

SUPPLEMENTARY MATERIAL

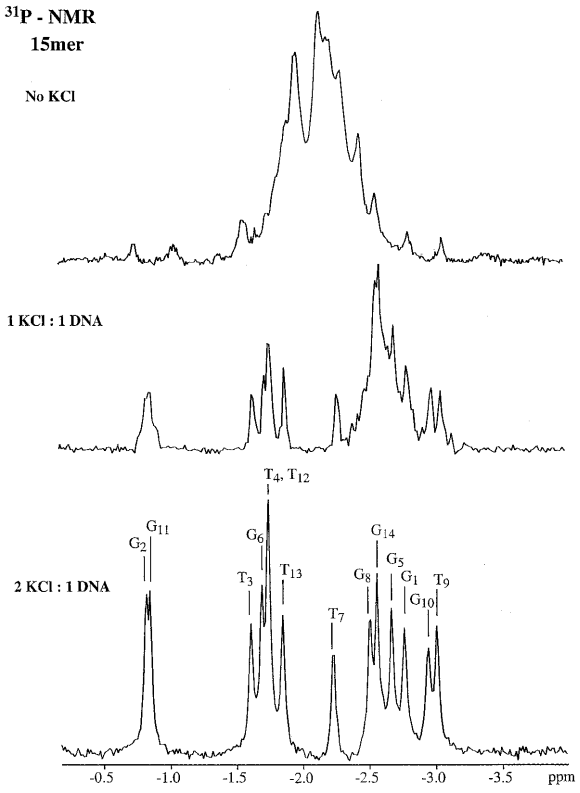

Figure S1. 161 MHz proton decoupled ^{31}P-NMR spectrum of d(GGTTGGTGTGGTTGG) at 0, 1 and 2 potassiums per DNA.

