

SUPPLEMENTARY MATERIAL

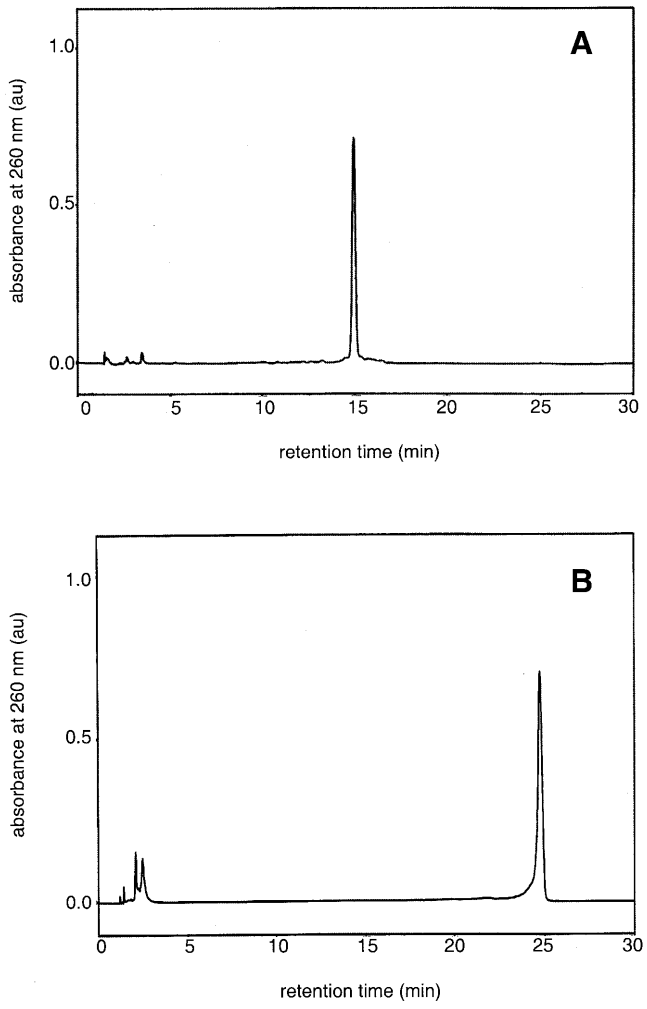

Figure S1. Anion exchange HPLC chromatograms for **4**. (**A**) Single-strand **4** eluted at 15 min. (**B**) Duplex **1** under the same elution conditions eluted at 25 min.

