Supplementary Material :

Table s1. Chemical shift assignments of ligand protons in the complexes with d(CGTGTATATCAGG)·d(CCTGATATACACG).[a]

	G_2 complex (298K)		G_2 complex (318K)		β_2 complex		$(Py)_2$ complex	
	ligand 1	**ligand 2**	**ligand 1**	**ligand 2**	**ligand 1**	**ligand 2**	**ligand 1**	**ligand 2**
ImPyPy								
H4-1	7.09	6.89	7.02	6.80	7.40	7.12	7.16	6.79
H5-1	7.14	6.96	7.04	6.88	7.08	6.93	7.04	6.87
NCH3-1	3.96	3.96	3.90	3.90	3.98	4.00	3.98	3.99
NH-1	-	-	-	-	9.63	10.89	9.73	10.85
H3-2	6.75	6.48	6.68	6.43	6.16	6.29	5.84	5.88
H5-2	7.35	7.43	7.27	7.35	7.58	7.63	7.55	7.67
NCH3-2	3.75	3.79	3.68	3.72	3.95	3.89	3.92	3.86
NH-2	-	-			9.09	8.63	10.06	9.27
H3-3	-	-	6.16?	6.22	5.92	5.95	5.68	5.93
H5-3	-	-	6.87?	6.84	7.54	7.28		
NCH3-3	-	-	3.55?	3.82	3.80	3.77		
Linker								
NH-3	-	-	-	-	6.95	8.01	9.05	9.99
C21-H1 or Py-H3	-	-	-	-	1.97	2.33	6.06	5.59
C21-H2	-	-	-	-	2.41	2.53		
C22-H1	n.a.	n.a.	n.a.	n.a.	2.53	2.89		
C22-H2	n.a.	n.a.	n.a.	n.a.	3.48	3.45		
PyPyPy								
NH-4	-	-	-	-	6.95	8.01	10.14	9.06
H3-1	6.38	5.75	6.28	5.64	6.14	5.90	5.87	6.17
H5-1	-	-	6.84?	7.16	7.50	7.38		
NCH3-1	-	-	3.82?	3.84	3.81	3.77	9.33	10.48
NH-5	-	-			9.29	10.94	6.37	6.30
H3-2	6.13	6.21	6.04	6.07	6.24	6.43		
H5-2	7.58	7.58	7.49	7.50	7.33	7.38		
NCH3-2	3.85	3.90	3.80	3.84	3.75	3.75	9.14	9.22
NH-6					9.04	9.20	6.34	6.41
H3-3	6.2	6.35	6.15	6.27	6.19	6.32		7.00
H5-3	7.22	7.19	7.14	7.12	7.16	7.12		
NCH3-3	3.71	3.69	3.65	3.63	3.71	3.67		
Tail [b]								
NH-7	-	-	-	-	8.73	9.05	8.88	9.30
C18-H1	2.97	2.99	2.91	3.05	2.91	2.66	2.99	3.08
C18-H2	3.46	3.54	3.40	3.47	3.35	3.40	3.44	3.45
C19-H1	1.63	1.64	1.59	1.61	1.52	1.56	1.52	1.63
C19-H2	1.74	1.82	1.69	1.80	1.69	1.79	1.68	1.75
C20-H1	2.80	2.85	2.34	2.78	2.74	2.80	2.31	2.75
C20-H2	-	-	2.92	2.94	2.80	2.81	2.31	2.75
$N(CH_3)_2$	2.74/2.80	2.80/2.85	2.71/2.75	2.79/2.81	2.75/2.80	2.80/2.85	2.90/2.86	2.80/2.84

[a]Chemical shifts are given in ppm (0.01 ppm) with the residual HDO signal referenced to 4.80 ppm (25 °C). n. a. = not applicable. [b]Not stereospecifically assigned. A ? following the value indicated assignment is probable but not certain.

Table s2. Ligand-DNA and inter-ligand NOE contacts for the G_2 complex with d(CGTGTATATCAGG)·d(CCTGATATACACG)[a,b] at 25 °C.

DNA to Lig.

