

The *cis*-(5*R*,6*S*)-Thymine Glycol Lesion Occupies the Wobble Position When Mismatched with dG in DNA

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Supporting Information

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Running Title: Wobble *cis*-(5*R*,6*S*)-Thymine Glycol:G Pairing

Table S1. Helicoidal Analysis of the Oligodeoxynucleotide Duplex Containing the Tg⁶•G¹⁹ Mismatch.

(a) Global Base-Axis Parameters

Residue	Xdisp	Ydisp	Incline	Tip	Residue	Xdisp	Ydisp	Incline	Tip
	(dx)	(dy)	(eta)	(theta)		(dx)	(dy)	(eta)	(theta)
G ¹	-1.18	-0.13	-8.04	-1.14	C ²⁴	-1.11	0.09	-0.18	-12.59
T ²	-0.84	-0.64	-10.0	-5.14	A ²³	-0.72	0.65	-0.97	-11.64
G ³	-1.22	-0.18	-0.69	-1.82	C ²²	-1.31	0.21	-4.26	-12.69
C ⁴	-0.93	-0.77	-7.84	-10.16	G ²¹	-0.86	0.83	1.10	-10.24
G ⁵	-1.66	-0.37	1.54	4.98	C ²⁰	-1.49	0.44	-8.24	-4.73
Tg ⁶	0.64	-0.58	-10.62	-20.57	G ¹⁹	-1.29	1.13	-9.29	-14.89
G ⁷	-1.76	-0.58	-7.40	-1.00	C ¹⁸	-1.59	0.69	1.32	-20.78
T ⁸	-1.20	-0.63	-9.46	-1.17	A ¹⁷	-0.99	0.82	1.00	-12.02
T ⁹	-1.59	-0.78	0.33	-3.14	A ¹⁶	-1.32	0.84	1.85	-14.29
T ¹⁰	-1.40	-0.48	8.90	-1.34	A ¹⁵	-1.21	0.61	-8.35	-18.64
G ¹¹	-1.39	-0.68	-10.61	-0.42	C ¹⁴	-1.41	0.86	8.15	-10.24
T ¹²	-1.53	-0.75	0.79	8.24	A ¹³	-1.37	0.75	2.73	-11.05

(b) Global Base pair - Axis Parameters

Residues	Xdisp	Ydisp	Incline	Tip
	(dx)	(dy)	(eta)	(theta)
G ¹ -C ²⁴	-1.15	-0.11	-4.11	5.73
T ² -A ²³	-0.78	-0.65	-5.49	3.25
G ³ -C ²²	-1.27	-0.19	-2.47	5.43
C ⁴ -G ²¹	-0.90	-0.80	-3.37	0.04

G ⁵ -C ²⁰	-1.58	-0.41	-3.35	4.86
Tg ⁶ -G ¹⁹	-0.33	-0.86	-9.96	-2.84
G ⁷ -C ¹⁸	-1.68	-0.63	-3.04	9.89
T ⁸ -A ¹⁷	-1.09	-0.72	-4.23	5.42
T ⁹ -A ¹⁶	-1.46	-0.81	1.09	5.57
T ¹⁰ -A ¹⁵	-1.30	-0.55	0.28	8.65
G ¹¹ -C ¹⁴	-1.40	-0.77	-1.23	4.91
T ¹² -A ¹³	-1.45	-0.75	1.76	9.65
Average:	-1.2	-0.6	-2.84	5.05

(c) Global Base-Base Parameters

Residues	Shear (Sx)	Stretch (Sy)	Stagger (Sz)	Buckle (kappa)	Propeller (omega)	Opening (sigma)
G ¹ -C ²⁴	-0.07	-0.05	-0.04	-7.87	-13.73	0.47
T ² -A ²³	-0.11	0.01	0.54	-9.03	-16.78	-0.11
G ³ -C ²²	0.08	0.03	0.07	3.58	-14.51	-1.38
C ⁴ -G ²¹	-0.07	0.06	0.32	-8.94	-20.41	-1.92
G ⁵ -C ²⁰	-0.16	0.07	0	9.78	0.25	-0.44
Tg ⁶ -G ¹⁹	1.93	0.55	1.36	-1.33	-35.46	27.57
G ⁷ -C ¹⁸	-0.17	0.11	0.05	-8.73	-21.78	1.72
T ⁸ -A ¹⁷	-0.21	0.19	0.22	-10.46	-13.18	4.95
T ⁹ -A ¹⁶	-0.28	0.06	-0.48	-1.51	-17.42	2.29
T ¹⁰ -A ¹⁵	-0.19	0.13	-0.42	17.25	-19.98	2.83
G ¹¹ -C ¹⁴	0.02	0.18	-0.13	-18.77	-10.67	2.87