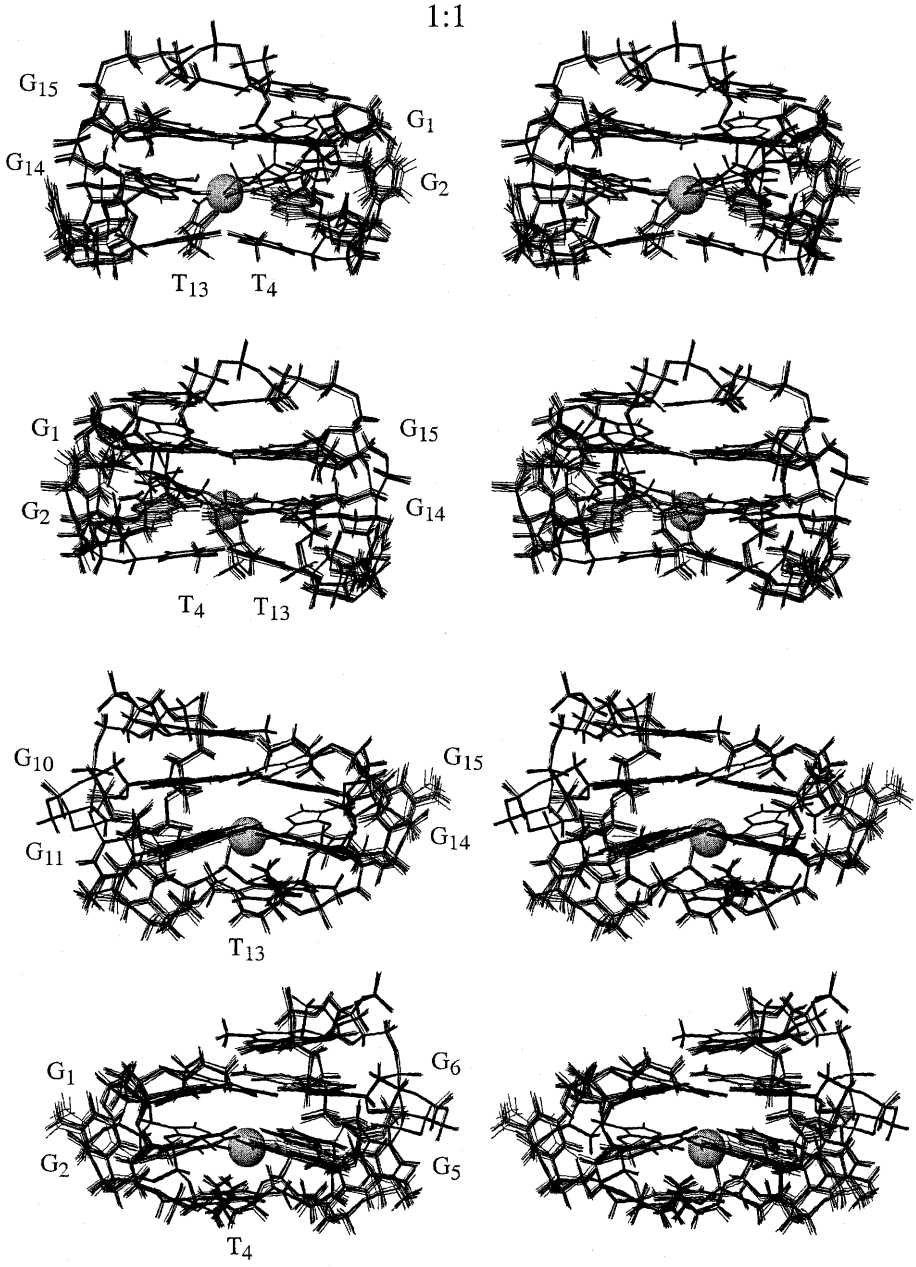

Figure S2. Ten structures from 80 to 100 ps extracted from the trajectory of the 2:1 potassium:DNA complex at 2 ps intervals. The structures are shown in stereo mode with the minimum energy potassium positions of the 100 ps structures presented in CPK format. The sphere depicting the potassium ions has a van der Waals radius of 1.96 Å.

