Base-Displaced Intercalated Structure of the N-(2′-Deoxyguanosin-8-yl)-3-aminobenzanthrone DNA Adduct

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Supporting Information

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Table S1. Pseudorotation angle restraints used in AMBER structural refinement calculations.

Nucleotide	Angle	Lower (º)	Upper (º)
T^2	ν_0	-44.7	-14.7
T^2	ν_1	18.1	48.1
T^2	ν_2	-37.2	-6.7
T^2	ν_3	-16.9	24.2
T^2	ν_4	-1.9	34.0
G^3	ν_0	-43.9	-13.9
G^3	ν_1	22.2	52.2
G^3	ν_2	-44.6	-14.6
G^3	ν_3	-3.2	26.8
G^3	ν_4	-4.4	25.6
G^7	ν_0	-43.9	-13.9
G^7	ν_1	22.2	52.2
G^7	ν_2	-44.6	-14.6
G^7	ν_3	-3.2	26.8
G^7	ν_4	-4.4	25.6
T^8	ν_0	-52.1	-22.1
T^8	ν_1	15.0	45.0
T^8	ν_2	-27.4	2.6
T^8	ν_3	-25.0	5.0
T^8	ν_4	13.5	43.5
T^9	ν_0	-52.1	-22.1

T^9	ν_1	15.0	45.0
T^9	ν_2	-27.4	2.6
T^9	ν_3	-25.0	5.0
T^9	ν_4	13.5	43.5
T^{10}	ν_0	-52.1	-22.1
T^{10}	ν_1	15.0	45.0
T^{10}	ν_2	-27.4	2.6
T^{10}	ν_3	-25.0	5.0
T^{10}	ν_4	13.5	43.5
G^{11}	ν_0	-44.7	-14.7
G^{11}	ν_1	18.1	48.1
G^{11}	ν_2	-37.2	-6.7
G^{11}	ν_3	-16.9	24.2
G^{11}	ν_4	-1.9	34.0
C^{14}	ν_0	-44.7	-14.7
C^{14}	ν_1	18.1	48.1
C^{14}	ν_2	-37.2	-6.7
C^{14}	ν_3	-16.9	24.2
C^{14}	ν_4	-1.9	34.0
A^{15}	ν_0	-43.9	-13.9
A^{15}	ν_1	22.2	52.2
A^{15}	ν_2	-44.6	-14.6

A^{15}	ν_3	-3.2	26.8
A^{15}	ν_4	-4.4	25.6
A^{16}	ν_0	-43.9	-13.9
A^{16}	ν_1	22.2	52.2
A^{16}	ν_2	-44.6	-14.6
A^{16}	ν_3	-3.2	26.8
A^{16}	ν_4	-4.4	25.6
A^{17}	ν_0	-43.9	-13.9
A^{17}	ν_1	22.2	52.2
A^{17}	ν_2	-44.6	-14.6
A^{17}	ν_3	-3.2	26.8
A^{17}	ν_4	-4.4	25.6
C^{18}	ν_0	-52.1	-22.1
C^{18}	ν_1	15.0	45.0
C^{18}	ν_2	-27.4	2.6
C^{18}	ν_3	-25.0	5.0
C^{18}	ν_4	13.5	43.5
G^{21}	ν_0	-43.9	-13.9
G^{21}	ν_1	22.2	52.2
G^{21}	ν_2	-44.6	-14.6
G^{21}	ν_3	-3.2	26.8
G^{21}	ν_4	-4.4	25.6
C^{22}	ν_0	-52.1	-22.1

C^{22}	ν_1	15.0	45.0
C^{22}	ν_2	-27.4	2.6
C^{22}	ν_3	-25.0	5.0
C^{22}	ν_4	13.5	43.5
A^{23}	ν_0	-44.7	-14.7
A^{23}	ν_1	18.1	48.1
A^{23}	ν_2	-37.2	-6.7
A^{23}	ν_3	-16.9	24.2
A^{23}	ν_4	-1.9	34.0

Table S2. Chemical Shifts (ppm) of the Non-exchangeable DNA Protons for the 5'-d(GTGCXTGTTTGT)-3':5'-d(ACAAACACGCAC)-3' Duplex; X = C8-dG-ABA Adduct. The temperature was 15 ºC. NA = not applicable; this proton does not exist in this nucleotide.

	Non-exchangeable Protons					
Nucleotide	H8/H6	H5/H2/CH_3	H1'	H2'	H2"	H3'
G^1	8.00	NA	6.04	2.71	2.83	4.84
T^2	7.42	1.41	6.01	2.24	2.62	4.95
G^3	7.88	NA	5.92	2.58	2.69	5.01
C^4	7.00	5.30	5.62	0.84	2.06	4.26
X^5	NA	NA	5.92	3.50	2.68	5.11
T^6	7.44	1.39	5.57	2.25	2.48	4.92
G^7	7.85	NA	6.00	2.64	2.82	4.99
T^8	7.26	1.33	6.02	2.14	2.58	4.88
T^9	7.46	1.60	6.11	2.16	2.60	4.91
T^{10}	7.32	1.71	5.84	2.00	2.39	4.92
G^{11}	7.99	NA	6.06	2.72	2.73	5.01
T^{12}	7.44	1.63	6.26	2.26	2.26	4.56
A^{13}	8.21	7.99	6.19	2.61	2.77	4.84
C^{14}	7.41	5.47	5.12	2.01	2.23	4.79
A^{15}	8.21	7.27	5.76	2.74	2.84	5.04
A^{16}	8.10	7.13	5.85	2.62	2.83	5.05
A^{17}	8.00	7.49	5.97	2.45	2.75	4.98
C^{18}	6.96	5.01	5.34	1.57	2.01	4.70
A^{19}	7.32	7.86	5.85	2.11	2.35	4.93
C^{20}	8.07	6.26	6.60	2.45	2.59	5.10

G[21]	7.35	NA	5.58	2.39	2.50	4.57
C[22]	7.35	5.16	5.50	2.02	2.34	4.74
A[23]	8.21	7.855	6.22	2.61	2.84	4.96
C[24]	7.37	5.37	6.09	2.09	2.12	4.47

Table S3. Chemical Shifts (ppm) of the DNA Protons for the Unmodified 5'-d(GTGCGTGTTTGT)-3':5'-d(ACAAACACGCAC)-3' Duplex. The temperature was 15 ºC. NA = not applicable; this proton does not exist in this nucleotide.

