Supporting Information

for manuscript entitled

High Fidelity Base Pairing at the 3'-Terminus

by

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1. One-Dimensional NMR Spectra of (1)₂

a)

b)

Figure S1. a) ¹H NMR spectrum of (1)₂ in phosphate-buffered saline, D₂O at 5°C, and b) Overlay of ¹H spectra from 5 °C to 90 °C (protons of nucleobases and anomeric protons).

2. HPLC Trace and MALDI spectrum of compound 1

Figure S2. Analytical HPLC chromatogram (Figure **a**) and MALDI-TOF mass spectrum (Figure **b**) of NMR sample of oligonucleotide ACGCG-Uaq. The HPLC was performed with a RP-C18 column using a mobile-phase, mixture of 0.1 M triethylammonium acetate, pH 7 and acetonitrile. The solvent gradient used for the HPLC analysis was 0% to 19% of CH₃CN in 68 min. The mass spectrum was recorded in linear negative mode. Calculated mass of oligonucleotide ACGCG-Uaq (**1**) for [M-H]⁻ 2026.3, observed 2028.6 Da.

Figure S3. Low field region of ^1H -NMR spectrum of $(\text{ACGCG-Uaq})_2$ (**1**)₂ in phosphate-buffered D_2O at 600 MHz and 278 K. Resonances of individual protons from major and minor conformations (labels of the latter written in italics along with primes) are labeled.

3. Protocol for Molecular Dynamics Calculations

Structure Calculation Protocol

Starting with an extended structure of the oligonucleotide backbone, calculations included the following stages:

1. Restrained TAMD for 0.005 ps at 20,000 K in 4000 steps
Bond*5, angle*5, van der Waals*0.1
 $K_{\text{NOE}}=150 \text{ kcal/mol}\text{\AA}^2$, $K_{\text{cdih}}=5 \text{ kcal/mol rad}^2$
2. Restrained TAMD for 0.15 ps during which the system is cooled to 0 K in 1000 steps
Bond*5, angle*5 van der Waals*0.1
 $K_{\text{NOE}}=150 \text{ kcal/mol}\text{\AA}^2$, $K_{\text{cdih}}=5 \text{ kcal/mol rad}^2$
3. 35 ps restrained MD starting at 1000 K and cooling to 0 K (second cooling step)
Bond*5, angle*5 van der Waals*0.1
 $K_{\text{NOE}}=150 \text{ kcal/mol}\text{\AA}^2$, $K_{\text{cdih}}=200 \text{ kcal/mol rad}^2$
4. 400 cycles of energy minimization of 800 steps (final minimization)
 $K_{\text{NOE}}=50 \text{ kcal/mol}\text{\AA}^2$, $K_{\text{cdih}}=300 \text{ kcal/mol rad}^2$

TAMD = Torsion Angle Molecular Dynamics

4. Overlays of Experimental and Back-Calculated NOESY Spectra

Figure S4. Overlay of experimental (red) and back-calculated (blue) NOESY spectrum of (ACGCG-Uaq)₂ (**1**)₂. The experimental spectrum was acquired in phosphate-buffered D₂O with 250 ms mixing time at 278 K. The back-calculated spectrum was generated from the average structure of the 10 lowest energy structures in CORMA. Note that resonances between 3 and 4 ppm were not assigned and that back-calculated peaks for minor conformation are not included.

Figure S5. Portion of the overlay of experimental (red) and back-calculated (blue) NOESY spectrum of (ACGCG-Uaq)₂ (**1**)₂ with crosspeaks for the protons of the minor conformation included (labels marked with primes). The experimental spectrum was acquired in phosphate-buffered D₂O with 250 ms mixing time at 278 K.

Table S1. Torsion angles of a representative low-energy structure of (ACGCG-Uaq)₂, as determined using the computer program CURVES¹.

Residue / Angle

	Gamma	Delta	Epsilon	Zeta	Alpha	Beta	Chi
A1	156.59	94.34	166.22	-57.00	-132.61	-96.18	-149.47
C2	96.32	97.79	179.92	-104.21	-33.11	169.24	-109.14
G3	33.36	138.85	172.28	-101.97	-26.48	-150.64	-95.83
C4	5.53	146.85	177.99	-86.52	-51.28	-167.31	-95.33
G5	24.77	140.68	-169.36	-93.08	107.50	-165.34	-93.03
U6	119.37	145.74	--	--	--	--	-130.22

6. Structure of the proposed minor conformation

Figure S6 shows the terminal region of the duplex formed by $(\mathbf{1})_2$ that was calculated using constraints from the minor set of signals in the ^1H NMR spectra for A1, U6 and AQ7, and unchanged constraints for the core tetramer (CGCG) $_2$. Due to the scarcity of constraints, no refinement was attempted.

a)

b)

Figure S6. Terminal region of the proposed minor conformation of (ACGCG-Uaq) $_2$ ($\mathbf{1}$) $_2$ that was generated by modeling, based on 48 constraints obtained for the terminal residues and the unchanged structure of the core tetramer or residues C2, G3, C4, and G5. This modeled, unrefined structure satisfies 38 of 48 NOE-based constraints obtained. According to this structure, the minor conformation differs from the major conformation by a 180° flip of the anthraquinone moiety, highlighted in Figure 6b.

