

Structure of (5'S)-8,5'-Cyclo-2'-Deoxyguanosine in DNA

Supporting Information

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Table of Contents

Complete Listing of Reference (77).

Scheme S1. Synthesis of phosphoramidite monomer for preparing oligonucleotide containing (5'*S*)-8,5'-cyclo-2'-deoxyguanosine.

Table S1. Chemical shifts of the non-exchangeable protons.

Table S2. 3J coupling constants and the pseudorotation of the deoxyribose

Table S3. NOE distance restraints used for the structural refinement

Figure S1. ^{31}P -H3' HMBC spectrum

Figure S2. Nucleotide-by-nucleotide sixth-root residuals (R_1^x).

Figure S3. Backbone torsion angles of the refined structure of the *S*-cdG containing duplex.

Figure S4. Base pairing and base stacking helicoidal parameters of the refined structure of the *S*-cdG containing duplex.

Figure S5. Calculated electrostatic potentials for the *S*-cdG nucleotide.

Complete listing of Reference (77).

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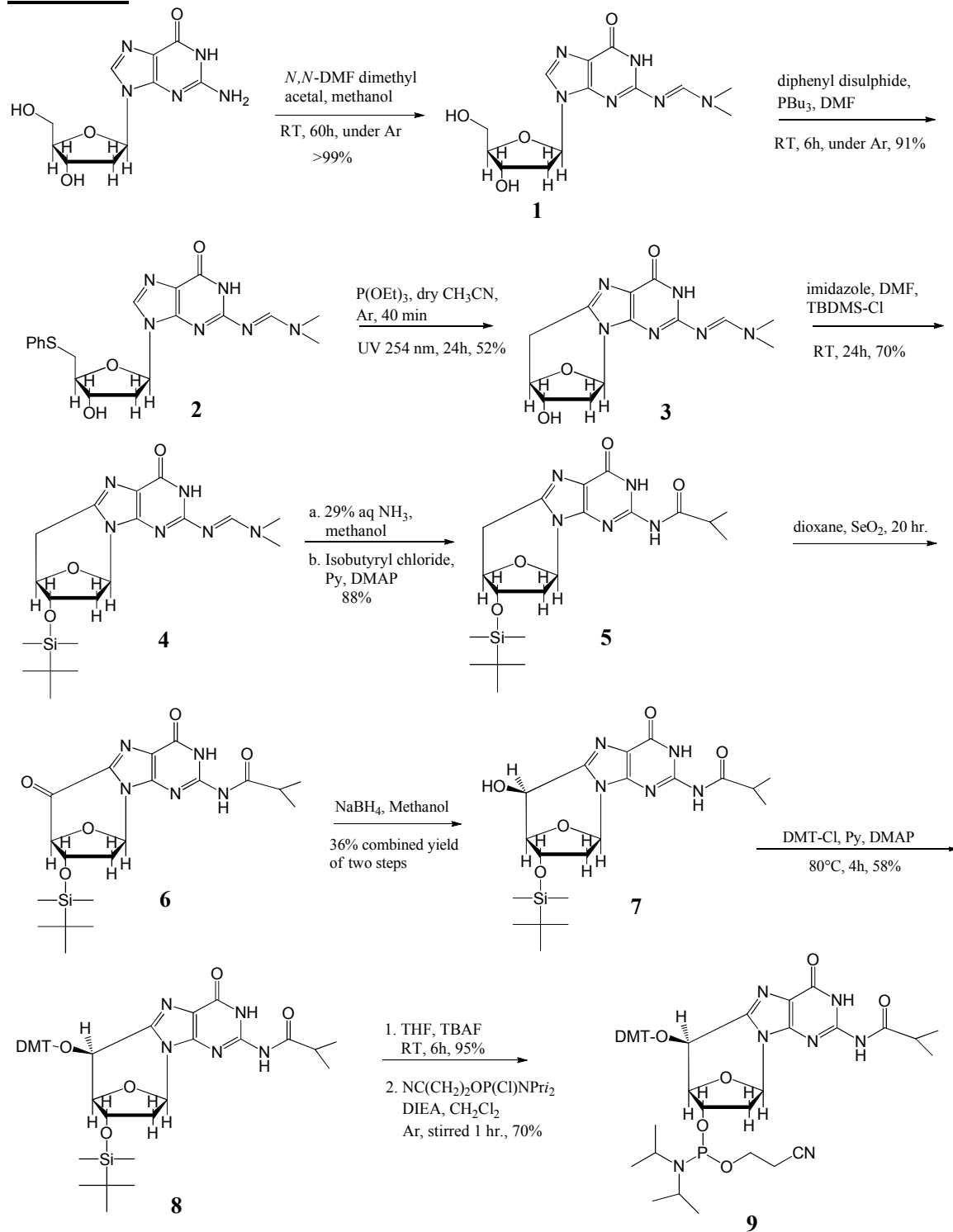
Synthesis of phosphoramidite monomer of (5'S)-8,5'-cyclo-2'-deoxyguanosine**Scheme S1**

Table S1. Chemical Shifts (ppm) of the Non-exchangeable Protons of the *S*-cdG Containing Duplex.

Nucleotide	H6/H8	H2/H5/CH ₃	H1'	H2'	H2''	H3'	H4'	H5'
G ¹	8.00		6.06	2.69	2.84	4.86	4.27	
T ²	7.40	1.43	6.00	2.22	2.59	4.96	4.29	
G ³	7.91		5.88	2.64	2.74	5.01	4.40	
C ⁴	7.55	5.43	6.12	2.22	3.44	5.01	4.40	
X ⁵			6.14	2.55	2.27	4.87	5.12	5.56
T ⁶	7.54	1.81	6.08	2.31	2.71	4.91	4.36	
G ⁷	7.78		6.00	2.56	2.82	4.94	4.38	
T ⁸	7.26	1.34	6.03	2.15	2.61	4.89	4.28	
T ⁹	7.47	1.63	6.16	2.19	2.63	4.92		
T ¹⁰	7.33	1.74	5.88	2.02	2.41	4.93		
G ¹¹	8.01		6.11	2.75	2.75	5.04	4.44	
T ¹²	7.47	1.67	6.28	2.29	2.29	4.58	4.13	
A ¹³	8.21		6.21	2.62	2.78	4.85	4.26	
C ¹⁴	7.43	5.52	5.17	2.02	2.25	4.81		
A ¹⁵	8.23		5.80	2.77	2.87	5.07	4.40	
A ¹⁶	8.15		5.92	2.69	2.89	5.09	4.48	
A ¹⁷	8.07	7.58	6.09	2.60	2.87	5.02	4.48	
C ¹⁸	7.17	5.18	5.66	1.99	2.41	4.77		
A ¹⁹	7.97		6.12	2.46	2.81	4.98	4.32	
C ²⁰	7.18	5.15	5.40	1.99	2.32	4.81		
G ²¹	7.81		5.83	2.52	2.70	4.93	4.30	
C ²²	7.34	5.37	5.61	2.06	2.39	4.85		
A ²³	8.27		6.28	2.69	2.90	5.03	4.41	