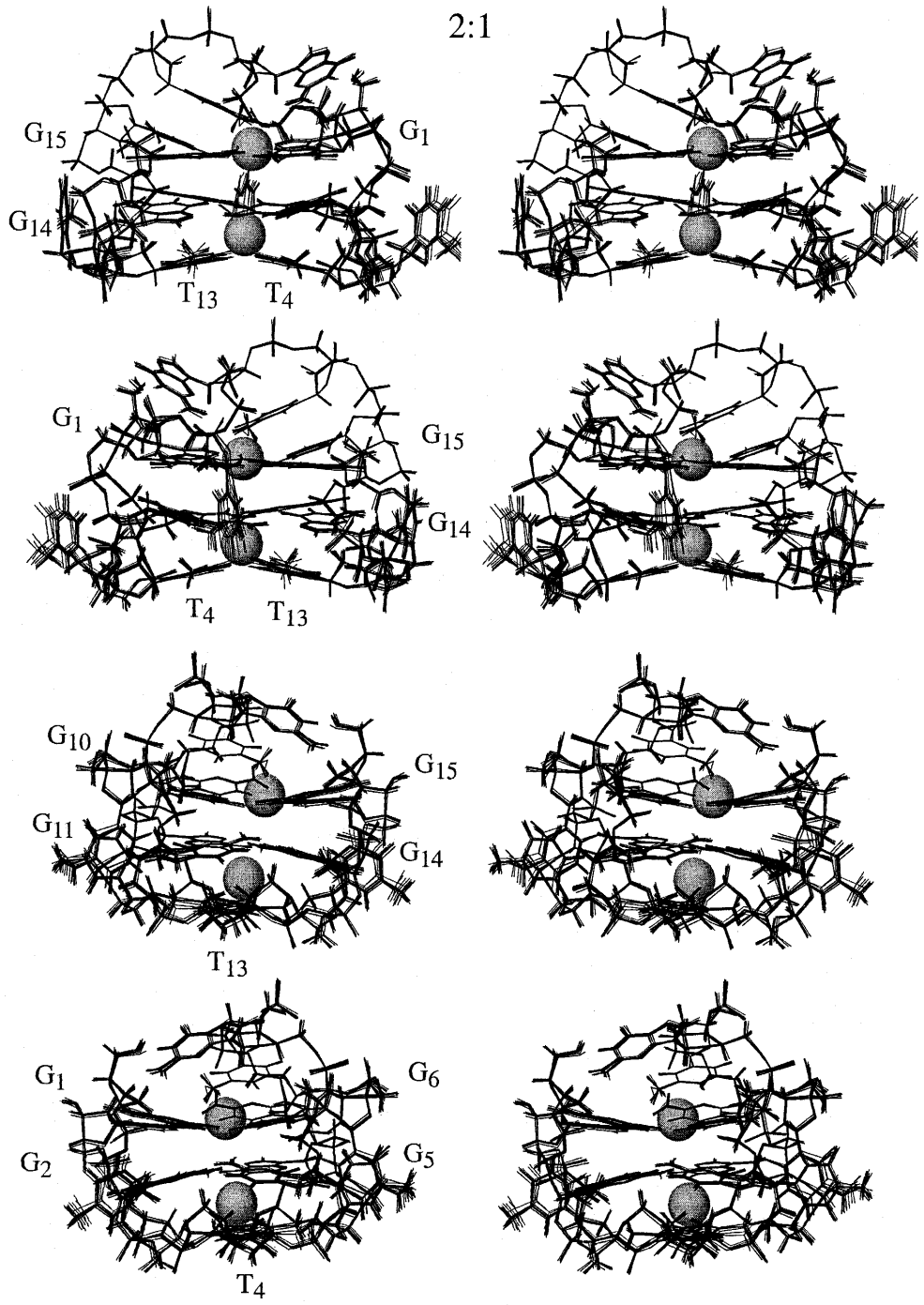

Figure S3. Ten structures from 80 to 100 ps extracted from the trajectory of the 1:1 potassium:DNA complex at 2 ps intervals. The structures are shown in stereo mode with the minimum energy potassium positions of the 100 ps structures presented in CPK format. The sphere depicting the potassium ions has a van der Waals radius of 1.96 Å.

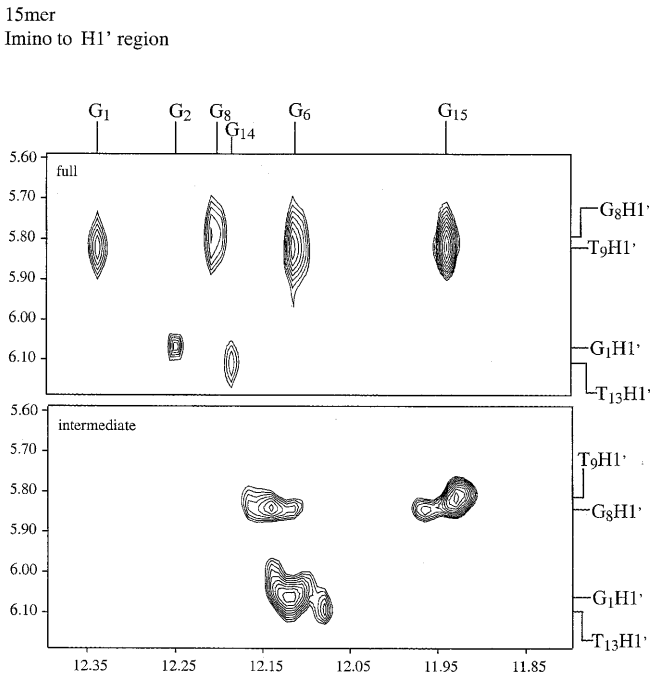

Figure S4. A portion of the 250 ms mixing time, 500 MHz NOESY spectra of the 15mer in H_2O is presented. The region contains some of the NOE crosspeaks of the imino protons of the residues 1, 6, 10 and 15. The spectrum obtained from the 2:1 sample is shown on top and the spectrum of the 1:1 sample at the bottom.

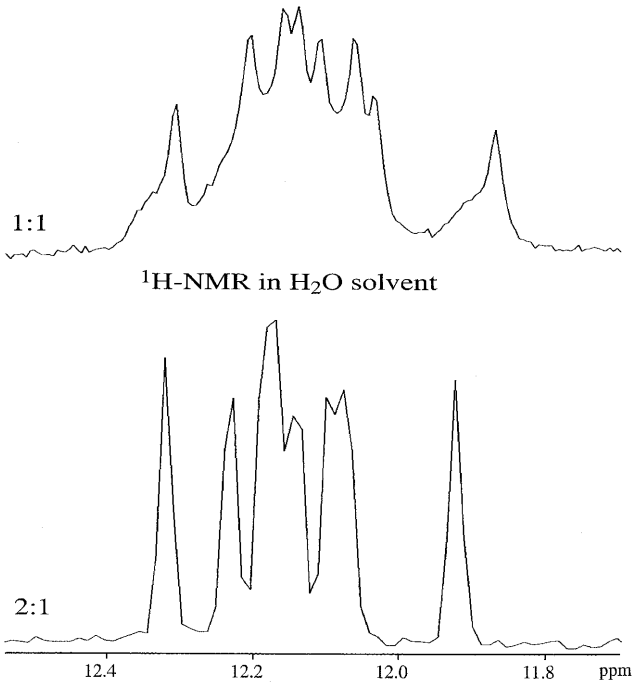

Figure S5. The ^{1}H-NMR spectrum in H_2O solvent, showing the imino region of the 1:1, top, and 2:1, bottom, potassium:DNA samples.