	Proton					
Nucleotide	**H8/H6**	**H5/H2/CH_3**	**H1'**	**H2'**	**H2"**	**H3'**
G^1	7.80	NA	6.04	2.69	2.83	4.85
T^2	7.41	1.39	5.95	2.25	2.60	4.94
G^3	7.90	NA	5.93	2.64	2.75	5.02
C^4	7.32	5.316	5.71	2.06	2.42	4.86
G^5	7.90	NA	5.98	2.63	2.80	4.99
T^6	7.18	1.48	5.83	2.15	2.53	4.89
G^7	7.85	NA	5.99	2.62	2.82	4.96
T^8	7.28	1.32	6.05	2.17	2.61	4.89
T^9	7.49	1.62	6.15	2.19	2.63	4.92
T^{10}	7.34	1.73	5.87	2.02	2.41	4.92
G^{11}	8.01	NA	6.08	2.72	2.74	5.03
T^{12}	7.44	1.64	6.28	2.27	2.27	4.57
A^{13}	8.22	8.01	6.21	2.62	2.79	4.85
C^{14}	7.42	5.48	5.13	2.03	2.24	4.80
A^{15}	8.23	Not Assigned	5.78	2.77	2.86	5.06
A^{16}	8.14	Not Assigned	5.90	2.67	2.87	5.08
A^{17}	8.07	7.56	6.07	2.54	2.87	5.01

C[18]	7.14	5.16	5.50	1.87	2.31	4.77
A[19]	8.16	7.61	6.147	2.64	2.85	5.00
C[20]	7.20	5.19	5.55	1.95	2.31	4.82
G[21]	7.84	NA	5.86	2.62	2.72	4.98
C[22]	7.36	5.42	5.62	2.04	2.40	4.84
A[23]	8.28	7.86	6.27	2.69	2.90	5.02
C[24]	7.39	5.43	6.10	2.10	2.14	4.50

Table S4. Chemical Shifts (ppm) of the Exchangeable DNA Protons for the 5'-d(GTGCXTGTTTGT)-3':5'-d(ACAAACACGCAC)-3' Duplex; X = C8-dG-ABA Adduct. The temperature was 15 ºC. NA = not applicable; this proton does not exist in this nucleotide.

	Exchangeable Protons		
Nucleotide	N1H/N3H	N^4H_a	N^4H_b
G^1	Not assigned	NA	NA
T^2	Not Assigned	NA	NA
G^3	12.57	NA	NA
C^4	NA	6.69	7.97
X^5	Not Assigned	NA	NA
T^6	12.95	NA	NA
G^7	12.27	NA	NA
T^8	13.86	NA	NA
T^9	13.93	NA	NA
T^{10}	13.87	NA	NA
G^{11}	12.64	NA	NA
T^{12}	Not Assigned	NA	NA
A^{13}	NA	NA	NA
C^{14}	NA	6.65	8.32
A^{15}	NA	NA	NA
A^{16}	NA	NA	NA
A^{17}	NA	NA	NA
C^{18}	NA	6.28	7.73
A^{19}	NA	NA	NA
C^{20}	NA	Not Assigned	Not Assigned

G^{21}	12.12	NA	NA
C^{22}	NA	6.54	8.29
A^{23}	NA	NA	NA
C^{24}	NA	Not Assigned	Not Assigned

Table S5. Chemical Shifts (ppm) of the Exchangeable DNA Protons for the unmodified 5'-d(GTGCGTGTTTGT)-3':5'-d(ACAAACACGCAC)-3' Duplex. The temperature was 15 ºC. NA = not applicable; this proton does not exist in this nucleotide.

	Exchangeable Protons		
Nucleotide	N1H/N3H	N^4H_a	N^4H_b
G^1	Not assigned	NA	NA
T^2	13.79	NA	NA
G^3	12.74	NA	NA
C^4	NA	6.39	8.27
G^5	12.78	NA	NA
T^6	13.56	NA	NA
G^7	12.50	NA	NA
T^8	13.95	NA	NA
T^9	13.98	NA	NA
T^{10}	13.91	NA	NA
G^{11}	12.68	NA	NA
T^{12}	Not Assigned	NA	NA
A^{13}	NA	NA	NA
C^{14}	NA	6.65	8.33
A^{15}	NA	NA	NA
A^{16}	NA	NA	NA
A^{17}	NA	NA	NA
C^{18}	NA	6.46	7.96
A^{19}	NA	NA	NA

C^{20}	NA	6.48	8.12
G^{21}	12.86	NA	NA
C^{22}	NA	6.48	8.38
A^{23}	NA	NA	NA
C^{24}	NA	6.85	8.16

Table S6. Chemical shifts (ppm) of the C8-dG-ABA Protons for the 5'-d(GTGCXTGTTTGT)-3':5'-d(ACAAACACGCAC)-3' Duplex; X = C8-dG-ABA Adduct. The temperature was 15 ºC.

C8-dG-ABA Proton	**Chemical Shift (ppm)**
H1	8.04
H2	8.25
H4	7.95
H5	7.61
H6	8.26
H8	7.43
H9	6.64
H10	7.20
H11	7.78

Table S7. NOE Distance Restraints Used for rMD Calculations for the 5'-d(GTGCXTGTTTGT)-3':5'-d(ACAAACACGCAC)-3' Duplex; X = C8-dG-ABA Adduct.

Nucleotide 1	Proton	Nucleotide 2	Proton	Lower (Å)	Upper (Å)	Window (Å)
G^1	H8	G^1	H1'	2.94	4.88	1.94
G^1	H8	G^1	H3'	2.89	4.68	1.79
G^1	H1'	G^1	H2'	2.80	3.32	0.52
G^1	H1'	G^1	H2"	1.92	2.51	0.59
G^1	H1'	G^1	H3'	3.63	3.92	0.29
G^1	H2'	G^1	H3'	1.95	2.68	0.73
G^1	H2"	G^1	H3'	2.49	3.02	0.53
G^1	H8	T^2	H6	3.33	5.16	1.83
G^1	H8	T^2	Me	2.50	3.62	1.12
G^1	H1'	T^2	H6	2.46	4.64	2.18
G^1	H1'	T^2	Me	2.63	5.93	3.30
G^1	H2'	T^2	Me	2.66	3.20	0.54
G^1	H2"	T^2	H6	2.09	3.75	1.66
G^1	H2"	T^2	Me	2.24	3.70	1.46
G^1	H3'	T^2	H6	3.64	5.79	2.15
T^2	H6	T^2	H1'	3.03	5.41	2.38
T^2	H6	T^2	H2"	1.86	3.46	1.60
T^2	H1'	T^2	H2'	2.69	3.51	0.82
T^2	H1'	T^2	H3'	2.63	4.45	1.82
T^2	H2'	T^2	H3'	2.16	3.26	1.10
T^2	H6	G^3	H8	3.51	5.53	2.02
T^2	Me	G^3	H8	3.75	5.76	2.01
T^2	H1'	G^3	H8	3.07	3.95	0.88