7. Sequence and compound number of the anthraquinone modified oligonucleotides

Figure S7. Oligonucleotides with Uaq residues synthesized with numbers assigned. Self-complementary deoxyoligonucleotides **1-4** and **6** were synthesized starting from anthraquinoyluridine-bearing solid support **5** (Scheme 1). Non-selfcomplementary DNAs **11-15** and RNA **16** were synthesized using reverse phosphoramidite building block **7** (Scheme 1).

8. Melting Point Data with Individual Standard Deviations

Table S2a. UV-melting points (°C) of duplexes of DNA-hybrids 5'-AGGTTGAN-Uaq-3' or control DNA strands 5'-AGGTTGAN-3' with complementary DNA target strands or target strands containing a mismatched terminal nucleotide. This is the same data as those in Table 3, except that experimental errors were included (one standard deviation).

Probe strand (5'-3')	5'-XTCAACCT-3' (Target strand)			
	X=T	X=G	X=C	X=A
AGGTTGAA-Uaq	41.8 ± 0.4	33.6 ± 0.8	25.8 ± 0.3	34.1 ± 0.4
AGGTTGAC-Uaq	30.4 ± 0.6	50.5 ± 0.8	21.0 ± 0.7	30.6 ± 0.6
AGGTTGAG-Uaq	28.3 ± 0.9	37.6 ± 0.9	47.5 ± 0.5	36.3 ± 0.4
AGGTTGAT-Uaq	31.8 ± 0.6	35.5 ± 0.3	29.5 ± 0.2	46.0 ± 0.4
AGGTTGAA	29.5 ± 0.6	25.1 ± 0.3	25.5 ± 0.2	27.4 ± 0.3
AGGTTGAC	23.4 ± 0.3	37.1 ± 0.5	23.2 ± 0.2	25.7 ± 0.3
AGGTTGAG	26.0 ± 0.2	26.7 ± 0.2	35.8 ± 0.1	27.7 ± 0.3
AGGTTGAT	25.6 ± 0.6	26.7 ± 0.3	24.6 ± 0.3	32.0 ± 0.3

Table S2b. UV melting points and hyperchromicities of octamer duplexes with or without mismatches at the 3'-terminus at different salt concentration for the sequence AGGTTGAT-Uaq and target strands of general sequence NTCAACCT or AACAACCT that produces a mismatch at the penultimate position. This table includes data points at 1 M NaCl, given in Table S1a.^a

Sequence (5'-3')	Target sequence (5'-3')	Mis- match	T _m at [NaCl] (°C) ^b			ΔT _m at 1 M [NaCl] ^c	Hyper. (%) ^d
			none	150 mM	1 M		
AGGTTGAT-Uaq	ATCAACCT	-	24.4 ± 0.3	40.1 ± 0.9	46.0 ± 0.4	--	7.7
AGGTTGAT-Uaq	CTCAACCT	T:C	<10	25.2 ± 0.3	29.5 ± 0.2	-16.5	7.0
AGGTTGAT-Uaq	GTCAACCT	T:G	13.3 ± 0.5	30.6 ± 0.6	35.5 ± 0.3	-10.5	8.4
AGGTTGAT-Uaq	TTCAACCT	T:T	<10	25.9 ± 0.4	31.8 ± 0.6	-14.2	6.9
AGGTTGAT-Uaq	AACAACCT	A:A	<10	26.0 ± 0.7	31.6 ± 0.8	-14.4	8.0

^a Conditions: 3.5 μM strand concentration in 10 mM phosphate buffer of pH 7.0 and NaCl concentration given. ^b Melting temperature (T_m) is the average of four to six experiments. ^c Melting point difference to fully complementary duplex. ^d Hyperchromicity between low- and high-temperature baseline at 260 nm for 1 M NaCl.

Table S3. UV-melting points (°C) of duplexes of DNA-hybrids 5'-AGGTTGAN-Uaq-3' or unmodified controls with complementary RNA target strands with three nucleotide overhang with or without mismatched nucleobases with individual errors.