C^{24}	7.42	5.45	6.14	2.13	2.17	4.51	4.05	
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Table S2. 3J Coupling Constants and the Deoxyribose Pseudorotation.

Nucleotide	$^3J_{\text{H1}'\text{-H2}'}$ (Hz)	$^3J_{\text{H1}'\text{-H2}''}$ (Hz)	P ($^\circ$)	τ_m ($^\circ$)	pseudorotation
G ¹	7.4	6.7	179.3	27.9	C2'-endo
T ²	9.6	6.2	131.0	40.2	C1'-exo
G ³	9.5	6.1	121.2	40.6	C1'-exo
C ⁴	10.7	6.4	147.7	42.1	C2'-endo
X ⁵	2.6	7.0	280.2	47.6	O4'-exo
T ⁶	9.1	6.6	161.6	34.2	C2'-endo
G ⁷	8.9	6.9	121.1	40.6	C1'-exo
T ⁸	9.4	6.6	133.2	35.6	C1'-exo
T ⁹	9.4	6.6	116.1	38.3	C1'-exo
T ¹⁰	9.2	7.1	118.8	37.9	C1'-exo
G ¹¹	8.5	6.2	145.0	35.6	C2'-endo
G ¹²	7.5	6.7	58.9	41.0	C4'-exo
A ¹³	8.9	6.0	167.9	29.3	C2'-endo
C ¹⁴	9.6	5.7	124.8	40.8	C1'-exo
A ¹⁵	9.7	6.2	151.1	33.5	C2'-endo
A ¹⁶	10.0	6.1	121.9	36.7	C1'-exo
A ¹⁷	9.7	6.3	139.2	36.3	C1'-exo
C ¹⁸	8.6	6.5	116.0	40.6	C1'-exo
A ¹⁹	8.9	6.7	125.5	37.7	C1'-exo
C ²⁰	10.2	6.0	131.7	44.5	C1'-exo
G ²¹	9.0	6.4	164.4	34.3	C2'-endo
C ²²	9.0	6.6	138.8	33.2	C1'-exo
A ²³	8.6	6.5	144.8	33.6	C2'-endo
C ²⁴	7.7	7.1	96.6	38.9	O4'-endo

Table S3. NOE Distance Restraints Used for the Structural Refinement.

Nucleotide I		Atom I	Nucleotide II		Atom II	Lower bound (Å)	Upper bound (Å)
1	DG5	H2''	1	DG5	H1'	1.95	2.47
1	DG5	H2'	1	DG5	H1'	2.19	3.97
1	DG5	H3'	1	DG5	H1'	3.94	4.44
1	DG5	H3'	1	DG5	H2''	2.78	4.49
1	DG5	H3'	1	DG5	H2'	2.12	2.67
1	DG5	H8	1	DG5	H1'	3.2	5.15
1	DG5	H8	1	DG5	H2''	3.64	6.42
1	DG5	H8	1	DG5	H2'	2.19	2.91
1	DG5	H8	1	DG5	H3'	3.00	4.00
1	DG5	H8	1	DG5	H4'	4.23	4.73
2	DT	H2''	2	DT	H1'	2.05	3.11
2	DT	H2'	2	DT	H1'	2.45	3.63
2	DT	H3'	2	DT	H1'	3.6	4.46
2	DT	H3'	2	DT	H2''	2.47	3.72
2	DT	H3'	2	DT	H2'	2.16	2.52
2	DT	H4'	2	DT	H1'	2.55	2.87
2	DT	H4'	2	DT	H2'	3.42	5.15
2	DT	H4'	2	DT	H3'	2.71	3.27
2	DT	H6	1	DG5	H1'	3.86	4.51
2	DT	H6	1	DG5	H2''	2.35	2.79
2	DT	H6	1	DG5	H3'	3.96	5.40
2	DT	H6	1	DG5	H8	3.93	6.78
2	DT	H6	2	DT	H1'	2.67	5.64
2	DT	H6	2	DT	H2''	2.50	5.39

2	DT	H6	2	DT	H2'	1.75	2.24
2	DT	H6	2	DT	H3'	3.42	5.02
2	DT	ME	1	DG5	H1'	4.91	7.21
2	DT	ME	1	DG5	H2''	3.70	4.13
2	DT	ME	1	DG5	H2'	3.15	3.65
2	DT	ME	1	DG5	H3'	3.94	4.36
2	DT	ME	1	DG5	H8	3.88	4.43
2	DT	ME	2	DT	H2'	4.30	5.39
2	DT	ME	2	DT	H3'	4.85	7.89
3	DG	H2''	3	DG	H1'	2.08	2.58
3	DG	H2'	3	DG	H1'	2.26	3.73
3	DG	H3'	3	DG	H1'	3.16	5.16
3	DG	H3'	3	DG	H2''	2.23	3.87
3	DG	H3'	3	DG	H2'	1.99	3.76
3	DG	H4'	3	DG	H1'	2.85	3.22
3	DG	H4'	3	DG	H2''	2.95	5.03
3	DG	H4'	3	DG	H2'	3.48	3.98
3	DG	H8	2	DT	H1'	3.65	4.27
3	DG	H8	2	DT	H2''	2.71	3.19
3	DG	H8	2	DT	H2'	3.26	4.91
3	DG	H8	2	DT	H3'	4.88	6.59
3	DG	H8	2	DT	H6	3.91	5.8
3	DG	H8	3	DG	H1'	3.54	5.44
3	DG	H8	3	DG	H2''	2.70	3.50
3	DG	H8	3	DG	H2'	2.21	2.79
3	DG	H8	3	DG	H3'	3.43	5.09