$T^{12}-A^{13}$	-0.17	0	0	-1.94	-2.81	0.51
Average:	0.05	0.11	0.12	-3.16	-15.54	3.28

(d) Global Inter-Base Parameters

	Shift (Dx)	Slide (Dy)	Rise (Dz)	Tilt (tau)	Roll (rho)	Twist (Omega)
G^1/T^2	0.21	-0.55	3.80	-0.88	-3.48	36.31
T^2/G^3	-0.67	0.41	2.90	11.74	2.90	32.23
G^3/C^4	-0.19	-0.54	3.76	-6.20	-1.84	34.43
C^4/G^5	-0.34	0.62	2.71	8.90	25.15	27.34
G^5/Tg^6	2.97	-0.37	5.01	-6.60	-23.43	52.39
Tg^6/G^7	-3.13	-0.55	2.54	6.56	25.53	15.61
G^7/T^8	0.02	-0.26	3.49	1.96	5.25	27.65
T^8/T^9	-0.33	-0.16	2.76	14.00	4.49	31.3
T^9/T^{10}	0.19	0.54	2.86	11.54	11.24	32.7
T^{10}/G^{11}	0.10	-0.36	4.45	-15.84	3.06	40.1
G^{11}/T^{12}	-0.23	-0.28	3.08	14.26	9.24	27.89

	Shift (Dx)	Slide (Dy)	Rise (Dz)	Tilt (tau)	Roll (rho)	Twist (Omega)
C^{24}/A^{23}	0.25	0.60	3.22	0.28	0.43	36.88
A^{23}/C^{22}	-0.86	-0.39	3.36	-0.86	-0.63	33.50
C^{22}/G^{21}	-0.03	0.57	3.51	6.32	-4.06	34.98
G^{21}/C^{20}	-0.24	-0.61	3.04	-9.83	-4.49	25.86

C^{20}/A^{19}	0.88	0.85	3.65	4.51	-12.29	24.38
A^{19}/C^{18}	-1.03	0.11	3.84	13.95	-11.85	41.46
C^{18}/A^{17}	0.06	0.34	3.32	3.69	3.35	24.42
A^{17}/A^{16}	-0.26	0.03	3.47	5.06	-8.73	33.96
A^{16}/A^{15}	0.10	-0.46	2.80	-7.22	-13.79	32.16
A^{15}/C^{14}	-0.11	0.40	4.15	20.18	6.25	40.06
C^{14}/A^{13}	-0.05	0.10	2.95	-2.56	-1.38	30.25

(e) Global Inter-Base Parameters

	Shift	Slide	Rise	Tilt	Roll	Twist
	(Dx)	(Dy)	(Dz)	(tau)	(rho)	(Omega)
G^1/T^2	0.23	-0.57	3.51	-0.30	-1.95	36.59
T^2/G^3	-0.77	0.4	3.13	5.44	1.77	32.86
G^3/C^4	-0.11	-0.55	3.64	0.06	1.11	34.7
C^4/G^5	-0.29	0.62	2.88	-0.47	14.82	26.6
G^5/Tg^6	1.93	-0.61	4.33	-1.05	-5.57	38.38
Tg^6/G^7	-2.08	-0.33	3.19	10.25	18.69	28.54
G^7/T^8	0.04	-0.30	3.41	2.82	0.95	26.03
T^8/T^9	-0.29	-0.09	3.11	9.53	6.61	32.63
T^9/T^{10}	0.14	0.50	2.83	2.16	12.51	32.43
T^{10}/G^{11}	-0.01	-0.38	4.30	2.17	-1.60	40.08
G^{11}/T^{12}	-0.14	-0.19	3.02	5.85	5.31	29.07
Average:	-0.12	-0.14	3.39	3.32	4.79	32.54