Ligand 1	DNA Strand 1	DNA Strand 2	Ligand 2
		A24 H1'	2H3-6
		A24 H2	2C18-H1/2 2C19-H1/2 2C20-H1/2
1H4-1	G4 H1'		
		C23 H1'	2H3-5
1H3-2		A22 H2	2H3-5
1H3-2	A6 H1'		
1H3-4		A8 H2	
		T19 H1'	2H3-2
1H3-4	T9 H1'		
1H3-5		A18 H2	2H3-2
1H3-5	C10 H1'		
1H3-6	A11 H1'		
1C18-H1/2 1C19-H1/2 1C20-H1/2		A11 H2	

Interligand

Ligand 1	Ligand 2
1H4-1 1H5-1	2C19-H1/2 2C20-H1/2 1N(CH_3)$_2$
1H3-2	2H3-5
1C19-H1/2	2H4-1
1C19-H1/2 1C20-H1/2 1N(CH_3)$_2$	2H4-1 2H5-1

[a] Identified in the D_2O NOESY acquired at 25 °C with 200 msec mixing time. [b] C18, C19 and C20 protons not stereospecifically assigned.

Table s3. Ligand-DNA and inter-ligand NOE contacts for the G_2 complex with d(CGTGTATATCAGG)·d(CCTGATATACACG)[a,b] at 45 °C.

DNA to Lig.

Ligand 1	DNA Strand 1	DNA Strand 2	Ligand 2
	T3 H1'		2N(CH_3)2
	T3 H4'		
		A24 H1'	2NH-7 2H3-6
1C18-H2 1C19-H1/2 1C20-H1		A24 H2	
1N(CH_3)2			
		A24 H4'	2H5-6
1H4-1	G4 H1'		
1NH-1		G4 NH1	2NH-7 2H3-6
1NH-1		G4 NH2	2H3-6
		C23 H1'	2NH-6 2H3-5
		C23 H4'	2H3-5 2H5-5
1H4-1 1NH-1	T5 H1'		
1H5-1	T5 H4'		
		A22 H1'	2NH-5 2H3-4
1NH-1 1H3-2 1NH-2		A22 H2	2H3-4 2NH-5 2H3-5
		A22 H4'	2H3-4
1NH-2 1H3-2	A6 H1'		
1NH-2 1H3-3		A6 H2	2H3-4
1H3-2 1H5-2	A6 H4'		
1H3-3	T7 H1'		
		A20 H1'	2H3-3
		A8 H2	2H3-3
		T19 H1'	2NH-2 2H3-2
		T19 H4'	2H5-2 2H3-2
1NH-5 1H3-4	T9 H1'		
1H3-4	T9 H4'		
		A18 H1'	2NH-1
1H3-4 1H3-5		A18 H2	2NH-1 2H3-2 2NH-2
1NH-6 1H3-5	C10 H1'		
1H5-5 1H3-5	C10 H4'		
		G17 H1'	2H4-1
1NH-7		G17 NH_2[c]	
1NH-7 1H3-6	A11 H1'		
		A11 H2	2C18-H2 2C19-H1/2 2C20-H2
			1N(CH_3)2
1H5-6 1H3-6	A11 H4'		
1N(CH_3)2		T16 H1'	
		T16 H4'	

Interligand

Ligand 1	Ligand 2
1H5-1	2C18 H1
1H4-1	2C18-H1/2 2C19-H1/2 2C20-H1/2 1N(CH_3)$_2$
1H3-2	2H3-4 2H3-5
1H3-5	2H3-2
1C19-H1/2	2H4-1
1C18-H1/2 1C20-H1/2 1N(CH_3)$_2$	2H4-1 2H5-1

[a] Identified in the NOESY acquired at 45 °C with 200 msec mixing time. [b] C18, C19 and C20 protons not stereospecifically assigned. [c] Not resolved.

