Stereochemistry Modulates Stability of Reduced Inter-Strand Cross-Links Arising From *R*- and S-α-CH_3-γ-OH-1,N^2-propano-2'-Deoxyguanosine in the 5'-CpG-3' DNA Sequence

Supporting Information

Revised Manuscript

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Running Title: Crotonaldehyde Interstrand DNA Cross-Link Structure

Table S1. Chemical Shifts (ppm) of Non-Exchangeable Protons in the Oligodeoxynucleotide 5'-d(GCTAGCXAGTCC)-3'•5'-(GGACTCYCTAGC)-3' Containing the 5'-Cp-N^2-dG-3'-*R*-(α)-CH_3-propyl-5'-Cp-N^2-dG-3' Inter-strand Cross-link **8a**.

Nucleotide	H1'	H2'	H2''	H3'	H4'	H5'	H5''	H6/H8	CH_3/H5
G[1]	6.02	2.68	2.79	4.85	4.26	3.75	n.a.	7.99	
C[2]	6.06	2.15	2.53	4.83	4.26	4.16	4.21	7.55	5.40
T[3]	5.58	2.16	2.43	4.88	4.15	4.09	4.10	7.43	1.69
A[4]	6.03	2.75	2.90	5.05	4.41	4.05	4.15	8.22	
G[5]	5.70	2.44	2.59	4.95	4.35	4.22	4.18	7.66	
C[6]	5.48	1.21	1.83	4.69	4.01	n.a.	4.18	7.07	5.17
X[7]	5.47	2.78	2.78	4.97	4.32	3.92	4.01	7.84	
A[8]	6.00	2.66	2.90	5.01	4.34	4.16	4.18	8.08	
G[9]	5.78	2.42	2.68	4.86	4.33	4.18	4.21	7.53	
T[10]	6.01	2.11	2.50	4.83	4.20	4.12	4.23	7.20	1.26
C[11]	6.09	2.24	2.49	4.84	4.17	4.09	4.06	7.60	5.70
C[12]	6.24	2.29	2.31	4.56	4.06	4.26	4.17	7.70	5.81
G[13]	5.64	2.47	2.64	4.81	4.17	3.66	n.a.	7.82	
G[14]	5.57	2.71	2.79	5.02	4.37	4.06	4.14	7.86	
A[15]	6.27	2.75	2.92	5.06	4.50	4.20	4.25	8.22	
C[16]	5.81	1.96	2.47	4.66	4.22	4.18	4.33	7.29	5.22
T[17]	6.03	2.09	2.43	4.85	4.18	4.06	4.09	7.37	1.50
C[18]	5.49	1.65	2.10	4.79	4.01	4.03	4.08	7.28	5.54
Y[19]	6.00	2.81	2.69	5.00	4.39	4.04	4.07	7.94	

C^{20}	5.84	1.98	2.46	4.67	4.17	4.17	4.28	7.43	5.39
T^{21}	5.56	2.08	2.39	4.84	4.11	4.03	4.39	7.40	1.69
A^{22}	6.02	2.73	2.87	5.03	4.38	4.03	4.11	8.21	
G^{23}	5.81	2.47	2.63	4.93	4.35	4.18	4.22	7.68	
C^{24}	6.12	2.13	2.20	4.46	4.22	4.03	4.26	7.40	5.36

Assignments of the 5'-Cp-N^2-dG-3'-*R*-(α)-CH_3-Propyl-5'- Cp-N^2-dG-3' Inter-strand Cross-link **8a** Protons:

Proton	**Chemical Shift (ppm)**
X^7 H_α	3.82
CH_3	1.03
$H_{\beta 1}$	1.82
$H_{\beta 2}$	1.63
$H_{\gamma 1}$	3.71
$H_{\gamma 2}$	2.82

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Table S2. Chemical Shifts (ppm) of Non-Exchangeable Protons in the Oligodeoxynucleotide 5'-d(GCTAGCXAGTCC)-3'•5'- (GGACTCYCTAGC)-3' Containing the 5'- Cp-N^2-dG-3'- *S*-(α)-CH_3-propyl-5'-Cp-N^2-dG-3' Inter-strand Cross-link **8b**.

Nucleotide	H1'	H2'	H2''	H3'	H4'	H5'	H5''	H6/H8	CH_3/H5
G[1]	6.00	2.67	2.77	4.84	4.26	3.73	n.a.	7.98	
C[2]	6.05	2.14	2.51	4.82	4.25	4.20	4.15	7.54	5.40
T[3]	5.55	2.15	2.41	4.87	4.13	n.a.	n.a.	7.42	1.68
A[4]	6.01	2.74	2.90	5.04	4.40	4.04	4.14	8.21	
G[5]	5.68	2.44	2.59	4.94	4.35	4.18	n.a.	7.65	
C[6]	5.49	1.33	2.00	4.71	3.99	4.20	4.04	7.07	5.19
X[7]	5.78	2.73	2.81	4.99	4.33	3.96	4.04	7.84	
A[8]	5.86	2.51	2.86	4.99	4.19	4.19	4.15	8.00	
G[9]	5.78	2.39	2.66	4.84	4.33	n.a.	n.a.	7.48	
T[10]	6.01	2.10	2.49	4.82	4.20	4.12	n.a.	7.20	1.23
C[11]	6.09	2.23	2.48	4.84	4.17	4.08	n.a.	7.60	5.70
C[12]	6.23	2.29	n.a.	4.55	4.05	4.26	4.17	7.71	5.81
G[13]	5.63	2.44	2.61	4.80	4.16	3.65	n.a.	7.80	
G[14]	5.55	2.70	2.78	5.01	4.36	4.05	4.13	7.85	
A[15]	6.26	2.75	2.91	5.05	4.50	4.19	4.24	8.22	
C[16]	5.80	1.99	2.50	4.65	4.23	4.33	4.19	7.27	5.20
T[17]	6.02	2.14	2.51	4.86	4.20	n.a.	n.a.	7.38	1.49
C[18]	5.61	1.73	2.30	4.83	4.03	n.a.	n.a.	7.28	5.52
Y[19]	5.96	2.76	2.64	4.99	4.39	4.09	4.03	7.93	

C^{20}	5.81	1.94	2.46	4.68	4.16	4.30	n.a.	7.42	5.34
T^{21}	5.55	2.09	2.39	4.84	4.11	n.a.	n.a.	7.40	1.66
A^{22}	6.01	2.72	2.86	5.03	4.38	4.02	4.12	8.20	
G^{23}	5.80	2.47	2.62	4.93	4.34	n.a.	n.a.	7.68	
C^{24}	6.11	2.12	2.20	4.45	4.03	4.45	n.a.	7.40	5.35

Assignments of the 5'-Cp-N^2-dG-3'-*S*-(α)-CH_3-Propyl-5'- Cp-N^2-dG-3' Inter-strand Cross-link **8b** Protons:

Proton	**Chemical Shift (ppm)**
X^7 H_α	3.28
CH_3	1.17
$H_{\beta 1}$	1.09
$H_{\beta 2}$	2.77
$H_{\gamma 1}$	4.06
$H_{\gamma 2}$	2.84

Table S3. ^{1}H Chemical Shifts (ppm) of Exchangeable Protons in the Oligodeoxynucleotide 5'-d(GCTAGCXAGTCC)-3'•5'-(GGACTCYCTAGC)-3'Containing the 5'-Cp-N^2-dG-3'-*R*-(α)-CH_3-propyl-5'-Cp-N^2-dG-3' Inter-strand Cross-link **8a**.