T^2	H2'	G^3	H8	3.30	3.96	0.66
T^2	H3'	G^3	H8	3.60	5.29	1.69
G^3	H8	G^3	H1'	3.35	5.29	1.94
G^3	H8	G^3	H3'	3.03	5.96	2.93
G^3	H1'	G^3	H2'	2.60	3.73	1.13
G^3	H1'	G^3	H2"	2.30	3.08	0.78
G^3	H1'	G^3	H3'	3.26	5.31	2.05
G^3	H8	C^4	H6	3.79	5.29	1.50
G^3	H8	C^4	H5	3.36	4.41	1.05
G^3	H1'	C^4	H6	3.16	3.67	0.51
G^3	H1'	C^4	H5	3.41	4.36	0.95
G^3	H2'	C^4	H6	3.21	5.89	2.68
G^3	H2'	C^4	H5	3.08	3.68	0.60
G^3	H2"	C^4	H6	2.38	2.95	0.57
G^3	H2"	C^4	H5	2.86	3.73	0.87
G^3	H3'	C^4	H5	4.13	6.60	2.47
C^4	H6	C^4	H1'	3.37	4.09	0.72
C^4	H6	C^4	H2'	2.47	2.92	0.45
C^4	H6	C^4	H2"	2.89	4.54	1.65
C^4	H6	C^4	H3'	3.23	4.25	1.02
C^4	H5	C^4	H2'	3.85	4.60	0.75
C^4	H1'	C^4	H2"	2.41	3.15	0.74
C^4	H2'	C^4	H3'	2.50	3.05	0.55
C^4	H2"	C^4	H3'	2.62	3.92	1.30
C^4	H5	X^5	ABA 2	3.90	4.83	0.93
C^4	H2'	X^5	H1'	3.70	4.30	0.60

C^4	H2"	X^5	H1'	3.70	4.15	0.45
X^5	ABA 4	X^5	H1'	2.30	4.55	2.25
X^5	ABA 4	X^5	H4'	3.07	4.17	1.10
X^5	ABA 4	X^5	H5'	2.84	4.54	1.70
X^5	ABA 4	X^5	H5"	3.31	5.65	2.34
X^5	ABA 5	X^5	H1'	3.47	5.85	2.38
X^5	H1'	X^5	H2'	2.48	4.16	1.68
X^5	H1'	X^5	H3'	2.79	4.52	1.73
X^5	H1'	X^5	H4'	2.71	3.32	0.61
X^5	H2'	X^5	H3'	2.15	2.78	0.63
X^5	H2'	X^5	H4'	3.05	5.44	2.39
X^5	H2"	X^5	H3'	2.40	3.84	1.44
X^5	H2"	X^5	H4'	3.22	5.09	1.87
X^5	H3'	X^5	H4'	2.55	3.15	0.60
X^5	ABA 2	T^6	Me	3.72	5.90	2.18
X^5	ABA 4	T^6	H6	3.51	5.06	1.55
X^5	ABA 4	T^6	Me	3.17	5.79	2.62
X^5	ABA 4	T^6	H1'	3.51	4.89	1.38
X^5	ABA 5	T^6	H1'	3.13	3.42	0.29
X^5	H1'	T^6	H6	2.84	4.37	1.53
X^5	H1'	T^6	Me	2.45	3.28	0.83
X^5	H2'	T^6	H6	3.03	4.85	1.82
X^5	H2'	T^6	Me	2.66	4.46	1.80
X^5	H3'	T^6	H6	3.11	4.26	1.15
X^5	H3'	T^6	Me	3.63	5.25	1.62
X^5	H4'	T^6	Me	4.51	6.77	2.26

X^5	ABA 8	A^{19}	H1'	3.55	4.14	0.59
X^5	ABA 8	A^{19}	H2'	2.93	4.75	1.82
X^5	ABA 8	A^{19}	H2"	2.69	3.76	1.07
X^5	ABA 9	A^{19}	H8	3.85	5.85	2.00
X^5	ABA 9	A^{19}	H1'	3.76	5.07	1.31
X^5	ABA 9	A^{19}	H2'	3.06	4.55	1.49
X^5	ABA 9	A^{19}	H2"	3.07	4.93	1.86
X^5	ABA 9	A^{19}	H3'	3.33	4.97	1.64
X^5	ABA 10	A^{19}	H1'	4.25	5.84	1.59
X^5	ABA 10	A^{19}	H2"	3.38	5.23	1.85
X^5	ABA 8	C^{20}	H6	3.77	4.50	0.73
X^5	ABA 9	C^{20}	H4'	3.30	5.70	2.40
X^5	ABA 6	G^{21}	H1'	3.06	3.45	0.39
T^6	H6	T^6	H2"	2.33	4.14	1.81
T^6	H1'	T^6	H2'	2.56	3.05	0.49
T^6	H1'	T^6	H3'	3.19	4.64	1.45
T^6	H2"	T^6	H3'	2.20	3.54	1.34
T^6	H6	G^7	H8	4.05	4.70	0.65
T^6	H1'	G^7	H8	3.18	3.70	0.52
T^6	H2'	G^7	H8	3.50	4.67	1.17
T^6	H2"	G^7	H8	2.58	3.45	0.87
T^6	H3'	G^7	H8	3.40	5.12	1.72
G^7	H8	G^7	H1'	2.93	4.78	1.85
G^7	H8	G^7	H2'	1.95	2.40	0.45
G^7	H8	G^7	H2"	2.92	3.85	0.93
G^7	H8	G^7	H3'	3.61	4.87	1.26