Probe strand (5'-3')	5'-r(GCA)XUr(CAACC)U-3' (RNA target strand)			
	X=U	X=rG	X=rC	X=rA
5'-AGGTTGAA-Uaq	38.8 ± 0.7	32.4 ± 0.9	28.3 ± 1.1	30.9 ± 1.2
5'-AGGTTGAC-Uaq	27.8 ± 1.4*	50.5 ± 0.6	30.5 ± 1.9*	37.3 ± 1.5*
5'-AGGTTGAG-Uaq	25.5 ± 1.2	23.3 ± 1.9	47.2 ± 0.8	35.5 ± 0.9
5'-AGGTTGAT-Uaq	33.2 ± 1.2	34.7 ± 1.0	32.3 ± 1.3	47.1 ± 0.8
5'-AGGTTGAA	24.7 ± 1.1	23.3 ± 1.2	23.2 ± 0.9	24.2 ± 1.1
5'-AGGTTGAC	20.1 ± 1.4	33.7 ± 0.7	21.8 ± 0.8	22.4 ± 1.0
5'-AGGTTGAG	23.5 ± 1.3	22.3 ± 1.2	34.4 ± 0.9	25.6 ± 1.0
5'-AGGTTGAT	23.0 ± 1.3	27.0 ± 1.0	23.3 ± 0.6	28.8 ± 0.9

* Broad transition.

Table S4. Thermodynamic parameters for duplex formation of oligonucleotides at 37 °C, as determined from UV-melting curves^a by using the program Meltwin.²

Probe Strand (5'-3')	Target strand (5'-3')	ΔH [kcal/mol]	ΔS [cal/K mol]	ΔG [kcal/mol]	Tm ^b (°C)
(ACGCG-Uaq) ₂ ^c	-	-49.8	-120.8	-12.3	63.7
(ACGCGT) ₂ ^c	-	-38.2	-97.4	-7.9	34.5
AGGTTGAT-Uaq	ATCAACCT	-62.8	-169.4	-10.2	45.4
AGGTTGAT	ATCAACCT	-46.6	-125.7	-7.6	30.9
AGGTTGAA-Uaq	r(GCAUUCAACCU)	-50.5	-134.4	-8.8	38.4
AGGTTGAA	r(GCAUUCAACCU)	-35.7	-93.9	-6.5	23.8
AGGTTGAC-Uaq	r(GCAGUCAACCU)	-57.3	-149.5	-10.9	50.1
AGGTTGAC	r(GCAGUCAACCU)	-44.8	-118.5	-8.0	33.5
AGGTTGAG-Uaq	r(GCACUCAACCU)	-57.1	-150.3	-10.5	47.5
AGGTTGAG	r(GCACUCAACCU)	-40.6	-104.9	-8.1	33.4
AGGTTGAT-Uaq	r(GCAAUCAACCU)	-54.7	-142.6	-10.4	48.0
AGGTTGAT	r(GCAAUCAACCU)	-38.1	-99.2	-7.3	27.4
r(AGGUUGAU)-Uaq	r(AUCAACCU)	-70.4	-189.6	-11.6	50.9
r(AGGUUGAU)	r(AUCAACCU)	-56.9	-154.8	-8.9	38.6
CTTTCTTTCT-Uaq	AGAAAGAAAG	-67.2	-182.2	-10.7	47.5
CTTTCTTTCT	AGAAAGAAAG	-44.3	-115.7	-8.3	35.9

^a Based on data acquired for 3.5 μ M strand concentration.

^b UV-melting point, as calculated by Meltwin for 3.5 μ M strand concentration, 10 mM phosphate buffer, 1 M NaCl, pH 7.0. These values differ slightly from those obtained from extrema of the first derivative of melting curves.

^c Thermodynamic parameters for self-complementary duplex with or without cap, calculated at 1.2 μ M strand concentration.

9. NMR Spectra of nucleosides

Figure S8. ¹H-NMR of 2'-(Anthraquinone-2-yl-carboxamido)-2'-deoxy-5'-O-(4,4'-dimethoxytrityl)-3'-O-acetyluridine.

Figure S9. ¹H-NMR of 2'-(Anthraquinone-2-yl-carboxamido)-2'-deoxy-3'-O-acetyluridine.

10. MALDI-TOF Mass Spectra of Modified Oligonucleotides

Figure S10. MALDI-TOF mass spectrum of compound 5'-GCGCG-Uaq (**2**).

Figure S11. MALDI-TOF mass spectrum of compound 5'-CCGCG-Uaq (**3**).

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Figure S12. MALDI-TOF mass spectrum of compound 5'-TCGCG-Uaq (**4**).

Figure S13. MALDI-TOF mass spectrum of compound 5'-CGCG-Uaq (**6**).

Figure S14. MALDI-TOF mass spectrum of compound 5'-AGGTTGAA-Uaq (**11**).

Figure S15. MALDI-TOF mass spectrum of compound 5'-AGGTTGAC-Uaq (**12**).

Figure S16. MALDI-TOF mass spectrum of compound 5'-AGGTTGAG-Uaq (**13**).

Figure S17. MALDI-TOF mass spectrum of compound 5'-AGGTTGAT-Uaq (**14**).

