with RMSD were for plotted (■ for mean and error bars for RMSD), also maximum deviation and minimum deviation were shown as ▲, and ▼, respectively. At each sampling %  $^{13}\text{C}$  (blue) and  $^1\text{H}$  (red) are shown individually. Y-axis on left represents mean and RMSD in Hz, scale on the right represent for minimum and maximum deviations in Hz. (C) Comparison of signal to noise ratio (S/N) for traces in the  $^{13}\text{C}$  dimension, for DNA<sup>control</sup> at 2.7 mM and 0.27 mM. With concentrated sample (2.7 mM) at 100% sampling S/N of 32.5 is observed, with low concentration (0.27 mM) sample S/N is 4.8 at 100% sampling and 64 scans, apparent S/N increased to 9.4 with one fourth sampling (25%) and 4 times more scans (ns 256) nearly doubled apparent S/N is observed with same amount experimental time.

## 2. HSQC spectra obtained for DNA<sup>F3</sup>



**Figure S2:** Overlaid  $^{13}\text{C}$ - $^1\text{H}$  spectra with F2-coupling acquired with 25% in  $^{13}\text{C}$  dimension for DNA<sup>F3</sup> sample. C1'-H1' region of spectra is shown. Data acquired in isotropic conditions used for measuring  $^1J_{\text{C1}'\text{-H1}'}$  is shown in blue and anisotropic conditions (~20-25 mg/mL Pf1-phage) used for  $^1(\text{J}+\text{D})_{\text{C1}'\text{-H1}'}$  measurements are shown in red.

### 3. NMR data tables for DNA and DNA<sup>N#</sup>

**Table S1:** NMR data tables for chemical shifts, J-couplings and dipolar couplings

DNA <sup>control</sup> d(CTACGCGCGTAG) <sub>2</sub>																							
Nt	C1'	H1'	C2'	H2'	H2''	C6/C8	H6/H8	C4'	H4'	C2/C5 /C7	H2/H5 /H7	N1/N3	H1/H3	H41	H42	<sup>1</sup> J <sub>C6/C8- H6/H8</sub>	<sup>1</sup> J <sub>C2-H2</sub>	<sup>1</sup> J <sub>C1'-H1'</sub>	<sup>1</sup> D <sub>C6/C8 -H6/H8</sub>	<sup>1</sup> D <sub>C2-H2</sub>	<sup>1</sup> D <sub>C1'- H1'</sub>	ΣH1' ( <sup>3</sup> J <sub>H2'- H1'</sub> )	ΣH1' ( <sup>3</sup> J <sub>H2''- H1'</sub> )
C1	88.3	5.91	40.7	2.15	2.56	143.2	7.85	88.2	4.11	99.4	5.96					182.7		172.2	15.7		-6.0	13.7	12.8
T2	85.9	5.69	39.0	2.23	2.52	139.7	7.55	86.4	4.19	14.50	1.73	159.3	13.69			179.2		165.9	12.3		11.0	13.3	17.0
A3	84.9	6.23	40.2	2.74	2.89	141.8	8.33	87.5	4.43	154.8	7.59					213.7	201.6	165.9	15.6	10.2	12.2	14.0	16.1
C4	86.1	5.55	39.8	1.93	2.31	142.1	7.24	85.2	4.16	98.4	5.27			8.17	6.51	178.6		165.9	20.0		3.5	-	16.5
G5	84.5	5.84	40.4	2.59	2.70	138.1	7.81	87.2	4.34			147.0	12.85			212.8		163.1	16.5		14.1	14.4	16.1
C6	86.3	5.64	39.9	1.95	2.35	142.2	7.23	85.4	4.13	98.5	5.28			8.27	6.33	178.2		166.4	21.0		12.6	13.1	16.8
G7	84.4	5.85	40.5	2.59	2.70	138.1	7.85	87.2	4.34			147.0	12.91			212.8		163.0	16.7		10.8	14.0	16.2
C8	86.3	5.65	40.0	2.00	2.36	142.2	7.25	85.4	4.14	98.6	5.31			8.27	6.34	177.8		166.1	18.8		11.3	13.4	16.9
G9	84.6	5.92	40.5	2.59	2.73	138.4	7.87	87.2	4.34			147.0	12.77			213.5		165.3	17.9		11.9	14.0	16.1
T10	85.2	5.57	39.1	1.94	2.25	138.5	7.20	85.4	4.12	14.5	1.53	158.5	13.64			177.1		167.6	14.6		9.5	13.7	16.8
A11	85.0	6.06	40.1	2.68	2.86	141.9	8.18	87.5	4.39	154.3	7.55					212.8	202.3	166.6	11.6	13.4	11.2	13.8	16.3
G12	84.2	6.01	42.4	2.26	2.43	138.5	7.71	87.4	4.17							211.4		163.8	9.0		7.6	16.1	13.8

DNA <sup>M6</sup> d(CTACG <sup>5m</sup> CGCGTAG) <sub>2</sub>																							
Nt	C1'	H1'	C2'	H2'	H2''	C6/C8	H6/H8	C4'	H4'	C2/C5 /C7	H2/H5 /H7	N1/N3	H1/H3	H41	H42	<sup>1</sup> J <sub>C6/C8- H6/H8</sub>	<sup>1</sup> J <sub>C2-H2</sub>	<sup>1</sup> J <sub>C1'-H1'</sub>	<sup>1</sup> D <sub>C6/C8- H6/H8</sub>	<sup>1</sup> D <sub>C2-H2</sub>	<sup>1</sup> D <sub>C1'- H1'</sub>	ΣH1' ( <sup>3</sup> J <sub>H2'- H1'</sub> )	ΣH1' ( <sup>3</sup> J <sub>H2'- H1'</sub> )
C1	88.3	5.91	40.7	2.14	2.56	143.2	7.85	88.2	4.11	99.4	5.97					181.5		173.3	15.2		-8.2	13.3	
T2	85.9	5.68	39.0	2.23	2.52	139.7	7.54	86.4	4.19	14.5	1.73	159.3	13.72			177.6		167.7	13.5		12.3	14.0	16.5
A3	84.9	6.23	40.2	2.74	2.89	141.8	8.32	87.5	4.43	154.8	7.58					212.8	200.6	166.3	14.0	12.3	14.2	14.7	16.4
C4	86.1	5.55	39.8	1.97	2.31	142.1	7.25	85.2	4.17	98.4	5.27			8.15	6.52	177.3		166.5	20.8		3.7	14.0	-
G5	84.6	5.92	40.5	2.53	2.78	138.2	7.80	87.2	4.34			147.0	12.85			212.1		164.9	17.5		14.4	13.4	16.5
<sup>5m</sup> C6	86.0	5.57	39.8	1.95	2.32	138.8	7.04	85.6	4.17	15.1	1.54			8.60	5.99	176.9		166.5	19.1		9.5	13.5	-
G7	84.5	5.84	40.5	2.61	2.69	138.1	7.83	87.2	4.34			147.1	12.94			212.0		164.0	15.7		13.9	14.3	15.9
C8	86.4	5.71	40.1	2.02	2.39	142.2	7.27	85.6	4.17	98.6	5.29			8.25	6.31	177.0		166.9	21.2		11.6	14.0	15.6
G9	84.6	5.91	40.5	2.59	2.73	138.3	7.86	87.2	4.33			146.9	12.75			213.7		163.7	15.9		14.8	14.1	15.9
T10	85.2	5.57	39.1	1.94	2.26	138.5	7.20	85.5	4.12	14.5	1.52	158.5	13.65			177.5		166.6	12.2		10.6	-	16.1
A11	85.0	6.06	40.1	2.68	2.86	141.9	8.18	87.4	4.39	154.3	7.55					213.8	204.0	166.2	8.8	13.77	12.3	14.0	15.8
G12	84.2	6.01	42.4	2.27	2.43	138.5	7.71	87.4	4.17							211.4		163.6	7.1		7.9	15.4	14.7

DNA <sup>M8</sup> d(CTACGCG <sup>5m</sup> CGTAG) <sub>2</sub>																							
Nt	C1'	H1'	C2'	H2'	H2''	C6/C8	H6/H8	C4'	H4'	C2/C5 /C7	H2/H5 /H7	N1/N3	H1/H3	H41	H42	<sup>1</sup> J <sub>C6/C8- H6/H8</sub>	<sup>1</sup> J <sub>C2-H2</sub>	<sup>1</sup> J <sub>C1'-H1'</sub>	<sup>1</sup> D <sub>C6/C8- H6/H8</sub>	<sup>1</sup> D <sub>C2-H2</sub>	<sup>1</sup> D <sub>C1'- H1'</sub>	ΣH1' ( <sup>3</sup> J <sub>H2'- H1'</sub> )	ΣH1' ( <sup>3</sup> J <sub>H2'- H1'</sub> )
C1	88.3	5.91	40.7	2.15	2.56	143.2	7.85	88.3	4.11	99.4	5.96					182.7		172.7	13.6		-6.5	14.0	
T2	85.9	5.69	39.0	2.24	2.52	139.8	7.55	86.4	4.19	14.5	1.73	159.2	13.71			178.8		166.0	13.6		11.1	13.6	17.5
A3	84.9	6.25	40.3	2.74	2.91	141.8	8.33	87.5	4.44	154.8	7.58					214.5	201.3	166.2	13.3	10.7	14.0	13.8	16.8
C4	86.1	5.56	39.7	1.93	2.33	142.0	7.23	85.2	4.16	98.4	5.28			8.21	6.50	178.6		165.3	16.3		5.7	13.3	17.1
G5	84.5	5.82	40.6	2.58	2.68	138.2	7.82	87.2	4.33			147.0	12.89			212.2		162.6	13.9		14.1	13.5	-
C6	86.3	5.68	39.9	2.01	2.38	142.2	7.26	85.6	4.16	98.4	5.27			8.24	6.31	177.1		168.5	19.9		11.8	12.7	17.5
G7	84.6	5.93	40.4	2.55	2.79	138.2	7.83	87.2	4.33			147.0	12.89			211.5		164.3	19.2		13.1	-	-
<sup>5m</sup> C8	86.1	5.56	39.8	1.98	2.31	138.9	7.06	85.6	4.16	15.1	1.57			8.55	6.05	176.6		165.7	20.0		9.1	13.7	16.5
G9	84.7	5.90	40.6	2.58	2.71	138.3	7.83	87.2	4.33			147.0	12.75			213.7		164.8	15.4		13.9	-	-
T10	85.3	5.60	39.1	1.96	2.27	138.6	7.21	85.6	4.13	14.5	1.51	158.5	13.63			177.9		167.6	11.5		11.7	13.3	17.4
A11	85.0	6.06	40.1	2.68	2.86	141.9	8.19	87.4	4.39	154.3	7.50					213.8	201.9	166.2	9.1	11.9	12.4	13.7	16.8
G12	84.2	6.01	42.4	2.27	2.43	138.5	7.71	87.4	4.17							212.2		164.0	7.8		7.9	16.8	13.3

**DNA<sup>M3</sup> d(CTA<sup>5m</sup>CG<sup>5m</sup>CG<sup>5m</sup>CGTAG)<sub>2</sub>**

Nt	C1'	H1'	C2'	H2'	H2''	C6/C8	H6/H8	C4'	H4'	C2/C5 /C7	H2/H5 /H7	N1/N3	H1/H3	H41	H42	<sup>1</sup> J <sub>C6/C8- H6/H8</sub>	<sup>1</sup> J <sub>C2-H2</sub>	<sup>1</sup> J <sub>C1'-H1'</sub>	<sup>1</sup> D <sub>C6/C8 -H6/H8</sub>	<sup>1</sup> D <sub>C2-H2</sub>	<sup>1</sup> D <sub>C1'- H1'</sub>	ΣH1' ( <sup>3</sup> J <sub>H2'- H1'</sub> )	ΣH1' ( <sup>3</sup> J <sub>H2'- H1'</sub> )
C1	88.3	5.91	40.7	2.15	2.56	143.2	7.85	88.3	4.11	99.4	5.96					173.0		173.0	14.3		-8.3	14.0	16.6
T2	85.9	5.71	39.0	2.24	2.52	139.7	7.55	86.4	4.19	14.5	1.73					164.7		164.7	12.3		13.7	13.6	16.2
A3	84.9	6.28	40.2	2.72	2.96	141.8	8.39	87.6	4.44	154.7	7.59					165.1	201.7	165.1	13.0	10.5	13.7	14.4	16.8
<sup>5m</sup> C4	85.9	5.50	39.7	1.97	2.29	138.9	7.07	85.2	4.14	14.9	1.57			8.43	6.17	164.7		164.7	17.4		1.7	14.3	-
G5	84.8	5.90	40.7	2.53	2.75	138.1	7.77	87.1	4.33			147.1	12.86			163.8		163.8	17.3		14.2	-	16.5
<sup>5m</sup> C6	86.2	5.61	39.8	2.03	2.34	138.9	7.08	85.6	4.14	15.0	1.50			8.55	5.96	167.4		167.4	18.2		10.8	12.4	-
G7	84.7	5.91	40.7	2.55	2.78	138.1	7.81	87.1	4.33			147.1	12.89			163.4		163.4	15.1		14.4	-	16.2
<sup>5m</sup> C8	86.2	5.62	39.8	2.05	2.36	138.9	7.09	85.6	4.14	15.1	1.54			8.56	5.95	166.2		166.2	17.0		11.0	13.7	-
G9	84.6	5.90	40.7	2.57	2.72	138.2	7.81	87.1	4.33			146.9	12.75			167.0		167.0	15.1		9.3	-	17.3
T10	85.3	5.61	39.2	1.99	2.30	138.6	7.23	85.6	4.14	14.4	1.48	158.5	13.61			165.9		165.9	16.8		11.9	13.9	16.1
A11	85.0	6.06	40.1	2.68	2.86	141.9	8.19	87.4	4.37	154.3	7.54					164.8	203.7	164.8	8.6	12.5	13.8	13.7	14.7
G12	84.2	6.01	42.4	2.26	2.43	138.5	7.71	87.4	4.17							164.0		164.0	7.0		6.9	16.1	



**DNA<sup>H6</sup> d(CTACG<sup>5hm</sup>CGCGTAG)<sub>2</sub>**

Nt	C1'	H1'	C2'	H2'	H2''	C6/C8	H6/H8	C4'	H4'	C2/C5 /C7	H2/H5 /H7	N1/N3	H1/H3	H41	H42	<sup>1</sup> J <sub>C6/C8- H6/H8</sub>	<sup>1</sup> J <sub>C2-H2</sub>	<sup>1</sup> J <sub>C1'-H1'</sub>	<sup>1</sup> D <sub>C6/C8 -H6/H8</sub>	<sup>1</sup> D <sub>C2-H2</sub>	<sup>1</sup> D <sub>C1'- H1'</sub>	ΣH1' ( <sup>3</sup> J <sub>H2'- H1'</sub> )	ΣH1' ( <sup>3</sup> J <sub>H2''- H1'</sub> )
C1	88.3	5.91	40.7	2.15	2.56	143.2	7.85	88.3	4.11	99.4	5.97					181.7		173.3	12.9		-7.2	14.0	
T2	85.9	5.68	39.0	2.23	2.52	139.7	7.55	86.4	4.19	14.5	1.73	159.2	13.71			177.9		167.0	11.8		10.9	13.9	16.6
A3	84.9	6.23	40.2	2.74	2.89	141.8	8.33	87.5	4.43	154.8	7.58					214.6	200.8	165.9	13.1	8.5	12.6	13.7	16.5
C4	86.1	5.54	39.8	1.96	2.31	142.1	7.25	85.2	4.16	98.3	5.27			8.14	6.52	178.0		166.7	18.3		2.1	13.8	16.9
G5	84.6	5.92	40.5	2.48	2.74	138.0	7.78	87.3	4.34			147.0	12.87			211.9		163.2	16.3		14.6	13.8	-
<sup>5hm</sup> C6	86.2	5.51	39.9	1.95	2.32	140.5	7.23	85.2	4.16	60.1	3.94			8.68	6.23	177.9		165.7	17.9		9.2	13.0	16.5
G7	84.5	5.87	40.5	2.63	2.72	138.4	7.89	87.3	4.35			146.8	12.86			212.8		163.0	15.6		12.6	13.8	15.7
C8	86.3	5.70	40.0	2.01	2.39	142.2	7.26	85.5	4.17	98.5	5.27			8.23	6.34	177.8		167.3	16.9		10.5	13.1	16.2
G9	84.6	5.91	40.5	2.59	2.74	138.4	7.87	87.2	4.33			146.9	12.91			212.8		164.3	16.7		12.9	-	-
T10	85.2	5.57	39.1	1.94	2.26	138.5	7.20	85.5	4.12	14.5	1.53	158.5	13.63			177.9		166.4	11.2		10.2	13.5	16.8
A11	85.0	6.06	40.1	2.68	2.86	141.9	8.18	87.5	4.39	154.3	7.55					213.7	201.7	166.0	9.0	13.2	12.6	13.3	16.8
G12	84.2	6.01	42.4	2.27	2.43	138.5	7.71	87.4	4.17							211.2		164.1	7.2		5.7	16.3	14.0

