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Table S-I

Exchangeable and A(H2) Proton Chemical Shifts of the
Control Duplex in H₂O Buffer, pH 6.5, at 0 °C

Chemical Shifts, (ppm)					
<u>Base pair</u>	<u>H3</u>	<u>H1</u>	<u>NH₂^b</u> ^a	<u>NH₂^e</u> ^b	<u>H2</u>
G1•C24			8.15	6.56	
C2•G23		12.78	8.40	6.54	
A3•T22	13.59				7.65
T4•A21	13.60				7.70
C5•G20		12.67	8.42	6.82	
G6•C19		12.98	8.46	6.76	
G7•C18		12.92	8.02	6.28	
C8•G17		12.78	8.12	6.51	
T9•A16	13.73				7.38
A10•T15	13.55				7.50
C11•G14		12.84	8.32	6.81	
G12•C13			7.97	7.02	

^aHydrogen-bonded cytosine amino protons.

^bExposed cytosine amino protons.

Table S-II
Chemical Shift Assignments for the Control
Duplex in D₂O Buffer at 25 °C

<u>Chemical Shift, (ppm)</u>								
<u>Base</u>	<u>H8/H6</u>	<u>H5/CH₃</u>	<u>H₂</u>	<u>H₁'</u>	<u>H₂'</u>	<u>H₂'</u>	<u>H₃'</u>	<u>H₄'</u>
G1	7.92			5.95	2.61	2.77	4.83	4.24
C2	7.46	5.41		5.67	2.17	2.48	4.89	4.21
A3	8.34		7.69	6.30	2.73	2.98	5.03	4.45
T4	7.16	1.40		5.89	2.02	2.43	4.84	4.18
C5	7.37	5.53		5.63	1.93	2.33		4.08
G6	7.82			5.60	2.65	2.72	4.98	4.32
G7	7.70			5.88	2.57	2.70	4.96	4.39
C8	7.36	5.24		5.84	1.99	2.44		4.16
T9	7.38	1.64		5.63	2.11	2.44	4.87	4.13
A10	8.31		7.54	6.19	2.70	2.84	5.02	4.42
C11	7.27	5.36		5.64	1.84	2.27		4.13
G12	7.87			6.11	2.58	2.35	4.64	4.15
C13	7.63	5.88		5.76	2.02	2.42	4.70	4.07
G14	7.98			5.97	2.68	2.78	4.97	4.36
T15	7.26	1.50		5.59	2.68	2.39	4.87	4.17
A16	8.17		7.42	6.06	2.72	2.91	5.05	4.41
G17	7.65			5.68	2.49	2.58	4.94	4.37
C18	7.29	5.17		5.88	1.99	2.41	4.70	4.19
C19	7.36	5.49		5.45	1.96	2.32	4.78	4.04
G20	7.88			5.62	2.70	2.80	5.00	4.34

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A21	8.19		7.74	6.21	2.60	2.91	5.00	4.44
T22	7.04	1.37		5.73	1.92	2.33	4.84	4.12
G23	7.82			5.90	2.57	2.67	4.96	4.33
C24	7.39	5.30		6.16	2.19	2.19	4.48	4.04

Table S-III

Exchangeable and A(H2) Proton Chemical Shifts of the
A1-bulge Duplex in H₂O buffer, pH 6.5, at 0 °C

Chemical Shifts, (ppm)					
Base pair	H3	H1	NH ₂ ^b ^a	NH ₂ ^b	H2
G1·C24			8.21	6.59	
C2·G23		12.82	8.45	6.56	
A3·T22	13.63				7.76
T4·A21	13.64				7.82
C5·G20		12.83	8.58	7.10	
G6·C19		12.91	8.58	7.33	
Ax					7.67
G7·C18		12.63	7.83	6.53	
C8·G17		12.74	8.12	6.54	
T9·A16	13.85				7.51
A10·T15	13.66				7.59
C11·G14		12.87	8.38	6.82	
G12·C13			8.13	7.06	

^aHydrogen-bonded cytosine amino protons.

^bExposed cytosine amino protons.