G^7	H1'	G^7	H2"	2.07	2.45	0.38
G^7	H8	T^8	H6	4.30	5.00	0.70
G^7	H8	T^8	Me	3.32	3.65	0.33
G^7	H1'	T^8	H6	3.18	4.33	1.15
G^7	H1'	T^8	Me	3.32	5.00	1.68
G^7	H2'	T^8	H6	2.39	4.14	1.75
G^7	H2'	T^8	Me	2.49	4.05	1.56
G^7	H2"	T^8	H6	2.25	2.69	0.44
G^7	H2"	T^8	Me	2.47	4.03	1.56
G^7	H3'	T^8	H6	3.84	4.90	1.06
G^7	H3'	T^8	Me	3.39	4.78	1.39
T^8	H6	T^8	H1'	2.57	4.84	2.27
T^8	H6	T^8	H2"	2.31	3.60	1.29
T^8	H6	T^8	H3'	3.04	4.64	1.60
T^8	H1'	T^8	H2'	2.50	3.40	0.90
T^8	H1'	T^8	H2"	2.12	2.45	0.33
T^8	H1'	T^8	H3'	2.94	4.91	1.97
T^8	H6	T^9	H6	2.90	5.37	2.47
T^8	H6	T^9	Me	3.11	4.88	1.77
T^8	H1'	T^9	H6	2.93	5.85	2.92
T^8	H1'	T^9	Me	3.13	5.54	2.41
T^8	H2'	T^9	Me	1.84	3.56	1.72
T^8	H3'	T^9	Me	3.12	5.19	2.07
T^9	H6	T^9	H1'	3.31	3.91	0.60
T^9	H1'	T^9	H2"	2.00	2.83	0.83
T^9	H1'	T^9	H3'	2.80	4.08	1.28

T^{9}	H6	T^{10}	H6	3.60	6.06	2.46
T^{9}	H6	T^{10}	Me	2.58	3.78	1.20
T^{9}	H1'	T^{10}	H6	2.76	3.48	0.72
T^{9}	H1'	T^{10}	Me	3.18	4.87	1.69
T^{9}	H2'	T^{10}	Me	2.45	3.28	0.83
T^{9}	H2"	T^{10}	H6	2.30	3.00	0.70
T^{9}	H2"	T^{10}	Me	2.49	3.67	1.18
T^{9}	H3'	T^{10}	Me	3.49	5.34	1.85
T^{10}	H6	T^{10}	H1'	2.91	5.67	2.76
T^{10}	H6	T^{10}	H2'	2.02	2.90	0.88
T^{10}	H6	T^{10}	H2"	2.08	3.87	1.79
T^{10}	Me	T^{10}	H2'	2.30	4.90	2.60
T^{10}	Me	T^{10}	H2"	2.64	5.13	2.49
T^{10}	H1'	T^{10}	H2'	2.08	3.48	1.40
T^{10}	H1'	T^{10}	H2"	1.77	2.70	0.93
T^{10}	H1'	T^{10}	H3'	2.48	4.08	1.60
T^{10}	H2'	T^{10}	H3'	2.35	2.75	0.40
T^{10}	H2"	T^{10}	H3'	2.25	3.57	1.32
T^{10}	H6	G^{11}	H8	3.42	5.18	1.76
T^{10}	H2'	G^{11}	H8	2.19	4.52	2.33
T^{10}	H2"	G^{11}	H8	2.39	4.41	2.02
T^{10}	H3'	G^{11}	H8	2.67	6.07	3.40
G^{11}	H8	G^{11}	H1'	2.56	4.84	2.28
G^{11}	H1'	G^{11}	H3'	2.96	3.96	1.00
G^{11}	H1'	G^{11}	H4'	2.51	3.39	0.88
G^{11}	H8	T^{12}	H6	3.01	5.41	2.40

G^{11}	H8	T^{12}	Me	2.66	3.68	1.02
G^{11}	H1'	T^{12}	Me	3.64	4.54	0.90
G^{11}	H2"	T^{12}	Me	2.80	3.40	0.60
G^{11}	H2"	T^{12}	H3'	3.39	4.92	1.53
G^{11}	H3'	T^{12}	H6	3.18	5.20	2.02
G^{11}	H3'	T^{12}	Me	4.07	6.40	2.33
T^{12}	H6	T^{12}	H3'	2.38	2.78	0.40
T^{12}	Me	T^{12}	H2'	2.13	4.05	1.92
T^{12}	Me	T^{12}	H3'	3.81	6.97	3.16
T^{12}	H1'	T^{12}	H3'	3.18	5.09	1.91
A^{13}	H8	A^{13}	H1'	2.38	5.09	2.71
A^{13}	H8	A^{13}	H3'	3.10	5.73	2.63
A^{13}	H1'	A^{13}	H2'	2.47	4.35	1.88
A^{13}	H1'	A^{13}	H2"	1.99	2.43	0.44
A^{13}	H1'	A^{13}	H3'	3.09	5.24	2.15
A^{13}	H2'	A^{13}	H3'	2.19	3.20	1.01
A^{13}	H2"	A^{13}	H3'	2.44	3.07	0.63
A^{13}	H2	C^{14}	H1'	3.66	4.79	1.13
A^{13}	H1'	C^{14}	H6	2.68	4.38	1.70
A^{13}	H1'	C^{14}	H5	2.57	4.72	2.15
A^{13}	H1'	C^{14}	H1'	3.56	4.95	1.39
A^{13}	H2'	C^{14}	H5	2.76	3.50	0.74
A^{13}	H2"	C^{14}	H6	2.16	2.89	0.73
A^{13}	H2"	C^{14}	H5	2.25	5.80	3.55
C^{14}	H6	C^{14}	H1'	2.90	4.10	1.20