DNA <sup>H8</sup> d(CTACGCG <sup>5hm</sup> CGTAG) <sub>2</sub>																							
Nt	C1'	H1'	C2'	H2'	H2''	C6/C8	H6/H8	C4'	H4'	C2/C5 /C7	H2/H5 /H7	N1/N3	H1/H3	H41	H42	<sup>1</sup> J <sub>C6/C8- H6/H8</sub>	<sup>1</sup> J <sub>C2-H2</sub>	<sup>1</sup> J <sub>C1'-H1'</sub>	<sup>1</sup> D <sub>C6/C8- H6/H8</sub>	<sup>1</sup> D <sub>C2-H2</sub>	<sup>1</sup> D <sub>C1'- H1'</sub>	$\Sigma$ H1' <sup>(3)</sup> J <sub>H2'-H1'</sub>	$\Sigma$ H1' <sup>(3)</sup> J <sub>H2''-H1'</sub>
C1	88.3	5.91	40.7	2.14	2.56	143.2	7.85	88.2	4.11	99.4	5.96					181.9		172.9	13.4		-5.9	13.3	
T2	85.9	5.69	39.0	2.23	2.52	139.7	7.54	86.4	4.19	14.5	1.73	159.2	13.70			177.6		167.0	13.9		8.5	13.3	16.5
A3	84.9	6.23	40.2	2.74	2.90	141.8	8.33	87.5	4.43	154.8	7.59					214.5	200.5	165.5	12.8	10.5	14.6	14.0	16.1
C4	86.1	5.57	39.7	1.91	2.34	142.0	7.22	85.2	4.16	98.5	5.25			8.19	6.53	178.2		167.4	16.8		2.7	14.9	15.6
G5	84.4	5.81	40.6	2.59	2.66	138.2	7.83	87.3	4.33			146.7	12.76			212.2		162.8	16.1		17.0	14.7	15.5
C6	86.3	5.68	40.0	2.00	2.37	142.3	7.26	85.6	4.16	98.4	5.27			8.21	6.32	177.6		166.8	23.7		12.2	13.9	15.9
G7	84.5	5.93	40.4	2.50	2.76	138.0	7.80	87.3	4.33			147.0	12.91			212.2		163.9	14.9		13.0	13.2	15.4
<sup>5hm</sup> C8	86.2	5.49	39.9	2.02	2.32	140.5	7.26	85.0	4.11	60.1	4.00			8.64	6.25	177.5		166.2	19.4		10.1	14.1	15.9
G9	84.8	5.94	40.6	2.58	2.75	138.5	7.87	87.3	4.36			146.9	12.79			212.2		164.8	18.2		13.2	13.8	15.4
T10	85.1	5.58	39.1	1.95	2.26	138.5	7.20	85.5	4.11	14.5	1.52	158.5	13.64			177.5		165.9	12.8		11.5	14.2	16.2
A11	85.0	6.06	40.1	2.68	2.86	141.9	8.19	87.4	4.39	154.3	7.54					213.1	202.6	165.7	10.6	11.8	12.2	13.7	16.1
G12	84.2	6.01	42.4	2.26	2.43	138.5	7.71	87.4	4.17							211.5		163.8	8.1		6.3	15.4	14.7

**DNA<sup>H3</sup> d(CTA<sup>5hm</sup>CG<sup>5hm</sup>CG<sup>5hm</sup>CGTAG)<sub>2</sub>**

Nt	C1'	H1'	C2'	H2'	H2''	C6/C8	H6/H8	C4'	H4'	C2/C5 /C7	H2/H5 /H7	N1/N3	H1/H3	H41	H42	<sup>1</sup> J <sub>C6/C8- H6/H8</sub>	<sup>1</sup> J <sub>C2-H2</sub>	<sup>1</sup> J <sub>C1'-H1'</sub>	<sup>1</sup> D <sub>C6/C8- H6/H8</sub>	<sup>1</sup> D <sub>C2-H2</sub>	<sup>1</sup> D <sub>C1'- H1'</sub>	ΣH1' ( <sup>3</sup> J <sub>H2'- H1'</sub> )	ΣH1' ( <sup>3</sup> J <sub>H2'- H1'</sub> )
C1	88.3	5.90	40.7	2.14	2.56	143.2	7.85	88.2	4.11	99.4	5.96					181.7		172.6	11.7		-5.9	13.8	
T2	85.9	5.69	39.0	2.24	2.51	139.7	7.54	86.4	4.19	14.5	1.72					178.5		167.1	10.2		9.6	13.4	16.8
A3	84.9	6.27	40.3	2.67	2.93	141.7	8.34	87.6	4.43	154.8	7.58					212.8	201.5	165.4	13.2	9.0	12.6	13.6	17.0
<sup>5hm</sup> C4	86.1	5.48	39.8	1.98	2.32	140.5	7.25	85.2	4.15	60.0	3.96			8.5	6.38	177.9		166.1	17.0		4.8	13.7	16.2
G5	84.7	5.90	40.8	2.48	2.74	138.3	7.80	87.3	4.34			146.8	12.79			211.8		162.1	13.8		14.8	13.6	-
<sup>5hm</sup> C6	86.2	5.55	39.9	2.03	2.35	140.5	7.26	85.2	4.14	60.0	3.84			8.61	6.2	178.0		167.5	16.8		10.2	13.6	-
G7	84.7	5.93	40.8	2.51	2.77	138.3	7.84	87.3	4.34			146.8	12.84			211.5		163.7	20.1		11.5	-	-
<sup>5hm</sup> C8	86.3	5.56	39.9	2.07	2.37	140.5	7.28	85.2	4.14	60.0	3.93			8.61	6.22	177.6		165.9	16.8		8.7	14.0	16.6
G9	84.8	5.93	40.8	2.57	2.74	138.5	7.87	87.3	4.34			146.6	12.68			212.4		164.9	13.6		11.1	14.6	-
T10	85.2	5.59	39.1	1.98	2.28	138.6	7.22	85.6	4.13	14.4	1.48	158.4	13.61			177.8		166.6	10.5		8.3	14.4	17.7
A11	85.0	6.06	40.1	2.68	2.87	141.9	8.19	87.5	4.39	154.3	7.50					213.3	201.2	166.2	8.2	10.7	8.5	13.7	16.4
G12	84.2	6.00	42.4	2.26	2.43	138.5	7.71	87.4	4.17							212.2		163.6	5.3		7.0	16.5	13.4

**DNA<sup>F6</sup> d(CTACG<sup>5f</sup>CGCGTAG)<sub>2</sub>**

Nt	C1'	H1'	C2'	H2'	H2''	C6/C8	H6/H8	C4'	H4'	C2/C5 /C7	H2/H5 /H7	N1/N3	H1/H3	H41	H42	<sup>1</sup> J <sub>C6/C8- H6/H8</sub>	<sup>1</sup> J <sub>C2-H2</sub>	<sup>1</sup> J <sub>C1'-H1'</sub>	<sup>1</sup> D <sub>C6/C8- H6/H8</sub>	<sup>1</sup> D <sub>C2-H2</sub>	<sup>1</sup> D <sub>C1'- H1'</sub>	ΣH1' ( <sup>3</sup> J <sub>H2'- H1'</sub> )	ΣH1' ( <sup>3</sup> J <sub>H2'- H1'</sub> )
C1	88.3	5.91	40.6	2.13	2.56	143.2	7.84	88.2	4.11	99.4	5.96					181.4		172.3	12.8		-6.6	13.3	14.0
T2	85.9	5.66	39.0	2.23	2.51	139.7	7.54	86.4	4.18	14.5	1.72	159.2	13.70			177.7		163.9	14.5		11.7	12.6	14.0
A3	84.9	6.22	40.2	2.73	2.88	141.8	8.32	87.5	4.43	154.7	7.58					213.8	200.9	165.2	12.9	8.7	14.6	14.3	14.3
C4	86.0	5.54	39.7	1.93	2.29	142.1	7.22	85.3	4.16	98.4	5.24			8.14	6.49	180.1		166.9	21.1		2.9	13.9	13.0
G5	84.4	5.93	40.6	2.56	2.78	137.9	7.73	87.3	4.34			147.1	12.92			210.6		164.3	14.2		15.2	-	14.3
<sup>5f</sup> C6	87.0	5.62	40.5	2.01	2.42	155.3	8.12	85.5	4.16	191.8	9.25			9.1	7.86	177.8		172.1	19.4		2.5	14.4	13.3
G7	84.5	5.89	40.7	2.61	2.73	138.6	7.90	87.3	4.36			146.3	12.55			212.0		163.0	19.3		11.2	14.3	14.5
C8	86.4	5.70	40.2	1.99	2.37	142.2	7.25	85.3	4.16	98.4	5.23			8.2	6.35	178.8		168.2	20.2		10.2	13.4	13.6
G9	84.6	5.92	40.4	2.60	2.74	138.4	7.87	87.3	4.34			146.9	12.74			211.7		164.8	18.8		12.4	13.4	14.5
T10	85.1	5.56	39.0	1.94	2.25	138.5	7.19	85.5	4.11	14.5	1.53	158.5	13.63			178.2		166.1	9.5		10.7	13.2	14.0
A11	85.0	6.05	40.1	2.68	2.86	141.9	8.18	87.5	4.38	154.3	7.55					213.6	201.3	166.7	8.1	12.3	11.8	14.0	14.7
G12	84.2	6.01	42.4	2.26	2.44	138.5	7.71	87.4	4.17							211.6		162.8	6.2		7.9	15.4	16.1

DNA <sup>F8</sup> d(CTACGCG <sup>5f</sup> CGTAG) <sub>2</sub>																							
Nt	C1'	H1'	C2'	H2'	H2''	C6/C8	H6/H8	C4'	H4'	C2/C5 /C7	H2/H5 /H7	N1/N3	H1/H3	H41	H42	<sup>1</sup> J <sub>C6/C8- H6/H8</sub>	<sup>1</sup> J <sub>C2-H2</sub>	<sup>1</sup> J <sub>C1'-H1'</sub>	<sup>1</sup> D <sub>C6/C8 -H6/H8</sub>	<sup>1</sup> D <sub>C2-H2</sub>	<sup>1</sup> D <sub>C1'- H1'</sub>	ΣH1' ( <sup>3</sup> J <sub>H2'- H1'</sub> )	ΣH1' ( <sup>3</sup> J <sub>H2'- H1'</sub> )
C1	88.3	5.91	40.7	2.14	2.56	143.2	7.84	88.2	4.11							181.9		171.7	13.8		-5.2	13.3	12.6
T2	85.9	5.69	39.0	2.24	2.51	139.7	7.53	86.4	4.19	14.5	1.72	159.3	13.69			177.8		165.7	11.5		11.9	16.4	16.5
A3	84.9	6.24	40.2	2.75	2.90	141.8	8.33	87.5	4.43	154.8	7.60					214.2	200.2	167.2	12.3	12.6	12.7	16.1	16.5
C4	86.1	5.51	39.7	1.94	2.34	142.1	7.25	85.3	4.16	98.4	5.29			8.18	6.57	179.0		165.9	18.1		4.4	16.1	16.1
G5	84.5	5.85	40.6	2.58	2.70	138.4	7.85	87.3	4.34			146.2	12.50			212.7		163.4	15.7		12.8	16.8	16.5
C6	86.2	5.66	40.0	1.92	2.32	142.2	7.21	85.5	4.13	98.4	5.21			8.2	6.35	178.0		168.2	18.4		9.5	14.5	15.9
G7	84.2	5.94	40.3	2.59	2.80	137.9	7.77	87.3	4.34			147.2	12.97			211.7		163.1	14.3		12.0	16.0	16.7
<sup>5f</sup> C8	87.1	5.61	40.4	2.05	2.41	155.3	8.12	85.4	4.18	191.9	9.27			9.1	7.81	178.2		171.1	16.6		6.1	15.5	15.1
G9	84.7	5.93	40.6	2.59	2.73	138.6	7.88	87.3	4.34			147.0	12.78			213.9		164.3	13.6		9.3	16.1	16.1
T10	85.2	5.57	39.0	1.96	2.25	138.6	7.21	85.5	4.12	14.4	1.51	158.5	13.66			178.0		166.8	11.5		7.8	16.5	16.1
A11	85.0	6.06	40.0	2.69	2.86	141.9	8.18	87.5	4.39	154.3	7.54					214.1	203.0	166.1	8.2	9.1	9.7	15.8	15.7
G12	84.2	6.01	42.4	2.27	2.44	138.5	7.71	87.4	4.17							213.0		165.1	5.8		5.1	15.4	14.7

DNA <sup>F3</sup> d(CTA <sup>5f</sup> CG <sup>5f</sup> CG <sup>5f</sup> CGTAG) <sub>2</sub>																							
Nt	C1'	H1'	C2'	H2'	H2''	C6/C8	H6/H8	C4'	H4'	C2/C5 /C7	H2/H5 /H7	N1/N3	H1/H3	H41	H42	<sup>1</sup> J <sub>C6/C8- H6/H8</sub>	<sup>1</sup> J <sub>C2-H2</sub>	<sup>1</sup> J <sub>C1'-H1'</sub>	<sup>1</sup> D <sub>C6/C8 -H6/H8</sub>	<sup>1</sup> D <sub>C2-H2</sub>	<sup>1</sup> D <sub>C1'- H1'</sub>	ΣH1' ( <sup>3</sup> J <sub>H2'- H1'</sub> )	ΣH1' ( <sup>3</sup> J <sub>H2''- H1'</sub> )
C1	88.3	5.90	40.6	2.12	2.54	143.2	7.83	88.3	4.10	99.4	5.96					182.4		171.9	12.65 5	-5.3	13.6	12.8	
T2	85.8	5.65	38.9	2.22	2.46	139.7	7.51	86.4	4.18	14.5	1.70	159.1	13.66			177.6		164.5	11.72 5	15.6	13.3	17.1	
A3	84.7	6.28	40.3	2.77	2.98	141.7	8.31	87.6	4.45	155.0	7.58					214.6	200.1	167.2	13.28	9.2	13.3	13.7	16.5
<sup>5f</sup> C4	86.8	5.57	40.3	2.01	2.39	155.4	8.14	85.5	4.22	191.7	9.23			8.97	7.91	178.0		171.0	19.18 5	-4.8	13.8	16.1	
G5	84.5	5.94	40.7	2.62	2.87	138.4	7.77	87.4	4.35			146.4	12.54			212.4		163.8	20.52 5	18.6	14.3	17.1	
<sup>5f</sup> C6	87.0	5.64	40.5	2.02	2.40	155.4	8.11	85.5	4.18	191.6	9.18			9.0	7.79	176.8		168.1	20.54	6.2	13.8	15.0	
G7	84.5	5.95	40.7	2.66	2.81	138.4	7.81	87.4	4.35			146.4	12.56			212.7		162.0	19.66	13.4	-	16.5	
<sup>5f</sup> C8	87.2	5.68	40.5	2.10	2.45	155.4	8.14	85.5	4.21	191.9	9.24			9.0	7.85	178.0		171.0	17.61 5	6.8	13.5	15.5	
G9	84.7	5.95	40.8	2.65	2.77	138.9	7.91	87.4	4.35			146.1	12.38			213.0		165.5	16.73	10.4	-	15.8	
T10	85.1	5.56	39.1	1.96	2.24	138.6	7.20	85.5	4.12	14.3	1.45	158.3	13.51			176.6		165.1	15.73	11.6	13.4	16.4	
A11	85.0	6.06	40.0	2.70	2.87	141.9	8.18	87.6	4.39	154.3	7.52					213.9	202.1	166.9	7.515	11.6	11.8	14.7	15.8
G12	84.2	6.00	42.4	2.25	2.44	138.5	7.71	87.4	4.17							211.8		164.0	6.455	5.2	16.1	14.0	

**Table S2:** The chemical shift perturbations (CSP) that arise due to the epigenetic modifications is tabulated. The presence of the modifications in 8<sup>th</sup> position (from DNA<sup>N8</sup>) provides the effect due to H-bonding (observed from **G5**) and stacking on the 5'-/3'-neighbors (G7/G9, respectively). Thus, for the 6<sup>th</sup> position modification (in DNA<sup>N6</sup>), we see that the CSP observed for G7 is a sum of H-bonding (as it pairs with C6) and stacking in the 3'-end (due to modification in the 6<sup>th</sup> position). For instance, the CSP of G5-N1 in DNA<sup>F8</sup> is -0.8 ppm, with G7 experiencing +0.1 ppm and no change for G5. Thus, the CSP of G7-N1 in DNA<sup>F6</sup> is -0.8+0.1 = -0.7 ppm. The same trend of such arithmetic sums of CSPs can be observed for <sup>13</sup>C-C6/C8 and <sup>13</sup>C-C1' resonances as well for the various cytosine modifications.