Table S-IV
Chemical Shift Assignments for the A1-bulge
Duplex in D₂O Buffer at 25 °C

<u>Chemical Shifts, (ppm)</u>								
<u>Base</u>	<u>H8/H6</u>	<u>H5/CH₃</u>	<u>H2</u>	<u>H1'</u>	<u>H2'</u>	<u>H2'</u>	<u>H3'</u>	<u>H4'</u>
G1	7.95			5.97	2.61	2.79	4.85	4.24
C2	7.49	5.44		5.68	2.19	2.50	4.90	4.22
A3	8.37		7.73	6.32	2.75	2.98	5.06	4.46
T4	7.20	1.44		5.92	2.02	2.42	4.85	4.15
C5	7.40	5.66		5.60	1.83	2.21		4.04
G6	7.85			5.59	2.34	2.38	4.95	4.17
Ax	7.93		7.62	5.75	2.51	2.61	4.90	4.27
G7	7.77			5.71	2.60	2.60	4.91	4.33
C8	7.34	5.24		5.84	1.99	2.43	4.67	4.18
T9	7.40	1.62		5.62	2.14	2.44	4.86	4.14
A10	8.31		7.55	6.20	2.72	2.85	5.03	4.42
C11	7.28	5.37		5.64	1.84	2.27		4.15
G12	7.88			6.12	2.56	2.34	4.64	4.15
C13	7.63	5.90		5.76	2.02	2.42	4.70	4.07
G14	7.97			5.98	2.67	2.77	4.97	4.36
T15	7.26	1.49		5.58	2.08	2.38	4.86	4.17
A16	8.16		7.42	6.05	2.70	2.87	5.05	4.40
G17	7.64			5.64	2.48	2.57	4.96	4.34
C18	7.28	5.33		6.04	1.63	2.11	4.66	4.20
C19	7.63	5.91		5.37	2.20	2.37	4.84	4.10

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G20	7.90			5.52	2.70	2.79	4.99	4.28
A21	8.21		7.74	6.22	2.62	2.91	5.00	4.42
T22	7.05	1.39		5.72	1.92	2.33	4.83	4.11
G23	7.84			5.91	2.57	2.68	4.95	4.34
C24	7.43	5.38		6.17	2.18	2.18	4.48	4.05

SUPPLEMENTARY FIGURE CAPTIONS

Figure S1: Expanded contour plot of the base to H1' region of the NOESY experiment (250 ms mixing time) on the control duplex in D₂O buffer at 25 °C. Sequential distance connectivities are traced out for the two strands separately in panels A and B. Intra-residue base to H1' cross peaks are labeled by residue. Asterices indicate the H6-H5 cross peak for cytosine residues.

Figure S2: Expanded contour plot of the base to H1' region of the NOESY experiment (250 ms mixing time) on the A1-bulge duplex in D₂O buffer at 25 °C. Sequential distance connectivities are traced out for the bulge-containing strand (panel A) and partner strand (panel B) separately. Intra-residue base to H1' cross peaks are labeled by residue. Asterices indicate the H6-H5 cross peak for cytosine residues.