C^{14}	H6	C^{14}	H2'	1.74	2.45	0.71
C^{14}	H6	C^{14}	H3'	2.91	4.41	1.50
C^{14}	H5	C^{14}	H1'	4.04	5.99	1.95
C^{14}	H5	C^{14}	H2'	3.26	4.82	1.56
C^{14}	H5	C^{14}	H2"	2.97	6.47	3.50
C^{14}	H1'	C^{14}	H2'	2.39	3.45	1.06
C^{14}	H1'	C^{14}	H2"	2.06	2.69	0.63
C^{14}	H1'	C^{14}	H3'	3.56	5.09	1.53
C^{14}	H2"	C^{14}	H3'	2.42	3.27	0.85
C^{14}	H1'	A^{15}	H8	2.92	3.78	0.86
C^{14}	H2"	A^{15}	H8	2.38	3.60	1.22
A^{15}	H8	A^{15}	H1'	3.00	3.98	0.98
A^{15}	H8	A^{15}	H3'	3.07	4.71	1.64
A^{15}	H2	A^{15}	H1'	3.93	4.87	0.94
A^{15}	H1'	A^{15}	H2'	2.20	3.04	0.84
A^{15}	H1'	A^{15}	H2"	1.92	3.67	1.75
A^{15}	H1'	A^{15}	H3'	2.23	4.02	1.79
A^{15}	H2"	A^{15}	H3'	2.31	3.41	1.10
A^{15}	H2	A^{16}	H2	3.70	4.10	0.40
A^{15}	H1'	A^{16}	H8	2.81	3.50	0.69
A^{15}	H2'	A^{16}	H8	3.60	5.83	2.23
A^{15}	H3'	A^{16}	H8	2.86	5.00	2.14
A^{16}	H8	A^{16}	H1'	3.21	5.60	2.39
A^{16}	H8	A^{16}	H2'	1.91	2.54	0.63
A^{16}	H8	A^{16}	H3'	2.98	5.20	2.22
A^{16}	H2	A^{16}	H1'	3.90	4.70	0.80

A^{16}	H1'	A^{16}	H2'	2.06	3.85	1.79
A^{16}	H1'	A^{16}	H2"	1.96	2.98	1.02
A^{16}	H1'	A^{16}	H3'	2.97	4.64	1.67
A^{16}	H2'	A^{16}	H3'	1.80	2.55	0.75
A^{16}	H2"	A^{16}	H3'	2.28	4.34	2.06
A^{16}	H2	A^{17}	H2	3.76	4.47	0.71
A^{16}	H2'	A^{17}	H8	3.09	4.85	1.76
A^{17}	H8	A^{17}	H1'	3.23	4.10	0.87
A^{17}	H8	A^{17}	H2'	2.12	4.02	1.90
A^{17}	H2	A^{17}	H1'	3.84	4.79	0.95
A^{17}	H1'	A^{17}	H2'	2.62	4.07	1.45
A^{17}	H1'	A^{17}	H2"	1.93	2.76	0.83
A^{17}	H2'	A^{17}	H3'	2.09	2.73	0.64
A^{17}	H2"	A^{17}	H3'	2.24	4.40	2.16
A^{17}	H8	C^{18}	H6	3.90	5.82	1.92
A^{17}	H2	C^{18}	H1'	4.00	5.42	1.42
A^{17}	H1'	C^{18}	H6	3.79	4.99	1.20
A^{17}	H2'	C^{18}	H6	3.07	6.09	3.02
A^{17}	H2"	C^{18}	H6	2.70	4.56	1.86
A^{17}	H2"	C^{18}	H5	2.62	4.67	2.05
A^{17}	H3'	C^{18}	H6	3.90	5.50	1.60
C^{18}	H6	C^{18}	H1'	3.25	4.03	0.78
C^{18}	H6	C^{18}	H2'	2.30	2.91	0.61
C^{18}	H6	C^{18}	H2"	3.50	4.05	0.55
C^{18}	H6	C^{18}	H3'	3.49	4.53	1.04
C^{18}	H5	C^{18}	H2'	3.28	5.37	2.09

C^{18}	H1'	C^{18}	H2'	2.74	3.16	0.42
C^{18}	H1'	C^{18}	H2"	2.50	2.96	0.46
C^{18}	H1'	C^{18}	H3'	3.24	4.94	1.70
C^{18}	H2'	C^{18}	H3'	2.35	2.97	0.62
C^{18}	H2"	C^{18}	H3'	2.60	3.49	0.89
C^{18}	H1'	A^{19}	H8	3.45	4.00	0.55
C^{18}	H2'	A^{19}	H8	3.40	4.20	0.80
C^{18}	H3'	A^{19}	H8	4.25	5.25	1.00
A^{19}	H8	A^{19}	H1'	3.68	4.73	1.05
A^{19}	H8	A^{19}	H2'	2.26	3.25	0.99
A^{19}	H8	A^{19}	H3'	3.08	4.85	1.77
A^{19}	H1'	A^{19}	H2'	2.96	3.36	0.40
A^{19}	H1'	A^{19}	H2"	2.22	3.09	0.87
A^{19}	H8	C^{20}	H6	3.84	5.79	1.95
A^{19}	H1'	C^{20}	H6	3.71	5.23	1.52
A^{19}	H2'	C^{20}	H6	2.57	3.78	1.21
A^{19}	H2'	C^{20}	H5	3.24	4.73	1.49
A^{19}	H2"	C^{20}	H6	2.89	4.21	1.32
A^{19}	H2"	C^{20}	H5	3.48	5.87	2.39
A^{19}	H3'	C^{20}	H6	3.06	3.68	0.62
A^{19}	H3'	C^{20}	H5	2.64	3.08	0.44
C^{20}	H6	C^{20}	H1'	3.04	5.00	1.96
C^{20}	H6	C^{20}	H2'	2.36	3.60	1.24
C^{20}	H6	C^{20}	H2"	2.33	3.70	1.37
C^{20}	H6	C^{20}	H3'	3.06	4.96	1.90
C^{20}	H6	C^{20}	H4'	3.52	5.55	2.03

C^{20}	H6	C^{20}	H5'	3.30	5.30	2.00
C^{20}	H6	C^{20}	H5"	3.30	5.30	2.00
C^{20}	H5	C^{20}	H2'	3.15	5.95	2.80
C^{20}	H1'	C^{20}	H2'	2.90	4.14	1.24
C^{20}	H1'	C^{20}	H2"	1.91	2.49	0.58
C^{20}	H1'	C^{20}	H3'	3.27	4.15	0.88
C^{20}	H1'	C^{20}	H4'	3.02	3.84	0.82
C^{20}	H2'	C^{20}	H3'	2.40	2.80	0.40
C^{20}	H2"	C^{20}	H3'	2.55	3.30	0.75
C^{20}	H1'	G^{21}	H8	3.36	3.81	0.45
G^{21}	H8	G^{21}	H1'	3.23	4.05	0.82
G^{21}	H8	G^{21}	H2"	2.85	4.26	1.41
G^{21}	H8	G^{21}	H3'	3.34	5.25	1.91
G^{21}	H1'	G^{21}	H2'	2.51	3.00	0.49
G^{21}	H1'	G^{21}	H3'	3.35	4.94	1.59
G^{21}	H2'	G^{21}	H3'	2.30	2.97	0.67
G^{21}	H2"	G^{21}	H3'	2.48	4.18	1.70
G^{21}	H1'	C^{22}	H6	4.30	5.20	0.90
G^{21}	H1'	C^{22}	H5	4.50	5.38	0.88
G^{21}	H2'	C^{22}	H6	2.64	4.87	2.23
G^{21}	H2'	C^{22}	H5	2.81	5.10	2.29
G^{21}	H2"	C^{22}	H6	2.50	3.12	0.62
G^{21}	H2"	C^{22}	H5	2.90	4.58	1.68
G^{21}	H3'	C^{22}	H6	2.95	4.78	1.83
G^{21}	H3'	C^{22}	H5	2.85	4.71	1.86
C^{22}	H6	C^{22}	H1'	2.97	4.11	1.14