3	DG	H8	3	DG	H4'	5.1	6.55
4	DC	H2''	4	DG	H3'	2.56	3.06
4	DC	H2''	4	DC	H1'	2.04	2.50
4	DC	H2'	4	DC	H1'	2.77	3.27
4	DC	H3'	4	DC	H1'	3.65	5.57
4	DC	H3'	4	DC	H2'	2.28	2.72
4	DC	H4'	4	DC	H2''	4.02	4.52
4	DC	H4'	4	DC	H2'	3.33	3.83
4	DC	H6	3	DG	H1'	3.54	5.18
4	DC	H6	3	DG	H2''	2.22	3.08
4	DC	H6	3	DG	H2'	2.82	5.68
4	DC	H6	3	DG	H8	4.00	6.77
4	DC	H6	4	DC	H1'	3.42	5.75
4	DC	H6	4	DC	H2''	2.72	3.32
4	DC	H6	4	DC	H2'	2.01	2.56
4	DC	H6	4	DC	H4'	3.79	6.22
4	DC	H5	3	DG	H1'	3.88	5.98
4	DC	H5	3	DG	H2''	2.89	3.55
4	DC	H5	3	DG	H2'	3.73	4.23
4	DC	H5	3	DG	H8	4.35	6.12
4	DC	H5	4	DC	H2''	3.51	6.19
4	DC	H5	4	DC	H2'	3.00	4.96
5	CDG	H2''	5	CDG	H1'	2.24	2.95
5	CDG	H2'	5	CDG	H1'	2.31	2.93
5	CDG	H3'	5	CDG	H1'	4.16	5.38
5	CDG	H3'	5	CDG	H2''	2.51	3.16

5	CDG	H3'	5	CDG	H2'	2.20	2.70
5	CDG	H4'	4	DC	H1'	4.30	5.66
5	CDG	H4'	4	DC	H2''	4.25	5.50
5	CDG	H4'	5	CDG	H1'	4.04	5.07
5	CDG	H4'	5	CDG	H2''	3.34	4.34
5	CDG	H4'	5	CDG	H2'	3.79	4.24
5	CDG	H4'	5	CDG	H3'	2.37	2.87
5	CDG	H5'	4	DC	H1'	2.21	2.71
5	CDG	H5'	4	DC	H2''	3.23	3.58
5	CDG	H5'	4	DC	H2'	4.46	4.96
5	CDG	H5'	4	DC	H3'	4.89	5.39
5	CDG	H5'	5	CDG	H3'	3.72	4.14
5	CDG	H5'	5	CDG	H4'	2.60	2.78
6	DT	H2''	6	DT	H1'	2.3	2.92
6	DT	H2'	6	DT	H1'	2.51	3.15
6	DT	H3'	6	DT	H1'	3.32	4.63
6	DT	H3'	6	DT	H2'	2.23	2.40
6	DT	H4'	5	CDG	H2''	3.5	5.84
6	DT	H4'	5	CDG	H2'	3.83	4.33
6	DT	H4'	6	DT	H2''	3.33	4.43
6	DT	H4'	6	DT	H2'	3.09	4.53
6	DT	H4'	6	DT	H3'	2.76	3.04
6	DT	H6	5	CDG	H1'	4.00	5.00
6	DT	H6	5	CDG	H2''	3.25	3.75
6	DT	H6	5	CDG	H3'	3.03	3.53
6	DT	H6	5	CDG	H5'	5.58	6.59

6	DT	H6	6	DT	H1'	3.34	5.02
6	DT	H6	6	DT	H2''	2.67	4.52
6	DT	H6	6	DT	H2'	1.92	2.14
6	DT	H6	6	DT	H3'	3.50	4.50
6	DT	H6	6	DT	H4'	4.33	6.04
6	DT	ME	4	DC	H1'	5.21	6.98
6	DT	ME	4	DC	H2''	3.88	4.34
6	DT	ME	4	DC	H2'	4.48	6.26
6	DT	ME	4	DC	H3'	5.56	7.50
6	DT	ME	5	CDG	H1'	4.50	5.50
6	DT	ME	5	CDG	H2''	3.71	5.10
6	DT	ME	5	CDG	H2'	3.94	4.44
6	DT	ME	5	CDG	H3'	3.05	3.25
6	DT	ME	5	CDG	H4'	4.97	6.13
6	DT	ME	5	CDG	H5'	4.65	5.02
6	DT	ME	6	DT	H2'	3.83	6.68
6	DT	ME	6	DT	H3'	4.53	5.58
7	DG	H2''	7	DG	H1'	1.93	2.32
7	DG	H2'	7	DG	H1'	2.51	5.11
7	DG	H3'	7	DG	H1'	3.52	4.09
7	DG	H3'	7	DG	H2''	2.34	2.78
7	DG	H3'	7	DG	H2'	2.34	2.95
7	DG	H4'	7	DG	H1'	2.93	3.18
7	DG	H4'	7	DG	H2''	3.32	5.21
7	DG	H4'	7	DG	H2'	3.70	4.99
7	DG	H4'	7	DG	H3'	2.85	3.04