Table s4. Chemical shift assignments of the d(CGTGTATATCAGG)·d(CCTGATATACACG) duplex, free and in the G_2 complex at 25 °C.[a]

	H6/H8			H1'			H2'/H2"		
	Free duplex	G_2 complex	Δδ	Free duplex	G_2 complex	Δδ	Free duplex	G_2 complex	Δδ
Strand 1									
C1	7.68	7.68	0.00	5.82	5.83	0.01	2.04/2.46	2.06/2.50	0.02/0.04
G2	8.00	8.07	0.07	6.03	6.08	0.05	2.70/2.83	2.74/2.87	0.04/0.04
T3	7.22	7.40	0.18	5.86	5.62	-0.24	2.53/2.18	2.39/2.58	0.21/0.05
G4	7.85	7.98	0.13	5.97	6.16	0.19	2.62/2.78	2.66/2.80	0.04/0.02
T5	7.22	6.99	-0.23	5.75	5.11	-0.64	2.14/2.52	1.42/2.04	-0.72/-0.48
A6	8.28	8.38	0.10	6.23	5.64	-0.59	2.65/2.93	2.23/2.72	-0.42/-0.21
T7	7.16	7.04	-0.12	5.68	-	-	2.13/2.51	1.93/2.24	-0.20/-0.27
A8	8.21	8.28	0.07	6.21	5.97	-0.24	2.61/2.92	2.06/2.17	-0.55/-0.75
T9	7.16	7.18	0.02	5.91	5.63	-0.28	2.01/2.42	2.26/2.26	0.25/-0.16
C10	7.49	7.10	-0.39	5.42	5.39	-0.03	1.97/2.28	1.50/2.29	-0.47/0.01
A11	8.18	8.17	-0.01	5.88	5.24	-0.64	2.65/2.81	2.29/2.29	-0.36/-0.52
G12	7.68	7.66	-0.02	5.61	5.41	-0.20	2.65/2.53	2.52/2.57	-0.01/-0.08
G13	7.73	7.78	0.05	6.13	6.17	0.04	2.36/2.45	2.35/2.51	-0.01/0.06
Strand 2									
C14	7.82	7.82	0.00	6.04	6.06	0.02	2.21/2.58	2.24/2.60	0.03/0.02
C15	7.67	7.71	0.04	6.05	6.15	0.10	2.15/2.49	2.15/2.57	0.00/0.08
T16	7.33	7.55	0.22	5.68	5.38	-0.30	2.08/2.41	2.40/2.40	0.32/-0.01
G17	7.92	7.94	0.02	5.63	5.28	-0.35	2.73/2.80	2.70/2.78	-0.03/-0.02
A18	8.18	8.07	-0.11	6.22	5.55	-0.67	2.61/2.92	2.08/2.67	-0.53/-0.25
T19	7.12	6.83	-0.29	5.67	5.26	-0.41	2.08/2.49	1.40/2.12	-0.68/-0.37
A20	8.20	8.30	0.10	6.20	5.68	-0.52	2.60/2.90	2.06/2.18	-0.54/-0.72
T21	7.14	7.42	0.28	5.67	5.28	-0.39	2.02/2.42	2.25/2.29	0.23/-0.13
A22	8.20	8.06	-0.14	6.15	5.69	-0.46	2.65/2.84	2.28/2.72	-0.37/-0.12
C23	7.29	6.86	-0.43	5.49	5.25	-0.24	1.97/2.33	1.37/2.22	-0.60/-0.11
A24	8.22	8.20	-0.02	6.17	5.39	-0.78	2.65/2.84	2.31/2.45	-0.34/-0.39
C25	7.28	7.17	-0.11	5.68	5.46	-0.22	1.88/2.29	1.89/2.16	0.01/-0.13
G26	7.90	7.89	-0.01	6.15	6.16	0.01	2.36/2.59	2.37/2.61	0.01/0.02

[a]Chemical shifts are given in ppm (0.01 ppm) with the residual HDO signal referenced to 4.80 ppm (25 °C)

Table s5. Chemical shift assignments of the d(CGTGTATATCAGG)·d(CCTGATATACACG) duplex in the G_2 complex at 45 °C.[a]