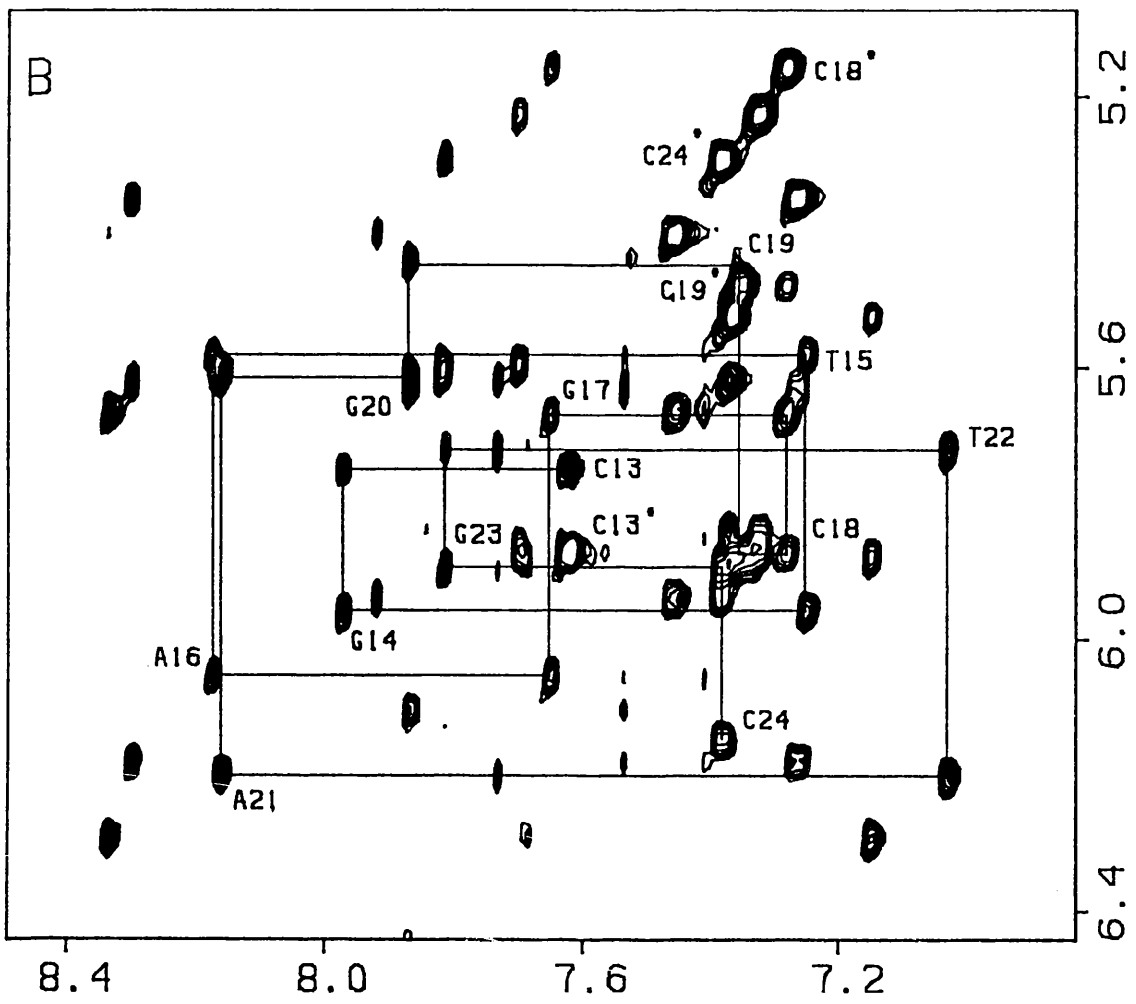
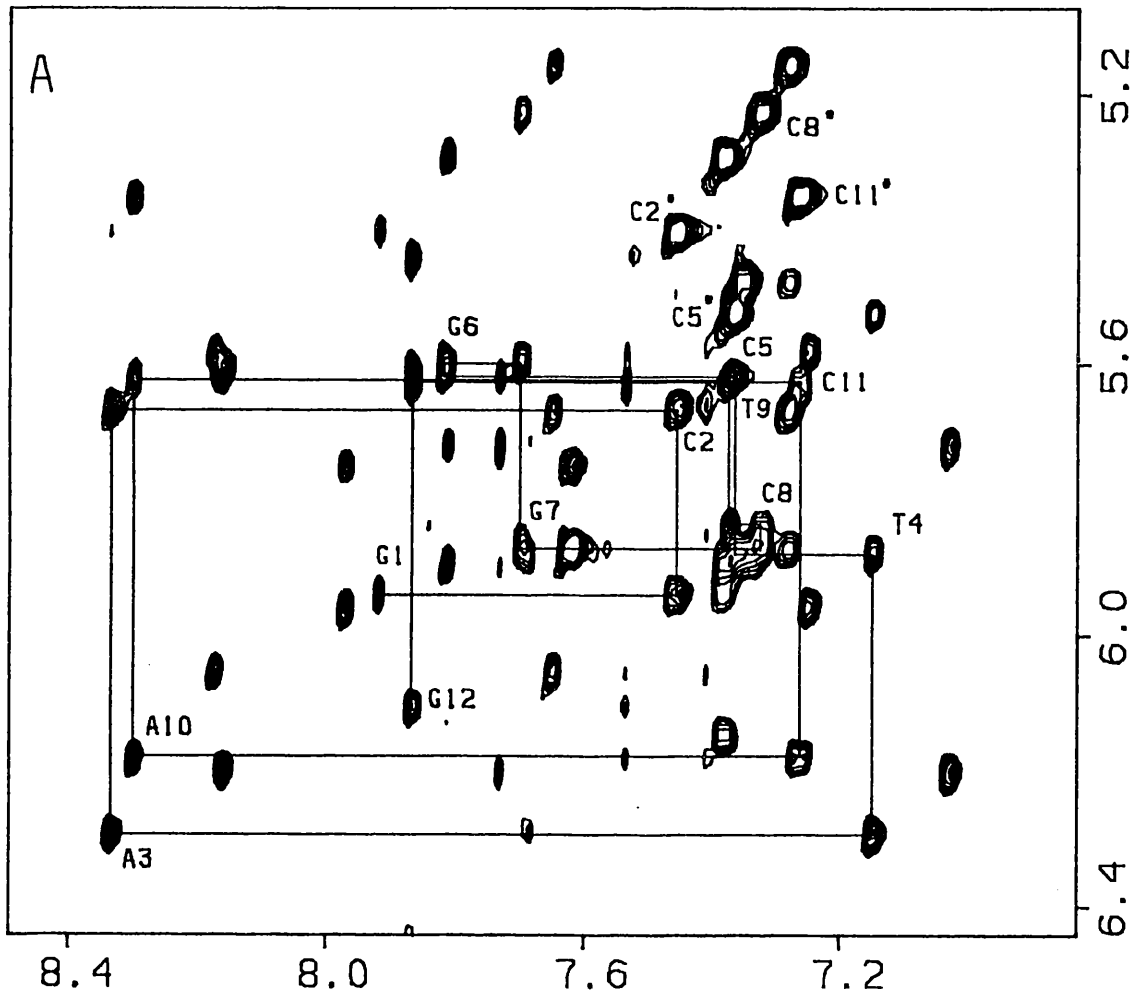