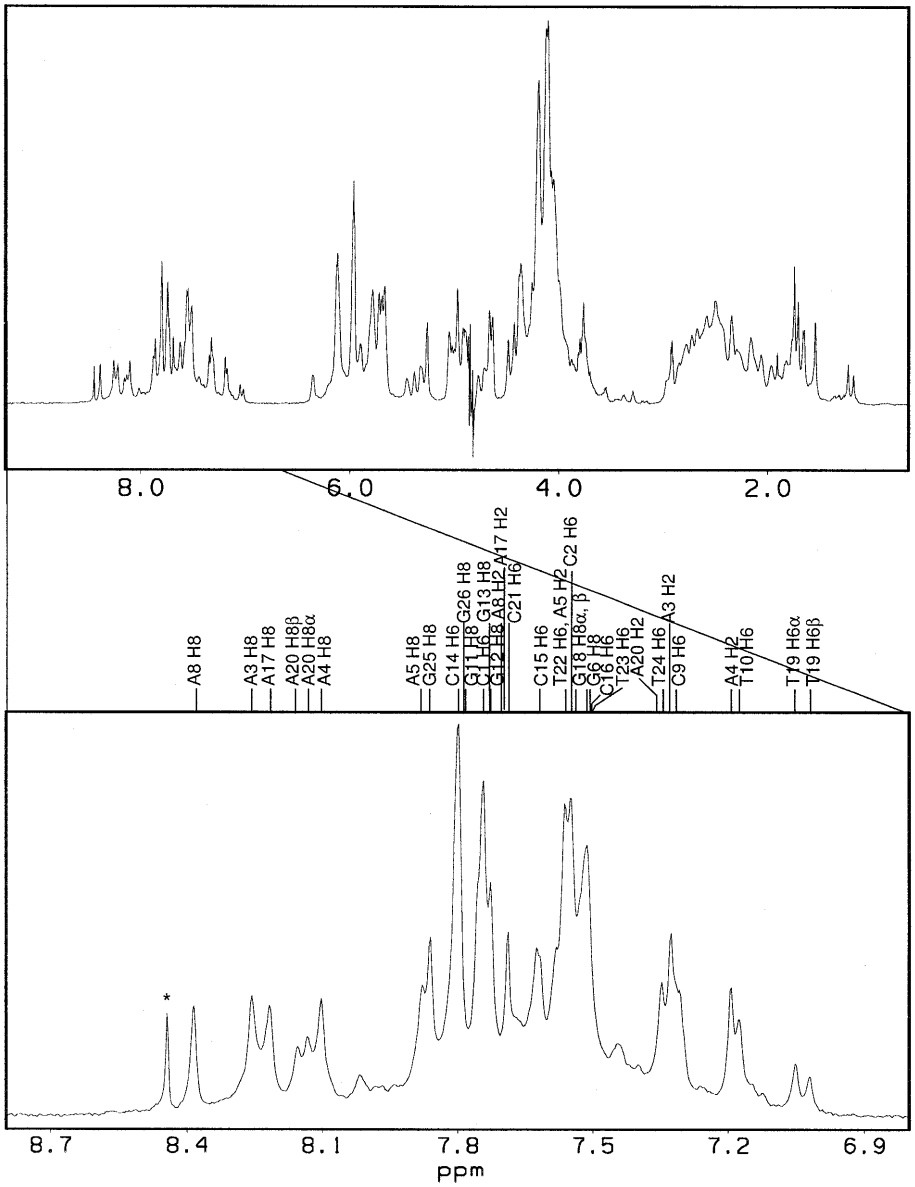

Figure S2. Proton NMR spectrum of the 2.5 mM sample of **1**. (Top) 1D NMR spectrum in D_2O at 750 MHz. (Bottom) Base proton region with chemical shift assignments. Both anomers are indicated where appropriate. The peak at 8.45 p.p.m. (*) is a minor non-nucleic acid contaminant which does not show any NOEs to **1**.