(f) Local Inter-Base Parameters

	Shift	Slide	Rise	Tilt	Roll	Twist
	(Dx)	(Dy)	(Dz)	(tau)	(rho)	(Omega)
G^1/T^2	0.64	-1.67	3.58	1.16	-8.89	36.03
T^2/G^3	-0.32	-0.47	2.87	13.29	-0.19	31.48
G^3/C^4	0.53	-1.34	3.76	-2.36	-3.97	35.27
C^4/G^5	0.03	-0.25	3.00	10.14	23.06	28.02
G^5/Tg^6	3.94	-0.80	4.57	1.84	-25.4	53.95
Tg^6/G^7	-2.51	-1.04	2.95	10.55	22.22	14.95
G^7/T^8	0.37	-1.46	3.40	2.69	1.07	28.06
T^8/T^9	0.10	-1.10	2.80	14.99	1.96	31.37
T^9/T^{10}	0.55	-0.08	3.10	12.75	13.58	31.63
T^{10}/G^{11}	0.81	-1.37	4.42	-13.99	2.3	40.66
G^{11}/T^{12}	-0.16	-1.29	2.96	12.05	6.47	28.95
	Shift	Slide	Rise	Tilt	Roll	Twist
	(Dx)	(Dy)	(Dz)	(tau)	(rho)	(Omega)
C^{24}/A^{23}	-0.18	-1.18	3.25	-7.30	-0.74	36.18
A^{23}/C^{22}	-1.22	-0.36	3.15	-7.66	-0.94	32.58
C^{22}/G^{21}	-0.49	-1.26	3.56	-0.84	3.21	35.67
G^{21}/C^{20}	-0.30	-0.09	3.25	-12.8	3.03	25.03
C^{20}/A^{19}	0.63	-1.90	3.53	0.03	8.98	24.94
A^{19}/C^{18}	-1.54	-1.56	3.54	-0.68	8.97	43.87
C^{18}/A^{17}	-0.60	-0.77	3.39	-3.41	-2.54	24.29

A^{17}/A^{16}	-0.54	-0.64	3.52	-2.91	9.59	34.06
A^{16}/A^{15}	-0.23	-0.45	3.02	-16.05	11.75	29.57
A^{15}/C^{14}	-0.77	-1.18	4.15	8.66	-5.58	43.98
C^{14}/A^{13}	-0.13	-0.57	3.02	-7.84	4.22	29.14

(g) Local Inter-Base pair Parameters

	Shift (Dx)	Slide (Dy)	Rise (Dz)	Tilt (tau)	Roll (rho)	Twist (Omega)
G^1/T^2	0.20	-1.41	3.44	-3.12	-4.81	36.60
T^2/G^3	-0.75	-0.42	3.03	2.84	-0.65	32.18
G^3/C^4	0	-1.31	3.69	-1.66	-0.36	35.95
C^4/G^5	-0.12	-0.17	3.10	-1.38	13.02	26.42
G^5/Tg^6	2.09	-1.20	4.31	3.06	-8.04	38.76
Tg^6/G^7	-1.90	-1.38	3.04	4.03	16.19	30.10
G^7/T^8	-0.12	-1.10	3.45	-0.40	-0.68	26.21
T^8/T^9	-0.18	-0.88	3.17	6.20	5.97	33.07
T^9/T^{10}	0.15	-0.26	3.07	-1.73	13.24	30.77
T^{10}/G^{11}	0	-1.25	4.34	-2.82	-1.97	42.43
G^{11}/T^{12}	-0.15	-0.93	3.00	2.10	5.44	28.75
Average:	-0.07	-0.94	3.42	0.65	3.4	32.84

(h) Global Axis Curvature

	Ax	Ay	Ainc	Atip	Adis	Angle	Path
G^1/T^2	-0.14	-0.04	1.07	0.52	0.14	1.19	3.51

T ² /G ³	-0.28	-0.06	2.43	-0.41	0.29	2.46	3.14
G ³ /C ⁴	-0.48	0.05	0.96	6.50	0.48	6.57	3.66
C ⁴ /G ⁵	0.39	0.23	-0.49	10.01	0.45	10.02	2.90
G ⁵ /Tg ⁶	0.68	-0.16	5.56	2.13	0.70	5.95	4.38
Tg ⁶ /G ⁷	-0.73	-0.55	3.33	5.96	0.92	6.83	3.31
G ⁷ /T ⁸	-0.55	-0.21	4.02	5.41	0.59	6.74	3.45
T ⁸ /T ⁹	0.07	0	4.21	6.46	0.07	7.71	3.11
T ⁹ /T ¹⁰	-0.01	0.23	2.97	9.43	0.23	9.89	2.83
T ¹⁰ /G ¹¹	0.09	-0.15	3.68	2.15	0.17	4.26	4.30
G ¹¹ /T ¹²	-0.09	-0.21	2.86	0.57	0.23	2.92	3.02

(i) Backbone Parameters

	C1'-C2'	C2'-C3'	Phase	Amplitude	Pucker	C1'	C2'	C3'
G ¹	25.89	-21.79	146.11	25.81	C2'- endo	100.8	112.0	101.6
T ²	14.21	2.22	85.48	28.91	O1'- endo	103.7	108.1	104.9
G ³	31.85	-31.78	162.66	33.66	C2'- endo	104.0	103.8	103.0
C ⁴	11.85	4.52	80.64	28.22	O1'- endo	103.7	108.2	105.2
G ⁵	36.80	-34.41	156.84	37.85	C2'- endo	103.3	103.0	102.7
Tg ⁶	-2.95	24.63	51.19	39.79	C4'-exo	104.9	105.5	102.4
G ⁷	28.45	-27.68	159.64	29.72	C2'- endo	104.0	104.9	103.9
T ⁸	-3.94	18.38	47.22	27.08	C4'-exo	103.8	109.7	103.7