Base-pair	**Imino Protons (G N1H/T N3H)**	**Cytosine Amino Proton C NH_{4a}**	**Cytosine Amino Proton C NH_{4b}**
C^2•G^{23}	12.91	8.39	6.73
T^3•A^{22}	13.88		
A^4•T^{21}	13.76		
G^5•C^{20}	12.73	8.09	6.51
C^6•Y^{19}	12.61	8.25	6.32
X^7•C^{18}	12.45	8.58	6.82
A^8•T^{17}	13.86		
G^9•C^{16}	12.83	7.96	6.71
T^{10}•A^{15}	13.68		
C^{11}•G^{14}	12.87	8.48	6.97

Table S4. ^{1}H Chemical Shifts (ppm) of Exchangeable Protons in the Oligodeoxynucleotide 5'-d(GCTAGCXAGTCC)-3'•5'-(GGACTCYCTAGC)-3'Containing the 5'-Cp-N^2-dG-3'-*S*-(α)-CH_3-propyl-5'-Cp-N^2-dG-3' Inter-strand Cross-link **8b**.

Base-pair	**Imino Protons (G N1H/T N3H)**	**Cytosine Amino Proton C NH_{4a}**	**Cytosine Amino Proton C NH_{4b}**
C^2•G^{23}	12.88	8.35	6.69
T^3•A^{22}	13.86		
A^4•T^{21}	13.71		
G^5•C^{20}	12.72	8.08	6.42
C^6•Y^{19}	12.52	8.30	6.28
X^7•C^{18}	12.29	8.39	6.73
A^8•T^{17}	13.87		
G^9•C^{16}	12.84	7.94	6.70
T^{10}•A^{15}	13.68		
C^{11}•G^{14}	12.85	8.44	6.93

Table S5. NOE Distance Restraints Used in rMD Calculations for the Oligodeoxynucleotide 5'-d(GCTAGCXAGTCC)-3'•5'-(GGACTCYCTAGC)-3'Containing the 5'-Cp-N^2-dG-3'-*R*-(α)-CH_3-propyl-5'-Cp-N^2-dG-3' Inter-strand Cross-link **8a**.

Class 1

res_#	res_name	atm_name	res_#	res_name	atm_name	low_bnd	up_bnd
1	GUA	H1'	1	GUA	H8	3.51	4.45
1	GUA	H2'2	1	GUA	H3'	2.61	3.35
1	GUA	H3'	1	GUA	H8	4.03	5.70
2	CYT	H5	1	GUA	H8	3.66	4.97
2	CYT	H2'1	2	CYT	H6	1.88	2.19
2	CYT	H2'2	2	CYT	H6	3.86	6.05
2	CYT	H4'	2	CYT	H2'1	3.76	5.32
2	CYT	H4'	2	CYT	H2'2	3.01	4.28
2	CYT	H5	2	CYT	H6	2.31	2.46
3	THY	M	2	CYT	H6	3.53	4.60
5	GUA	H3'	5	GUA	H1'	3.37	3.68
5	GUA	H8	5	GUA	H1'	3.33	3.98
5	GUA	H2'1	6	CYT	H6	3.62	5.46
6	CYT	H5	5	GUA	H2'2	2.73	2.92
6	CYT	H5	5	GUA	H8	3.51	3.90
6	CYT	H6	5	GUA	H1'	3.02	3.22
6	CYT	H6	5	GUA	H2'2	2.47	2.65
6	CYT	H1'	6	CYT	H2'1	2.76	3.88
6	CYT	H1'	6	CYT	H2'2	2.02	2.25
6	CYT	H1'	6	CYT	H3'	3.70	4.71
6	CYT	H1'	6	CYT	H6	3.17	3.81

6	CYT	H2'1	6	CYT	H3'	2.38	2.58
6	CYT	H2'1	6	CYT	H6	2.21	2.45
6	CYT	H2'2	6	CYT	H3'	2.61	3.20
6	CYT	H2'2	6	CYT	H6	2.95	4.39
6	CYT	H3'	6	CYT	H6	3.17	3.52
6	CYT	H5	6	CYT	H6	2.29	2.42
7	X	H2x1	7	X	H1x	2.16	2.98
7	X	H2x1	7	X	M	2.63	3.79
7	X	H2x2	7	X	H1x	2.30	3.05
7	X	H2x2	7	X	M	2.67	3.78
7	X	M	7	X	H1x	2.15	2.86
8	ADE	H2	7	X	M	4.00	5.09
8	ADE	H4'	7	X	M	4.11	5.57
8	ADE	H8	7	X	H1'	2.88	3.16
8	ADE	H2'1	8	ADE	H8	2.10	2.42
8	ADE	H2'2	8	ADE	H8	3.30	4.85
8	ADE	H8	8	ADE	H1'	3.42	4.06
9	GUA	H8	9	GUA	H1'	3.38	4.00
10	THY	H6	9	GUA	H1'	2.67	3.43
10	THY	M	9	GUA	H1'	4.58	6.91
10	THY	M	9	GUA	H2'1	3.47	4.48
10	THY	M	9	GUA	H3'	4.20	5.42
10	THY	M	9	GUA	H8	3.53	4.48
10	THY	H1'	10	THY	H6	3.58	4.35
10	THY	M	10	THY	H6	2.81	3.54
10	THY	H1'	11	CYT	H6	3.41	4.38
11	CYT	H5	10	THY	H2'1	3.18	5.55

11	CYT	H5	10	THY	H6	3.29	3.59
11	CYT	H2'1	11	CYT	H5	4.05	5.89
11	CYT	H5	11	CYT	H6	2.25	2.38
11	CYT	H1'	15	ADE	H2	3.72	4.20
12	CYT	H3'	12	CYT	H1'	3.96	5.79
12	CYT	H4'	12	CYT	H1'	3.06	3.23
12	CYT	H6	12	CYT	H1'	3.47	4.61
13	GUA	H1'	13	GUA	H3'	3.82	5.06
13	GUA	H3'	13	GUA	H8	4.62	7.30
13	GUA	H1'	14	GUA	H8	3.43	3.91
14	GUA	H1'	14	GUA	H8	3.50	5.14
14	GUA	H3'	14	GUA	H8	3.81	5.59
15	ADE	H8	14	GUA	H8	4.54	6.59
15	ADE	H2	15	ADE	H1'	4.03	5.08
15	ADE	H2'1	15	ADE	H1'	2.95	3.45
15	ADE	H2'2	15	ADE	H1'	2.30	2.40
15	ADE	H3'	15	ADE	H1'	3.54	4.41
15	ADE	H4'	15	ADE	H1'	3.07	3.21
15	ADE	H8	15	ADE	H1'	3.47	4.31
16	CYT	H1'	15	ADE	H2	3.32	3.52
16	CYT	H5	15	ADE	H2'2	3.46	4.44
16	CYT	H5	15	ADE	H8	3.40	3.66
16	CYT	H6	15	ADE	H1'	3.15	3.38
16	CYT	H6	15	ADE	H2'1	3.18	3.85
16	CYT	H6	15	ADE	H2'2	2.00	2.66
16	CYT	H6	15	ADE	H8	3.73	5.10
16	CYT	H2'1	16	CYT	H6	1.82	2.47