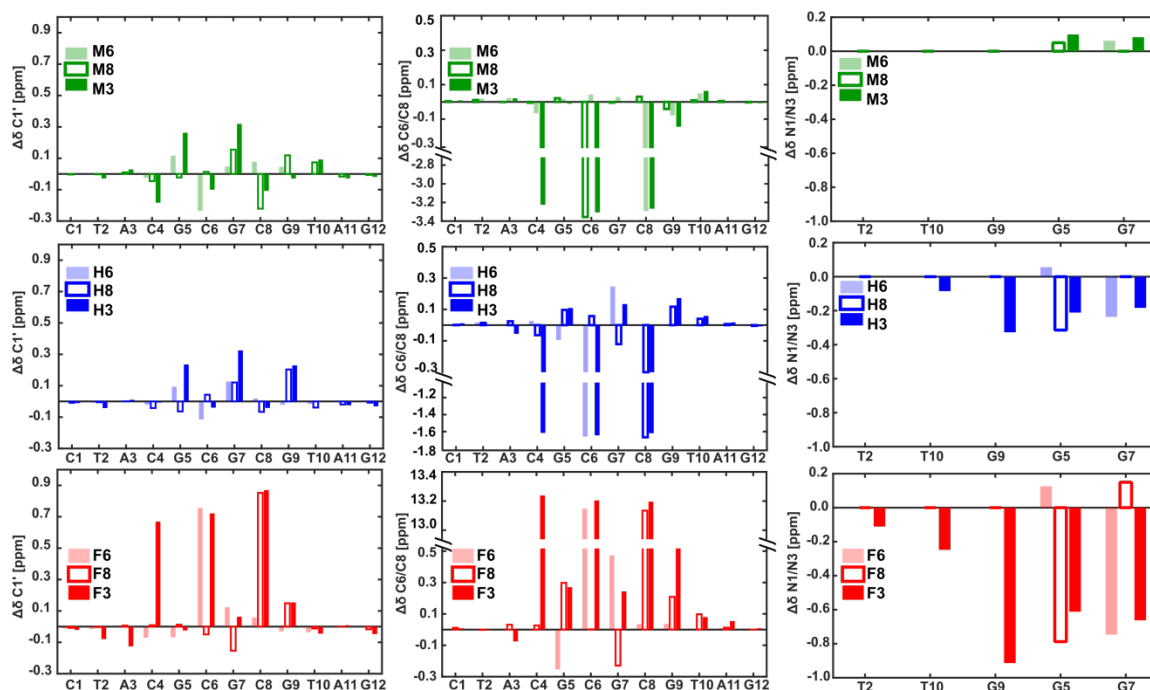
Modified-Control DNA $\Delta\delta$ (ppm)										
N3/N1	DNA <sup>control</sup>	DNA <sup>M6</sup>	DNA <sup>M8</sup>	DNA <sup>M3</sup>	DNA <sup>H6</sup>	DNA <sup>H8</sup>	DNA <sup>H3</sup>	DNA <sup>F6</sup>	DNA <sup>F8</sup>	DNA <sup>F3</sup>
<b>T2-A11</b>	159.3	0.0	0.0	-	0.0	0.0	-	0.0	0.0	-0.1
<b>A3-T10</b>	158.5	0.0	0.0	0.0	0.0	0.0	-0.1	0.0	0.0	-0.2
<b>C4-G9</b>	147.0	0.0	0.0	0.0	0.0	0.0	-0.3	-0.1	0.0	-0.9
<b>G5-C8</b>	147.0	0.0	0.1	0.1	0.1	-0.3	-0.2	0.1	-0.8	-0.6
<b>C6-G7</b>	147.0	0.1	0.0	0.1	-0.2	0.0	-0.2	-0.7	0.1	-0.7

Modified-Control DNA $\Delta\delta$ (ppm)										
C1'	DNA <sup>control</sup>	DNA <sup>M6</sup>	DNA <sup>M8</sup>	DNA <sup>M3</sup>	DNA <sup>H6</sup>	DNA <sup>H8</sup>	DNA <sup>H3</sup>	DNA <sup>F6</sup>	DNA <sup>F8</sup>	DNA <sup>F3</sup>
<b>TSP</b>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<b>C1</b>	88.3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<b>T2</b>	85.9	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.1
<b>A3</b>	84.9	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.1
<b>C4</b>	86.1	0.0	0.0	-0.2	0.0	0.0	0.0	-0.1	0.0	0.7
<b>G5</b>	84.5	0.1	0.0	0.3	0.1	-0.1	0.2	-0.1	0.0	0.0
<b>C6</b>	86.3	-0.2	0.0	-0.1	-0.1	0.0	0.0	0.8	0.0	0.7
<b>G7</b>	84.4	0.0	0.2	0.3	0.1	0.1	0.3	0.1	-0.2	0.1
<b>C8</b>	86.3	0.1	-0.2	-0.1	0.0	-0.1	0.0	0.1	0.9	0.9
<b>G9</b>	84.6	0.0	0.1	0.0	0.0	0.2	0.2	0.0	0.1	0.2
<b>T10</b>	85.2	0.0	0.1	0.1	0.0	0.0	0.0	0.0	0.0	0.0
<b>A11</b>	85.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<b>G12</b>	84.2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

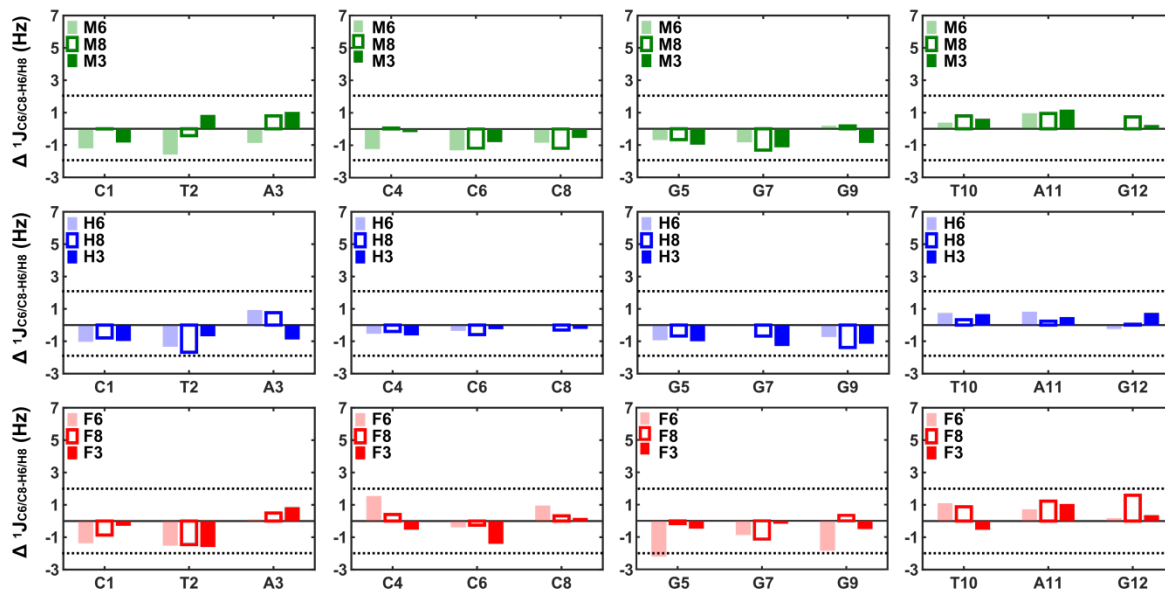
Modified-Control DNA $\Delta\delta$ (ppm)										
<b>C6/C8</b>	<b>DNA<sup>control</sup></b>	<b>DNA<sup>M6</sup></b>	<b>DNA<sup>M8</sup></b>	<b>DNA<sup>M3</sup></b>	<b>DNA<sup>H6</sup></b>	<b>DNA<sup>H8</sup></b>	<b>DNA<sup>H3</sup></b>	<b>DNA<sup>F6</sup></b>	<b>DNA<sup>F8</sup></b>	<b>DNA<sup>F3</sup></b>
<b>C1</b>	143.2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<b>T2</b>	139.7	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<b>A3</b>	141.8	0.0	0.0	0.0	0.0	0.0	-0.1	0.0	0.0	-0.1
<b>C4</b>	142.1	0.0	-0.1	-3.2	0.0	-0.1	-1.6	0.0	0.0	13.2
<b>G5</b>	138.1	0.0	0.0	0.0	-0.1	0.1	0.1	-0.3	0.3	0.3
<b>C6</b>	142.2	-3.4	0.0	-3.3	-1.7	0.1	-1.6	13.1	0.0	13.2
<b>G7</b>	138.1	0.0	0.0	0.0	0.2	-0.1	0.1	0.5	-0.2	0.2
<b>C8</b>	142.2	0.0	-3.3	-3.3	0.0	-1.7	-1.6	0.0	13.1	13.2
<b>G9</b>	138.4	0.0	-0.1	-0.1	0.0	0.1	0.2	0.0	0.2	0.5
<b>T10</b>	138.5	0.0	0.0	0.1	0.0	0.0	0.1	0.0	0.1	0.1
<b>A11</b>	141.9	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1
<b>G12</b>	138.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0



4.  $^{13}\text{C}/^{15}\text{N}$  chemical shift and  $^1\text{J}_{\text{C-H}}$  perturbations for all the nucleotides across samples ( $\text{DNA}^{\text{N\#}}$ ) compared to  $\text{DNA}^{\text{control}}$



**Figure S3:** Chemical shift differences of  $\text{DNA}^{\text{N\#}}$  compared to  $\text{DNA}^{\text{control}}$ . Left panel: changes to sugar  $^{13}\text{C}\text{-C1'}$  chemical shifts magnitudes ( $\Delta\delta \text{C1'}$ , in ppm). Middle panel: changes to aromatic  $^{13}\text{C}\text{-C6/C8}$  chemical shifts magnitudes ( $\Delta\delta \text{C6/C8}$ , in ppm); Right panel: changes to imino  $^{15}\text{N}\text{-N1/N3}$  chemical shifts magnitudes ( $\Delta\delta \text{N1/N3}$ , in ppm) for all nucleotide positions from 1-12 upon cytosine modification across  $\text{DNA}^{\text{N\#}}$  samples. With  $\text{DNA}^{\text{M6/M8/M3}}$  (in green),  $\text{DNA}^{\text{H6/H8/H3}}$  (in blue), and  $\text{DNA}^{\text{F6/F8/F3}}$  (in red) showing significant changes relative to  $\text{DNA}^{\text{control}}$ .



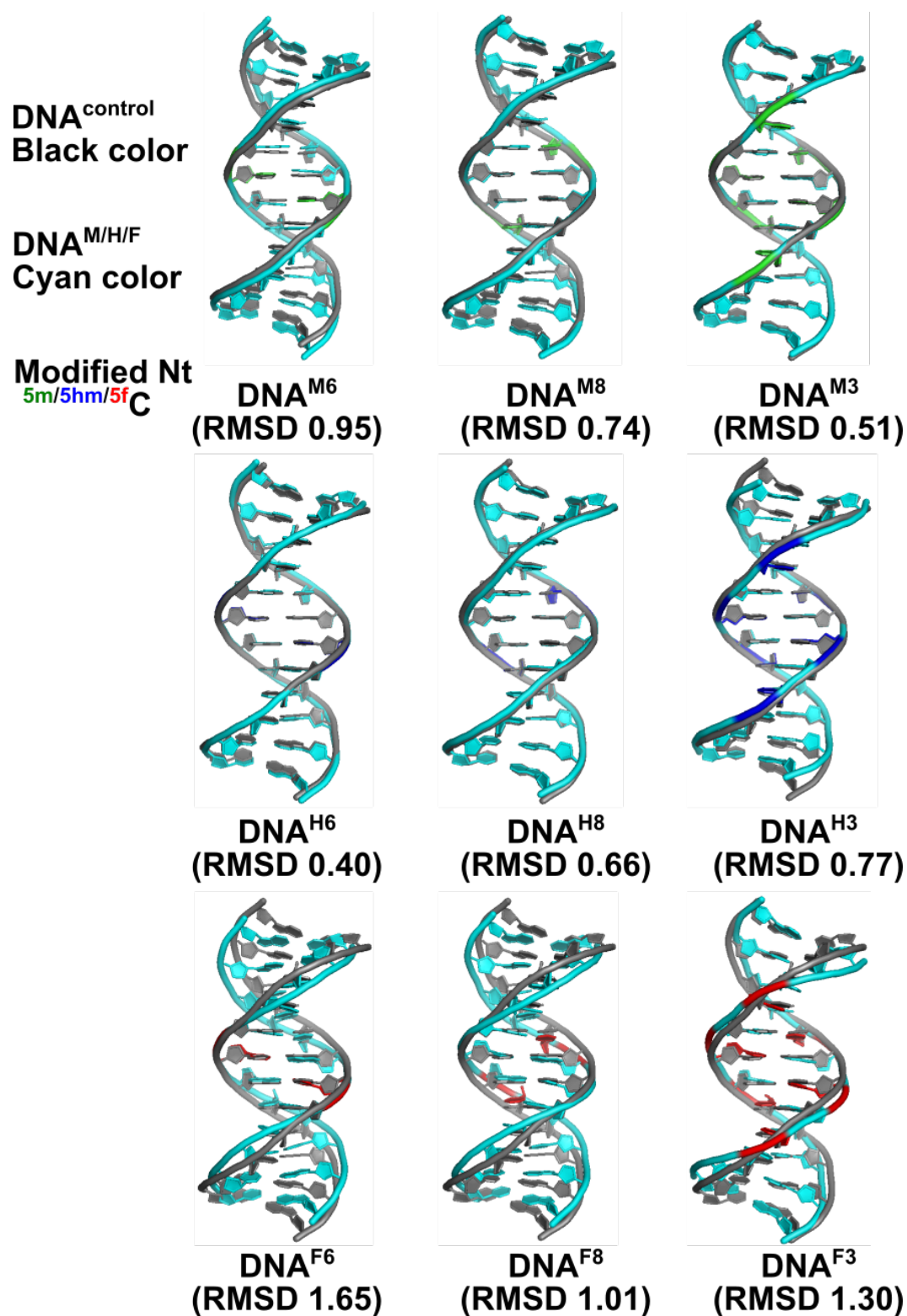
**Figure S4:** Changes to one-bond  $^{13}\text{C}$ - $^1\text{H}$  C6/C8-H6/H8 heteronuclear scalar coupling magnitudes ( $\Delta^1J_{\text{C6/C8-H6/H8}}$ , in Hz) for all nucleotide positions 1-12 upon cytosine modification across DNA<sup>N#</sup> samples. Measurement uncertainty (2 Hz) is marked with dotted lines, with DNA<sup>M6/M8/M3</sup> (in green, upper panel), DNA<sup>H6/H8/H3</sup> (in blue, middle panel), and DNA<sup>F6/F8/F3</sup> (in red, lower panel) showing significant changes relative to DNA<sup>control</sup>.