Figure S1

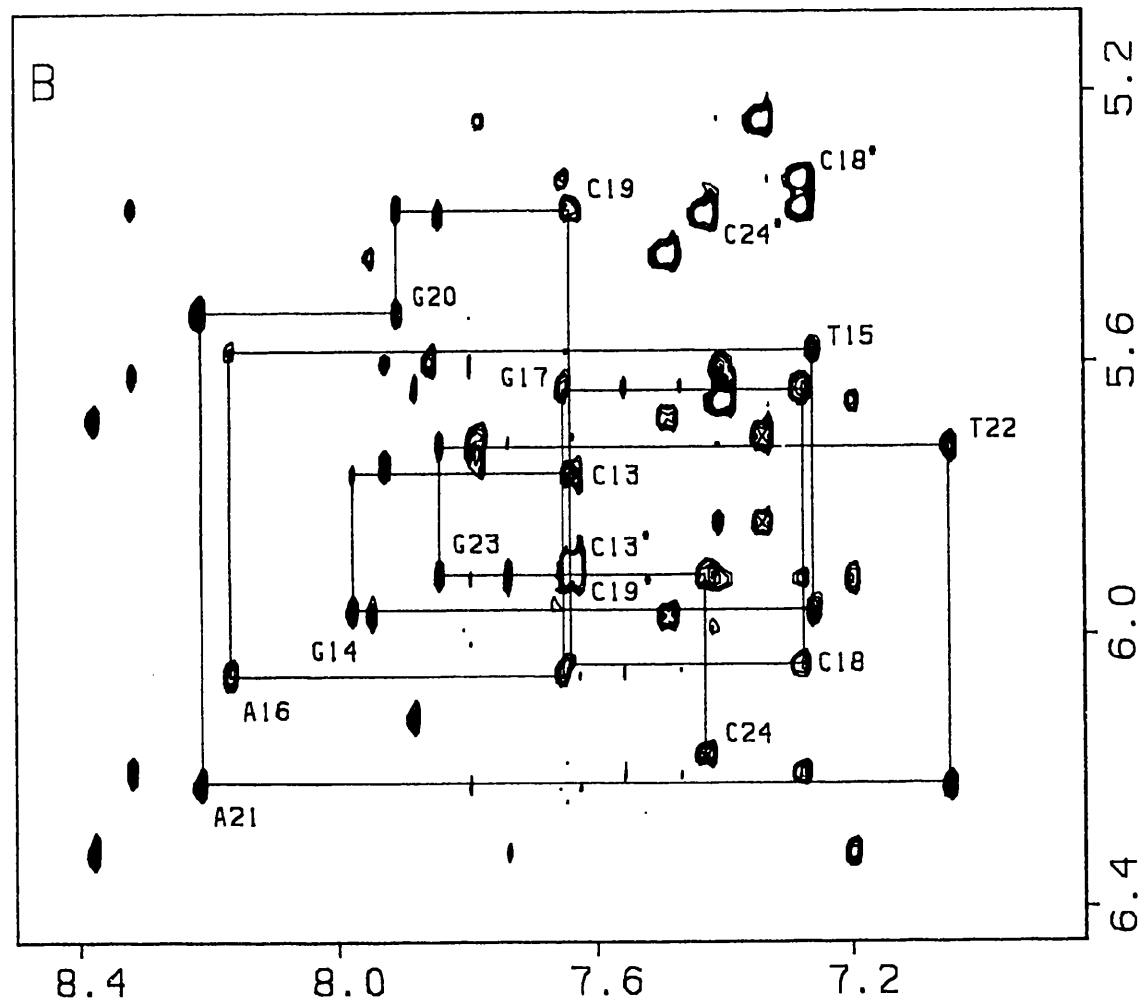