16	CYT	H3'	16	CYT	H6	3.31	4.07
16	CYT	H4'	16	CYT	H2'1	3.76	4.81
16	CYT	H5	16	CYT	H6	2.36	2.48
16	CYT	H6	16	CYT	H1'	3.36	3.70
16	CYT	H2'2	17	THY	M	3.90	6.82
17	THY	H6	16	CYT	H1'	4.00	5.41
17	THY	H6	16	CYT	H3'	4.14	6.00
17	THY	M	16	CYT	H3'	3.69	4.67
17	THY	M	16	CYT	H5	4.06	5.13
17	THY	M	16	CYT	H6	3.49	4.44
17	THY	H1'	17	THY	H6	3.08	3.79
17	THY	M	17	THY	H6	2.83	3.57
17	THY	H1'	18	CYT	H6	3.79	4.87
18	CYT	H5	17	THY	H6	3.12	3.44
18	CYT	H2'1	18	CYT	H1'	2.92	6.26
18	CYT	H2'2	18	CYT	H1'	2.25	2.35
18	CYT	H3'	18	CYT	H6	3.54	4.48
19	Y	H3x1	7	X	H2x1	2.08	2.92
19	Y	H3x1	7	X	H2x2	2.06	2.81
19	Y	H3x1	7	X	M	3.29	6.38
19	Y	H3x2	7	X	H2x2	2.16	2.88
19	Y	H3x2	7	X	M	2.83	4.59
19	Y	H8	18	CYT	H1'	3.72	4.85
19	Y	H8	18	CYT	H2'2	3.01	3.43
19	Y	H1'	19	Y	H8	3.56	5.13
20	CYT	H1'	19	Y	H3x2	2.26	2.62
20	CYT	H5	19	Y	H8	3.53	4.52

20	CYT	H6	19	Y	H2'1	3.12	3.93
21	THY	H5'1	20	CYT	H1'	3.39	5.13
22	ADE	H8	21	THY	H2'1	4.01	6.51
22	ADE	H3'	23	GUA	H8	3.81	5.02
23	GUA	H1'	23	GUA	H3'	3.58	4.16
24	CYT	H1'	24	CYT	H3'	3.65	4.57

Class 2

res_#	res_name	atm_name	res_#	res_name	atm_name	low_bnd	up_bnd
1	GUA	H2'1	1	GUA	H8	2.12	2.30
1	GUA	H2'2	1	GUA	H8	2.97	4.96
1	GUA	H4'	1	GUA	H2'1	2.94	3.96
2	CYT	H6	1	GUA	H2'2	2.40	2.60
2	CYT	H1'	2	CYT	H6	3.19	3.81
3	THY	M	2	CYT	H2'2	3.70	5.24
3	THY	H1'	3	THY	H6	3.14	3.79
3	THY	H2'1	4	ADE	H8	3.07	3.35
4	ADE	H4'	4	ADE	H2'1	3.24	4.01
4	ADE	H4'	4	ADE	H2'2	3.45	4.39
4	ADE	H1'	5	GUA	H8	2.76	3.33
4	ADE	H3'	5	GUA	H8	3.68	4.59
5	GUA	H8	4	ADE	H2'1	2.81	3.38
5	GUA	H8	4	ADE	H2'2	2.37	2.83
5	GUA	H2'2	5	GUA	H8	2.73	4.16
5	GUA	H4'	5	GUA	H1'	2.77	2.97
5	GUA	H2'1	6	CYT	H5	4.00	6.14
6	CYT	H5	5	GUA	H1'	3.61	4.61
6	CYT	H2'2	6	CYT	H2'1	1.80	2.10

7	X	H8	6	CYT	H2'2	3.09	3.58
7	X	H3'	7	X	H1'	3.13	4.01
7	X	H3'	7	X	H8	3.43	4.71
8	ADE	H3'	8	ADE	H8	3.32	4.66
9	GUA	H8	8	ADE	H3'	4.43	5.72
9	GUA	H8	8	ADE	H8	3.79	5.70
9	GUA	H2'1	9	GUA	H8	2.24	2.40
9	GUA	H3'	9	GUA	H1'	3.51	4.31
9	GUA	H2'2	10	THY	H6	2.06	2.74
9	GUA	H2'2	10	THY	M	3.32	4.52
10	THY	H6	9	GUA	H2'1	2.75	3.49
10	THY	H6	9	GUA	H8	3.72	5.16
10	THY	H2'1	10	THY	H6	2.08	2.28
10	THY	H2'2	10	THY	H6	3.00	4.63
10	THY	H3'	10	THY	H6	3.17	4.28
11	CYT	H5	10	THY	H3'	3.65	5.42
11	CYT	H5	10	THY	M	4.33	5.84
11	CYT	H6	10	THY	H2'1	3.03	4.45
11	CYT	H6	10	THY	H6	3.67	5.67
11	CYT	H1'	11	CYT	H2'1	2.59	5.47
11	CYT	H1'	11	CYT	H2'2	2.04	2.19
11	CYT	H2'1	11	CYT	H6	2.00	2.17
11	CYT	H4'	11	CYT	H2'1	3.12	4.04
12	CYT	H5	11	CYT	H6	3.39	4.34
12	CYT	H3'	12	CYT	H6	2.77	3.09
12	CYT	H4'	12	CYT	H3'	2.47	2.92
13	GUA	H1'	13	GUA	H8	3.21	3.91

13	GUA	H2'1	13	GUA	H8	2.10	2.30
13	GUA	H2'2	13	GUA	H8	2.70	4.06
14	GUA	H8	13	GUA	H2'2	2.31	2.52
14	GUA	H1'	14	GUA	H3'	3.26	3.97
14	GUA	H2'1	14	GUA	H8	2.00	2.29
16	CYT	H5	15	ADE	H2'1	3.29	4.12
16	CYT	H6	15	ADE	H3'	3.84	5.01
17	THY	H6	16	CYT	H2'1	2.87	4.16
17	THY	M	16	CYT	H1'	4.90	7.90
17	THY	M	16	CYT	H2'1	3.02	3.93
17	THY	H2'1	17	THY	H6	1.94	2.09
18	CYT	H1'	8	ADE	H2	3.81	4.48
18	CYT	H2'1	18	CYT	H3'	2.43	2.85
18	CYT	H2'1	18	CYT	H5	3.70	5.24
18	CYT	H2'1	18	CYT	H6	2.10	2.24
18	CYT	H2'2	18	CYT	H3'	2.85	3.35
18	CYT	H6	18	CYT	H1'	3.19	3.96
19	Y	H3x1	7	X	H1x	2.16	2.42
19	Y	H3x2	7	X	H2x1	2.09	2.59
19	Y	H8	18	CYT	H2'1	2.85	3.13
19	Y	H2'1	19	Y	H8	2.10	2.29
19	Y	H2'2	19	Y	H8	2.50	3.54
19	Y	H3'	19	Y	H8	3.53	4.95
20	CYT	H6	19	Y	H2'2	2.05	2.82
20	CYT	H5	20	CYT	H6	2.26	2.42
20	CYT	H2'2	21	THY	M	3.69	6.24
21	THY	M	20	CYT	H2'1	3.07	4.04

21	THY	M	20	CYT	H3'	3.79	4.90
21	THY	H1'	21	THY	H6	3.16	4.65
22	ADE	H1'	23	GUA	H8	3.04	3.34
22	ADE	H2'1	23	GUA	H8	2.77	3.20
22	ADE	H2'2	23	GUA	H8	2.27	2.83
23	GUA	H2'2	23	GUA	H8	2.79	4.05
24	CYT	H1'	24	CYT	H2'1	2.87	4.32
24	CYT	H1'	24	CYT	H2'2	2.12	2.29
24	CYT	H2'1	24	CYT	H3'	2.42	2.64
24	CYT	H3'	24	CYT	H6	2.94	3.29
24	CYT	H5	24	CYT	H6	2.43	2.57