## 5. Statistics of structure refinement constraints

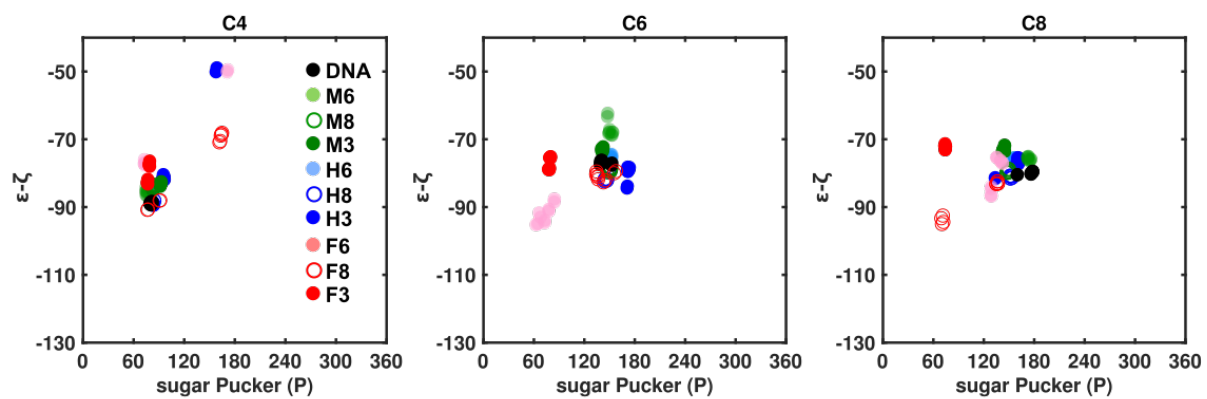
	DNA <sup>control</sup>	DNA <sup>M6</sup>	DNA <sup>M8</sup>	DNA <sup>M3</sup>	DNA <sup>H6</sup>	DNA <sup>H8</sup>	DNA <sup>H3</sup>	DNA <sup>F6</sup>	DNA <sup>F8</sup>	DNA <sup>F3</sup>
Dihedral restraints	116	116	116	116	116	116	116	116	116	116
H-bond restraints	72	72	72	72	72	72	72	72	72	72
Base-pair planarity restraints	26	26	26	26	26	26	26	26	26	26
NOE restraints	324	276	288	262	286	289	292	282	282	288
RDC restraints	44	44	44	44	44	44	44	44	44	44
D <sub>a</sub> , R	-20.0, 0.26	-20.0, 0.26	-20.0, 0.26	-20.0, 0.26	-20.0, 0.26	-20.0, 0.26	-20.0, 0.26	-20.0, 0.26	-20.0, 0.26	-20.0, 0.26
Dihedral angle violations (>6°)	0	0	0	0	0	0	0	0	0	0
NOE violations (>0.5 Å)	0	0	0	0	0	0	0	0	0	0
RDC RMSD (Hz)	1.81 ± 0.07	1.55 ± 0.08	1.09 ± 0.01	1.21 ± 0.01	1.46 ± 0.00	1.54 ± 0.03	1.22 ± 0.11	1.75 ± 0.03	1.33 ± 0.13	1.75 ± 0.01

**Table S3:** Statistics on the structure refinement of DNA<sup>control</sup>, and DNA<sup>N#</sup> systems.

6. Cartoon model comparison of DNA<sup>control</sup> and DNA<sup>N#</sup>



**Figure S5:** Aligned structures of DNA<sup>N#</sup> with respect to DNA<sup>control</sup>, only heavy atoms of nucleotides 3-10 and 15-22 were aligned using pymol, root mean square deviation (RMSD) calculated for aligned structures for all heavy atoms of 3-10, 15-22 were provided for each overlaid structures. DNA<sup>control</sup> is shown in grey and DNA<sup>N#</sup> shown as cyan, with modification sites being represented in specific colors, <sup>5m</sup>C (green), <sup>5hm</sup>C (blue), and <sup>5f</sup>C (red)



**Figure S6:** Correlation of  $\varepsilon\text{-}\zeta$  values to the sugar pucker (P) for DNA<sup>control</sup> and DNA<sup>N#</sup>. Backbone conformation defined by  $\varepsilon\text{-}\zeta < 0$  for BI and  $\varepsilon\text{-}\zeta > 0$  for BII. Here **C4**, **C6**, **C8** nucleotides sample BI conformation canonical to B-DNA

**Table S4:** Structural parameters for Xplor-NIH refined structures of DNA<sup>control</sup> and DNA<sup>N#</sup>. Average (Avg) and standard deviation (std) are for ensemble of 5 structures

Tip (°)																				
Base Steps	DNA <sup>control</sup>		DNA <sup>M6</sup>		DNA <sup>M8</sup>		DNA <sup>M3</sup>		DNA <sup>H6</sup>		DNA <sup>H8</sup>		DNA <sup>H3</sup>		DNA <sup>F6</sup>		DNA <sup>F8</sup>		DNA <sup>F3</sup>	
	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std
01CT/11AG	-0.32	0.49	-4.74	0.44	0.59	0.17	-1.31	2.15	-3.43	0.28	0.46	1.08	-7.33	1.32	-1.56	2.71	-0.57	0.83	-4.53	1.87
02TA/10TA	1.91	0.48	2.9	0.32	-0.41	0.1	4.61	0.18	0.85	0.09	-0.67	0.23	0.47	0.4	-1.69	1.04	-1.7	0.57	9.47	0.42
03AC/09GT	-1.26	1.53	2.16	1.06	-0.01	0.35	-2.52	0.19	7.97	0.1	1.35	0.49	2.43	0.41	0.39	4.3	-0.12	2.46	-1.28	0.18
04CG/08CG	-6.36	0.12	-6.96	0.12	-5.91	0.21	-6.65	0.11	-6.82	0.09	-5.97	0.19	-1.66	4.51	5.3	1.64	6.88	6.2	-2.91	0.17
05GC/07GC	-0.57	0.86	8.86	0.52	2.88	0.08	3.1	0.16	1.99	0.17	1.92	0.19	2.8	1.19	2.33	0.63	-0.46	1.19	3.11	0.13
06CG/06CG	-0.05	0.01	0	0.02	-0.04	0.02	-0.04	0.02	-0.02	0.01	-0.06	0.01	-0.03	0.01	1.3	1.81	-0.03	2.12	0.34	0.01
07GC/05GC	0.21	0.86	-9.2	0.54	-3.28	0.06	-3.53	0.16	-2.41	0.18	-2.28	0.19	-3.12	1.19	-2.45	0.31	0.05	1.33	-1.78	0.13
08CG/04CG	6.28	0.11	6.27	0.12	5.79	0.21	6.56	0.1	6.73	0.09	5.81	0.19	1.45	4.49	-4.91	2.23	-6.98	6.25	3.68	0.18
09GT/03AC	1.3	1.52	-1.37	1.02	0.09	0.35	2.62	0.19	-7.89	0.1	-1.22	0.48	-2.34	0.41	-3.95	0.66	0.19	2.64	0.1	0.19
10TA/02TA	-2.15	0.48	-3.16	0.31	0.2	0.1	-4.84	0.19	-1.09	0.1	0.43	0.22	-0.65	0.4	-0.17	1.23	1.49	0.53	-8.3	0.4
11AG/01CT	0.29	0.48	4.68	0.44	-0.65	0.17	1.23	2.14	3.37	0.27	-0.53	1.07	7.25	1.32	2.45	1.87	0.49	1	4.54	1.9

X-displacement (Å)																				
Base Steps	DNA <sup>control</sup>		DNA <sup>M6</sup>		DNA <sup>M8</sup>		DNA <sup>M3</sup>		DNA <sup>H6</sup>		DNA <sup>H8</sup>		DNA <sup>H3</sup>		DNA <sup>F6</sup>		DNA <sup>F8</sup>		DNA <sup>F3</sup>	
	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std
01CT/11AG	-2.76	0.06	-2.79	0.16	-2.29	0.05	-1.67	0.22	-2.44	0.04	-2.06	0.13	-1.85	0.28	-1.23	0.51	-1.88	0.31	-2.23	0.14
02TA/10TA	-1.59	0.23	-1.18	0.16	-0.88	0.04	-0.95	0.07	-1.49	0.03	-1.69	0.15	-0.85	0.04	-2.24	0.47	-0.89	0.36	-0.54	0.04
03AC/09GT	-2.64	0.46	-2.52	0.45	-2.44	0.05	-2.78	0.06	-1.95	0.03	-2.82	0.20	-2.30	0.93	0.43	0.19	-0.28	0.75	-2.92	0.04
04CG/08CG	1.28	0.18	0.79	0.13	0.79	0.02	1.22	0.02	1.60	0.02	0.58	0.03	0.32	0.19	0.58	0.55	0.32	0.29	-0.23	0.05
05GC/07GC	1.30	0.08	1.21	0.12	0.60	0.04	0.03	0.02	0.47	0.02	1.05	0.05	0.63	0.15	1.03	0.18	0.56	0.37	-0.43	0.08
06CG/06CG	-0.57	0.12	1.58	0.36	0.70	0.04	0.34	0.04	-0.03	0.03	-0.56	0.05	1.04	0.37	0.72	0.14	0.70	0.17	-1.01	0.06
07GC/05GC	1.30	0.08	1.23	0.11	0.60	0.04	0.03	0.03	0.46	0.02	1.04	0.05	0.62	0.15	1.03	0.17	0.46	0.23	-0.29	0.08
08CG/04CG	1.28	0.19	0.71	0.12	0.78	0.02	1.22	0.03	1.59	0.02	0.58	0.03	0.32	0.19	0.57	0.54	0.44	0.12	-0.29	0.05
09GT/03AC	-2.64	0.46	-2.45	0.46	-2.42	0.05	-2.78	0.06	-1.94	0.03	-2.82	0.20	-2.30	0.94	0.44	0.17	-0.33	0.83	-2.72	0.05
10TA/02TA	-1.59	0.23	-1.19	0.16	-0.88	0.04	-0.96	0.07	-1.49	0.03	-1.69	0.14	-0.86	0.04	-2.24	0.48	-0.81	0.48	-0.59	0.04
11AG/01CT	-2.77	0.06	-2.79	0.16	-2.29	0.05	-1.67	0.22	-2.45	0.03	-2.07	0.14	-1.86	0.28	-1.23	0.51	-2.01	0.21	-2.22	0.13

Y-displacement (Å)																				
Base Steps	DNA <sup>control</sup>		DNA <sup>M6</sup>		DNA <sup>M8</sup>		DNA <sup>M3</sup>		DNA <sup>H6</sup>		DNA <sup>H8</sup>		DNA <sup>H3</sup>		DNA <sup>F6</sup>		DNA <sup>F8</sup>		DNA <sup>F3</sup>	
	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std
01CT/11AG	0.80	0.08	1.17	0.05	0.71	0.03	0.93	0.27	0.99	0.04	0.79	0.18	1.53	0.17	1.04	0.14	0.96	0.32	1.14	0.28
02TA/10TA	-0.05	0.04	-0.10	0.03	0.15	0.01	-0.49	0.03	0.09	0.02	0.02	0.06	-0.07	0.05	0.12	0.17	0.34	0.09	-0.75	0.04
03AC/09GT	0.56	0.26	0.04	0.07	-0.01	0.02	0.15	0.08	-0.37	0.01	-0.18	0.10	-0.17	0.21	0.31	0.52	0.37	0.23	-0.08	0.04
04CG/08CG	0.69	0.05	0.75	0.04	0.74	0.01	0.75	0.02	0.79	0.01	0.86	0.02	0.48	0.31	0.01	0.59	-0.17	0.05	0.08	0.01
05GC/07GC	-0.50	0.20	-1.45	0.09	0.07	0.02	-0.29	0.02	-0.49	0.02	0.18	0.04	0.41	0.11	-0.10	0.15	0.14	0.26	-0.26	0.07
06CG/06CG	-0.01	0.00	-0.02	0.01	-0.01	0.00	-0.01	0.01	-0.01	0.00	-0.01	0.00	-0.01	0.00	-0.01	0.22	-0.14	0.18	0.02	0.00
07GC/05GC	0.51	0.20	1.45	0.09	-0.05	0.02	0.30	0.02	0.51	0.02	-0.17	0.04	-0.40	0.11	0.12	0.12	-0.16	0.32	0.17	0.07
08CG/04CG	-0.70	0.05	-0.69	0.04	-0.74	0.01	-0.76	0.02	-0.79	0.01	-0.86	0.02	-0.47	0.31	-0.01	0.59	0.11	0.14	-0.08	0.01
09GT/03AC	-0.58	0.26	-0.14	0.08	-0.02	0.03	-0.17	0.08	0.35	0.01	0.15	0.10	0.15	0.21	-0.32	0.52	-0.03	0.70	0.23	0.04
10TA/02TA	0.05	0.04	0.11	0.03	-0.15	0.01	0.50	0.04	-0.09	0.02	-0.02	0.05	0.08	0.05	-0.12	0.17	-0.24	0.07	0.68	0.03
11AG/01CT	-0.82	0.08	-1.18	0.05	-0.72	0.03	-0.94	0.26	-1.00	0.04	-0.80	0.18	-1.54	0.17	-1.05	0.15	-1.09	0.21	-1.10	0.29



Helical Rise (Å)																				
Base Steps	DNA <sup>control</sup>		DNA <sup>M6</sup>		DNA <sup>M8</sup>		DNA <sup>M3</sup>		DNA <sup>H6</sup>		DNA <sup>H8</sup>		DNA <sup>H3</sup>		DNA <sup>F6</sup>		DNA <sup>F8</sup>		DNA <sup>F3</sup>	
	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std
01CT/11AG	3.14	0.01	3.15	0.04	3.23	0.02	3.22	0.02	2.95	0.08	3.21	0.01	3.15	0.07	3.20	0.06	3.38	0.08	3.17	0.06
02TA/10TA	3.35	0.12	3.34	0.03	3.48	0.08	3.62	0.02	3.40	0.05	3.46	0.02	3.23	0.10	3.20	0.01	2.85	0.18	3.50	0.06
03AC/09GT	3.55	0.02	3.77	0.02	3.63	0.05	3.70	0.02	3.27	0.14	3.71	0.01	3.49	0.02	3.42	0.03	3.15	0.36	3.20	0.17
04CG/08CG	3.30	0.03	3.23	0.02	3.48	0.02	3.52	0.01	3.23	0.03	3.26	0.02	3.22	0.02	3.20	0.02	3.33	0.06	3.53	0.19
05GC/07GC	3.36	0.02	3.46	0.01	3.71	0.06	3.72	0.02	3.49	0.19	3.67	0.01	3.20	0.01	3.69	0.02	3.43	0.17	3.42	0.05
06CG/06CG	3.83	0.03	3.71	0.01	4.69	0.12	3.84	0.02	3.30	0.06	3.73	0.01	4.19	0.02	3.45	0.02	3.20	0.07	3.13	0.17
07GC/05GC	3.36	0.02	3.46	0.01	3.71	0.06	3.71	0.02	3.49	0.19	3.66	0.01	3.20	0.01	3.72	0.02	3.42	0.17	3.56	0.24
08CG/04CG	3.30	0.03	3.24	0.02	3.51	0.02	3.53	0.01	3.23	0.03	3.26	0.01	3.23	0.01	3.19	0.01	3.34	0.06	3.38	0.02
09GT/03AC	3.55	0.02	3.77	0.02	3.62	0.04	3.70	0.02	3.27	0.15	3.71	0.01	3.49	0.03	3.46	0.03	3.14	0.36	3.26	0.26
10TA/02TA	3.34	0.12	3.33	0.02	3.47	0.08	3.61	0.01	3.39	0.05	3.45	0.02	3.23	0.10	3.20	0.01	2.84	0.19	3.49	0.05
11AG/01CT	3.14	0.01	3.15	0.04	3.22	0.02	3.22	0.02	2.95	0.09	3.21	0.01	3.16	0.07	3.23	0.05	3.38	0.08	3.17	0.07