7	DG	H8	6	DT	H1'	3.16	3.46
7	DG	H8	6	DT	H2''	2.24	2.84
7	DG	H8	6	DT	H2'	2.95	3.77
7	DG	H8	6	DT	H3'	4.67	6.01
7	DG	H8	6	DT	H6	3.99	6.48
7	DG	H8	7	DG	H1'	3.47	4.67
7	DG	H8	7	DG	H2''	2.87	4.87
7	DG	H8	7	DG	H2'	2.23	2.54
7	DG	H8	7	DG	H3'	3.50	4.50
7	DG	H8	7	DG	H4'	4.54	6.52
8	DT	H2''	8	DT	H1'	2.03	2.66
8	DT	H2'	8	DT	H1'	2.28	3.51
8	DT	H3'	8	DT	H1'	3.46	3.96
8	DT	H3'	8	DT	H2''	2.38	3.62
8	DT	H3'	8	DT	H2'	2.15	2.58
8	DT	H4'	8	DT	H3'	2.58	2.82
8	DT	H6	7	DG	H1'	3.08	4.57
8	DT	H6	7	DG	H2''	2.33	2.72
8	DT	H6	7	DG	H2'	2.91	5.24
8	DT	H6	7	DG	H3'	4.72	6.07
8	DT	H6	7	DG	H8	4.29	6.23
8	DT	H6	8	DT	H1'	3.28	4.72
8	DT	H6	8	DT	H2''	2.45	5.19
8	DT	H6	8	DT	H2'	2.01	2.46
8	DT	H6	8	DT	H3'	4.14	4.64
8	DT	H6	8	DT	H4'	3.93	5.73

8	DT	ME	7	DG	H1'	4.15	5.13
8	DT	ME	7	DG	H2''	3.51	3.91
8	DT	ME	7	DG	H2'	3.32	3.82
8	DT	ME	7	DG	H3'	4.19	4.67
8	DT	ME	7	DG	H8	3.51	3.78
8	DT	ME	8	DT	H2'	4.68	5.40
8	DT	ME	8	DT	H3'	5.05	6.66
9	DT	H2''	9	DT	H1'	2.26	2.76
9	DT	H2'	9	DT	H1'	2.00	3.00
9	DT	H3'	9	DT	H1'	3.22	4.49
9	DT	H3'	9	DT	H2''	2.39	3.55
9	DT	H3'	9	DT	H2'	2.14	2.68
9	DT	H6	8	DT	H1'	4.54	5.10
9	DT	H6	8	DT	H2'	2.37	4.87
9	DT	H6	8	DT	H3'	3.40	6.54
9	DT	H6	8	DT	H6	3.42	6.42
9	DT	H6	9	DT	H1'	3.24	4.52
9	DT	H6	9	DT	H2'	2.11	2.61
9	DT	H6	9	DT	H3'	3.23	4.97
9	DT	ME	8	DT	H1'	4.11	5.03
9	DT	ME	8	DT	H2''	3.21	4.62
9	DT	ME	8	DT	H2'	3.11	3.62
9	DT	ME	8	DT	H3'	4.24	6.08
9	DT	ME	8	DT	H6	3.67	4.24
9	DT	ME	9	DT	H2'	3.38	4.89
9	DT	ME	9	DT	H3'	4.78	6.02

10	DT	H2''	10	DT	H1'	1.95	2.29
10	DT	H2'	10	DT	H1'	2.50	3.50
10	DT	H3'	10	DT	H1'	3.63	5.37
10	DT	H3'	10	DT	H2''	2.53	2.81
10	DT	H3'	10	DT	H2'	2.27	2.66
10	DT	H6	9	DT	H1'	3.71	4.41
10	DT	H6	9	DT	H2''	2.22	2.81
10	DT	H6	9	DT	H2'	2.97	4.21
10	DT	H6	10	DT	H1'	3.41	4.22
10	DT	H6	10	DT	H2'	2.33	2.88
10	DT	ME	9	DT	H1'	4.36	5.57
10	DT	ME	9	DT	H2''	3.62	4.38
10	DT	ME	9	DT	H2'	3.37	3.61
10	DT	ME	9	DT	H3'	4.19	4.91
10	DT	ME	9	DT	H6	3.54	3.75
10	DT	ME	10	DT	H2'	3.79	5.16
11	DG	H2'	11	DG	H1'	2.38	2.88
11	DG	H3'	11	DG	H1'	3.78	5.06
11	DG	H3'	11	DG	H2'	2.41	2.82
11	DG	H4'	11	DG	H1'	3.02	3.52
11	DG	H4'	11	DG	H2'	3.61	4.18
11	DG	H4'	11	DG	H3'	2.69	3.48
11	DG	H8	10	DT	H1'	3.81	4.51
11	DG	H8	10	DT	H2''	2.31	2.96
11	DG	H8	10	DT	H2'	2.95	3.45
11	DG	H8	10	DT	H3'	4.23	4.93

11	DG	H8	10	DT	H6	4.86	6.14
11	DG	H8	11	DG	H1'	3.51	4.01
11	DG	H8	11	DG	H2'	2.55	3.14
11	DG	H8	11	DG	H3'	3.39	4.36
11	DG	H8	11	DG	H4'	4.75	6.58
12	DT3	H2'	12	DT3	H1'	2.53	2.67
12	DT3	H3'	12	DT3	H1'	3.00	4.00
12	DT3	H3'	12	DT3	H2'	2.59	2.82
12	DT3	H4'	12	DT3	H1'	2.6	3.12
12	DT3	H4'	12	DT3	H3'	2.72	3.22
12	DT3	H6	11	DG	H1'	3.69	4.19
12	DT3	H6	11	DG	H2'	3.14	3.69
12	DT3	H6	11	DG	H3'	4.53	6.40
12	DT3	H6	11	DG	H8	4.06	5.44
12	DT3	H6	12	DT3	H1'	3.62	5.68
12	DT3	H6	12	DT3	H2'	2.98	3.41
12	DT3	H6	12	DT3	H3'	2.99	3.21
12	DT3	ME	11	DG	H1'	5.04	5.89
12	DT3	ME	11	DG	H2'	3.79	4.15
12	DT3	ME	11	DG	H3'	4.9	5.86
12	DT3	ME	11	DG	H8	3.91	4.22
12	DT3	ME	12	DT3	H2'	5.00	6.00
12	DT3	ME	12	DT3	H3'	5.47	7.61
13	DA5	H2''	13	DA5	H1'	1.95	2.34
13	DA5	H2'	13	DA5	H1'	2.47	5.44
13	DA5	H3'	13	DA5	H1'	3.88	5.54