Class 3

res_#	res_name	atm_name	res_#	res_name	atm_name	low_bnd	up_bnd
1	GUA	H4'	1	GUA	H2'2	3.21	4.12
2	CYT	H6	1	GUA	H8	3.56	5.01
2	CYT	H2'1	2	CYT	H5	3.66	5.24
5	GUA	H3'	5	GUA	H8	3.33	5.03
6	CYT	H6	5	GUA	H3'	3.70	4.75
7	X	H5'1	6	CYT	H2'2	2.89	3.50
7	X	H8	6	CYT	H2'1	2.97	3.56
7	X	H1x	7	X	H1'	3.29	4.55
8	ADE	H1'	7	X	H1x	3.33	4.96
8	ADE	H1'	7	X	M	2.94	4.35
9	GUA	H1'	8	ADE	H2	3.54	3.93
10	THY	H6	9	GUA	H3'	3.34	4.99
10	THY	H2'1	10	THY	M	4.49	7.47
11	CYT	H1'	11	CYT	H6	3.30	3.81

11	CYT	H1'	12	CYT	H6	3.70	5.93
14	GUA	H8	13	GUA	H2'1	2.88	4.21
14	GUA	H8	13	GUA	H3'	3.52	4.70
15	ADE	H4'	15	ADE	H2'1	3.29	4.66
15	ADE	H4'	15	ADE	H2'2	3.47	4.71
15	ADE	H4'	15	ADE	H8	4.05	5.75
16	CYT	H1'	15	ADE	H1'	3.37	4.70
16	CYT	H5	15	ADE	H1'	3.82	4.79
17	THY	H2'1	17	THY	M	4.31	7.30
17	THY	H3'	18	CYT	H6	4.00	5.82
18	CYT	H5	17	THY	M	4.82	7.75
19	Y	H3x2	19	Y	H3x1	1.65	1.88
20	CYT	H6	19	Y	H8	3.50	4.98
21	THY	H6	20	CYT	H2'1	2.42	3.80
21	THY	H2'1	21	THY	H6	1.82	2.05
23	GUA	H3'	23	GUA	H8	3.29	5.05
24	CYT	H1'	24	CYT	H6	3.46	4.77

Class 4

res_#	res_name	atm_name	res_#	res_name	atm_name	low_bnd	up_bnd
4	ADE	H8	3	THY	H3'	3.98	5.93
6	CYT	H4'	6	CYT	H2'2	2.66	3.02
7	X	H1'	7	X	M	4.04	5.62
7	X	H2x2	7	X	H2x1	1.65	1.84
7	X	H3'	8	ADE	H8	3.89	5.53
11	CYT	H3'	12	CYT	H6	3.50	4.73
12	CYT	H6	11	CYT	H2'1	3.04	5.53
16	CYT	H2'1	16	CYT	H5	3.92	5.32

18	CYT	H4'	18	CYT	H2'1	3.73	5.91
19	Y	H8	18	CYT	H6	3.79	5.26
20	CYT	H1'	7	X	M	5.19	8.54
20	CYT	H6	19	Y	H3'	3.83	5.32
20	CYT	H2'1	20	CYT	H5	4.22	6.60
21	THY	H3'	22	ADE	H8	3.54	5.01
24	CYT	H5	23	GUA	H8	3.46	4.24
24	CYT	H6	23	GUA	H3'	3.92	5.93

Class 5

res_#	res_name	atm_name	res_#	res_name	atm_name	low_bnd	up_bnd
2	CYT	H3'	3	THY	H6	3.47	4.83
3	THY	H3'	3	THY	H6	2.86	4.21
6	CYT	H2'1	6	CYT	H5	4.30	5.68
20	CYT	H1'	7	X	H1x	3.54	5.07
20	CYT	H4'	7	X	M	4.91	8.03
20	CYT	H3'	20	CYT	H6	2.94	4.28
21	THY	H6	20	CYT	H3'	3.07	4.38

Table S6. NOE Distance Restraints Used in rMD Calculations for the Oligodeoxynucleotide 5'-d(GCTAGCXAGTCC)-3'•5'-(GGACTCYCTAGC)-3'Containing the 5'-Cp-N^2-dG-3'-*S*-(α)-CH_3-propyl-5'-Cp-N^2-dG-3' Inter-strand Cross-link **8b**.

Class 1

res_#	res_name	atm_name	res_#	res_name	atm_name	low_bnd	up_bnd
1	GUA	H1'	1	GUA	H4'	3.11	3.38
1	GUA	H2'1	1	GUA	H8	2.02	2.44
1	GUA	H2'2	1	GUA	H8	3.03	3.77
1	GUA	H3'	1	GUA	H8	3.38	4.52
1	GUA	H8	1	GUA	H1'	3.20	4.08
2	CYT	H5	1	GUA	H8	3.49	4.01
2	CYT	H5	1	GUA	H2'2	3.10	3.38
2	CYT	H6	1	GUA	H1'	2.93	3.17
2	CYT	H6	1	GUA	H2'2	2.60	2.75
2	CYT	H1'	2	CYT	H4'	2.90	3.09
2	CYT	H2'2	2	CYT	H6	3.05	3.86
2	CYT	H5	2	CYT	H6	2.36	2.47
3	THY	H6	2	CYT	H1'	3.50	4.06
3	THY	M	2	CYT	H6	3.51	3.67
3	THY	M	2	CYT	H5	4.10	4.43
5	GUA	H8	4	ADE	H1'	3.19	3.48
5	GUA	H8	4	ADE	H2'2	2.23	2.93
5	GUA	H1'	5	GUA	H4'	2.99	3.19
5	GUA	H2'1	5	GUA	H8	2.33	2.45
5	GUA	H2'2	5	GUA	H1'	2.38	2.53
5	GUA	H2'2	5	GUA	H8	3.12	3.73
5	GUA	H3'	5	GUA	H8	3.72	4.86

5	GUA	H8	5	GUA	H1'	3.40	3.93
6	CYT	H5	5	GUA	H8	3.44	3.90
6	CYT	H6	5	GUA	H1'	3.03	3.26
6	CYT	H6	5	GUA	H2'2	2.45	2.93
6	CYT	H1'	6	CYT	H4'	2.74	2.94
6	CYT	H2'1	6	CYT	H1'	2.88	3.06
6	CYT	H2'1	6	CYT	H6	2.53	2.65
6	CYT	H2'1	6	CYT	H3'	2.03	2.64
6	CYT	H2'2	6	CYT	H4'	3.09	3.37
6	CYT	H2'2	6	CYT	H1'	2.30	2.41
6	CYT	H2'2	6	CYT	H2'1	1.80	2.19
6	CYT	H3'	6	CYT	H6	3.11	3.40
6	CYT	H5	6	CYT	H6	2.41	2.51
7	X	H3'	7	X	H5'1	2.93	3.85
7	X	H4'	7	X	H5'1	2.42	2.55
8	ADE	H1'	7	X	M	3.13	3.28
8	ADE	H8	7	X	H1'	3.05	3.29
8	ADE	H1'	8	ADE	H4'	2.71	2.86
8	ADE	H2'1	8	ADE	H8	2.46	2.58
8	ADE	H2'1	8	ADE	H3'	2.11	2.54
8	ADE	H2'2	8	ADE	H1'	2.39	2.52
8	ADE	H2'2	8	ADE	H2'1	1.81	2.08
9	GUA	H8	8	ADE	H2'1	2.90	3.10
9	GUA	H8	8	ADE	H2'2	2.15	2.81
9	GUA	H2'1	9	GUA	H8	2.51	2.65
9	GUA	H2'2	9	GUA	H2'1	1.80	2.08
9	GUA	H8	9	GUA	H1'	3.27	4.03