Helical Twist (°)																				
Base Steps	DNA <sup>control</sup>		DNA <sup>M6</sup>		DNA <sup>M8</sup>		DNA <sup>M3</sup>		DNA <sup>H6</sup>		DNA <sup>H8</sup>		DNA <sup>H3</sup>		DNA <sup>F6</sup>		DNA <sup>F8</sup>		DNA <sup>F3</sup>	
	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std
01CT/11AG	32.8	0.2	33.9	0.2	32.2	0.1	32.3	0.6	33.3	0.2	32.8	1.3	31.9	0.6	31.9	0.5	33.4	1.9	34.4	2.8
02TA/10TA	36.3	0.5	35.1	0.5	37.1	0.2	34.6	0.2	36.0	0.1	35.5	0.4	38.1	0.3	39.1	0.7	35.4	1.4	35.7	0.4
03AC/09GT	30.8	0.3	30.4	0.1	30.4	0.1	30.7	0.1	30.3	0.1	31.0	0.3	32.0	1.2	35.3	0.5	34.3	1.9	28.9	0.1
04CG/08CG	36.8	0.6	35.2	0.6	34.1	0.2	38.8	0.1	37.4	0.2	35.6	0.2	36.9	2.4	44.0	2.5	38.2	3.0	39.9	0.1
05GC/07GC	39.0	0.1	37.2	0.5	37.0	0.1	35.6	0.1	37.6	0.1	38.1	0.2	39.7	1.6	39.2	1.6	38.5	1.2	31.2	0.2
06CG/06CG	36.3	0.2	35.0	1.2	35.5	0.3	38.9	0.3	35.1	0.2	37.1	0.4	37.9	0.3	37.4	0.7	38.8	0.2	39.3	0.1
07GC/05GC	39.0	0.1	37.2	0.5	37.0	0.2	35.6	0.1	37.5	0.1	38.0	0.2	39.6	1.6	39.2	1.6	38.3	1.3	31.3	0.2
08CG/04CG	36.8	0.6	35.0	0.5	34.1	0.2	38.8	0.1	37.4	0.1	35.6	0.2	36.9	2.4	44.0	2.6	38.1	3.1	40.2	0.1
09GT/03AC	30.8	0.3	30.4	0.1	30.4	0.1	30.7	0.1	30.3	0.1	31.0	0.4	32.0	1.2	35.3	0.6	34.1	2.2	28.8	0.1
10TA/02TA	36.3	0.5	35.1	0.5	37.0	0.2	34.6	0.2	36.1	0.1	35.5	0.4	38.1	0.3	39.1	0.7	35.3	1.3	35.6	0.4
11AG/01CT	32.7	0.2	33.9	0.2	32.2	0.2	32.2	0.6	33.3	0.2	32.7	1.3	31.8	0.6	31.9	0.5	33.7	1.8	34.5	2.8

Inclination (°)																				
Base Steps	DNA <sup>control</sup>		DNA <sup>M6</sup>		DNA <sup>M8</sup>		DNA <sup>M3</sup>		DNA <sup>H6</sup>		DNA <sup>H8</sup>		DNA <sup>H3</sup>		DNA <sup>F6</sup>		DNA <sup>F8</sup>		DNA <sup>F3</sup>	
	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std
01CT/11AG	25.2	0.2	30.5	1.4	17.8	0.5	13.8	1.9	25.0	0.4	14.5	3.0	8.0	2.7	7.0	3.8	22.6	4.2	28.4	1.8
02TA/10TA	17.7	4.7	15.8	3.3	9.5	0.2	8.8	1.4	20.4	0.1	15.6	3.2	4.2	1.4	29.2	2.6	13.0	4.9	11.6	0.8
03AC/09GT	10.4	4.1	11.9	3.9	10.5	0.2	9.2	0.5	5.3	0.1	10.4	2.4	6.9	7.6	-16.6	7.7	-1.6	5.7	6.9	0.4
04CG/08CG	-1.3	0.8	4.5	1.1	2.5	0.1	-4.1	0.2	-6.3	0.3	0.9	0.3	1.0	4.1	-3.0	5.5	1.1	7.8	11.3	0.5
05GC/07GC	-2.9	0.3	0.2	0.4	4.3	0.2	4.8	0.2	3.8	0.2	-2.6	0.2	-0.3	5.9	-14.0	2.0	-8.1	0.9	-16.5	0.4
06CG/06CG	13.5	0.9	-3.3	1.4	4.1	0.1	2.5	0.4	5.8	0.2	13.6	0.8	-4.0	0.4	-0.4	2.0	-6.9	1.4	16.9	0.2
07GC/05GC	-2.8	0.3	0.0	0.4	4.4	0.2	4.9	0.2	3.9	0.2	-2.5	0.2	-0.2	5.9	-13.9	2.0	-8.2	0.7	-17.6	0.4
08CG/04CG	-1.2	0.8	5.4	1.0	2.7	0.1	-3.9	0.2	-6.1	0.3	1.0	0.3	1.0	4.1	-2.8	5.5	-1.3	4.2	11.6	0.5
09GT/03AC	10.4	4.2	11.5	4.0	10.4	0.2	9.2	0.6	5.2	0.2	10.4	2.4	6.9	7.7	-16.8	7.6	-2.4	4.8	5.2	0.4
10TA/02TA	17.7	4.7	15.8	3.3	9.6	0.2	8.8	1.5	20.4	0.1	15.6	3.2	4.2	1.5	29.2	2.4	12.8	5.4	12.4	0.8
11AG/01CT	25.2	0.2	30.5	1.5	17.8	0.5	13.8	1.9	25.0	0.4	14.5	3.0	8.0	2.7	7.0	3.8	24.3	3.0	28.1	1.8

Shear (Å)																				
Base Pair	DNA <sup>control</sup>		DNA <sup>M6</sup>		DNA <sup>M8</sup>		DNA <sup>M3</sup>		DNA <sup>H6</sup>		DNA <sup>H8</sup>		DNA <sup>H3</sup>		DNA <sup>F6</sup>		DNA <sup>F8</sup>		DNA <sup>F3</sup>	
	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std
01C-12G	0.11	0.01	0.09	0.00	0.09	0.00	0.08	0.01	0.08	0.01	0.10	0.00	0.09	0.01	0.04	0.01	0.08	0.00	0.09	0.01
02T-11A	-0.03	0.01	-0.06	0.01	-0.05	0.01	-0.05	0.01	-0.04	0.00	-0.05	0.01	-0.02	0.01	-0.04	0.01	-0.03	0.01	-0.03	0.00
03A-10T	-0.01	0.03	-0.01	0.02	0.02	0.01	0.03	0.00	-0.06	0.00	-0.01	0.01	0.01	0.01	0.01	0.01	-0.03	0.01	0.00	0.00
04C-09G	0.02	0.01	0.04	0.01	0.08	0.00	0.08	0.00	0.05	0.00	0.09	0.01	0.07	0.01	0.12	0.04	0.13	0.01	0.10	0.01
05G-08C	-0.06	0.00	-0.03	0.01	-0.05	0.00	-0.11	0.01	-0.10	0.01	-0.05	0.00	-0.06	0.01	-0.07	0.04	-0.10	0.02	-0.05	0.01
06C-07G	0.08	0.00	0.07	0.01	0.08	0.00	0.11	0.00	0.07	0.00	0.10	0.00	0.07	0.01	0.11	0.02	0.07	0.01	0.08	0.00
07G-06C	-0.09	0.01	-0.07	0.01	-0.09	0.01	-0.11	0.00	-0.08	0.01	-0.11	0.00	-0.08	0.01	-0.12	0.02	-0.06	0.01	-0.07	0.00
08C-05G	0.06	0.00	0.03	0.01	0.05	0.01	0.10	0.01	0.09	0.00	0.05	0.00	0.06	0.01	0.07	0.04	0.09	0.01	0.05	0.00
09G-04C	-0.02	0.01	-0.05	0.01	-0.08	0.01	-0.08	0.00	-0.05	0.00	-0.09	0.01	-0.07	0.01	-0.13	0.03	-0.11	0.02	-0.08	0.01
10T-03A	0.01	0.03	0.01	0.02	-0.02	0.01	-0.03	0.00	0.06	0.00	0.01	0.01	-0.01	0.01	-0.02	0.01	0.03	0.00	0.01	0.00
11A-02T	0.04	0.01	0.06	0.00	0.05	0.01	0.05	0.01	0.04	0.00	0.05	0.00	0.02	0.01	0.04	0.01	0.03	0.01	0.03	0.00
12G-01C	-0.10	0.01	-0.08	0.00	-0.09	0.01	-0.07	0.01	-0.08	0.00	-0.09	0.01	-0.09	0.01	-0.04	0.01	-0.08	0.01	-0.09	0.00

Stretch (Å)																				
Base Pair	DNA <sup>control</sup>		DNA <sup>M6</sup>		DNA <sup>M8</sup>		DNA <sup>M3</sup>		DNA <sup>H6</sup>		DNA <sup>H8</sup>		DNA <sup>H3</sup>		DNA <sup>F6</sup>		DNA <sup>F8</sup>		DNA <sup>F3</sup>	
	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std
01C-12G	-0.20	0.01	-0.16	0.00	-0.20	0.00	-0.16	0.01	-0.17	0.00	-0.19	0.01	-0.18	0.01	-0.17	0.00	-0.17	0.00	-0.17	0.00
02T-11A	-0.08	0.01	-0.08	0.00	-0.09	0.00	-0.08	0.00	-0.08	0.00	-0.10	0.00	-0.12	0.01	-0.18	0.03	-0.10	0.01	-0.10	0.00
03A-10T	-0.13	0.01	-0.12	0.01	-0.12	0.00	-0.11	0.01	-0.15	0.01	-0.12	0.01	-0.12	0.01	-0.11	0.01	-0.14	0.01	-0.13	0.01
04C-09G	-0.20	0.00	-0.20	0.00	-0.18	0.00	-0.18	0.00	-0.18	0.00	-0.19	0.00	-0.18	0.00	-0.22	0.04	-0.18	0.00	-0.18	0.00
05G-08C	-0.18	0.00	-0.18	0.01	-0.17	0.00	-0.19	0.00	-0.18	0.00	-0.17	0.01	-0.18	0.02	-0.24	0.03	-0.22	0.00	-0.21	0.01
06C-07G	-0.18	0.00	-0.26	0.01	-0.19	0.00	-0.20	0.00	-0.19	0.00	-0.19	0.00	-0.21	0.04	-0.26	0.02	-0.23	0.03	-0.17	0.00
07G-06C	-0.18	0.00	-0.26	0.01	-0.19	0.00	-0.20	0.00	-0.19	0.00	-0.19	0.00	-0.21	0.04	-0.26	0.02	-0.24	0.01	-0.17	0.00
08C-05G	-0.18	0.00	-0.19	0.00	-0.17	0.00	-0.19	0.00	-0.18	0.00	-0.18	0.01	-0.18	0.02	-0.24	0.02	-0.22	0.01	-0.21	0.01
09G-04C	-0.20	0.00	-0.20	0.00	-0.18	0.00	-0.19	0.01	-0.18	0.00	-0.19	0.00	-0.18	0.01	-0.22	0.04	-0.18	0.01	-0.18	0.00
10T-03A	-0.13	0.01	-0.12	0.01	-0.12	0.00	-0.11	0.00	-0.14	0.00	-0.12	0.01	-0.12	0.01	-0.10	0.01	-0.14	0.01	-0.14	0.01
11A-02T	-0.08	0.01	-0.08	0.00	-0.09	0.00	-0.08	0.00	-0.08	0.00	-0.10	0.00	-0.12	0.01	-0.18	0.03	-0.10	0.02	-0.10	0.00
12G-01C	-0.20	0.01	-0.16	0.00	-0.20	0.00	-0.17	0.01	-0.17	0.00	-0.19	0.01	-0.18	0.01	-0.17	0.00	-0.17	0.00	-0.17	0.00

Stagger (Å)																				
Base Pair	DNA <sup>control</sup>		DNA <sup>M6</sup>		DNA <sup>M8</sup>		DNA <sup>M3</sup>		DNA <sup>H6</sup>		DNA <sup>H8</sup>		DNA <sup>H3</sup>		DNA <sup>F6</sup>		DNA <sup>F8</sup>		DNA <sup>F3</sup>	
	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std
01C-12G	-0.19	0.02	0.18	0.03	-0.14	0.01	0.04	0.09	0.06	0.01	-0.11	0.02	-0.03	0.06	-0.13	0.01	0.01	0.04	0.05	0.02
02T-11A	0.13	0.10	0.06	0.08	0.25	0.01	0.12	0.03	0.01	0.01	0.26	0.01	0.16	0.03	0.32	0.09	0.09	0.07	-0.13	0.05
03A-10T	0.12	0.09	0.07	0.04	0.18	0.01	0.23	0.02	-0.16	0.01	0.12	0.03	0.06	0.08	0.06	0.09	-0.10	0.06	0.25	0.01
04C-09G	0.44	0.04	0.36	0.04	0.26	0.03	0.24	0.01	0.44	0.01	0.36	0.02	0.25	0.19	0.12	0.14	-0.16	0.13	0.14	0.01
05G-08C	-0.11	0.02	-0.29	0.04	-0.13	0.01	-0.09	0.01	-0.02	0.01	-0.06	0.01	0.11	0.19	0.51	0.23	0.29	0.18	0.09	0.01
06C-07G	0.06	0.02	0.63	0.04	0.17	0.00	0.19	0.01	0.24	0.01	-0.01	0.01	0.29	0.13	0.43	0.13	0.40	0.20	0.20	0.01
07G-06C	0.06	0.02	0.64	0.04	0.18	0.01	0.19	0.01	0.25	0.01	-0.01	0.02	0.30	0.13	0.43	0.15	0.54	0.02	0.18	0.01
08C-05G	-0.12	0.02	-0.31	0.04	-0.14	0.01	-0.10	0.01	-0.03	0.01	-0.07	0.01	0.10	0.18	0.51	0.23	0.43	0.03	0.13	0.01
09G-04C	0.43	0.05	0.32	0.04	0.25	0.03	0.23	0.01	0.43	0.01	0.35	0.02	0.24	0.18	0.11	0.15	0.05	0.16	0.16	0.01
10T-03A	0.13	0.08	0.08	0.04	0.19	0.01	0.23	0.02	-0.15	0.01	0.12	0.03	0.06	0.08	0.07	0.08	-0.11	0.04	0.21	0.01
11A-02T	0.13	0.09	0.06	0.08	0.25	0.01	0.12	0.03	0.01	0.01	0.26	0.01	0.16	0.03	0.32	0.09	0.03	0.02	-0.11	0.05
12G-01C	-0.18	0.02	0.18	0.03	-0.13	0.02	0.05	0.08	0.06	0.01	-0.11	0.01	-0.03	0.06	-0.13	0.01	0.01	0.03	0.04	0.02

