Solution Structure of a DNA Duplex Containing a Guanine-Difluorotoluene Pair: A Wobble Pair Without Hydrogen Bonding?

Danielle A. Pfaff, Kristine M. Clarke, Timothy A. Parr, Joanna M. Cole, Bernhard H. Geierstanger[†], Deborah C. Tahmassebi, Tammy J. Dwyer**

Supporting Information Table 1. Proton chemical shift assignments (ppm) for the G-T duplex at 20°C[a].

Nucleotide	H6/H8	H5	Methyl	H1'	H2'	H2''	H3'	H4'	NH[b]
C1	7.77	5.98	na[c]	5.99	2.09	2.52	3.79	4.11	
C2	7.58	5.76	na	5.38	2.07	2.33	--[d]	--	
A3	8.29	na	na	5.94	2.84	2.96	5.11	4.02	
A4	8.15	na	na	6.06	2.68	2.83	5.07	4.29	
G5	7.53	na	na	5.87	2.54	2.66	5.08	4.27	10.70
C6	7.32	5.21	na	5.86	2.04	2.51	5.21	4.17	
T7	7.54	na	1.60	6.17	2.25	2.65	4.94	4.12	14.10
T8	7.48	na	1.73	6.15	2.24	2.63	4.94	4.24	13.95
C9	7.63	5.83	na	6.13	2.27	2.54	4.90	4.24	
C10	7.70	5.84	na	6.28	2.33	2.33	4.54	4.10	
G11	7.84	na	na	5.65	2.43	2.56	3.68	4.14	12.90
G12	7.86	na	na	5.42	2.67	2.75	5.03	4.03	12.85
A13	8.21	na	na	5.95	2.76	2.94	5.12	--	
A14	8.06	na	na	6.08	2.63	2.92	5.10	4.27	
G15	7.51	na	na	5.87	2.46	2.69	5.09	4.25	13.05
T16	7.19	na	1.65	5.77	1.94	2.45	4.92	4.14	11.55
T17	7.56	na	1.62	6.15	2.29	2.53	4.93	4.11	14.55
T18	7.35	na	1.75	5.72	2.01	2.31	4.89	4.12	14.15
G19	7.90	na	na	5.73	2.70	2.74	5.02	4.08	13.05
G20	7.84	na	na	5.19	2.44	2.58	4.26	--	13.25

[a]Chemical shifts are referenced to residual HOD resonance.
[b]Chemical shifts for imino protons are reported for the duplex at 5°C.
[c]Not applicable.
[d]Not assigned due to overlap.

Supporting Information Table 2. Proton chemical shift assignments (ppm) for the G-F duplex at 15°C[a].

Nucleotide	H6/H8	H5	Methyl	H1'	H2'	H2''	H3'	H4'	NH[b]
C1	7.66	5.86	na[c]	5.87	1.98	2.41	4.53	3.68	
C2	7.49	5.64	na	5.19	1.98	2.22	4.58	3.92	
A3	8.16	na	na	5.77	2.66	2.74	4.96	4.30	
A4	7.79	na	na	5.86	1.86	2.12	4.95	4.29	
G5	7.91	na	na	5.58	2.56	2.64	4.89	4.24	10.80
C6	7.43	5.16	na	5.79	2.06	2.45	4.46	4.04	
T7	7.47	na	1.48	6.03	2.15	2.54	4.46	4.18	14.15
T8	7.37	na	1.58	6.05	2.14	2.52	4.83	4.10	13.90
C9	7.51	5.68	na	5.97	2.13	2.39	--[d]	4.11	
C10	7.55	5.66	na	6.15	2.20	2.39	4.48	3.93	
G11	7.73	na	na	5.53	2.06	2.38	--	--	12.95
G12	7.74	na	na	5.30	2.38	2.61	--	3.57	12.85
A13	8.08	na	na	5.85	2.62	2.82	5.00	4.36	
A14	7.95	na	na	5.95	2.51	2.78	4.99	4.37	
G15	7.39	na	na	5.55	2.21	2.56	4.98	4.21	13.30
F16	6.90	na	1.37	6.02	2.35	2.54	4.98	4.10	
T17	7.11	na	1.36	5.91	1.97	2.37	4.98	4.09	13.95
T18	7.28	na	1.59	5.61	1.96	2.22	4.53	4.02	14.25
G19	7.79	na	na	5.59	2.43	2.63	4.92	--	13.05
G20	7.72	na	na	6.07	2.27	2.44	4.57	4.15	13.20

[a]Chemical shifts are referenced to residual HOD resonance.
[b]Chemical shifts for imino protons are reported for the duplex at 5°C.
[c]Not applicable.
[d]Not assigned due to overlap.

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