	H6/H8	H1'	H2'/H2"
	G_2 complex	G_2 complex	G_2 complex
Strand 1			
C1	7.60	5.81	1.96/2.41
G2	7.96	6.02	2.66/2.82
T3	7.30	5.58	2.32/2.49
G4	7.90	6.09	2.59/2.72
T5	6.90	5.05	1.35/1.96
A6	8.22	5.59	2.17/2.64
T7	6.92	4.80	1.54/1.83
A8	8.20	5.91	2.49/2.72
T9	7.09	5.56	1.67/2.27
C10	7.01	5.33	1.43/2.21
A11	8.07	5.19	2.25/2.25
G12	7.54	5.40	2.43/2.50
G13	7.69	6.09	2.32/2.46
Strand 2			
C14	7.72	6.00	2.17/2.57
C15	7.63	6.07	2.10/2.52
T16	7.45	5.35	2.33/2.33
G17	7.85	5.26	2.64/2.73
A18	7.99	5.47	2.05/2.61
T19	6.74	5.22	1.34/1.99
A20	8.19	5.45	1.98/2.17
T21	7.32	5.27	2.21/2.21
A22	7.99	5.65	2.22/2.64
C23	6.77	5.19	1.31/2.17
A24	8.09	5.40	2.22/2.40
C25	7.07	5.45	1.82/2.11
G26	7.80	6.09	2.33/2.53

[a]Chemical shifts are given in ppm (0.01 ppm) with the residual HDO signal referenced to 4.52 ppm (45 °C)

Table s6. Chemical shift assignments of the d(CGTGTATATCAGG)·d(CCTGATATACACG) duplex, free and in the β_2 complex.[a]

	H6/H8			H1'			H2'/H2"		
	Free duplex	β_2 complex	$\Delta\delta$	Free duplex	β_2 complex	$\Delta\delta$	Free duplex	β_2 complex	$\Delta\delta$
Strand 1									
C1	7.68	7.67	-0.01	5.82	5.83	0.01	2.04/2.46	2.04/2.47	0.00/0.01
G2	8.00	8.07	0.07	6.03	6.07	0.04	2.70/2.83	2.73/2.84	0.03/0.01
T3	7.22	7.42	0.20	5.86	5.54	-0.32	2.53/2.18	2.39/2.51	0.21/-0.02
G4	7.85	7.97	0.12	5.97	6.03	0.06	2.62/2.78	2.58/2.69	-0.04/-0.09
T5	7.22	6.99	-0.23	5.75	5.24	-0.51	2.14/2.52	1.54/2.01	-0.60/-0.51
A6	8.28	8.36	0.08	6.23	5.69	-0.54	2.65/2.93	2.31/2.72	-0.34/-0.21
T7	7.16	6.89	-0.27	5.68	5.05	-0.63	2.13/2.51	1.54/1.89	-0.59/-0.62
A8	8.21	8.37	0.16	6.21	5.92	-0.29	2.61/2.92	2.69/2.71	0.08/-0.21
T9	7.16	7.08	-0.08	5.91	5.48	-0.43	2.01/2.42	1.62/2.23	-0.39/-0.19
C10	7.49	7.07	-0.42	5.42	5.43	0.01	1.97/2.28	1.49/2.26	-0.48/-0.02
A11	8.18	8.19	0.01	5.88	5.21	-0.67	2.65/2.81	2.27/2.29	-0.38/-0.52
G12	7.68	7.65	-0.03	5.61	5.42	-0.19	2.65/2.53	2.56/2.58	0.03/-0.07
G13	7.73	7.78	0.05	6.13	6.16	0.03	2.36/2.45	2.36/2.51	0.00/0.06
Strand 2									
C14	7.82	7.81	-0.01	6.04	6.05	0.01	2.21/2.58	2.22/2.60	0.01/0.43
C15	7.67	7.70	0.03	6.05	6.13	0.08	2.15/2.49	2.15/2.55	0.00/0.06
T16	7.33	7.55	0.22	5.68	5.29	-0.39	2.08/2.41	2.36/2.40	0.28/-0.01
G17	7.92	7.98	0.06	5.63	5.27	-0.36	2.73/2.80	2.75/2.80	0.02/0.00
A18	8.18	8.14	-0.04	6.22	5.71	-0.51	2.61/2.92	2.23/2.73	-0.38/-0.19
T19	7.12	6.88	-0.24	5.67	5.25	-0.42	2.08/2.49	1.54/1.89	-0.54/-0.60
A20	8.20	8.36	0.16	6.20	5.58	-0.62	2.60/2.90	2.36/2.51	-0.24/-0.39
T21	7.14	7.34	0.20	5.67	5.35	-0.32	2.02/2.42	2.22/2.33	0.20/-0.09
A22	8.20	8.06	-0.14	6.15	5.55	-0.60	2.65/2.84	2.17/2.66	-0.48/-0.18
C23	7.29	6.87	-0.42	5.49	5.34	-0.15	1.97/2.33	1.38/2.21	-0.59/-0.12
A24	8.22	8.19	-0.03	6.17	5.43	-0.74	2.65/2.84	2.24/2.37	-0.41/-0.47
C25	7.28	7.18	-0.10	5.68	5.38	-0.30	1.88/2.29	1.91/2.14	0.03/-0.15
G26	7.90	7.90	0.00	6.15	6.17	0.02	2.36/2.59	2.37/2.61	0.01/0.02