C^{22}	H6	C^{22}	H2'	1.91	2.94	1.03
C^{22}	H6	C^{22}	H2"	2.23	4.11	1.88
C^{22}	H6	C^{22}	H3'	2.61	4.04	1.43
C^{22}	H5	C^{22}	H2'	3.20	4.45	1.25
C^{22}	H1'	C^{22}	H2'	2.25	3.23	0.98
C^{22}	H1'	C^{22}	H2"	2.06	2.40	0.34
C^{22}	H1'	C^{22}	H3'	3.50	5.47	1.97
C^{22}	H2'	C^{22}	H3'	2.30	3.00	0.70
C^{22}	H2"	C^{22}	H3'	2.60	4.18	1.58
C^{22}	H1'	A^{23}	H8	2.85	3.40	0.55
C^{22}	H2'	A^{23}	H8	3.60	4.20	0.60
C^{22}	H3'	A^{23}	H8	4.45	5.15	0.70
A^{23}	H8	A^{23}	H1'	3.00	3.79	0.79
A^{23}	H8	A^{23}	H3'	2.97	4.26	1.29
A^{23}	H2	A^{23}	H1'	3.56	4.87	1.31
A^{23}	H1'	A^{23}	H2'	2.34	3.50	1.16
A^{23}	H1'	A^{23}	H2"	1.83	2.32	0.49
A^{23}	H1'	A^{23}	H3'	3.36	5.38	2.02
A^{23}	H2"	A^{23}	H3'	1.87	2.64	0.77
A^{23}	H8	C^{24}	H5	3.63	4.10	0.47
A^{23}	H1'	C^{24}	H6	3.00	3.99	0.99
A^{23}	H1'	C^{24}	H5	3.19	5.25	2.06
A^{23}	H2'	C^{24}	H6	2.36	3.95	1.59
A^{23}	H2'	C^{24}	H5	2.91	4.69	1.78
A^{23}	H2"	C^{24}	H6	1.98	2.86	0.88
A^{23}	H2"	C^{24}	H5	2.87	4.59	1.72

A^{23}	H2"	C^{24}	H3'	2.28	5.30	3.02
A^{23}	H3'	C^{24}	H6	2.72	5.46	2.74
C^{24}	H6	C^{24}	H1'	2.68	4.83	2.15
C^{24}	H6	C^{24}	H2'	1.80	2.20	0.40
C^{24}	H6	C^{24}	H3'	2.62	3.80	1.18
C^{24}	H5	C^{24}	H1'	3.82	5.92	2.10
C^{24}	H5	C^{24}	H2'	2.98	5.44	2.46
C^{24}	H1'	C^{24}	H2'	2.05	5.06	3.01
C^{24}	H1'	C^{24}	H2"	1.62	2.20	0.58
C^{24}	H1'	C^{24}	H3'	2.92	5.14	2.22
C^{24}	H2'	C^{24}	H3'	1.91	2.55	0.64
C^{24}	H2"	C^{24}	H3'	2.28	2.75	0.47

Table S8. Anti-distance restraints used for rMD calculations for the 5'-d(GTGCXTGTTTGT)-3':5'-d(ACAAACACGCAC)-3' duplex; X = C8-dG-ABA adduct.

Nucleotide 1	Proton	Nucleotide 2	Proton	Lower (Å)	Upper (Å)
X^5	ABA H8	C^{20}	H1'	5.00	9.99
X^5	ABA H8	C^{20}	H2'	5.00	9.99
X^5	ABA H9	C^{20}	H1'	5.00	9.99
X^5	ABA H9	C^{20}	H2"	5.00	9.99
X^5	ABA H10	C^{20}	H6	5.00	9.99
X^5	ABA H10	G^{21}	H8	5.00	9.99
A^{19}	H2'	C^{20}	H1'	5.00	9.99
A^{19}	H2"	C^{20}	H1'	5.00	9.99
C^{20}	H1'	G^{21}	H5'	5.00	9.99
C^{20}	H1'	G^{21}	H5"	5.00	9.99

Table S9. RMS differences and sixth root residual R^X_1 values calculated for the average structure without including anti-distance restraints.

Average structure (calculated from ten structures emergent from the simulated annealing rMD calculations)			
rms pairwise difference between structures	0.575		
rms difference from average structure	0.389		
	Complete Relaxation Matrix Analysis for the Calculated Average Structure, Using the Program CORMA[a]		
	Intranucleotide	Internucleotide	Total
R^X_1[b]	0.080	0.089	0.084
Average error[c]			0.019

[a]Mixing time was 250 ms

[b]R^X_1 is the sixth root R factor: $\sum[((I_o)_i^{1/6})-((I_c)_i^{1/6})/\sum((I_o)_i^{1/6})]$

[c]Average error: $\sum(I_c-I_o)/n$ where I_c are NOE intensities calculated from the refined structure and I_o are experimental NOE intensities

Table S10. Comparison of restraints used in rMD calculations to measured distances in refined structure for lesion site.