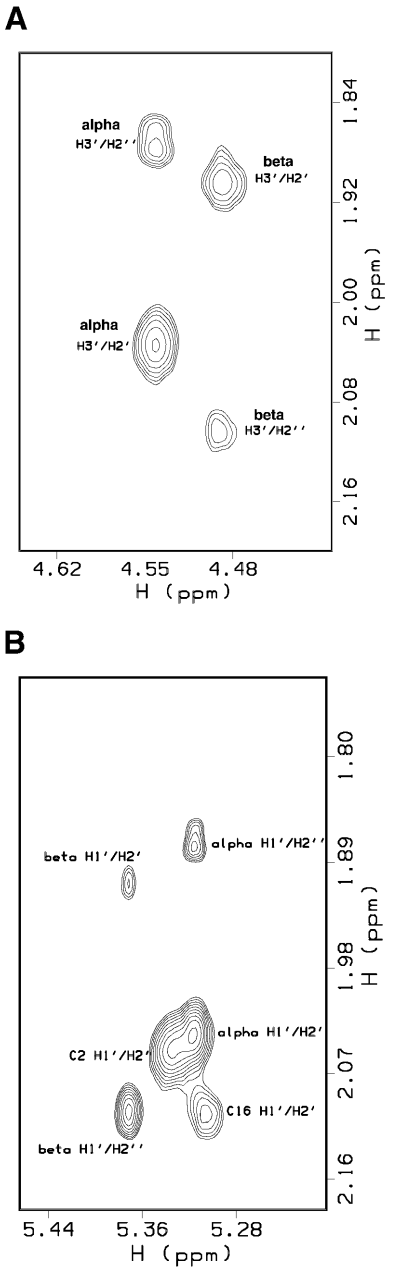

Figure S3. (**A**) H3′ to H2′/H2″ region for both anomers of the abasic site duplex. Since the H3′ to H2′ distance is shorter than the H3′ to H2″ distance for all sugar puckers, the H3′ to H2′ NOE is expected to be larger than the H3′ to H2″ NOE. (**B**) H1′ to H2′/H2″ region for both anomers of the abasic site. The H1′ to H2′ distance is shorter than the H1′ to H2″ distance for the α anomer, so the H1′ to H2′ NOE is expected to be larger than the H1′ to H2″ NOE. The opposite is true for the β anomer.

Table S1. ESI-MS results

	4	3	1
Theoretical mass	1290.85 (–3 ion)	1307.53 (–3 ion)	1559.23 (–5 ion)
Observed mass	1290.7 ± 0.3	1307.3 ± 0.3	1558.9 ± 0.3
Theoretical mass	967.89 (–4 ion)	980.40 (–4 ion)	
Observed mass	968.0 ± 0.3	980.6 ± 0.3	

Table S2. Chemical shift assignments in p.p.m. for the 2.5 mM sample of the abasic site duplex

Base	H1'	H2'	H2''	H3'	H4'	H8/H6	H2/H5/Me	NH imino	NH_2
C1	5.97	2.06	2.49	4.66	4.11	7.75	5.97		7.08 8.01
C2	5.31	2.05	2.31	4.82	4.07	7.55	5.72		6.97 8.74
A3	5.79	2.77	2.85	5.04	4.37	8.26	7.33		
A4	5.79	2.58	2.76	5.02	4.39	8.10	7.19		
A5	5.89	2.38	2.68	4.97	4.35	7.88	7.57		
G6 α	5.67	2.41	2.42	4.89	4.29	7.52		12.73	
β	5.67	2.41	2.42	4.92	4.29	7.55			
Abasic α	5.26	1.96	1.83	4.49	4.38				
β	5.33	1.87	2.06	4.42	4.05				
A8	6.35	2.81	2.96	5.00	4.48	8.39	7.70		
C9	5.81	1.90	2.45	4.72	4.22	7.31	5.26		6.73 8.07
T10	5.45	1.82	2.12	4.77	4.28	7.18	1.55	14.14	
G11	5.38	2.61	2.63	4.91	4.34	7.79		13.04	
G12	5.76	2.59	2.73	4.97	4.38	7.73		13.17	
G13	6.13	2.34	2.49	4.63	4.19	7.74			
C14	5.97	2.16	2.54	4.66	4.12	7.80	5.96		7.12 7.82
C15	5.98	2.16	2.43	4.85	4.18	7.62	5.67		6.87 8.51
C16	5.26	2.10	2.34	4.83	4.09	7.52	5.70		6.95 8.64
A17	6.10	2.80	2.92	5.05	4.43	8.22	7.71		
G18 α	5.79	2.41	2.57	4.87	4.36	7.55		12.66	
β	5.79	2.40	2.56	4.87	4.36	7.53		12.66	
T19 α	5.74	1.95	2.29	4.72	4.21	7.05	1.23	14.16	
β	5.73	1.94	2.26	4.70	4.21	7.02	1.18	14.16	
A20 α	6.10	2.52	2.68	4.92	4.35	8.14	7.37		
β	6.11	2.51	2.68	4.92	4.35	8.16	7.37		
C21 α	5.91	2.23	2.51	4.76	4.28	7.67	5.67		
β	5.91	2.22	2.51	4.76	4.26	7.67	5.67		
T22	6.11	2.25	2.62	4.89	4.26	7.57	1.66	14.08	
T23	6.10	2.14	2.57	4.89	4.19	7.51	1.71	14.12	
T24	5.68	1.97	2.29	4.86	4.09	7.35	1.74	14.14	
G25	5.65	2.67	2.71	4.97	4.35	7.86		13.00	
G26	6.13	2.34	2.52	4.63	4.20	7.80			

All chemical shifts are referenced to an internal standard, sodium 3-(trimethylsilyl)-1-propanesulfonate at 0.00 p.p.m.