13	DA5	H3'	13	DA5	H2''	2.36	3.50
13	DA5	H3'	13	DA5	H2'	2.14	3.28
13	DA5	H4'	13	DA5	H1'	3.07	3.37
13	DA5	H4'	13	DA5	H3'	2.33	2.89
13	DA5	H8	13	DA5	H1'	3.53	4.03
13	DA5	H8	13	DA5	H2''	2.71	4.03
13	DA5	H8	13	DA5	H2'	2.48	3.06
13	DA5	H8	13	DA5	H3'	3.00	4.00
13	DA5	H8	13	DA5	H4'	4.00	5.00
14	DC	H2''	14	DC	H1'	2.02	2.37
14	DC	H2'	14	DC	H1'	2.64	3.14
14	DC	H3'	14	DC	H2''	2.39	3.07
14	DC	H3'	14	DC	H2'	2.22	2.72
14	DC	H6	13	DA5	H1'	4.06	4.51
14	DC	H6	13	DA5	H2''	2.47	3.02
14	DC	H6	13	DA5	H2'	2.52	3.49
14	DC	H6	13	DA5	H3'	4.71	6.21
14	DC	H6	13	DA5	H8	4.50	5.50
14	DC	H6	14	DC	H1'	2.62	3.91
14	DC	H6	14	DC	H2''	2.81	4.6
14	DC	H6	14	DC	H2'	1.77	2.21
14	DC	H5	13	DA5	H2''	3.50	5.21
14	DC	H5	13	DA5	H2'	3.16	3.93
14	DC	H5	13	DA5	H8	4.31	6.75
14	DC	H5	14	DC	H2''	3.22	5.86
14	DC	H5	14	DC	H2'	3.04	6.14

15	DA	H2''	15	DA	H1'	1.92	2.42
15	DA	H2'	15	DA	H1'	2.59	5.09
15	DA	H3'	15	DA	H1'	3.25	5.08
15	DA	H3'	15	DA	H2''	2.31	3.18
15	DA	H3'	15	DA	H2'	2.24	2.82
15	DA	H4'	15	DA	H1'	3.07	3.40
15	DA	H4'	15	DA	H2''	3.08	4.99
15	DA	H4'	15	DA	H2'	2.99	4.60
15	DA	H4'	15	DA	H3'	2.60	2.76
15	DA	H8	14	DC	H1'	3.71	4.26
15	DA	H8	14	DC	H2''	2.66	3.16
15	DA	H8	14	DC	H2'	3.78	4.78
15	DA	H8	14	DC	H6	4.75	6.30
15	DA	H8	15	DA	H1'	3.61	5.40
15	DA	H8	15	DA	H2''	2.92	3.38
15	DA	H8	15	DA	H2'	2.04	2.54
15	DA	H8	15	DA	H3'	3.54	5.47
15	DA	H8	15	DA	H4'	5.09	6.76
16	DA	H2''	16	DA	H1'	2.06	2.44
16	DA	H2'	16	DA	H1'	2.35	4.64
16	DA	H3'	16	DA	H1'	3.49	3.97
16	DA	H3'	16	DA	H2''	2.50	3.50
16	DA	H3'	16	DA	H2'	2.09	2.45
16	DA	H4'	16	DA	H1'	2.97	3.11
16	DA	H4'	16	DA	H2'	3.50	5.70
16	DA	H4'	16	DA	H3'	2.82	2.96

16	DA	H8	15	DA	H1'	3.23	3.74
16	DA	H8	15	DA	H2'	2.67	3.37
16	DA	H8	15	DA	H3'	4.19	5.98
16	DA	H8	16	DA	H1'	3.48	5.15
16	DA	H8	16	DA	H2''	2.26	4.70
16	DA	H8	16	DA	H2'	2.11	2.48
16	DA	H8	16	DA	H3'	3.39	5.96
16	DA	H8	16	DA	H4'	4.50	5.50
17	DA	H2''	17	DA	H1'	2.15	2.65
17	DA	H2'	17	DA	H1'	2.47	4.20
17	DA	H3'	17	DA	H1'	3.87	5.56
17	DA	H3'	17	DA	H2''	2.72	4.81
17	DA	H3'	17	DA	H2'	2.17	2.86
17	DA	H4'	17	DA	H1'	3.20	3.59
17	DA	H4'	17	DA	H2'	3.45	4.04
17	DA	H4'	17	DA	H3'	2.86	3.36
17	DA	H8	16	DA	H1'	3.20	3.79
17	DA	H8	16	DA	H2'	2.83	3.32
17	DA	H8	16	DA	H3'	3.96	4.65
17	DA	H8	17	DA	H1'	3.50	5.26
17	DA	H8	17	DA	H2''	2.60	5.60
17	DA	H8	17	DA	H2'	2.04	2.52
17	DA	H8	17	DA	H3'	3.42	4.58
17	DA	H8	17	DA	H4'	4.42	6.24
18	DC	H1'	17	DA	H2	3.49	3.68
18	DC	H2''	18	DC	H1'	1.95	2.32

18	DC	H2'	18	DC	H1'	2.50	3.50
18	DC	H6	17	DA	H1'	3.25	4.05
18	DC	H6	17	DA	H2''	2.48	3.00
18	DC	H6	17	DA	H2'	2.90	3.72
18	DC	H6	17	DA	H3'	3.94	5.60
18	DC	H6	17	DA	H8	4.38	4.88
18	DC	H6	18	DC	H1'	2.64	3.70
18	DC	H6	18	DC	H2''	2.50	3.50
18	DC	H5	17	DA	H2''	3.86	4.36
18	DC	H5	17	DA	H2'	3.51	4.21
18	DC	H5	17	DA	H8	3.99	4.57
18	DC	H5	18	DC	H2'	3.50	4.50
19	DA	H2''	19	DA	H1'	1.99	2.55
19	DA	H2'	19	DA	H1'	2.35	4.52
19	DA	H3'	19	DA	H1'	3.46	5.12
19	DA	H3'	19	DA	H2''	2.49	4.65
19	DA	H3'	19	DA	H2'	2.09	2.45
19	DA	H4'	18	DC	H2''	4.57	5.64
19	DA	H4'	19	DA	H2''	3.10	3.80
19	DA	H4'	19	DA	H2'	3.46	5.78
19	DA	H4'	19	DA	H3'	2.84	3.52
19	DA	H8	18	DC	H1'	3.53	4.27
19	DA	H8	18	DC	H2''	2.53	2.93
19	DA	H8	18	DC	H2'	2.74	3.38
19	DA	H8	19	DA	H1'	3.45	3.98
19	DA	H8	19	DA	H2''	3.19	3.67