10	THY	H6	9	GUA	H1'	3.24	3.81
10	THY	H6	9	GUA	H2'1	2.94	3.42
10	THY	H6	9	GUA	H2'2	2.30	2.88
10	THY	M	9	GUA	H8	3.65	3.87
10	THY	M	9	GUA	H2'2	3.66	3.95
10	THY	H2'1	10	THY	H6	2.24	2.36
10	THY	H2'2	10	THY	H6	3.10	3.81
10	THY	H6	10	THY	H1'	3.32	3.71
10	THY	M	10	THY	H6	2.67	3.71
11	CYT	H5	10	THY	H6	3.37	3.81
11	CYT	H6	10	THY	H2'1	3.15	3.83
11	CYT	H1'	11	CYT	H4'	2.80	3.00
11	CYT	H2'1	11	CYT	H1'	2.95	3.15
11	CYT	H2'1	11	CYT	H6	2.25	2.37
11	CYT	H2'1	11	CYT	H3'	2.20	2.64
11	CYT	H5	11	CYT	H6	2.42	2.55
12	CYT	H6	11	CYT	H2'2	2.31	3.02
12	CYT	H1'	12	CYT	H4'	2.65	3.19
12	CYT	H3'	12	CYT	H5'2	2.98	3.23
12	CYT	H3'	12	CYT	H6	2.83	2.99
12	CYT	H6	12	CYT	H1'	3.31	3.72
13	GUA	H2'1	13	GUA	H8	2.36	2.49
13	GUA	H2'2	13	GUA	H8	3.23	3.98
13	GUA	H2'2	13	GUA	H3'	2.57	3.07
13	GUA	H8	13	GUA	H1'	3.35	4.32
14	GUA	H8	13	GUA	H2'1	3.16	3.55
14	GUA	H8	13	GUA	H2'2	2.57	3.05

14	GUA	H1'	14	GUA	H4'	3.03	3.25
14	GUA	H8	14	GUA	H1'	3.33	4.00
15	ADE	H3'	15	ADE	H5'2	2.57	2.75
15	ADE	H3'	15	ADE	H4'	2.62	2.76
15	ADE	H4'	15	ADE	H5'1	2.52	2.65
15	ADE	H4'	15	ADE	H5'2	2.42	2.55
15	ADE	H8	15	ADE	H1'	3.45	4.02
16	CYT	H5	15	ADE	H8	3.39	3.88
16	CYT	H6	15	ADE	H1'	3.00	3.27
16	CYT	H6	15	ADE	H2'2	2.59	2.68
16	CYT	H2'1	16	CYT	H6	2.52	2.67
16	CYT	H2'1	16	CYT	H3'	2.01	2.63
16	CYT	H3'	16	CYT	H5'1	3.25	3.65
16	CYT	H3'	16	CYT	H5'2	2.84	2.99
16	CYT	H3'	16	CYT	H6	3.18	3.44
16	CYT	H5	16	CYT	H6	2.44	2.54
16	CYT	H6	16	CYT	H1'	3.26	3.90
17	THY	H6	16	CYT	H2'1	2.85	3.09
17	THY	M	16	CYT	H6	3.56	3.78
17	THY	M	16	CYT	H5	4.09	4.38
17	THY	M	16	CYT	H3'	3.67	3.95
17	THY	M	16	CYT	H2'1	3.16	4.08
17	THY	M	17	THY	H6	2.69	3.75
18	CYT	H5	17	THY	H6	3.25	3.51
18	CYT	H2'1	18	CYT	H1'	2.72	3.52
18	CYT	H2'1	18	CYT	H6	2.09	2.52
18	CYT	H2'2	18	CYT	H1'	2.39	2.52

18	CYT	H2'2	18	CYT	H2'1	1.80	2.22
18	CYT	H3'	18	CYT	H6	3.10	3.55
18	CYT	H5	18	CYT	H6	2.47	2.56
19	Y	H8	18	CYT	H2'1	2.83	3.00
19	Y	H8	18	CYT	H2'2	2.84	3.03
19	Y	H1'	19	Y	H4'	3.09	3.33
19	Y	H2'2	19	Y	H3'	2.70	2.91
19	Y	H3'	19	Y	H4'	2.65	2.79
19	Y	H8	19	Y	H2'2	2.89	3.15
19	Y	H8	19	Y	H2'1	2.28	2.40
20	CYT	H5	19	Y	H8	3.44	3.94
20	CYT	H6	19	Y	H1'	2.67	2.84
20	CYT	H1'	20	CYT	H4'	2.88	3.06
20	CYT	H2'1	20	CYT	H3'	1.97	2.63
21	THY	M	20	CYT	H5	4.09	4.47
21	THY	M	20	CYT	H2'1	2.89	3.42
23	GUA	H8	22	ADE	H1'	2.84	3.36
23	GUA	H8	22	ADE	H2'1	3.09	3.36
23	GUA	H8	22	ADE	H2'2	2.21	2.85
23	GUA	H2'1	23	GUA	H8	2.09	2.42
23	GUA	H2'2	23	GUA	H8	3.08	3.71
23	GUA	H3'	23	GUA	H8	3.45	4.32
24	CYT	H5	23	GUA	H8	3.34	3.79
24	CYT	H1'	24	CYT	H4'	2.88	3.08
24	CYT	H3'	24	CYT	H6	3.00	3.31

Class2

res_#	res_name	atm_name	res_#	res_name	atm_name	low_bnd	up_bnd

2	CYT	H2'1	2	CYT	H6	2.21	2.37
2	CYT	H6	2	CYT	H1'	3.42	4.26
3	THY	M	2	CYT	H3'	4.02	4.51
3	THY	M	2	CYT	H2'1	2.98	3.26
3	THY	M	2	CYT	H2'2	3.66	4.17
3	THY	H2'2	3	THY	H2'1	1.80	2.12
3	THY	H3'	3	THY	H6	3.19	4.15
5	GUA	H8	4	ADE	H2'1	3.10	3.59
6	CYT	H5	5	GUA	H2'2	3.10	3.55
6	CYT	H3'	6	CYT	H4'	2.76	2.97
7	X	H2x1	7	X	H1x	2.59	2.84
7	X	H2x1	7	X	M	2.63	2.89
7	X	H2x1	7	X	H2x2	1.80	2.11
7	X	H2x2	7	X	M	2.76	3.05
7	X	H4'	7	X	H5'2	2.37	2.59
7	X	M	7	X	H1'	3.98	4.44
7	X	M	7	X	H1x	2.21	2.48
8	ADE	H4'	7	X	M	3.28	3.66
8	ADE	H8	7	X	H2'2	2.62	2.86
8	ADE	H2'2	8	ADE	H8	3.11	4.07
9	GUA	H2'1	9	GUA	H1'	2.85	3.20
10	THY	M	9	GUA	H3'	4.18	4.86
10	THY	M	9	GUA	H2'1	3.06	4.38
11	CYT	H6	10	THY	H1'	3.36	4.20
11	CYT	H2'2	11	CYT	H2'1	1.80	2.19
12	CYT	H6	11	CYT	H1'	3.27	3.86
12	CYT	H6	11	CYT	H2'1	2.84	3.16