Table S1. The assignments of the saturated and intermediate forms of the 15mer are listed

1:1	H6/H8	H1′	H2′	H2″	H3′	H4′	H5′/H5″	CH_3
$\underline{G}_1$	7.44	5.99	3.21	3.21	5.24	4.64	4.27/	
G_2	8.22	5.96	3.26	2.44	5.25	4.52	4.31	
T_3	7.95	6.14	2.31	2.45	5.02			1.98
T_4	7.19	6.08	2.18	2.78	4.97	4.29	4.01	1.01
$\underline{G}_5$	7.46	6.10	3.68	3.11	4.89	4.42	4.24/4.30	
G_6	7.74	5.93	3.00	2.76	5.27	4.60	4.28	
T_7	7.98	6.53	2.77	2.66	4.91			2.01
G_8	7.50	5.74	1.99	2.76	5.21	4.33	3.96/4.05	
T_9	7.28	5.76	1.98	2.49	4.71	3.81	3.06/3.62	1.79
$\underline{G}_{10}$	7.47	5.97	3.81	3.11	4.94	4.31	4.17	
G_{11}	8.33	5.95	3.25	2.43	5.23	4.48	4.31	
T_{12}	7.95	6.14	2.31	2.45	4.76			2.02
T_{13}	7.27	6.14	2.11	2.87	5.04	4.26	3.96	1.05
$\underline{G}_{14}$	7.51	5.99	3.67	3.18	4.70	4.31	4.19	
G_{15}	8.12	6.13	2.79	2.56	4.91	4.76	4.08/4.10	

saturated	H6/H8	H1′	H2′	H2″	H3′	H4′	H5′/H5″	CH_3
$\underline{G}_1$	7.42	6.08	2.96	2.96	4.99	4.40	4.03/4.12	
G_2	8.20	6.03	3.04	2.34	5.15	4.41	4.23	
T_3	7.90	6.19	2.22	2.56	4.91	4.29	4.24/4.32	1.98
T_4	7.18	6.07	2.06	2.66	4.88	4.20	3.92	0.98
$\underline{G}_5$	7.43	6.04	3.38	2.91	4.87	4.41	4.23/4.28	
G_6	7.70	5.95	2.79	2.61	5.12	4.45	4.23	
T_7	7.93	6.49	2.51	2.61	4.86	4.43	4.24/4.28	1.98
G_8	7.47	5.77	1.98	2.32	4.77	3.98	4.01/4.10	
T_9	7.26	5.82	1.96	2.41	4.62	3.79	3.01/3.55	1.79
$\underline{G}_{10}$	7.45	6.06	3.72	2.93	4.92	4.28	4.14	
G_{11}	8.23	6.02	2.98	2.33	5.14	4.39	4.22	
T_{12}	7.90	6.19	2.20	2.58	4.91	4.29	4.24/4.32	1.98
T_{13}	7.25	6.11	2.08	2.72	4.90	4.22	3.92	1.03
$\underline{G}_{14}$	7.48	6.08	3.51	2.96	4.92	4.42	4.30/4.37	
G_{15}	8.09	6.16	2.69	2.44	4.80	4.25	4.12/4.18	

Table S2. The intraresidue and interesidue NOEs with the largest percentage difference between the saturated and intermediate forms of the 15mer are presented in this table

intraresidue

	H8/H6 – H1′		H8/H6 – H2′		H8/H6 – H2″		H8/H6 – H3′	
	full	inter	full	inter	full	inter	full	inter
T_3	93.3	61.6	106.8	140.9	85.2	45.1	37.5	26.8
T_7	107.6	112.0	489.1	501.8	419.1	434.6	34.2	41.6
G_8	92.0	57.7	317.9	209.8	306.6	202.3	127.2	86.0
T_9	93.9	66.9	375.0	247.5	102.7	68.8	31.0	22.5
$\underline{G}_{10}$	897.1	691.0	50.5	33.3	50.6	34.4	143.5	93.7
T_{12}	93.3	60.5	106.8	140.9	85.2	45.1	37.5	24.7

interesidue

	H8/H6 – H1′		H8/H6 – H2′		H8/H6 – H2″	
	Full	Inter	Full	Inter	Full	inter
T_7 to G_6	35.9	23.7	102.7	87.8	122.3	70.7
G_8 to G_6	27.7	38.8	94.6	121.2	181.0	219.4
G_8 to T_7					122.3	69.9
T_9 to G_8	83.2	94.9	182.6	190.5	92.6	111.1
G_{15} to G_9					79.9	52.7