19	DA	H8	19	DA	H2'	2.01	2.58
19	DA	H8	19	DA	H3'	3.56	5.28
19	DA	H8	19	DA	H4'	4.36	6.19
20	DC	H2''	20	DC	H1'	2.11	2.58
20	DC	H2'	20	DC	H1'	3.09	4.75
20	DC	H3'	20	DC	H2''	2.38	3.11
20	DC	H3'	20	DC	H2'	2.41	3.72
20	DC	H6	19	DA	H1'	3.24	4.10
20	DC	H6	19	DA	H2''	2.24	2.86
20	DC	H6	19	DA	H2'	2.57	4.15
20	DC	H6	19	DA	H3'	3.50	6.31
20	DC	H6	20	DC	H1'	3.21	3.78
20	DC	H6	20	DC	H2''	2.18	5.43
20	DC	H5	19	DA	H2''	3.64	4.69
20	DC	H5	19	DA	H2'	2.98	4.31
20	DC	H5	19	DA	H8	3.79	4.63
20	DC	H5	20	DC	H2''	4.76	5.22
20	DC	H5	20	DC	H2'	3.70	5.96
21	DG	H2''	21	DG	H1'	1.85	2.35
21	DG	H2'	21	DG	H1'	2.27	4.97
21	DG	H3'	21	DG	H1'	3.66	5.72
21	DG	H3'	21	DG	H2'	2.02	2.52
21	DG	H4'	21	DG	H1'	3.15	3.37
21	DG	H4'	21	DG	H3'	2.86	3.39
21	DG	H8	20	DC	H1'	3.55	4.43
21	DG	H8	20	DC	H2''	2.31	2.82

21	DG	H8	20	DC	H2'	3.75	5.29
21	DG	H8	20	DC	H6	4.88	5.38
21	DG	H8	21	DG	H1'	3.41	5.94
21	DG	H8	21	DG	H2''	2.36	4.23
21	DG	H8	21	DG	H2'	2.09	2.55
21	DG	H8	21	DG	H3'	3.44	4.80
21	DG	H8	21	DG	H4'	4.35	6.07
22	DC	H2''	22	DC	H1'	1.98	2.27
22	DC	H2'	22	DC	H1'	2.50	3.50
22	DC	H3'	22	DC	H1'	3.80	4.30
22	DC	H3'	22	DC	H2''	2.81	3.38
22	DC	H3'	22	DC	H2'	2.39	2.61
22	DC	H6	21	DG	H1'	3.49	4.24
22	DC	H6	21	DG	H2''	2.13	2.73
22	DC	H6	21	DG	H2'	2.94	5.87
22	DC	H6	21	DG	H8	3.56	6.17
22	DC	H6	22	DC	H1'	3.33	4.25
22	DC	H6	22	DC	H2'	2.09	2.72
22	DC	H6	22	DC	H3'	3.66	5.25
22	DC	H5	21	DG	H1'	3.96	5.52
22	DC	H5	21	DG	H2''	3.31	4.63
22	DC	H5	21	DG	H2'	3.01	3.58
22	DC	H5	21	DG	H3'	4.86	6.79
22	DC	H5	21	DG	H8	3.65	4.52
22	DC	H5	22	DC	H2''	5.00	6.00
22	DC	H5	22	DC	H2'	3.43	4.42

23	DA	H2''	23	DA	H1'	1.97	2.35
23	DA	H2'	23	DA	H1'	2.99	5.07
23	DA	H3'	23	DA	H1'	3.20	3.83
23	DA	H3'	23	DA	H2''	2.79	5.57
23	DA	H3'	23	DA	H2'	2.12	2.71
23	DA	H4'	23	DA	H1'	2.83	3.31
23	DA	H4'	23	DA	H2''	3.21	4.16
23	DA	H4'	23	DA	H2'	3.61	4.11
23	DA	H8	22	DC	H1'	3.54	4.08
23	DA	H8	22	DC	H2''	2.40	2.90
23	DA	H8	22	DC	H2'	3.22	3.74
23	DA	H8	22	DC	H3'	4.96	6.72
23	DA	H8	22	DC	H6	4.23	6.36
23	DA	H8	23	DA	H1'	3.20	4.59
23	DA	H8	23	DA	H2''	2.93	5.48
23	DA	H8	23	DA	H2'	2.06	2.35
23	DA	H8	23	DA	H3'	3.36	5.48
23	DA	H8	23	DA	H4'	4.55	6.23
24	DC3	H2''	24	DC3	H1'	2.23	3.06
24	DC3	H2'	24	DC3	H1'	2.51	4.17
24	DC3	H3'	24	DC3	H1'	3.45	4.35
24	DC3	H3'	24	DC3	H2''	2.00	3.00
24	DC3	H3'	24	DC3	H2'	1.98	2.81
24	DC3	H4'	24	DC3	H2''	3.00	4.96
24	DC3	H4'	24	DC3	H2'	3.28	4.89
24	DC3	H6	23	DA	H1'	3.29	4.34

24	DC3	H6	23	DA	H2''	2.69	2.97
24	DC3	H6	23	DA	H3'	4.22	6.43
24	DC3	H6	23	DA	H8	4.10	6.12
24	DC3	H6	24	DC3	H1'	3.38	3.95
24	DC3	H6	24	DC3	H2''	2.71	5.00
24	DC3	H6	24	DC3	H2'	2.21	2.78
24	DC3	H6	24	DC3	H3'	2.88	3.58
24	DC3	H5	23	DA	H2''	3.14	4.45
24	DC3	H5	23	DA	H2'	3.24	5.57
24	DC3	H5	23	DA	H8	3.51	3.91
24	DC3	H5	24	DC3	H2''	3.00	5.70
24	DC3	H5	24	DC3	H2'	3.42	5.50