Buckle (°)																				
Base Pair	DNA <sup>control</sup>		DNA <sup>M6</sup>		DNA <sup>M8</sup>		DNA <sup>M3</sup>		DNA <sup>H6</sup>		DNA <sup>H8</sup>		DNA <sup>H3</sup>		DNA <sup>F6</sup>		DNA <sup>F8</sup>		DNA <sup>F3</sup>	
	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std
01C-12G	-9.0	0.4	-11.1	0.1	-10.9	0.5	-11.9	2.2	-10.7	0.6	-8.0	0.8	-5.8	1.7	-0.9	1.2	-6.7	0.7	-9.9	0.4
02T-11A	-3.7	0.3	-7.7	0.5	-5.6	0.1	-5.0	0.3	-5.1	0.0	-4.9	0.3	-0.4	2.6	3.0	1.0	1.2	0.2	-4.2	0.1
03A-10T	-1.5	0.3	-3.8	0.3	-4.8	0.1	1.9	0.1	-3.7	0.1	-2.6	0.3	-3.8	3.1	5.0	1.6	-0.7	1.2	6.5	0.2
04C-09G	-11.5	0.5	-9.7	0.7	-9.5	0.2	-8.4	0.1	-12.0	0.1	-9.6	0.2	-5.0	8.2	13.3	7.0	8.3	3.6	-5.8	0.2
05G-08C	-0.8	0.5	-0.7	0.7	-0.4	0.1	3.0	0.1	1.6	0.1	0.7	0.2	0.9	3.1	4.7	3.7	2.6	1.7	7.6	0.2
06C-07G	3.7	0.2	4.3	0.3	0.6	0.1	3.0	0.1	1.1	0.1	8.2	0.2	-1.0	2.3	-0.7	1.3	-1.0	2.3	-1.0	0.1
07G-06C	-4.1	0.2	-4.7	0.3	-1.0	0.1	-3.5	0.1	-1.5	0.1	-8.7	0.2	0.5	2.3	0.3	1.4	2.8	0.9	2.0	0.1
08C-05G	0.6	0.5	0.6	0.7	0.2	0.1	-3.2	0.1	-1.8	0.1	-1.0	0.2	-1.3	3.1	-4.9	3.7	-3.9	0.4	-7.4	0.2
09G-04C	11.3	0.4	8.8	0.7	9.3	0.2	8.2	0.1	11.8	0.1	9.4	0.2	4.7	8.2	-13.5	7.0	-5.9	7.3	6.6	0.3
10T-03A	1.2	0.3	3.5	0.3	4.6	0.1	-2.2	0.1	3.4	0.1	2.4	0.3	3.6	3.1	-5.2	1.6	0.9	1.8	-5.7	0.2
11A-02T	3.7	0.3	7.6	0.5	5.6	0.1	5.0	0.3	5.1	0.1	4.8	0.3	0.3	2.6	-3.1	1.0	0.1	2.0	4.9	0.1
12G-01C	8.9	0.4	11.0	0.1	10.8	0.5	11.7	2.2	10.5	0.6	7.9	0.8	5.7	1.7	0.7	1.2	6.5	0.8	10.2	0.5

Propeller (°)																				
Base Pair	DNA <sup>control</sup>		DNA <sup>M6</sup>		DNA <sup>M8</sup>		DNA <sup>M3</sup>		DNA <sup>H6</sup>		DNA <sup>H8</sup>		DNA <sup>H3</sup>		DNA <sup>F6</sup>		DNA <sup>F8</sup>		DNA <sup>F3</sup>	
	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std
01C-12G	-12.5	0.8	-1.9	0.9	-13.9	0.4	-6.7	0.3	-8.2	0.4	-11.7	2.2	-10.4	2.6	-5.5	1.1	-5.7	2.4	-7.9	1.8
02T-11A	-5.8	0.8	-6.3	0.6	-5.0	0.3	-8.4	0.6	-6.0	0.3	-8.4	1.1	-16.2	1.0	-24.8	3.7	-9.4	2.4	-11.6	0.9
03A-10T	-14.8	5.2	-12.1	4.2	-10.5	0.4	-7.8	0.5	-20.9	0.3	-12.8	2.7	-11.8	2.6	-9.0	4.3	-18.7	1.6	-17.4	0.5
04C-09G	-14.9	0.7	-14.1	0.3	-11.0	0.4	-10.3	0.4	-10.2	0.3	-11.3	0.3	-10.3	1.8	-25.7	4.8	-16.5	3.3	-11.1	0.2
05G-08C	-9.0	0.5	-4.8	1.0	-5.5	0.3	-15.4	0.3	-10.2	0.3	-9.7	0.2	-9.4	4.2	-18.8	1.9	-18.7	0.8	-19.6	0.4
06C-07G	-12.1	0.8	4.6	0.7	-9.8	0.4	-14.2	0.4	-8.2	0.2	-13.9	0.2	-13.4	5.3	-23.5	1.5	-18.5	1.3	-2.3	0.8
07G-06C	-12.3	0.8	4.5	0.7	-10.0	0.4	-14.4	0.4	-8.4	0.2	-14.1	0.2	-13.6	5.3	-23.7	1.4	-17.5	2.7	-2.1	0.8
08C-05G	-8.7	0.6	-4.1	1.0	-5.1	0.3	-15.1	0.3	-9.8	0.3	-9.4	0.2	-9.0	4.2	-18.5	2.1	-16.1	2.3	-20.3	0.4
09G-04C	-14.9	0.7	-14.6	0.3	-11.0	0.4	-10.3	0.4	-10.2	0.2	-11.4	0.3	-10.4	1.9	-25.8	4.7	-15.8	4.3	-12.4	0.2
10T-03A	-14.8	5.2	-12.2	4.2	-10.6	0.4	-7.9	0.5	-20.9	0.3	-12.8	2.7	-11.8	2.5	-9.1	4.2	-19.0	1.2	-16.9	0.5
11A-02T	-5.7	0.8	-6.3	0.6	-5.0	0.3	-8.2	0.6	-5.9	0.3	-8.3	1.1	-16.1	1.0	-24.7	3.8	-11.0	4.7	-11.7	0.9
12G-01C	-12.6	0.8	-2.0	0.9	-14.0	0.4	-6.8	0.4	-8.3	0.4	-11.8	2.2	-10.5	2.6	-5.6	1.1	-5.8	2.4	-7.9	1.8



Opening (°)																				
Base Pair	DNA <sup>control</sup>		DNA <sup>M6</sup>		DNA <sup>M8</sup>		DNA <sup>M3</sup>		DNA <sup>H6</sup>		DNA <sup>H8</sup>		DNA <sup>H3</sup>		DNA <sup>F6</sup>		DNA <sup>F8</sup>		DNA <sup>F3</sup>	
	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std
01C-12G	1.4	0.3	-1.2	0.1	1.4	0.2	-0.5	0.2	-0.5	0.1	0.8	0.3	-0.1	0.4	-1.7	0.2	-1.0	0.2	-0.7	0.1
02T-11A	-2.7	0.1	-1.8	0.1	-2.9	0.1	-2.2	0.1	-2.3	0.1	-3.1	0.2	-3.6	0.3	-5.2	1.4	-2.7	0.1	-1.7	0.3
03A-10T	-2.4	0.9	-2.9	0.6	-3.1	0.1	-3.3	0.2	-0.3	0.1	-3.3	0.5	-3.3	0.4	-2.4	0.6	-1.6	0.6	-3.2	0.1
04C-09G	-3.4	0.4	-2.8	0.3	-2.0	0.2	-1.8	0.1	-3.1	0.1	-2.4	0.1	-2.3	0.2	-3.3	0.5	-1.2	0.9	-1.4	0.1
05G-08C	-2.2	0.2	-2.3	0.1	-2.2	0.1	-0.4	0.1	-1.5	0.0	-2.0	0.1	-2.0	0.3	-3.7	1.2	-2.3	0.8	-0.9	0.1
06C-07G	-1.8	0.2	-0.4	0.2	-2.5	0.0	-2.5	0.1	-2.5	0.1	-2.5	0.1	-3.3	1.1	-3.5	1.0	-3.5	0.7	-2.3	0.1
07G-06C	-1.8	0.2	-0.4	0.2	-2.5	0.0	-2.5	0.1	-2.5	0.1	-2.5	0.1	-3.4	1.1	-3.5	1.1	-3.9	0.2	-2.4	0.1
08C-05G	-2.2	0.2	-2.4	0.1	-2.2	0.1	-0.4	0.1	-1.6	0.0	-2.1	0.1	-2.1	0.3	-3.7	1.2	-2.6	0.3	-1.0	0.1
09G-04C	-3.5	0.4	-2.7	0.2	-2.1	0.2	-1.9	0.1	-3.1	0.1	-2.5	0.1	-2.4	0.2	-3.3	0.5	-2.0	0.1	-1.6	0.1
10T-03A	-2.4	0.8	-2.9	0.5	-3.1	0.1	-3.3	0.2	-0.4	0.1	-3.3	0.4	-3.3	0.4	-2.4	0.6	-1.7	0.7	-2.9	0.1
11A-02T	-2.7	0.1	-1.8	0.1	-2.9	0.1	-2.2	0.1	-2.3	0.1	-3.1	0.2	-3.6	0.3	-5.2	1.4	-2.5	0.3	-1.7	0.3
12G-01C	1.3	0.3	-1.3	0.1	1.4	0.2	-0.5	0.2	-0.5	0.1	0.8	0.3	-0.1	0.4	-1.7	0.2	-1.1	0.2	-0.7	0.1

Shift (Å)																				
Base Pair	DNA <sup>control</sup>		DNA <sup>M6</sup>		DNA <sup>M8</sup>		DNA <sup>M3</sup>		DNA <sup>H6</sup>		DNA <sup>H8</sup>		DNA <sup>H3</sup>		DNA <sup>F6</sup>		DNA <sup>F8</sup>		DNA <sup>F3</sup>	
	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std
01CT/11AG	-0.44	0.03	-0.40	0.02	-0.43	0.01	-0.45	0.04	-0.37	0.02	-0.48	0.05	-0.46	0.02	-0.54	0.08	-0.47	0.05	-0.43	0.10
02TA/10TA	-0.08	0.01	-0.11	0.01	-0.07	0.01	0.03	0.02	-0.11	0.01	0.02	0.02	0.02	0.05	0.01	0.09	-0.11	0.03	-0.05	0.01
03AC/09GT	-0.22	0.23	-0.16	0.10	0.01	0.03	0.09	0.04	-0.31	0.01	0.01	0.09	-0.05	0.09	-0.18	0.40	-0.23	0.38	0.11	0.02
04CG/08CG	-0.09	0.02	-0.05	0.02	-0.08	0.01	-0.14	0.01	-0.13	0.01	-0.20	0.02	-0.21	0.05	-0.36	0.13	-0.19	0.04	0.10	0.01
05GC/07GC	0.36	0.18	0.37	0.08	-0.22	0.01	0.00	0.02	0.20	0.02	-0.22	0.03	-0.44	0.14	0.09	0.06	-0.22	0.20	-0.05	0.04
06CG/06CG	0.01	0.00	0.01	0.00	0.01	0.00	0.01	0.00	0.01	0.00	0.01	0.00	0.01	0.00	0.01	0.02	0.02	0.02	-0.03	0.00
07GC/05GC	-0.35	0.18	-0.35	0.09	0.24	0.02	0.02	0.02	-0.18	0.02	0.23	0.03	0.45	0.14	-0.08	0.07	0.25	0.22	0.02	0.04
08CG/04CG	0.10	0.02	0.05	0.02	0.09	0.01	0.15	0.01	0.14	0.01	0.21	0.02	0.21	0.05	0.37	0.14	0.20	0.04	-0.14	0.01
09GT/03AC	0.22	0.23	0.16	0.10	0.00	0.03	-0.08	0.04	0.31	0.01	0.00	0.09	0.06	0.09	0.18	0.40	0.26	0.35	-0.12	0.02
10TA/02TA	0.09	0.02	0.12	0.01	0.08	0.01	-0.02	0.02	0.12	0.01	-0.01	0.02	-0.01	0.05	0.00	0.10	0.15	0.05	0.03	0.01
11AG/01CT	0.45	0.03	0.41	0.01	0.44	0.01	0.46	0.04	0.38	0.02	0.49	0.05	0.47	0.02	0.55	0.08	0.50	0.04	0.40	0.10

Slide (Å)																				
Base Pair	DNA <sup>control</sup>		DNA <sup>M6</sup>		DNA <sup>M8</sup>		DNA <sup>M3</sup>		DNA <sup>H6</sup>		DNA <sup>H8</sup>		DNA <sup>H3</sup>		DNA <sup>F6</sup>		DNA <sup>F8</sup>		DNA <sup>F3</sup>	
	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std
01CT/11AG	-0.13	0.01	0.18	0.03	-0.27	0.01	-0.18	0.02	0.03	0.01	-0.38	0.05	-0.61	0.05	-0.27	0.06	0.16	0.04	0.31	0.04
02TA/10TA	0.02	0.10	0.21	0.07	0.02	0.02	-0.07	0.04	0.29	0.01	-0.17	0.06	-0.32	0.09	0.00	0.22	0.23	0.10	0.29	0.03
03AC/09GT	-0.76	0.06	-0.57	0.03	-0.60	0.01	-0.87	0.02	-0.69	0.01	-0.88	0.03	-0.85	0.07	-0.64	0.58	-0.22	0.13	-1.05	0.02
04CG/08CG	0.74	0.09	0.74	0.03	0.61	0.02	0.60	0.01	0.68	0.01	0.41	0.02	0.26	0.08	0.29	0.12	0.31	0.27	0.44	0.01
05GC/07GC	0.71	0.04	0.79	0.06	0.65	0.01	0.30	0.01	0.53	0.01	0.55	0.02	0.43	0.19	-0.11	0.14	-0.10	0.27	-1.24	0.04
06CG/06CG	0.51	0.04	0.68	0.09	0.69	0.02	0.38	0.01	0.34	0.01	0.59	0.05	0.46	0.21	0.45	0.04	0.12	0.17	0.29	0.04
07GC/05GC	0.71	0.04	0.79	0.06	0.65	0.01	0.30	0.01	0.53	0.01	0.55	0.02	0.43	0.19	-0.11	0.14	-0.19	0.14	-1.24	0.04
08CG/04CG	0.74	0.10	0.74	0.04	0.62	0.02	0.60	0.02	0.68	0.01	0.41	0.01	0.26	0.08	0.29	0.12	0.22	0.14	0.41	0.01
09GT/03AC	-0.76	0.05	-0.56	0.03	-0.60	0.02	-0.87	0.02	-0.69	0.01	-0.88	0.03	-0.85	0.07	-0.63	0.58	-0.28	0.21	-1.05	0.01
10TA/02TA	0.02	0.10	0.21	0.07	0.01	0.02	-0.07	0.04	0.28	0.01	-0.17	0.06	-0.33	0.08	0.00	0.23	0.26	0.05	0.30	0.03
11AG/01CT	-0.13	0.01	0.18	0.03	-0.27	0.01	-0.18	0.02	0.03	0.01	-0.38	0.05	-0.61	0.05	-0.27	0.07	0.18	0.02	0.31	0.04

Roll (°)																				
Base Pair	DNA <sup>control</sup>		DNA <sup>M6</sup>		DNA <sup>M8</sup>		DNA <sup>M3</sup>		DNA <sup>H6</sup>		DNA <sup>H8</sup>		DNA <sup>H3</sup>		DNA <sup>F6</sup>		DNA <sup>F8</sup>		DNA <sup>F3</sup>	
	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std
01CT/11AG	13.8	0.1	17.0	0.8	9.8	0.3	7.6	0.9	13.9	0.3	8.1	1.9	4.4	1.5	3.8	2.0	12.7	2.8	16.3	2.1
02TA/10TA	10.9	2.9	9.4	2.1	6.0	0.1	5.2	0.8	12.4	0.1	9.4	2.0	2.7	1.0	18.8	1.3	7.8	2.7	7.0	0.5
03AC/09GT	5.5	2.2	6.2	2.0	5.5	0.1	4.9	0.3	2.8	0.1	5.5	1.3	3.6	4.3	-9.9	4.3	-1.1	3.3	3.4	0.2
04CG/08CG	-0.8	0.5	2.7	0.6	1.5	0.0	-2.7	0.1	-4.0	0.2	0.6	0.2	0.5	2.8	-2.4	4.1	0.4	4.9	7.7	0.3
05GC/07GC	-2.0	0.2	0.2	0.3	2.7	0.1	3.0	0.1	2.4	0.1	-1.7	0.1	-0.3	4.2	-9.3	1.7	-5.3	0.7	-8.8	0.2
06CG/06CG	8.4	0.5	-2.0	0.8	2.5	0.1	1.7	0.3	3.5	0.1	8.6	0.4	-2.6	0.2	-0.3	1.3	-4.6	1.0	11.2	0.1
07GC/05GC	-1.9	0.2	0.0	0.2	2.8	0.1	3.0	0.1	2.5	0.1	-1.6	0.1	-0.2	4.2	-9.3	1.6	-5.4	0.6	-9.4	0.2
08CG/04CG	-0.7	0.5	3.3	0.6	1.6	0.0	-2.6	0.1	-3.9	0.2	0.6	0.2	0.5	2.8	-2.2	4.1	-1.0	2.7	7.9	0.3
09GT/03AC	5.5	2.2	6.0	2.0	5.4	0.1	4.9	0.3	2.7	0.1	5.5	1.3	3.6	4.3	-9.9	4.3	-1.5	2.8	2.6	0.2
10TA/02TA	10.9	2.9	9.4	2.1	6.1	0.1	5.2	0.9	12.4	0.1	9.4	2.0	2.7	1.0	18.8	1.1	7.6	3.0	7.5	0.5
11AG/01CT	13.8	0.1	17.0	0.8	9.8	0.3	7.6	0.9	13.9	0.3	8.1	1.9	4.4	1.5	3.8	2.0	13.8	2.2	16.1	2.1