[a]Chemical shifts are given in ppm (0.01 ppm) with the residual HDO signal referenced to 4.80 ppm (25 °C)

Table s7. Listings of all restraints used to derive the molecular model of the β_2 complex with d(CGTGTATATCAGG)·d(CCTGATATACACG) and achieved distances.[a]

Ligand to DNA restraints: Force constant: 25 kcal/mole*Å^2

Atom1		Atom2				
InsightII	Atom	InsightII	Atom	Lower	Upper	Dist
1:DIA_48:H1	1H4-1	1:G_4:H1'	G4-H1'	2.50	3.70	2.85
1:DIB_49:H3	1NH-1	1:T_5:H1'	T5-H1'	2.50	3.70	3.22
1:DIB_49:H3	1NH-1	1:G_4:H21	G4-H21	3.70	5.00	3.63
1:DIC_50:H7	1H3-2	1:A_9B:H2	A22-H2	2.50	3.70	3.26
1:DIC_50:H8	1H5-2	1:A_6:H4'	A6-H4'	2.50	3.70	3.26
1:DID_51:H5	1NH-2	1:A_6:H1'	A6-H1'	2.50	3.70	2.63
1:DID_51:H5	1NH-2	1:A_6:H2	A6-H2	3.70	5.00	3.95
1:DIE_52:H13	1H3-3	1:T_7:H1'	T7-H1'	2.50	3.70	2.87
1:DIE_52:H14	1H5-3	1:T_7:H4'	T7-H4'	2.50	3.70	3.50
1:DIE_52:H13	1H3-3	1:A_6:H2	A6-H2	2.50	3.70	2.83
1:DIJ_56:HN	1NH-4	1:A_8:H1'	A8-H1'	1.80	2.50	2.56
1:DIJ_56:HN	1NH-4	1:A_8:H2	A8-H2	2.50	3.70	2.92
1:DIK_57:H2	1H3-4	1:T_9:H1'	T9-H1'	2.50	3.70	2.45
1:DIK_57:H2	1H3-4	1:A_8:H2	A8-H2	2.50	3.70	2.58
1:DIL_58:H2	1NH-5	1:T_9:H1'	T9-H1'	2.50	3.70	2.46
1:DIL_58:H2	1NH-5	1:A_8:H2	A8-H2	3.70	5.00	3.89
1:DIM_59:H3	1H3-5	1:C_10:H1'	C10-H1'	2.50	3.70	3.71
1:DIM_59:H8	1H5-5	1:C_10:H4'	C10-H4'	2.50	3.70	3.72
1:DIN_60:H5	1NH-6	1:C_10:H1'	C10-H1'	2.50	3.70	2.64
1:DIN_60:H5	1NH-6	1:A_5B:H2	A18-H2	3.70	5.00	3.85
1:DIN_60:H5	1NH-6	1:G_4B:H21	G17-H21	2.50	3.70	3.74
1:DIO_61:H13	1H3-6	1:A_11:H1'	A11-H1'	2.50	3.70	3.43
1:DIP_62:H7	1NH-7	1:A_11:H2	A11-H2	2.50	3.70	3.26
1:DIP_62:H7	1NH-7	1:A_11:H1'	A11-H1'	2.50	3.70	2.83
1:DIA_48B:H1	2H4-1	1:G_4B:H1'	G17-H1'	2.50	3.70	2.43
1:DIB_49B:H3	2NH-1	1:A_5B:H1'	A18-H1'	2.50	3.70	3.18
1:DIB_49B:H3	2NH-1	1:A_5B:H2	A18-H2	2.50	3.70	2.71
1:DIB_49B:H3	2NH-1	1:G_4B:H21	G17-H21	2.50	3.70	3.11
1:DIC_50B:H7	2H3-2	1:T_6B:H1'	T19-H1'	2.50	3.70	2.51
1:DIC_50B:H7	2H3-2	1:A_5B:H2	A18-H2	1.80	2.50	2.50
1:DID_51B:H5	2NH-2	1:T_6B:H1'	T19-H1'	2.50	3.70	2.77
1:DIE_52B:H13	2H3-3	1:A_7B:H1'	A20-H1'	3.70	5.00	3.65
1:DIE_52B:H14	2H5-3	1:A_7B:H4'	A20-H4'	2.50	3.70	2.64
1:DIE_52B:H13	2H3-3	1:A_8:H2	A8-H2	2.50	3.70	2.96
1:DIF_53C:H7	2NH-3	1:A_7B:H1'	A20-H1'	2.50	3.70	3.39
1:DIK_57B:H2	2H3-4	1:A_9B:H2	A22-H2	2.50	3.70	3.65
1:DIK_57B:H2	2H3-4	1:A_6:H2	A6-H2	2.50	3.70	2.61
1:DIK_57B:H2	2H3-4	1:A_9B:H1'	A22-H1'	3.70	5.00	3.62
1:DIL_58B:H2	2NH-5	1:A_9B:H1'	A22-H1'	2.50	3.70	2.70
1:DIL_58B:H2	2NH-5	1:A_6:H2	A6-H2	2.50	3.70	3.69
1:DIL_58B:H2	2NH-5	1:A_9B:H2	A22-H2	2.50	3.70	2.86
1:DIM_59B:H3	2H3-5	1:C_10B:H1'	C23-H1'	2.50	3.70	2.49
1:DIM_59B:H3	2H3-5	1:A_9B:H2	A22-H2	1.80	2.50	2.51
1:DIN_60B:H5	2NH-6	1:A_9B:H2	A22-H2	3.70	5.00	3.87
1:DIN_60B:H5	2NH-6	1:G_4:H21	G4-H21	3.70	5.00	3.71
1:DIO_61B:H13	2H3-6	1:A_11B:H1'	A24-H1'	2.50	3.70	3.55
1:DIP_62B:H7	2NH-7	1:A_11B:H2	A24-H2	2.50	3.70	2.49