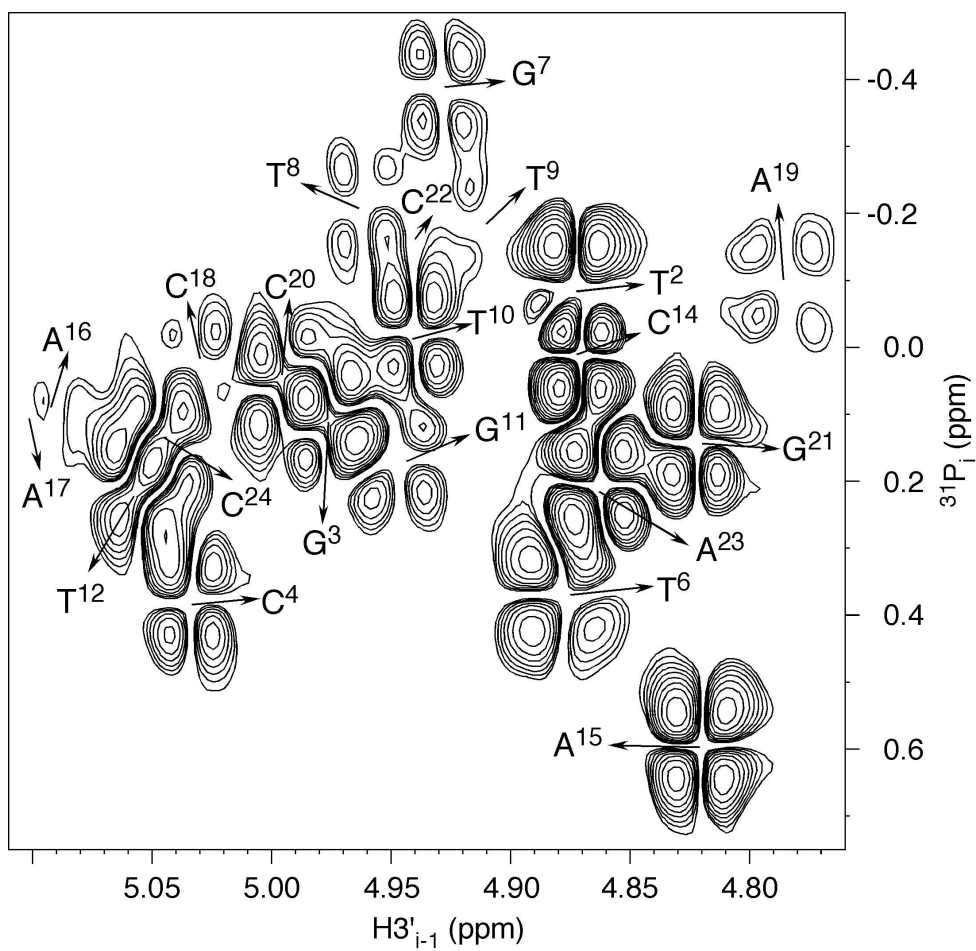


Figure S1. ^{31}P - $\text{H}3'$ HMBC spectrum showing the assignment of the ^{31}P resonances.

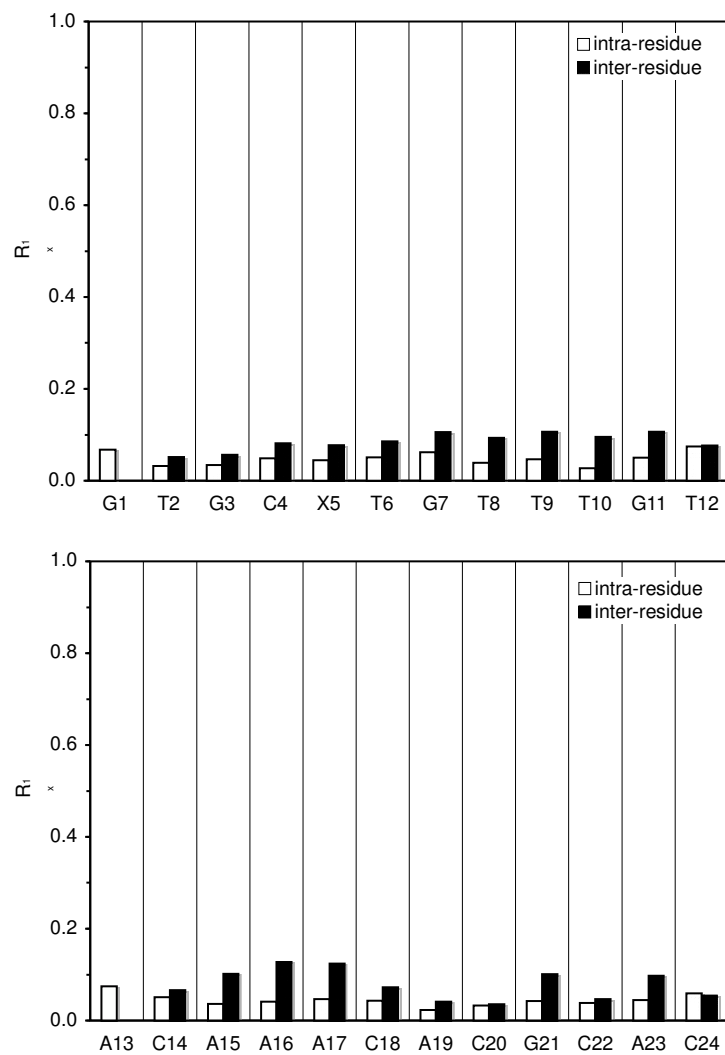


Figure S2. Nucleotide-by-nucleotide sixth-root residuals (R_1^x) for the refined structure obtained by CORMA calculation.