Tilt (°)																				
Base Pair	DNA <sup>control</sup>		DNA <sup>M6</sup>		DNA <sup>M8</sup>		DNA <sup>M3</sup>		DNA <sup>H6</sup>		DNA <sup>H8</sup>		DNA <sup>H3</sup>		DNA <sup>F6</sup>		DNA <sup>F8</sup>		DNA <sup>F3</sup>	
	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std
01CT/11AG	0.2	0.3	2.6	0.3	-0.3	0.1	0.7	1.2	1.9	0.2	-0.2	0.6	4.0	0.6	0.3	0.5	0.9	1.5	2.7	1.2
02TA/10TA	-1.2	0.3	-1.7	0.2	0.3	0.1	-2.7	0.1	-0.5	0.1	0.4	0.1	-0.3	0.3	1.1	0.4	1.0	0.7	-5.8	0.2
03AC/09GT	0.7	0.8	-1.1	0.6	0.0	0.2	1.3	0.1	-4.2	0.1	-0.7	0.3	-1.3	0.2	0.1	1.4	-0.3	2.5	0.6	0.1
04CG/08CG	4.0	0.1	4.2	0.1	3.5	0.1	4.4	0.1	4.4	0.1	3.7	0.1	0.9	3.0	-5.3	4.8	-3.5	1.3	2.0	0.1
05GC/07GC	0.4	0.6	-5.6	0.4	-1.8	0.1	-1.9	0.1	-1.3	0.1	-1.3	0.1	-1.9	0.9	0.3	0.8	-1.5	0.4	-1.7	0.1
06CG/06CG	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.3	-0.9	1.2	-0.2	0.0
07GC/05GC	-0.1	0.6	5.9	0.4	2.1	0.1	2.2	0.1	1.6	0.1	1.5	0.1	2.1	0.9	-0.1	0.9	1.6	0.2	0.9	0.1
08CG/04CG	-4.0	0.1	-3.8	0.1	-3.4	0.1	-4.4	0.1	-4.3	0.1	-3.6	0.1	-0.8	3.0	5.4	4.9	3.3	1.7	-2.5	0.1
09GT/03AC	-0.7	0.8	0.7	0.5	-0.1	0.2	-1.4	0.1	4.1	0.1	0.7	0.3	1.3	0.2	-0.1	1.5	2.3	0.2	-0.1	0.1
10TA/02TA	1.3	0.3	1.9	0.2	-0.1	0.1	2.9	0.1	0.7	0.1	-0.3	0.1	0.4	0.3	-1.0	0.4	0.1	0.8	5.0	0.2
11AG/01CT	-0.2	0.3	-2.6	0.3	0.4	0.1	-0.7	1.2	-1.9	0.2	0.3	0.6	-4.0	0.6	-0.3	0.5	-1.4	1.1	-2.7	1.2

$\alpha$ Torsion Angle (°)																				
Nucleotide	DNA <sup>control</sup>		DNA <sup>M6</sup>		DNA <sup>M8</sup>		DNA <sup>M3</sup>		DNA <sup>H6</sup>		DNA <sup>H8</sup>		DNA <sup>H3</sup>		DNA <sup>F6</sup>		DNA <sup>F8</sup>		DNA <sup>F3</sup>	
	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std
02T	-66	0	-64	0	-65	0	-62	2	-65	0	-65	0	-63	1	-69	1	-64	0	-63	0
03A	-66	0	-66	0	-66	0	-63	0	-65	0	-66	0	-63	1	-61	1	-63	1	-63	1
04C	-68	1	-67	1	-67	0	-65	1	-66	0	-66	0	-64	5	-59	3	-60	4	-66	0
05G	-57	1	-59	1	-58	1	-56	1	-57	1	-56	1	-58	2	-58	3	-55	1	-59	2
06C	-57	1	-62	1	-60	1	-60	1	-60	1	-59	1	-59	1	-65	1	-59	1	-63	1
07G	-62	1	-59	1	-60	1	-59	0	-61	0	-61	0	-60	2	-58	1	-59	1	-62	1
08C	-58	0	-59	1	-59	0	-60	0	-60	0	-56	0	-58	0	-59	1	-59	3	-56	1
09G	-57	1	-58	0	-56	0	-57	0	-58	0	-55	0	-58	0	-58	1	-58	1	-65	0
10T	-63	0	-64	0	-62	0	-62	0	-64	0	-61	2	-59	1	-64	1	-62	1	-65	0
11A	-64	1	-63	1	-61	0	-63	0	-64	0	-62	0	-57	1	-60	1	-60	1	-63	1

<b><math>\beta</math> Torsion Angle (°)</b>																				
<b>Nucleotide</b>	<b>DNA<sup>control</sup></b>		<b>DNA<sup>M6</sup></b>		<b>DNA<sup>M8</sup></b>		<b>DNA<sup>M3</sup></b>		<b>DNA<sup>H6</sup></b>		<b>DNA<sup>H8</sup></b>		<b>DNA<sup>H3</sup></b>		<b>DNA<sup>F6</sup></b>		<b>DNA<sup>F8</sup></b>		<b>DNA<sup>F3</sup></b>	
	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std
02T	184	1	184	1	181	0	187	0	183	0	183	0	181	0	165	2	184	3	184	3
03A	174	2	176	1	179	0	176	1	175	0	177	1	179	3	179	1	176	5	171	1
04C	171	0	170	0	173	0	170	0	170	0	172	0	176	4	170	14	179	4	165	0
05G	183	1	182	0	181	0	184	0	182	0	184	0	178	6	173	10	175	1	179	1
06C	174	1	180	1	179	0	176	0	181	0	176	1	182	1	164	4	178	2	169	1
07G	179	1	177	1	180	0	179	0	178	0	181	1	180	2	172	2	178	2	181	1
08C	183	1	183	0	183	0	179	0	181	0	182	0	179	5	173	1	170	7	160	0
09G	177	1	175	1	175	0	177	0	176	0	176	0	176	1	172	2	176	1	183	0
10T	169	10	175	7	179	0	182	0	164	0	178	7	181	4	173	4	172	7	166	0
11A	182	1	182	1	182	0	182	0	181	0	181	0	177	4	174	2	175	2	181	0

<b><math>\gamma</math> Torsion Angle (°)</b>																				
<b>Nucleotide</b>	<b>DNA<sup>control</sup></b>		<b>DNA<sup>M6</sup></b>		<b>DNA<sup>M8</sup></b>		<b>DNA<sup>M3</sup></b>		<b>DNA<sup>H6</sup></b>		<b>DNA<sup>H8</sup></b>		<b>DNA<sup>H3</sup></b>		<b>DNA<sup>F6</sup></b>		<b>DNA<sup>F8</sup></b>		<b>DNA<sup>F3</sup></b>	
	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std
02T	51	1	52	0	54	0	47	2	52	0	50	2	54	1	61	1	52	2	51	3
03A	55	1	53	1	54	0	53	1	55	0	51	1	53	2	59	1	54	2	56	1
04C	57	1	57	1	54	1	58	1	57	1	55	1	51	3	60	11	50	4	57	1
05G	55	1	54	1	56	1	56	1	57	1	53	1	55	2	54	3	58	2	58	1
06C	56	1	54	1	55	1	53	1	52	1	54	1	54	1	60	1	54	2	56	1
07G	53	1	60	1	54	0	56	0	55	0	53	0	54	1	61	1	55	2	53	1
08C	52	0	53	0	48	0	51	0	53	0	47	0	52	4	59	2	58	2	68	0
09G	57	0	58	0	57	0	57	0	58	0	54	0	55	2	62	1	57	1	50	0
10T	53	7	49	6	48	0	47	0	60	0	47	6	46	5	54	3	53	4	59	0
11A	49	1	51	0	51	0	50	0	52	0	49	1	56	3	56	4	56	1	52	0



<b>δ Torsion Angle (°)</b>																					
<b>Nucleotide</b>	<b>DNA<sup>control</sup></b>		<b>DNA<sup>M6</sup></b>		<b>DNA<sup>M8</sup></b>		<b>DNA<sup>M3</sup></b>		<b>DNA<sup>H6</sup></b>		<b>DNA<sup>H8</sup></b>		<b>DNA<sup>H3</sup></b>		<b>DNA<sup>F6</sup></b>		<b>DNA<sup>F8</sup></b>		<b>DNA<sup>F3</sup></b>		
	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	
02T	135	1	134	1	134	1	134	1	132	0	133	2	134	1	88	1	133	2	134	4	
03A	127	1	124	0	130	0	127	0	126	0	127	0	132	3	140	3	128	5	127	0	
04C	95	1	94	1	97	0	101	0	96	0	96	0	111	14	123	31	123	20	90	1	
05G	135	1	134	1	132	0	136	0	135	0	136	0	137	2	139	3	135	4	139	0	
06C	128	2	129	1	128	1	129	0	131	0	127	1	137	0	99	5	128	3	91	0	
07G	132	0	131	1	130	0	132	0	130	0	131	0	134	2	134	3	133	1	140	0	
08C	133	1	134	1	127	0	129	0	130	0	129	0	133	3	127	3	114	16	88	0	
09G	138	0	137	1	136	0	140	0	136	0	137	1	136	1	135	1	131	4	141	0	
10T	105	17	113	12	123	1	122	1	90	0	116	13	125	4	100	3	104	13	90	0	
11A	135	0	134	1	137	0	133	0	133	0	135	1	132	2	133	2	128	4	132	1	

$\epsilon$ Torsion Angle ( $^{\circ}$ )																				
Nucleotide	DNA <sup>control</sup>		DNA <sup>M6</sup>		DNA <sup>M8</sup>		DNA <sup>M3</sup>		DNA <sup>H6</sup>		DNA <sup>H8</sup>		DNA <sup>H3</sup>		DNA <sup>F6</sup>		DNA <sup>F8</sup>		DNA <sup>F3</sup>	
	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std
02T	-171	1	-171	1	-171	0	-174	0	-171	0	-171	1	-177	0	-154	1	-175	2	-173	1
03A	-172	1	-172	1	-172	0	-173	1	-173	0	-175	1	-176	5	-178	1	-180	5	-174	0
04C	-181	0	-176	1	-178	0	-182	0	-180	0	-181	0	-179	1	-171	5	-184	1	-172	1
05G	-182	0	-175	0	-179	0	-180	0	-180	0	-181	0	-181	1	-175	1	-182	1	-182	0
06C	-176	0	-176	0	-177	0	-180	0	-178	0	-176	0	-182	1	-180	2	-181	1	-169	1
07G	-182	0	-180	1	-178	0	-179	0	-178	0	-181	0	-183	0	-180	2	-181	5	-185	0
08C	-181	0	-180	0	-182	0	-181	1	-180	0	-183	0	-181	2	-183	1	-181	2	-158	1
09G	-176	1	-173	0	-174	0	-179	0	-174	0	-177	1	-180	2	-180	3	-175	1	-178	0
10T	-167	5	-172	3	-175	0	-173	0	-165	0	-172	2	-182	1	-176	3	-175	1	-166	0
11A	-172	1	-166	1	-176	0	-176	0	-169	0	-175	1	-176	1	-171	1	-166	1	-168	0

$\zeta$ Torsion Angle ( $^{\circ}$ )																				
Nucleotide	DNA <sup>control</sup>		DNA <sup>M6</sup>		DNA <sup>M8</sup>		DNA <sup>M3</sup>		DNA <sup>H6</sup>		DNA <sup>H8</sup>		DNA <sup>H3</sup>		DNA <sup>F6</sup>		DNA <sup>F8</sup>		DNA <sup>F3</sup>	
	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std
02T	-107	1	-100	1	-106	0	-101	1	-102	0	-100	1	-107	1	-76	1	-99	3	-102	3
03A	-93	1	-92	0	-93	0	-95	1	-91	0	-94	0	-96	1	-94	1	-97	4	-89	0
04C	-93	0	-91	1	-94	0	-99	0	-96	0	-92	0	-104	12	-118	26	-107	9	-92	2
05G	-102	2	-103	2	-107	1	-97	0	-97	0	-108	0	-109	1	-95	3	-98	1	-92	0
06C	-99	0	-109	3	-98	0	-107	0	-103	0	-95	1	-102	3	-87	2	-100	1	-92	1
07G	-107	3	-105	1	-95	0	-95	0	-104	0	-94	0	-97	0	-96	3	-99	2	-95	0
08C	-101	0	-104	0	-102	0	-108	0	-104	0	-102	0	-104	1	-103	5	-94	7	-85	0
09G	-92	1	-91	0	-93	0	-94	0	-92	0	-94	0	-95	1	-95	2	-92	1	-95	0
10T	-90	10	-97	7	-104	0	-101	0	-84	0	-97	7	-106	4	-86	2	-91	8	-85	1
11A	-99	1	-95	0	-99	0	-101	1	-96	0	-101	1	-93	1	-90	2	-89	2	-94	1

### X Torsion Angle (°)

Nucleotide	DNA <sup>control</sup>		DNA <sup>M6</sup>		DNA <sup>M8</sup>		DNA <sup>M3</sup>		DNA <sup>H6</sup>		DNA <sup>H8</sup>		DNA <sup>H3</sup>		DNA <sup>F6</sup>		DNA <sup>F8</sup>		DNA <sup>F3</sup>	
	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std
02T	-108	1	-110	0	-114	0	-108	1	-111	0	-113	1	-111	1	-147	1	-109	1	-106	1
03A	-115	0	-114	0	-113	1	-113	1	-113	0	-112	0	-114	2	-122	1	-112	5	-112	0
04C	-133	0	-133	1	-128	0	-133	0	-136	0	-133	1	-125	10	-120	31	-109	10	-143	1
05G	-103	1	-105	1	-105	0	-101	1	-103	1	-104	0	-110	3	-116	5	-115	1	-105	1
06C	-108	0	-110	1	-110	1	-108	0	-107	1	-110	1	-109	3	-132	3	-118	5	-142	0
07G	-109	0	-115	1	-108	1	-112	1	-112	1	-112	0	-107	4	-118	2	-110	2	-113	1
08C	-106	0	-102	0	-105	1	-107	0	-108	0	-103	0	-107	6	-119	2	-123	6	-158	0
09G	-103	1	-104	0	-106	0	-103	0	-105	0	-105	0	-108	3	-113	3	-115	3	-102	0
10T	-130	13	-116	10	-112	1	-118	0	-134	1	-118	10	-112	5	-127	5	-120	7	-143	1
11A	-104	1	-100	1	-104	0	-102	1	-105	1	-105	1	-115	3	-115	2	-115	1	-102	0