12	CYT	H3'	12	CYT	H4'	2.48	3.17
12	CYT	H5	12	CYT	H6	2.42	2.64
13	GUA	H1'	13	GUA	H4'	3.28	3.73
13	GUA	H2'1	13	GUA	H3'	2.44	2.69
13	GUA	H2'2	13	GUA	H1'	2.41	2.61
14	GUA	H4'	14	GUA	H5'1	2.39	2.63
14	GUA	H4'	14	GUA	H5'2	2.33	2.52
15	ADE	H1'	15	ADE	H4'	3.08	3.42
15	ADE	H2'2	15	ADE	H1'	2.36	2.58
15	ADE	H3'	15	ADE	H5'1	2.96	3.91
15	ADE	H3'	15	ADE	H1'	3.38	4.19
16	CYT	H6	15	ADE	H2'1	3.20	3.86
16	CYT	H2'2	16	CYT	H3'	3.01	3.30
16	CYT	H2'2	16	CYT	H2'1	1.80	2.18
16	CYT	H3'	16	CYT	H4'	2.49	2.95
17	THY	M	16	CYT	H2'2	3.74	4.21
17	THY	H3'	17	THY	H6	3.23	4.25
17	THY	H6	17	THY	H1'	3.09	3.76
19	Y	H3x1	7	X	H1x	2.37	2.59
19	Y	H3x1	7	X	H2x1	2.38	2.88
19	Y	H3x2	7	X	H2x1	2.32	2.57
19	Y	H1'	19	Y	H2'2	2.44	2.62
19	Y	H3x1	19	Y	H3x2	1.80	2.05
19	Y	H8	19	Y	H3'	3.46	4.63
20	CYT	H6	19	Y	H2'2	2.61	2.86
20	CYT	H2'1	20	CYT	H1'	2.69	2.95
20	CYT	H2'2	20	CYT	H2'1	1.80	2.16

20	CYT	H5	20	CYT	H6	2.30	2.49
21	THY	M	20	CYT	H3'	3.67	4.12
21	THY	H2'2	21	THY	H6	2.95	3.56
23	GUA	H2'2	23	GUA	H1'	2.30	2.49
23	GUA	H8	23	GUA	H1'	3.23	3.96
24	CYT	H6	23	GUA	H2'2	2.28	2.81
24	CYT	H2'2	24	CYT	H1'	2.21	2.40
24	CYT	H2'2	24	CYT	H3'	2.97	3.53
24	CYT	H5	24	CYT	H6	2.41	2.59
24	CYT	H6	24	CYT	H1'	3.30	3.81

Class3

res_#	res_name	atm_name	res_#	res_name	atm_name	low_bnd	up_bnd
2	CYT	H5	1	GUA	H2'1	3.46	5.15
2	CYT	H6	1	GUA	H2'1	3.14	4.04
3	THY	H2'2	3	THY	H4'	3.19	4.28
3	THY	M	3	THY	H6	2.66	2.99
5	GUA	H3'	5	GUA	H1'	3.38	4.39
6	CYT	H5'1	5	GUA	H1'	3.02	3.53
6	CYT	H3'	6	CYT	H5'2	2.68	3.03
7	X	H8	6	CYT	H2'1	2.91	3.42
7	X	H8	6	CYT	H2'2	3.13	3.55
7	X	H1'	7	X	H2'2	2.22	2.53
7	X	H1'	7	X	H2'1	2.75	3.35
8	ADE	H2'1	8	ADE	H1'	2.73	3.13
8	ADE	H3'	8	ADE	H8	3.43	4.37
9	GUA	H8	8	ADE	H1'	2.64	3.65
9	GUA	H2'2	9	GUA	H4'	3.29	4.04

9	GUA	H2'2	9	GUA	H1'	2.21	2.45
9	GUA	H2'2	9	GUA	H8	3.31	4.26
9	GUA	H3'	9	GUA	H8	3.29	4.46
10	THY	H2'2	11	CYT	H5	3.24	4.46
11	CYT	H5	10	THY	H2'1	3.19	4.42
11	CYT	H6	11	CYT	H1'	3.20	3.76
14	GUA	H2'1	14	GUA	H8	2.07	2.33
14	GUA	H3'	14	GUA	H1'	3.39	4.13
18	CYT	H2'2	18	CYT	H6	2.98	3.98
19	Y	H3x2	7	X	H1x	2.62	3.73
19	Y	H3x2	7	X	M	3.37	4.07
19	Y	H1'	19	Y	H3'	3.37	4.21
19	Y	H1'	19	Y	H2'1	2.92	3.56
19	Y	H8	19	Y	H1'	3.45	4.40
20	CYT	H5	19	Y	H2'2	2.41	3.14
20	CYT	H5	19	Y	H1'	3.06	3.59
20	CYT	H3'	20	CYT	H6	3.06	4.06
21	THY	M	20	CYT	H2'2	3.82	4.72
21	THY	H2'2	21	THY	H4'	3.15	4.13
21	THY	H3'	21	THY	H6	3.14	4.21

Class4

res_#	res_name	atm_name	res_#	res_name	atm_name	low_bnd	up_bnd
2	CYT	H5	1	GUA	H1'	3.38	4.38
2	CYT	H2'1	2	CYT	H4'	3.16	4.52
2	CYT	H2'2	2	CYT	H4'	3.08	3.80
3	THY	H2'1	3	THY	H4'	2.88	3.90
3	THY	H2'2	3	THY	H3'	2.50	2.99

4	ADE	H8	3	THY	H2'1	3.53	6.96
6	CYT	H5	5	GUA	H1'	3.37	4.48
6	CYT	H2'2	6	CYT	H6	3.23	4.05
6	CYT	H2'2	6	CYT	H3'	2.79	3.29
6	CYT	H3'	6	CYT	H5'1	3.12	3.94
6	CYT	H6	6	CYT	H1'	3.28	4.36
7	X	H2x2	7	X	H1x	2.71	3.21
7	X	H8	7	X	H3'	3.23	4.53
8	ADE	H2	7	X	M	4.41	6.86
8	ADE	H3'	8	ADE	H1'	3.35	4.76
11	CYT	H5	10	THY	M	4.55	7.46
11	CYT	H2'2	11	CYT	H1'	2.18	2.54
12	CYT	H5	11	CYT	H6	3.35	4.55
13	GUA	H3'	13	GUA	H8	3.58	5.68
14	GUA	H2'2	14	GUA	H8	2.59	3.47
14	GUA	H3'	14	GUA	H8	3.31	4.63
16	CYT	H5	15	ADE	H2'2	3.11	4.03
16	CYT	H6	15	ADE	H8	3.56	5.94
17	THY	H2'2	17	THY	H3'	2.53	3.15
17	THY	H1'	18	CYT	H6	3.27	4.12
18	CYT	H5	17	THY	H2'1	2.93	3.56
18	CYT	H5	17	THY	H2'2	3.31	4.96
18	CYT	H6	17	THY	H2'1	3.22	6.00
19	Y	H3x1	7	X	H2x2	2.71	3.35
20	CYT	H5	19	Y	H2'1	3.42	5.46
20	CYT	H2'2	20	CYT	H1'	2.29	2.71
20	CYT	H2'2	20	CYT	H3'	2.85	3.53