Ligand to ligand restraints: Force constant: 25 kcal/mole*Å2

1:DID_51:H5	1NH-2	1:DIE_52:H13	1H3-3	2.50	3.70	2.50
1:DIE_52:H13	1H3-3	1:DIF_53B:H7	1NH-3	1.80	3.70	2.31
1:DIJ_56:HN	1NH-4	1:DIK_57:H2	1H3-4	2.50	3.70	2.58
1:DIK_57:H2	1H3-4	1:DIL_58:H2	1NH-5	1.80	2.50	2.12
1:DIL_58:H2	1NH-5	1:DIM_59:H3	1H3-5	2.50	3.70	2.58
1:DIM_59:H3	1H3-5	1:DIN_60:H5	1NH-6	1.80	2.50	2.13
1:DIN_60:H5	1NH-6	1:DIO_61:H13	1H3-6	1.80	2.50	2.52
1:DIO_61:H13	1H3-6	1:DIP_62:H7	1NH-7	1.80	2.50	2.00
1:DIB_49B:H3	2NH-1	1:DIC_50B:H7	2H3-2	2.50	3.70	2.54
1:DIC_50B:H7	2H3-2	1:DID_51B:H5	2NH-2	1.80	2.50	2.01
1:DID_51B:H5	2NH-2	1:DIE_52B:H13	2H3-3	2.50	3.70	2.53
1:DIE_52B:H13	2H3-3	1:DIF_53C:H7	2NH-3	1.80	2.50	2.05
1:DIJ_56B:HN	1NH-4	1:DIK_57B:H2	2H3-4	2.50	3.70	2.57
1:DIK_57B:H2	2H3-4	1:DIL_58B:H2	2NH-5	1.80	2.50	2.17
1:DIL_58B:H2	2NH-5	1:DIM_59B:H3	2H3-5	2.50	3.70	2.59
1:DIM_59B:H3	2H3-5	1:DIN_60B:H5	2NH-6	1.80	2.50	2.13
1:DIN_60B:H5	2NH-6	1:DIO_61B:H13	2H3-6	2.50	3.70	2.56
1:DIO_61B:H13	2H3-6	1:DIP_62B:H7	2NH-7	1.80	2.50	2.04
1:DIP_62:H18*	1C18*	1:A_11:H2	A11-H2	3.50	5.00	3.58
1:DIP_62:H19*	1C19*	1:A_11:H2	A11-H2	2.20	4.20	2.83
1:DIP_62B:H18*	2C18*	1:A_11B:H2	A24-H2	3.50	5.00	3.41
1:DIP_62B:H19*	2C19*	1:A_11B:H2	A24-H2	2.20	4.20	3.87