Nucleotide 1	Proton	Nucleotide 2	Proton	Lower (Å)	Upper (Å)	Measured (Å)
C^4	H5	X^5	ABA 2	3.90	4.83	4.67
C^4	H2'	X^5	H1'	3.70	4.30	4.37*
C^4	H2"	X^5	H1'	3.70	4.15	4.15
X^5	ABA 4	X^5	H1'	2.30	4.55	3.26
X^5	ABA 4	X^5	H4'	3.07	4.17	3.70
X^5	ABA 4	X^5	H5'	2.84	4.55	4.55
X^5	ABA 4	X^5	H5"	3.31	5.65	5.70*
X^5	ABA 5	X^5	H1'	3.47	5.85	5.78
X^5	H1'	X^5	H2'	2.48	4.16	3.03
X^5	H1'	X^5	H3'	2.79	4.52	3.77
X^5	H1'	X^5	H4'	2.71	3.32	2.69*
X^5	H2'	X^5	H3'	2.15	2.78	2.28
X^5	H2'	X^5	H4'	3.05	5.44	3.84
X^5	H2"	X^5	H3'	2.40	3.84	2.80
X^5	H2"	X^5	H4'	3.22	5.09	3.85
X^5	H3'	X^5	H4'	2.55	3.15	2.92
X^5	ABA 2	T^6	Me	3.72	5.90	5.23
X^5	ABA 4	T^6	H6	3.51	5.06	4.31
X^5	ABA 4	T^6	Me	3.17	5.79	5.44
X^5	ABA 4	T^6	H1'	3.51	4.89	3.95

X^5	ABA 5	T^6	H1'	3.13	3.42	3.44*
X^5	H1'	T^6	H6	2.84	4.37	2.83*
X^5	H1'	T^6	Me	2.45	3.28	2.81
X^5	H2'	T^6	H6	3.03	4.85	4.88*
X^5	H2'	T^6	Me	2.66	4.46	4.40
X^5	H3'	T^6	H6	3.11	4.30	4.33*
X^5	H3'	T^6	Me	3.63	5.25	4.94
X^5	H4'	T^6	Me	4.51	6.77	4.69
X^5	ABA 8	A^{19}	H1'	3.55	4.14	3.84
X^5	ABA 8	A^{19}	H2'	2.93	4.75	4.03
X^5	ABA 8	A^{19}	H2"	2.69	3.76	2.69
X^5	ABA 9	A^{19}	H8	3.85	5.85	4.15
X^5	ABA 9	A^{19}	H1'	3.76	5.07	4.89
X^5	ABA 9	A^{19}	H2'	3.06	4.55	3.06
X^5	ABA 9	A^{19}	H2"	3.07	4.93	3.02*
X^5	ABA 9	A^{19}	H3'	3.33	4.97	4.84
X^5	ABA 10	A^{19}	H1'	4.25	5.84	5.88*
X^5	ABA 10	A^{19}	H2"	3.38	5.23	4.84
X^5	ABA 8	C^{20}	H6	3.77	4.50	4.43
X^5	ABA 9	C^{20}	H4'	3.30	5.70	5.53
X^5	ABA 6	G^{21}	H1'	3.06	3.45	3.43

* indicates values outside of imposed distance restraints

Figure S1. Structure of the C8-dG-ABA adduct, depicting bond lengths and partial charges used for rMD calculations. **A.** Calculated bond lengths (Å) for the C8-dG-ABA adduct. **B.** Calculated partial charges for atoms of the C8-dG-ABA adduct. All calculations were performed in GAUSSIAN.