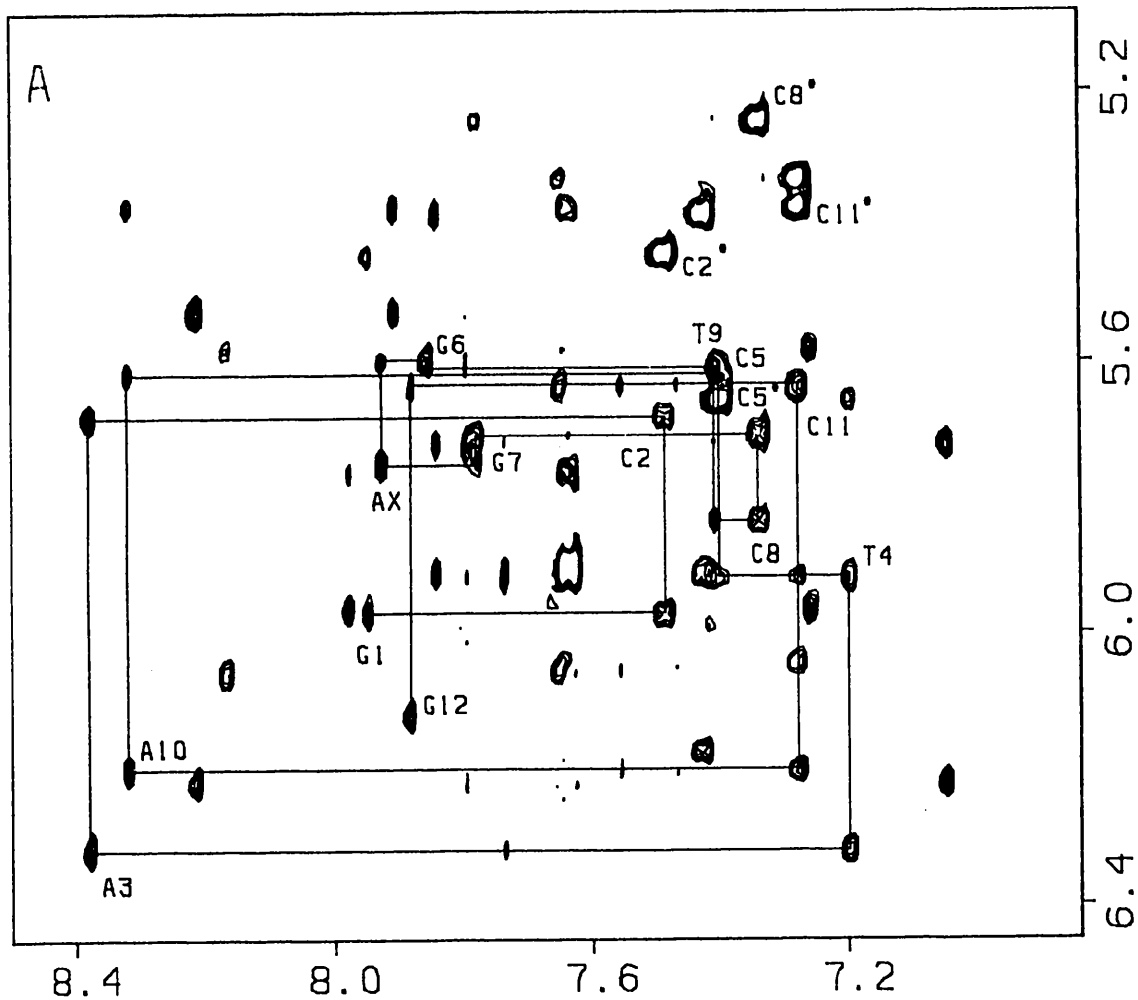


Figure S2