Watson-Crick Base Pairs: Force constant: 200 kcal/mole*Å2

1:C_1:O2	C1-O2	1:G_13B:H22	G26-H22	1.65	2.05	1.88
1:C_1:N3	C1-N3	1:G_13B:H1	G26-H1	1.65	2.05	1.86
1:C_1:H42	C1-H42	1:G_13B:O6	G26-O6	1.65	2.05	1.83
1:G_2:H22	G2-H22	1:C_12B:O2	C25-O2	1.65	2.05	1.82
1:G_2:H1	G2-H1	1:C_12B:N3	C25-N3	1.65	2.05	1.83
1:G_2:O6	G2-O6	1:C_12B:H42	C25-H42	1.65	2.05	1.82
1:T_3:H3	T3-H3	1:A_11B:N1	A24-N1	1.65	2.05	1.83
1:T_3:O4	T3-O4	1:A_11B:H61	A24-H61	1.65	2.05	1.89
1:G_4:O6	G4-O6	1:C_10B:H42	C23-H42	1.65	2.05	1.84
1:G_4:H1	G4-H1	1:C_10B:N3	C23-N3	1.65	2.05	1.85
1:G_4:H22	G4-H22	1:C_10B:O2	C23-O2	1.65	2.05	1.82
1:T_5:H3	T5-H3	1:A_9B:N1	A22-N1	1.65	2.05	1.95
1:T_5:O4	T5-O4	1:A_9B:H61	A22-H61	1.65	2.05	1.81
1:A_6:H61	A6-H61	1:T_8B:O4	T21-O4	1.65	2.05	1.84
1:A_6:N1	A6-N1	1:T_8B:H3	T21-H3	1.65	2.05	1.83
1:T_7:H3	T7-H3	1:A_7B:N1	A20-N1	1.65	2.05	1.84
1:T_7:O4	T7-O4	1:A_7B:H61	A20-H61	1.65	2.05	1.85
1:A_8:N1	A8-N1	1:T_6B:H3	T19-H3	1.65	2.05	1.82
1:A_8:H61	A8-H61	1:T_6B:O4	T19-O4	1.65	2.05	1.83
1:T_9:H3	T9-H3	1:A_5B:N1	A18-N1	1.65	2.05	1.89
1:T_9:O4	T9-O4	1:A_5B:H61	A18-H61	1.65	2.05	1.81
1:C_10:O2	C10-O2	1:G_4B:H22	G17-H22	1.65	2.05	1.84
1:C_10:N3	C10-N3	1:G_4B:H1	G17-H1	1.65	2.05	1.84
1:C_10:H42	C10-H42	1:G_4B:O6	G17-O6	1.65	2.05	1.83
1:A_11:N1	A11-N1	1:T_3B:H3	T16-H3	1.65	2.05	1.80
1:A_11:H61	A11-H61	1:T_3B:O4	T16-O4	1.65	2.05	1.86
1:G_12:H22	G12-H22	1:C_2B:O2	C15-O2	1.65	2.05	1.84

1:G_12:H1	G12-H1	1:C_2B:N3	C15-N3	1.65	2.05	1.84
1:G_12:O6	G12-O6	1:C_2B:H42	C15-H42	1.65	2.05	1.82
1:G_13:H22	G13-H22	1:C_1E:O2	C14-O2	1.65	2.05	1.89
1:G_13:H1	G13-H1	1:C_1E:N3	C1-N3	1.65	2.05	1.87
1:G_13:O6	G13-O6	1:C_1E:H42	C1-H42	1.65	2.05	1.83

[a] Derived from H_2O NOESY data acquired at 100 msec mixing time. Restraints defined to pseudo-atoms (*).