Table S3. Coupling constants (in Hz) derived from a PECOSY experiment

	C1	**C2**	**A3**	**A4**	**A5**	**G6**	**AB**	**A8**	**C9**	**T10**	**G11**	**G12**	**G13**
$J_{H1'-H2'}$	8.2	8.9	8.1	7.8	8.0	9.2	2.6 (α)	8.0	8.0	8.0	8.4	8.8	7.8
$J_{H1'-H2''}$	5.9	4.7	3.7	3.9	4.6	6.4	3.4 (β) Nd (α) 3.0 (β)	5.0	5.0	5.8	5.1	5.3	5.9
	C14	**C15**	**C16**	**A17**	**G18**	**T19**	**A20**	**C21**	**T22**	**T23**	**T24**	**G25**	**G26**
$J_{H1'-H2'}$	7.5	9.0	9.0	Nd	7.8	8.9	7.8	Nd	7.8	Nd	8.8	9.8	7.8
$J_{H1'-H2''}$	6.0	6.0	4.1	5.8	4.9	5.4	4.1	4.5	4.2	5.6	5.8	5.2	6.5

Precision of coupling constants is ±0.5 Hz. Coupling constants except for the abasic site are consistent with the C2′ *endo* conformation. Nd, not determined.

Table S4. H3′-^{31}P coupling constants derived from a ^{31}P-HCOSY experiment (41,42)

	C1	**C2**	**A3**	**A4**	**A5**	**G6**	**AB**	**A8**	**C9**	**T10**	**G11**	**G12**
$J_{H3'-P}$ in Hz	6.8	7.6	9.3	7.6	6.8	6.8	8.8 (α) 8.3 (β)	7.8	8.6	8.0	8.1	8.1
	C14	**C15**	**C16**	**A17**	**G18**	**T19**	**A20**	**C21**	**T22**	**T23**	**T24**	**G25**
$J_{H3'-P}$ in Hz	8.0	6.8	8.0	9.8	Nd	8.5	6.4	8.0	7.8	8.8	7.8	8.0

All coupling constants were determined with an accuracy of ±0.5 Hz. Nd, not determined due to overlap.

Table S5. Summary of results of modeling runs

	α (10 structures)	β (20 structures)
Rms deviation to average structure for all atoms (Å)	0.51	0.78
Rms deviation to average structure for all residues except the ones at the ends and the abasic site (Å)	0.40	0.66
Average NOE violation (Å)	0.024	0.031
Average dihedral angle violation (degrees)	0.24	0.22
Number of NOE violations >0.5 Å	0	0
Number of dihedral angle violations >5°	0	0
Average distance between abasic H3' and neighboring A H8 (Å)	3.02	2.80
Average distance between abasic H2' and neighboring A H8 (Å)	4.71	4.03
Average distance between abasic H2" and neighboring A H8 (Å)	5.58	4.88
Average abasic dihedral H1'-C1'-C2'-H2' (degrees)	9.8	153.2
Average abasic dihedral H1'-C1'-C2'-H2" (degrees)	-108.0	33.9
Average abasic dihedral H2'-C2'-C3'-H3' (degrees)	8.06	-5.8
Average abasic dihedral H2"-C2'-C3'-H3' (degrees)	130.3	114.7
Average abasic dihedral H3'-C3'-C4'-H4' (degrees)	-145.4	-147.4
Average abasic dihedral nH3'-nC3'-nO3'-(n+1)P (degrees)	-9.8	-7.6