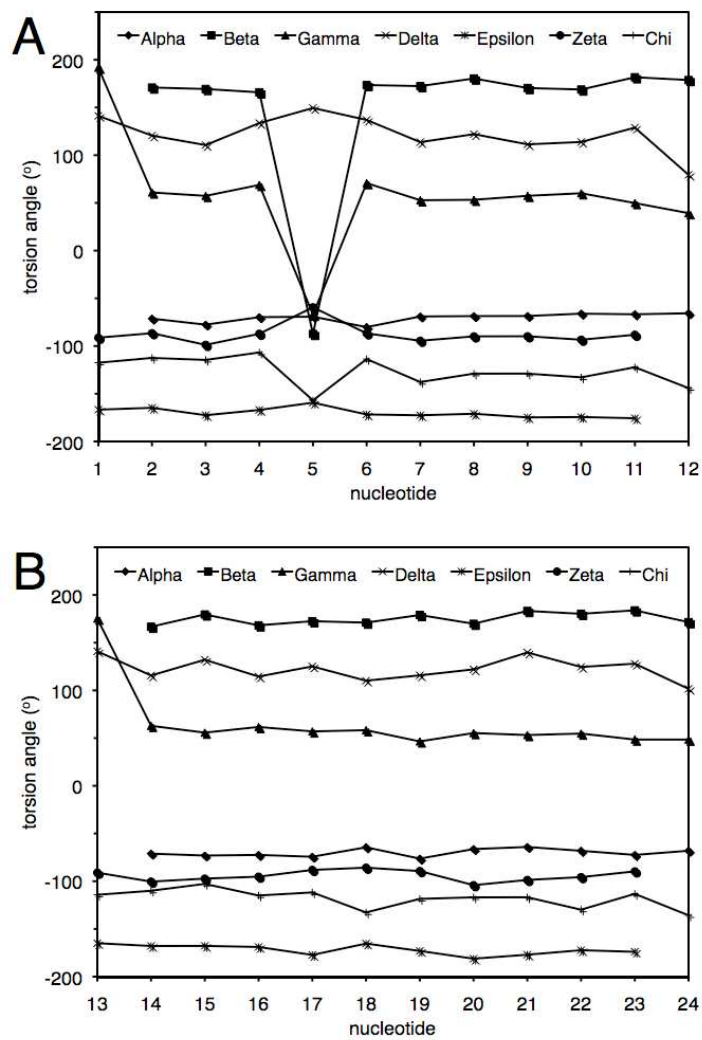


Figure S3. Backbone torsion angles of the refined structure of the *S*-cdG containing duplex. **A.** Modified strand. **B.** Complementary strand.

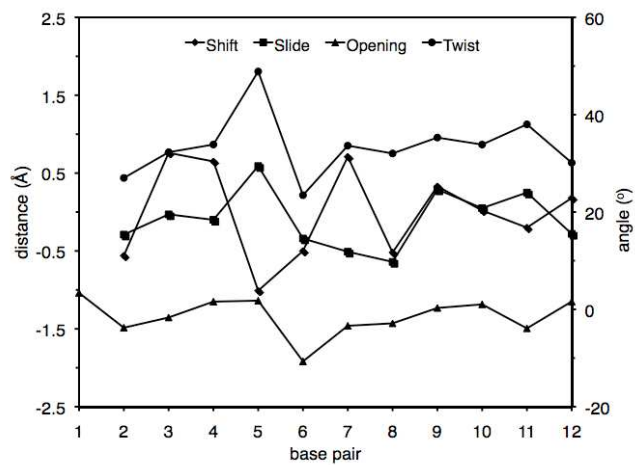


Figure S4. Base pairing and base stacking parameters of the refined structure of the S-cdG containing duplex.

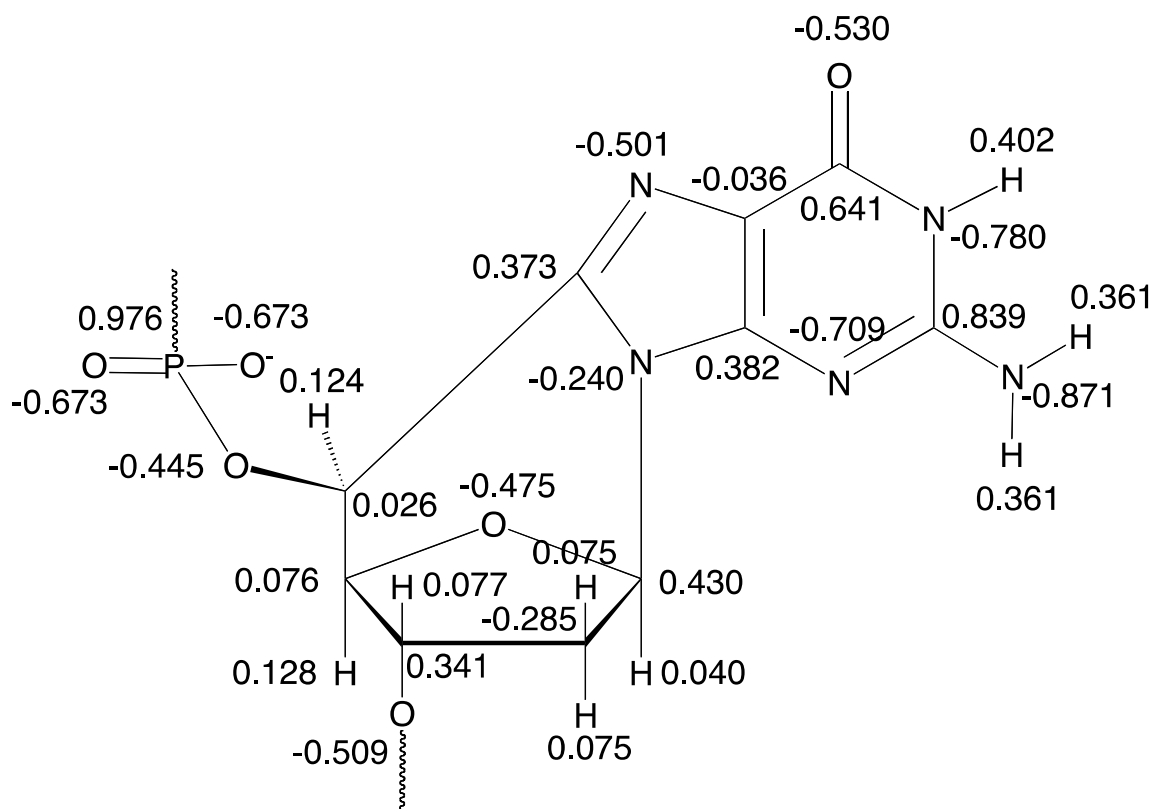


Figure S5. Partial charges of the *S*-cdG 5'-phosphate nucleotide.