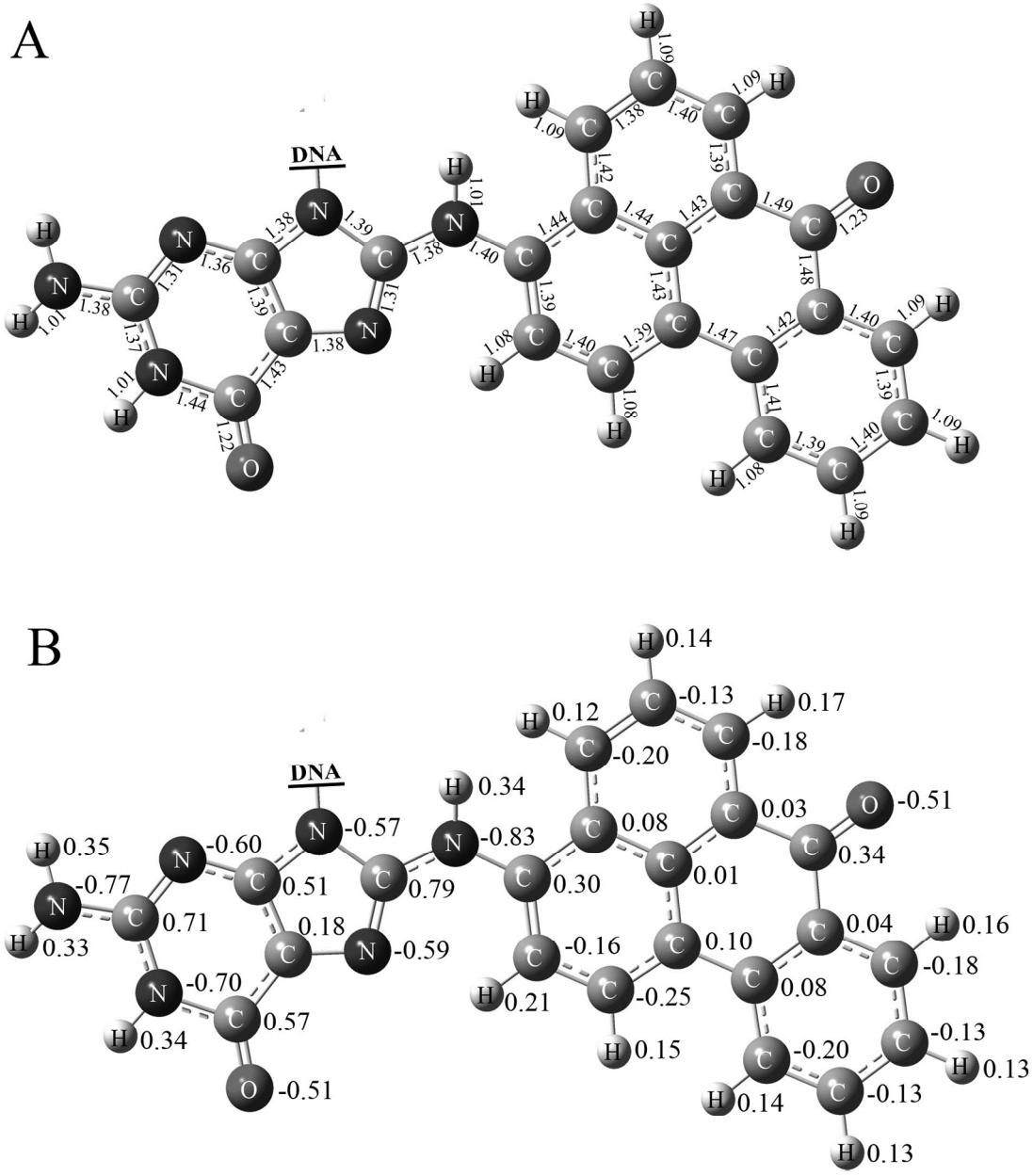

Figure S2. Expanded plots of NOESY spectra comparing chemical shift overlaps for the C8-dG-ABA adduct H8, T^6 H6 and G^{21} H8 protons in the regions of the spectra showing NOEs between base aromatic and deoxyribose H1' proton resonances. The duplex is 5'-d(GTGCXTGTTTGT)-3':5'-d(ACAAACACGCAC)-3'; X = C8-dG-ABA Adduct**. Left Panel:** The NOESY spectrum at 15 ºC. **Right Panel:** The NOESY spectrum at 25 ºC. The improved spectral resolution obtained at 15 ºC spectrum allowed unequivocal assignment of these resonances.

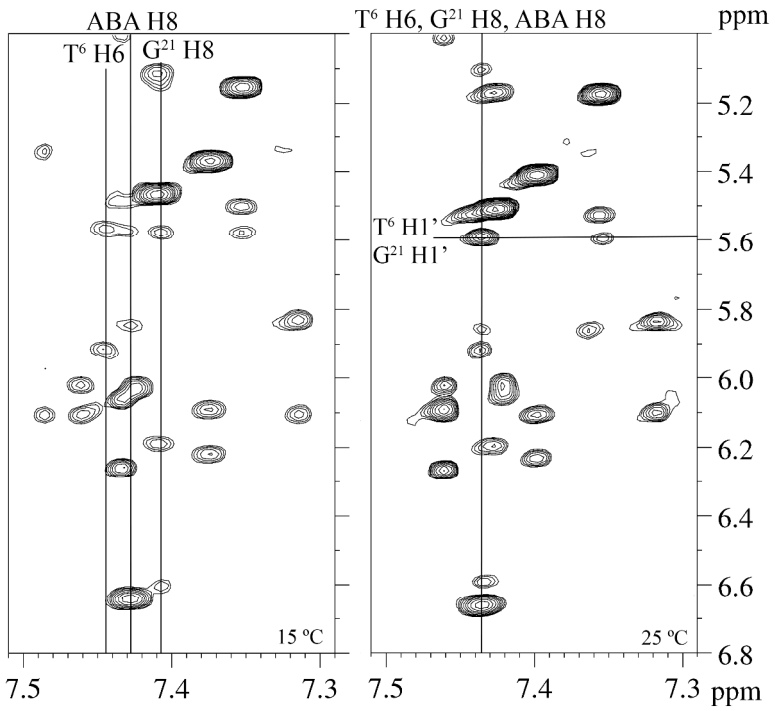

Figure S3. Expanded plots from a NOESY spectrum of the 5'-d(GTGCGTGTTTGT)-3':5'-d(ACAAACACGCAC)-3' duplex showing the sequential NOE connectivity between aromatic H8/H6 protons and deoxyribose H1' protons. **Left Panel.** The primary strand, showing bases G^1 through T^{12}. **Right Panel.** The complementary strand connectivity showing assignments for bases A^{13} through C^{24}. The 900 MHz spectrum was acquired at 15 ºC using a 250 ms mixing time.

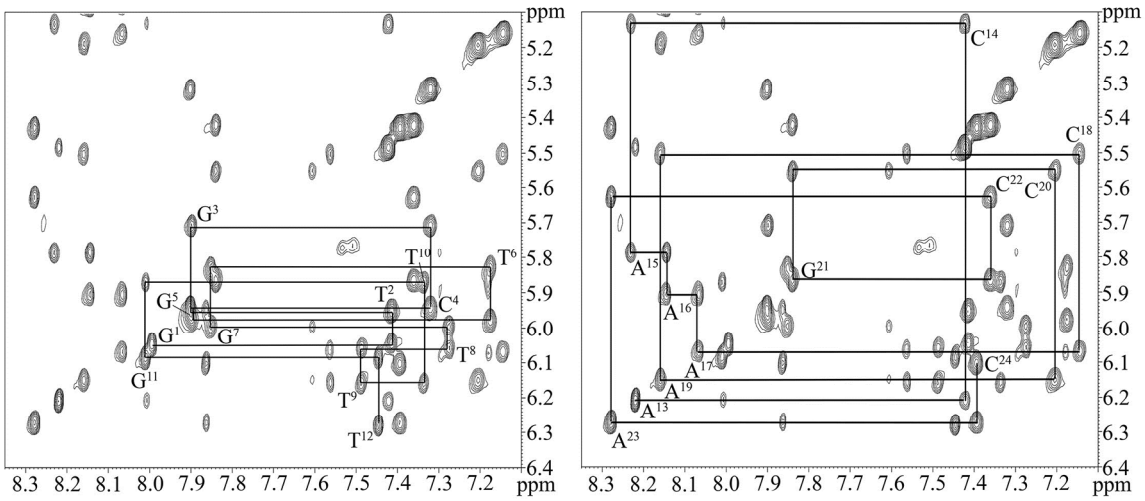
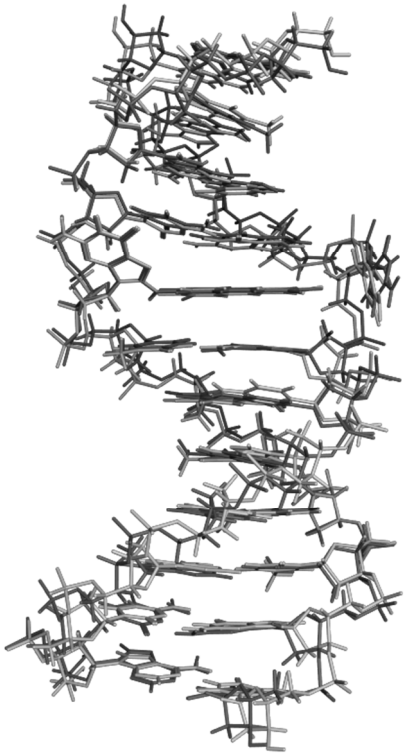
Figure S4. Overlay of lowest energy refined structure with anti-distance restraints in dark grey with the lowest energy refined structure without negative restraints in light grey. Major structural features are unchanged and the maximum pairwise difference of the two structures is 0.475 Å.