T ⁹	6.24	4.42	75.7	18.07	O1'- endo	103.6	111.3	104.9
T ¹⁰	32.42	-30.79	157.98	33.56	C2'- endo	103.7	103.9	103.3
G ¹¹	-4.89	21.16	46.51	31.04	C4'-exo	104.3	108.4	103.2
T ¹²	-10.77	25.61	36.41	32.26	C4'-exo	104.8	107.2	101.1

	Chi	Gamma	Delta	Epsilon	Zeta	Alpha	Beta
	C1'-N	C5'-C4'	C4'-C3'	C3'-O3'	O3'-P	P-O5'	O5'-C5'
G ¹	-134.41	-174.37	132.03	-168.86	-90.08	-76.62	177.21
T ²	-140.37	62.11	101.78	-173.28	-92.95	-68.83	178.92
G ³	-111.12	64.78	141.78	-174.71	-98.81	-76.91	178.97
C ⁴	-135.23	57.70	100.26	-158.97	-84.65	-80.24	175.59
G ⁵	-106.31	62.44	142.01	-177.25	-91.25	-67.53	167.46
Tg ⁶	-146.28	76.68	81.32	-168.77	-91.09	-75.17	-170.79
G ⁷	-115.91	60.65	138.03	-166.50	-108.8	124.65	-165.23
T ⁸	-152.99	-171.89	96.99	-162.78	-79.83	-77.60	175.30
T ⁹	-132.81	66.74	108.14	-164.28	-84.70	-74.75	176.17
T ¹⁰	-106.08	66.31	140.26	-174.29	-101.79	-85.01	175.95
G ¹¹	-152.41	61.23	90.56	-160.39	-78.31	-80.70	177.39
T ¹²	-140.43	61.40	90.14				

	C1'-C2'	C2'-C3'	Phase	Amplitude	Pucker	C1'	C2'	C3'
C ²⁴	18.15	-2.40	94.37	29.13	O1'- endo	103.1	109.7	101.4
A ²³	29.38	-25.97	150.42	29.97	C2'-	103.4	105.2	104.2

					endo			
C ²²	39.07	-30.58	141.42	39.46	C1'-exo	101.6	103.9	102.9
G ²¹	31.89	-34.74	169.51	35.49	C2'- endo	103.5	103.3	103.1
C ²⁰	23.92	-9.27	108.06	29.88	C1'-exo	102.0	111.1	103.3
A ¹⁹	18.79	-7.19	107.14	24.20	O1'- endo	103.2	109.4	105.4
C ¹⁸	37.42	-33.59	152.68	38.15	C2'- endo	102.7	103.1	102.8
A ¹⁷	37.89	-32.99	150.31	38.39	C2'- endo	102.8	102.9	103.0
A ¹⁶	29.36	-32.50	171.55	33.08	C2'- endo	104.4	104.0	103.4
A ¹⁵	-16.53	29.98	25.80	33.62	C3'- endo	105.0	105.8	102.5
C ¹⁴	33.40	-25.13	137.82	34.01	C1'-exo	102.2	106.0	103.1
A ¹³	25.10	-22.56	152.61	25.50	C2'- endo	103.3	107.3	103.1

	Chi	Gamma	Delta	Epsilon	Zeta	Alpha	Beta
	C1'-N	C5'-C4'	C4'-C3'	C3'-O3'	O3'-P	P-O5'	O5'-C5'
C ²⁴	-121.47	58.98	107.19				
A ²³	-150.01	168.36	136.50	-151.82	-83.08	-93.83	177.43
C ²²	-109.14	50.17	134.81	-146.21	-73.21	-107.58	66.46
G ²¹	-136.79	166.25	148.89	-160.18	-84.96	-87.20	-177.72
C ²⁰	-132.74	56.40	114.78	-127.44	-71.07	-106.64	65.39
A ¹⁹	-141.67	-173.94	115.21	-163.74	-85.63	-81.47	-177.89

C ¹⁸	-154.27	171.61	143.70	-153.35	-83.40	111.82	-175.06
A ¹⁷	-100.40	50.27	140.50	-147.61	-78.98	-101.57	65.21
A ¹⁶	-113.16	71.58	146.17	-168.56	-94.50	-79.94	-173.37
A ¹⁵	-151.13	59.41	87.57	-163.13	-76.18	-69.35	177.54
C ¹⁴	-114.24	64.38	128.12	-178.68	-103.53	-81.54	178.81
A ¹³	-109.97	-175.85	129.76	-173.21	-98.45	-75.29	172.04