21	THY	H2'1	21	THY	H4'	3.09	3.88
22	ADE	H1'	22	ADE	H3'	3.46	4.48
23	GUA	H8	22	ADE	H8	3.64	5.23

Class5

res_#	res_name	atm_name	res_#	res_name	atm_name	low_bnd	up_bnd
4	ADE	H8	3	THY	H1'	2.50	3.50
7	X	H8	7	X	H1'	3.19	4.06
8	ADE	H2	8	ADE	H1'	3.54	6.33
8	ADE	H8	8	ADE	H1'	3.50	5.44
14	GUA	H8	13	GUA	H1'	3.10	4.30
18	CYT	H6	18	CYT	H1'	3.27	4.44
19	Y	H3x1	7	X	M	3.92	5.73
19	Y	H8	18	CYT	H1'	3.56	6.26

res_#	res_name	atm_name	res_#	res_name	atm_name	low_bnd	up_bnd
1	GUA	H8	1	GUA	H4'	4.00	5.50
1	GUA	H8	2	CYT	H6	4.50	5.50
2	CYT	H6	1	GUA	H3'	4.00	5.50
2	CYT	H6	2	CYT	H3'	3.50	5.00
2	CYT	H1'	3	THY	M	3.50	5.00
3	THY	H6	2	CYT	H3'	4.00	5.50
3	THY	H6	3	THY	H3'	3.50	5.00
3	THY	H6	4	ADE	H8	4.50	5.50
4	ADE	H8	3	THY	H3'	4.50	5.50
4	ADE	H8	3	THY	H2'	3.00	4.00
4	ADE	H8	3	THY	H2"	2.00	3.50
4	ADE	H8	4	ADE	H1'	3.50	4.50

4	ADE	H8	4	ADE	H3'	4.00	5.00
4	ADE	H8	4	ADE	H2'	2.00	4.00
4	ADE	H8	4	ADE	H2"	3.50	4.50
4	ADE	H8	5	GUA	H8	4.50	5.50
5	GUA	H8	4	ADE	H3'	4.50	5.50
5	GUA	H8	5	GUA	H4'	4.00	5.50
5	GUA	H8	6	CYT	H6	4.50	5.50
6	CYT	H6	5	GUA	H3'	4.50	5.50
6	CYT	H6	5	GUA	H2'	3.00	5.00
6	CYT	H5	6	CYT	H2'	4.00	5.00
6	CYT	H6	7	X	H8	4.50	5.50
7	X	H8	6	CYT	H1'	3.50	5.00
7	X	H8	6	CYT	H3'	4.50	5.50
7	X	H8	8	ADE	H8	4.50	5.50
8	ADE	H1'	7	X	H1x	3.00	6.00
8	ADE	H8	7	X	H3'	4.50	5.50
8	ADE	H8	7	X	M	4.00	5.50
8	ADE	H2	8	ADE	H1'	4.00	5.50
8	ADE	H2	9	GUA	H1'	4.00	5.50
8	ADE	H8	9	GUA	H8	4.50	5.50
8	ADE	H2	17	THY	H1'	4.00	5.50
8	ADE	H2	18	CYT	H1'	4.00	5.50
9	GUA	H8	8	ADE	H3'	4.50	5.50
9	GUA	H8	9	GUA	H4'	4.00	5.50
9	GUA	H1'	10	THY	M	3.00	4.50
9	GUA	H8	10	THY	H6	4.50	5.50
10	THY	H6	9	GUA	H3'	4.00	5.50

10	THY	H6	10	THY	H3'	3.50	5.00
10	THY	H6	11	CYT	H6	4.50	5.50
11	CYT	H6	10	THY	H3'	4.00	5.50
11	CYT	H5	11	CYT	H2'	3.50	5.00
11	CYT	H6	11	CYT	H3'	3.50	5.00
11	CYT	H6	12	CYT	H6	4.50	5.50
12	CYT	H6	11	CYT	H3'	4.00	5.50
13	GUA	H8	13	GUA	H4'	4.00	5.50
13	GUA	H8	14	GUA	H8	4.50	5.50
14	GUA	H8	13	GUA	H3'	4.50	5.50
14	GUA	H8	15	ADE	H8	4.50	5.50
15	ADE	H2	10	THY	H1'	4.00	5.50
15	ADE	H2	11	CYT	H1'	4.00	5.50
15	ADE	H8	14	GUA	H3'	4.50	5.50
15	ADE	H2	15	ADE	H1'	4.00	5.50
15	ADE	H8	15	ADE	H3'	4.00	5.00
15	ADE	H8	15	ADE	H4'	4.00	5.50
15	ADE	H2	16	CYT	H1'	3.70	5.50
15	ADE	H2	16	CYT	H2"	4.00	6.00
16	CYT	H6	15	ADE	H3'	4.50	5.50
16	CYT	H6	16	CYT	H4'	4.00	5.50
16	CYT	H1'	17	THY	M	3.50	4.50
16	CYT	H6	17	THY	H6	4.50	5.50
17	THY	H6	16	CYT	H3'	4.00	5.50
18	CYT	H5	17	THY	M	4.00	5.00
18	CYT	H6	17	THY	H6	4.50	5.50
18	CYT	H6	17	THY	H3'	4.00	5.50

19	Y	H1'	7	X	H1x	3.00	6.00
19	Y	H8	18	CYT	H6	4.50	5.50
19	Y	H8	18	CYT	H3'	4.50	5.50
19	Y	H8	19	Y	H4'	4.00	5.50
20	CYT	H1'	7	X	M	3.00	6.00
20	CYT	H1'	7	X	H2x1	3.00	6.00
20	CYT	H1'	19	Y	H3x1	3.00	4.50
20	CYT	H1'	19	Y	H3x2	3.00	4.50
20	CYT	H6	19	Y	H8	4.50	5.50
20	CYT	H6	19	Y	H3'	4.50	5.50
20	CYT	H6	20	CYT	H1'	3.50	4.50
20	CYT	H1'	21	THY	M	3.50	5.00
21	THY	H6	20	CYT	H1'	2.50	4.00
21	THY	H6	20	CYT	H3'	4.00	5.50
21	THY	H6	21	THY	H1'	3.50	4.50
22	ADE	H8	21	THY	H1'	2.50	3.50
22	ADE	H8	21	THY	H6	4.50	5.50
22	ADE	H8	21	THY	H3'	4.00	5.50
22	ADE	H8	21	THY	H2'	3.00	4.00
22	ADE	H8	21	THY	H2"	2.00	3.50
22	ADE	H8	22	ADE	H1'	3.50	4.50
22	ADE	H8	22	ADE	H3'	4.00	5.00
22	ADE	H8	22	ADE	H2'	2.00	4.00
22	ADE	H8	22	ADE	H2"	3.50	4.50
23	GUA	H8	22	ADE	H3'	4.50	5.50
23	GUA	H8	23	GUA	H4'	4.00	5.50
24	CYT	H6	23	GUA	H8	4.50	5.50

24	CYT	H6	23	GUA	H3'	4.50	5.50

Figure S1. Chemical shift differences of non-exchangeable aromatic protons of the un-adducted and cross-linked oligodeoxynucleotides. **A.** The *R*-α-CH_3-γ-OH-1,N^2-propano-2'-deoxyguanosine cross-linked adduct. **B.** The *S*-α-CH_3-γ-OH-1,N^2-propano-2'-deoxyguanosine cross-linked adduct. Black bars represent the H1' resonances, grey bars represent the H2' resonances, and stippled bars represent the H2" resonances. $\Delta\delta$ (ppm) = $\delta_{\text{unmodified oligodeoxynucleotide}} - \delta_{\text{cross-linked oligodeoxynucleotide}}$.