Sugar Phase Angle P (°)																				
Nucleotide	DNA <sup>control</sup>		DNA <sup>M6</sup>		DNA <sup>M8</sup>		DNA <sup>M3</sup>		DNA <sup>H6</sup>		DNA <sup>H8</sup>		DNA <sup>H3</sup>		DNA <sup>F6</sup>		DNA <sup>F8</sup>		DNA <sup>F3</sup>	
	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std
01C	69	1	67	1	64	1	101	36	64	1	92	41	79	1	33	4	87	55	92	56
02T	153	0	159	1	150	1	157	4	154	1	149	6	147	1	10	4	162	7	158	11
03A	133	1	130	1	141	1	135	1	134	1	134	1	147	4	184	12	140	11	133	0
04C	81	1	76	1	83	1	92	1	84	0	83	1	108	27	131	50	132	41	78	1
05G	172	4	165	2	157	1	171	1	168	1	169	1	164	3	180	6	163	7	169	2
06C	142	5	151	2	150	2	141	1	152	1	146	2	172	1	73	8	141	9	79	1
07G	153	1	158	3	154	1	156	2	147	1	157	1	161	9	156	7	153	3	175	1
08C	174	7	174	2	149	1	144	1	156	1	152	1	155	11	135	6	110	34	74	0
09G	167	2	159	1	159	0	167	1	162	0	160	0	156	3	150	5	149	12	171	1
10T	99	28	111	20	128	1	127	2	74	0	118	21	133	8	86	5	93	26	74	1
11A	153	0	151	2	158	1	149	1	150	1	152	0	147	6	144	4	137	10	151	1
12G	150	0	154	1	150	0	152	1	152	0	148	1	146	1	148	1	152	2	152	2

Major groove (Å)																				
Nt	DNA <sup>control</sup>		DNA <sup>M6</sup>		DNA <sup>M8</sup>		DNA <sup>M3</sup>		DNA <sup>H6</sup>		DNA <sup>H8</sup>		DNA <sup>H3</sup>		DNA <sup>F6</sup>		DNA <sup>F8</sup>		DNA <sup>F3</sup>	
	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std
4CG	17.2	0.3	17.6	0.1	16.7	0.1	17.4	0.1	17.6	0.1	17.7	0.1	17.0	0.6	17.4	0.2	17.0	0.6	14.7	0.9
5GC	17.2	0.2	17.3	1.0	15.8	1.0	18.9	0.2	17.3	0.1	16.5	0.1	16.3	1.1	18.2	0.2	16.3	1.1	15.0	0.8
6CG	15.7	0.2	15.9	1.3	14.4	1.3	17.5	0.2	15.9	0.1	14.7	0.1	14.9	0.4	17.3	0.2	14.9	0.4	13.9	1.2
7GC	17.2	0.2	17.3	1.1	15.8	1.1	19.0	0.2	17.3	0.1	16.5	0.1	16.3	1.1	18.2	0.2	16.3	1.1	15.0	0.8
8CG	17.2	0.3	17.6	0.1	16.7	0.1	17.5	0.1	17.6	0.1	17.7	0.1	17.0	0.5	17.4	0.2	17.0	0.5	14.6	0.9
Minor groove (Å)																				
Nt	DNA <sup>control</sup>		DNA <sup>M6</sup>		DNA <sup>M8</sup>		DNA <sup>M3</sup>		DNA <sup>H6</sup>		DNA <sup>H8</sup>		DNA <sup>H3</sup>		DNA <sup>F6</sup>		DNA <sup>F8</sup>		DNA <sup>F3</sup>	
	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std	Avg	Std
4CG	14.0	0.2	15.1	1.9	12.8	1.9	13.7	0.1	15.1	0.1	13.8	0.1	11.7	1.4	15.6	0.2	11.7	1.4	10.4	0.5
5GC	13.8	0.1	15.1	1.7	12.5	1.7	13.1	0.1	15.1	0.1	13.7	0.1	11.0	1.6	15.6	0.2	11.0	1.6	10.2	0.7
6CG	14.0	0.1	15.3	1.5	12.5	1.5	13.0	0.0	15.3	0.1	14.0	0.1	11.0	1.7	15.8	0.3	11.0	1.7	10.3	0.7
7GC	13.8	0.1	15.1	1.7	12.5	1.7	13.1	0.1	15.1	0.1	13.7	0.1	11.0	1.6	15.6	0.2	11.0	1.6	10.2	0.7
8CG	14.0	0.2	15.1	1.9	12.8	1.9	13.7	0.1	15.1	0.0	13.8	0.1	11.7	1.4	15.6	0.2	11.7	1.4	10.4	0.5

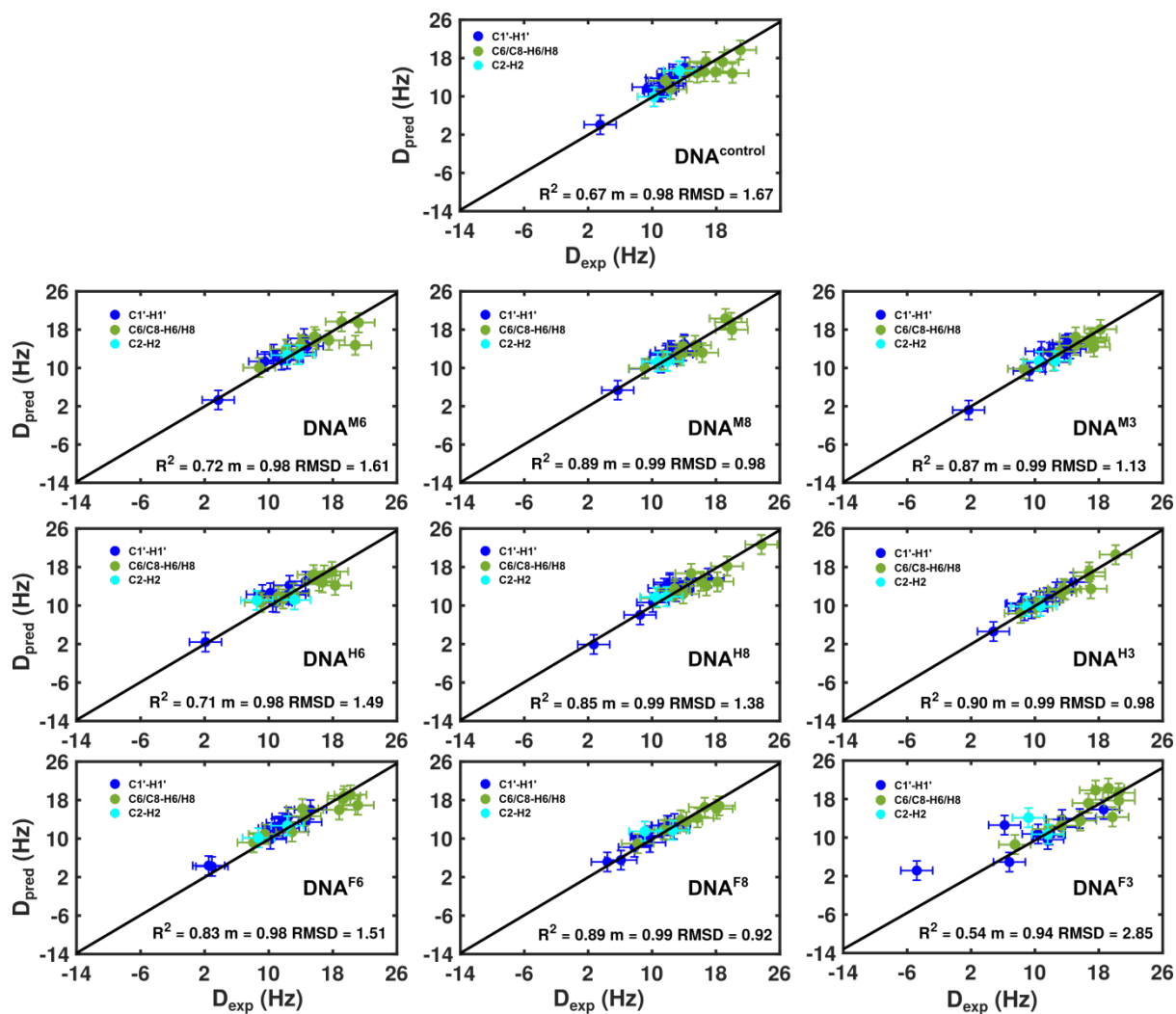
DNA helical parameters from Curves+										
Sys/S.No	DNA <sup>control</sup>	DNA <sup>M6</sup>	DNA <sup>M8</sup>	DNA <sup>M3</sup>	DNA <sup>H6</sup>	DNA <sup>H8</sup>	DNA <sup>H3</sup>	DNA <sup>F6</sup>	DNA <sup>F8</sup>	DNA <sup>F3</sup>
1	5.9	11.3	6.6	6.2	1.8	6.7	8.3	11.8	3.4	6.9
2	11.3	3.1	6.5	5.7	1.6	3	10.6	8.9	3.4	6.6
3	5.8	11.4	6.6	5.3	1.9	7.1	10.4	10.7	3.3	6.9
4	11.9	11.4	6.3	4.7	1.6	6.7	10.7	10.7	7.6	7.3
5	5.2	10.9	6.3	5	1.5	6.6	10.3	11.7	7.2	6.8
<b>Avg</b>	8	9.6	6.5	5.4	1.7	6	10.1	10.8	5	6.9
<b>Stdev</b>	3.3	3.7	0.2	0.6	0.2	1.7	1	1.2	2.2	0.3

## 7. RDC RMSD tables

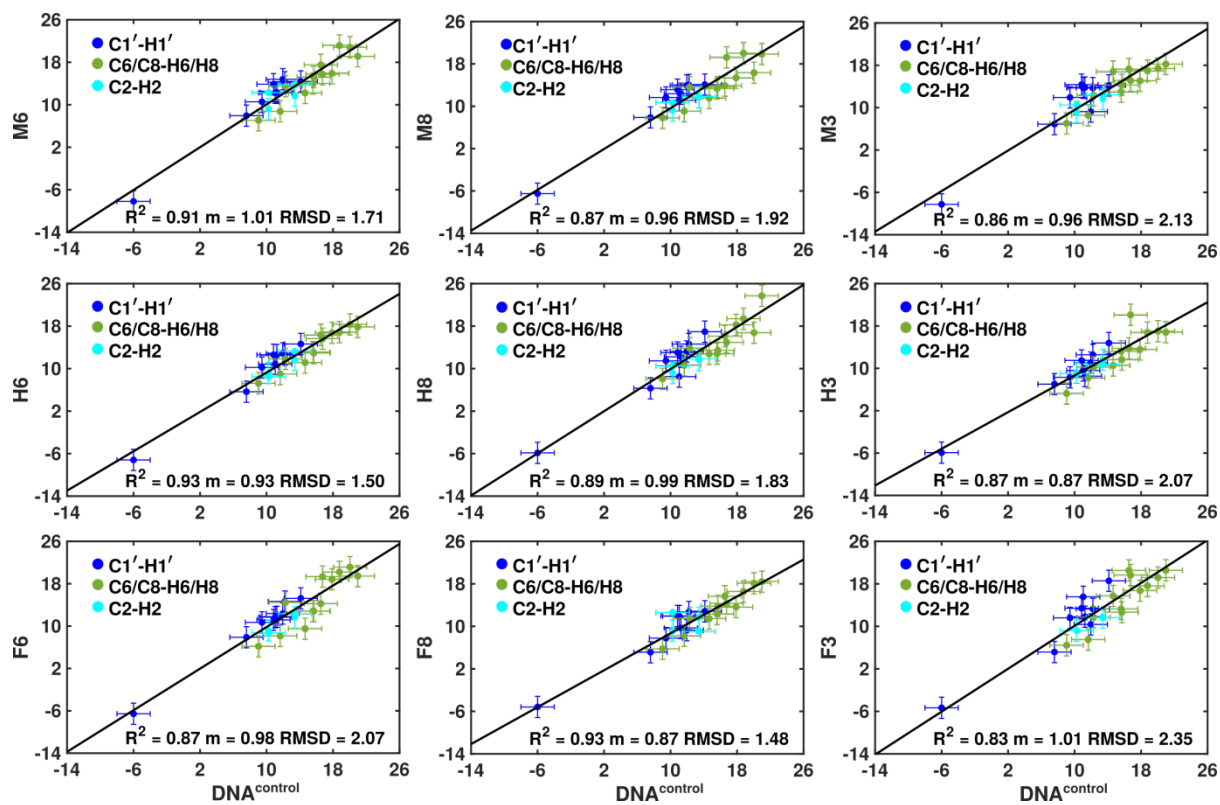
Structure used to predict (↓)	RDC RMSD (Hz)									
	DNA <sup>control</sup>	DNA <sup>M6</sup>	DNA <sup>M8</sup>	DNA <sup>M3</sup>	DNA <sup>H6</sup>	DNA <sup>H8</sup>	DNA <sup>H3</sup>	DNA <sup>F6</sup>	DNA <sup>F8</sup>	DNA <sup>F3</sup>
DNA <sup>control</sup>	1.81 ± 0.07	2.59 ± 0.04	1.91 ± 0.04	2.15 ± 0.03	2.01 ± 0.04	2.12 ± 0.05	2.08 ± 0.06	3.58 ± 0.02	2.51 ± 0.03	3.57 ± 0.06
DNA <sup>M6</sup>	1.88 ± 0.05	1.73 ± 0.06	1.37 ± 0.03	1.73 ± 0.05	1.34 ± 0.06	1.61 ± 0.09	1.97 ± 0.05	2.75 ± 0.06	2.19 ± 0.04	2.81 ± 0.16
DNA <sup>M8</sup>	2.26 ± 0.01	2.42 ± 0.01	1.09 ± 0.01	2.22 ± 0.01	1.87 ± 0.01	2.04 ± 0.01	1.72 ± 0.01	3.16 ± 0.02	2.37 ± 0.01	3.39 ± 0.02
DNA <sup>M3</sup>	2.33 ± 0.01	2.54 ± 0.01	2.07 ± 0.01	1.21 ± 0.01	1.99 ± 0.01	2.44 ± 0.02	2.33 ± 0.01	3.57 ± 0.01	2.38 ± 0.00	2.61 ± 0.01
DNA <sup>H6</sup>	2.04 ± 0.07	2.14 ± 0.00	1.52 ± 0.00	1.89 ± 0.00	1.46 ± 0.00	1.98 ± 0.01	1.97 ± 0.01	3.02 ± 0.00	2.41 ± 0.00	3.08 ± 0.00
DNA <sup>H8</sup>	2.17 ± 0.05	2.48 ± 0.03	1.68 ± 0.00	2.22 ± 0.01	1.98 ± 0.03	1.54 ± 0.03	2.27 ± 0.02	3.60 ± 0.01	2.53 ± 0.03	3.78 ± 0.01
DNA <sup>H3</sup>	2.21 ± 0.11	2.44 ± 0.10	1.42 ± 0.03	2.22 ± 0.12	1.93 ± 0.07	2.38 ± 0.07	1.22 ± 0.11	3.13 ± 0.09	2.26 ± 0.04	3.21 ± 0.18
DNA <sup>F6</sup>	2.54 ± 0.05	1.81 ± 0.10	1.86 ± 0.20	2.47 ± 0.02	1.48 ± 0.06	2.19 ± 0.03	2.10 ± 0.08	1.75 ± 0.03	2.29 ± 0.01	2.75 ± 0.15
DNA <sup>F8</sup>	2.31 ± 0.05	2.20 ± 0.04	2.08 ± 0.25	2.18 ± 0.03	2.22 ± 0.05	2.59 ± 0.23	2.25 ± 0.07	3.43 ± 0.13	1.33 ± 0.13	3.43 ± 0.21
DNA <sup>F3</sup>	3.12 ± 0.01	3.15 ± 0.01	2.79 ± 0.00	2.25 ± 0.01	2.43 ± 0.01	3.08 ± 0.01	2.77 ± 0.01	3.15 ± 0.01	2.16 ± 0.01	1.75 ± 0.01

**Table S5:** RMSD between predicted RDCs and experimentally derived RDCs. RDCs predicted for structures refined with Xplor-NIH 2.4.1 were correlated with each of set measured RDCs of DNA<sup>control</sup> and DNA<sup>N#</sup>. Here mean ± standard deviation, represents average RMSD for 5 structures and standard deviation of RMSDs.





**Figure S8:** Correlation of predicted RDCs of Xplor-NIH structures with measured RDCs of respective DNA<sup>control</sup> and DNA<sup>N#</sup>, correlation coefficient ( $R^2$ ), and root mean square deviation (RMSD) between predicted and measured RDCs with slope ( $m$ ) is also provided.



**Figure S9:** Correlation of measured RDCs of DNA<sup>N#</sup> with respect to DNA<sup>control</sup> sans modified nucleotides C1'-H1'

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