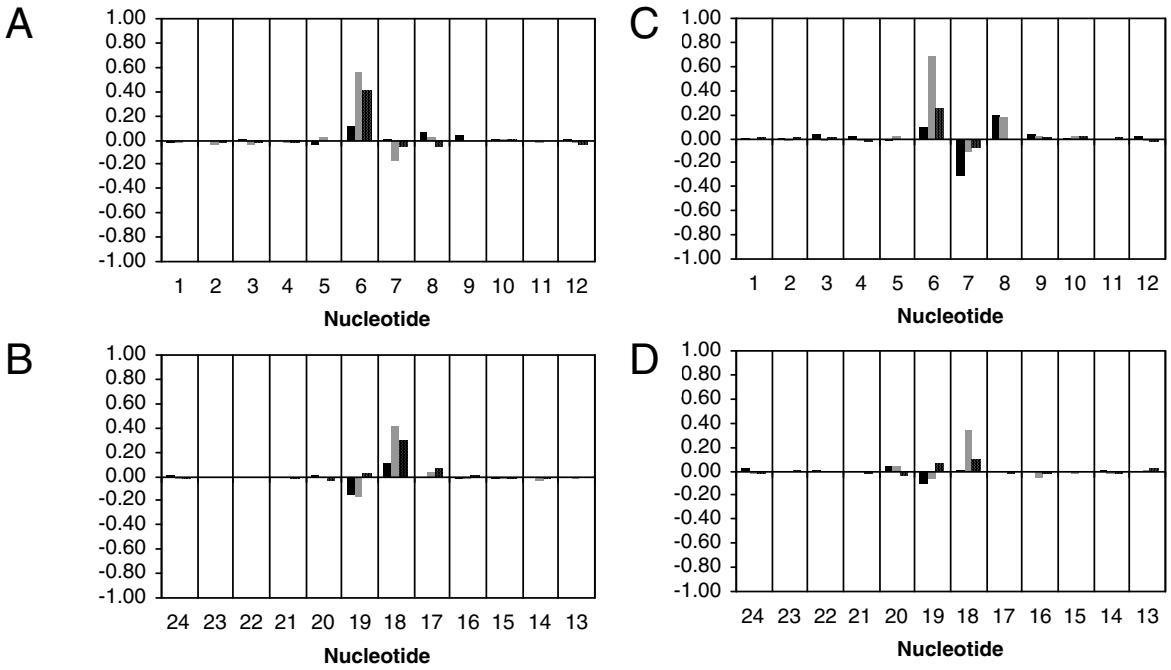

Figure S2. Parameterization of the 5'- Cp-N^2-dG-3'-*R*-(α)-CH_3-propyl-5'-Cp-N^2-dG-3' and Containing the 5'- Cp-N^2-dG-3'- *S*-(α)-CH_3-propyl-5'-Cp-N^2-dG-3' Inter-strand Cross-links **8a** and **8b** in the AMBER 8.0 Forcefield.

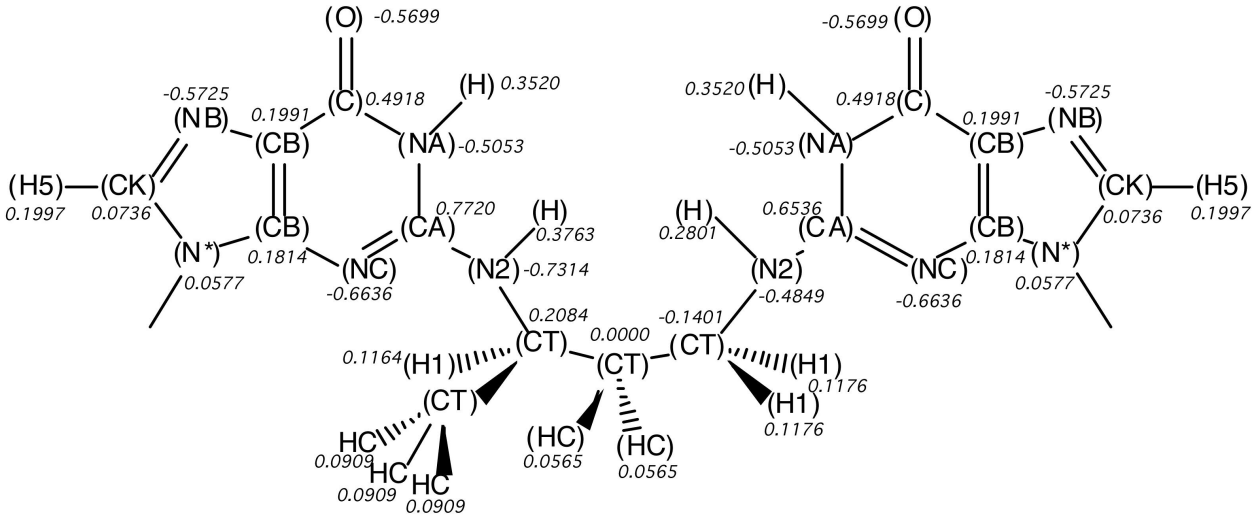

Figure S3. Stereoviews of superimposed structures that emerged from randomly seeded rMD calculations of the cross-linked oligodeoxynucleotides. **A.** The *R*-α-CH_3-γ-OH-1,N^2-propano-2'-deoxyguanosine cross-linked adduct. **B.** The *S*-α-CH_3-γ-OH-1,N^2-propano-2'-deoxyguanosine cross-linked adduct.

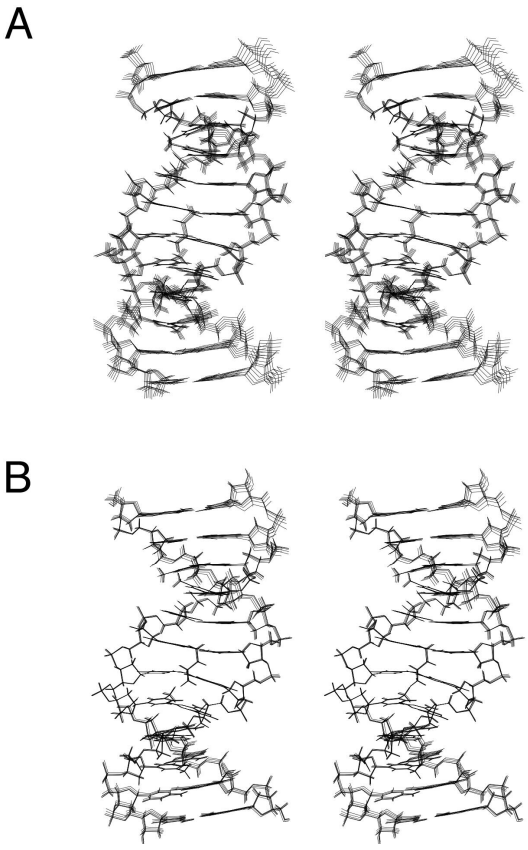

Figure S4. Complete relaxation matrix calculations on the average structures that emerged from randomly seeded rMD calculations of the cross-linked oligodeoxynucleotides, showing sixth root residuals (R_1^x) for each nucleotide. **A.** The *R*-α-CH_3-γ-OH-1,N^2-propano-2'-deoxyguanosine cross-linked adduct. The adducted strand (top); the complementary strand (bottom). **B.** The *S*-α-CH_3-γ-OH-1,N^2-propano-2'- deoxyguanosine cross-linked adduct. The adducted strand (top); the complementary strand (bottom). The black bars represent intranucleotide R_1^x values, and the gray bars represent internucleotide R_1^x values.