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Figure S18. MALDI-TOF mass spectrum of compound 5'-CTTTCTTTCT-Uaq (**15**).

Figure S19. MALDI-TOF mass spectrum of RNA strand 5'-r(AGGUUGAU-Uaq) (**16**).

11. Resonance assignments for the ^1H -NMR spectrum of (1)₂.

Group	Atom	Chemical Shift (ppm)
A1	H1'	6.274
A1	H2	7.212
A1	H2'	2.811
A1	H2''	2.912
A1	H3'	4.994
A1	H4'	4.314
A1	H5'/5''	3.819*
A1	H8	7.867
C2	H1'	5.522
C2	H2'	2.185
C2	H2''	2.404
C2	H3'	4.796
C2	H4'	4.313
C2	H5	5.396
C2	H5'	4.159
C2	H5''	4.256
C2	H6	7.484
G3	H1'	5.851
G3	H2'	2.612
G3	H2''	2.651
G3	H3'	4.995
G3	H4'	4.41
G3	H5'	4.117
G3	H5''	4.154
G3	H8	7.854
C4	H1'	5.56
C4	H2'	1.729
C4	H2''	2.259
C4	H3'	4.804

C4	H4'	4.138
C4	H5	5.229
C4	H5'	4.131
C4	H5''	4.217
C4	H6	7.222
G5	H1'	5.811
G5	H2'	2.865
G5	H2''	2.919
G5	H3'	5.145
G5	H4'	4.473
G5	H5'	4.084
G5	H5''	4.147
G5	H8	8.012
U6	H1'	6.509
U6	H2'	4.55
U6	H3'	4.595
U6	H4'	4.516
U6	H5	6.042
U6	H5'	4.346
U6	H5''	4.236
U6	H6	8.212
AQ7	H1	7.701
AQ7	H3	7.813
AQ7	H4	7.597
AQ7	H5	7.626
AQ7	H6	7.687
AQ7	H7	7.756
AQ7	H8	8.014

Exchangable protons (in H₂O/D₂O)

C2	H41	6.165
C2	H42	7.583

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G3	H1	12.802
C4	H41	6.291
C4	H42	8.129
G5	H1	11.963
AQ7	H'N	8.836

* No stereospecific assignment (appear as single peak).

12. Coordinates of the lowest energy structure of (1)₂ (pdb format)

ATOM	1	H5T	DA	A	1	1.165	13.250	-6.758	1.00	0.00	H
ATOM	2	O5'	DA	A	1	0.681	13.575	-5.994	1.00	0.00	O
ATOM	3	H5'	DA	A	1	-1.119	12.849	-5.284	1.00	0.00	H
ATOM	4	H5''	DA	A	1	0.330	12.088	-4.602	1.00	0.00	H
ATOM	5	H4'	DA	A	1	-1.023	11.641	-7.221	1.00	0.00	H
ATOM	6	H1'	DA	A	1	1.828	9.660	-8.221	1.00	0.00	H
ATOM	7	N9	DA	A	1	2.569	9.728	-6.272	1.00	0.00	N
ATOM	8	C4	DA	A	1	3.610	8.832	-6.348	1.00	0.00	C
ATOM	9	N3	DA	A	1	3.832	7.914	-7.304	1.00	0.00	N
ATOM	10	C2	DA	A	1	4.940	7.221	-7.040	1.00	0.00	C
ATOM	11	H2	DA	A	1	5.189	6.446	-7.763	1.00	0.00	H
ATOM	12	N1	DA	A	1	5.787	7.335	-6.012	1.00	0.00	N
ATOM	13	C6	DA	A	1	5.535	8.266	-5.069	1.00	0.00	C
ATOM	14	N6	DA	A	1	6.379	8.376	-4.042	1.00	0.00	N
ATOM	15	H61	DA	A	1	6.210	9.064	-3.323	1.00	0.00	H
ATOM	16	H62	DA	A	1	7.185	7.770	-3.986	1.00	0.00	H
ATOM	17	C5	DA	A	1	4.390	9.065	-5.229	1.00	0.00	C
ATOM	18	N7	DA	A	1	3.853	10.088	-4.461	1.00	0.00	N
ATOM	19	C8	DA	A	1	2.778	10.444	-5.119	1.00	0.00	C
ATOM	20	H8	DA	A	1	2.116	11.225	-4.784	1.00	0.00	H
ATOM	21	H2'	DA	A	1	0.468	8.131	-6.414	1.00	0.00	H
ATOM	22	C2'	DA	A	1	0.227	9.074	-6.901	1.00	0.00	C
ATOM	23	C5'	DA	A	1	-0.116	12.490	-5.511	1.00	0.00	C
ATOM	24	C4'	DA	A	1	-0.210	11.387	-6.538	1.00	0.00	C
ATOM	25	O4'	DA	A	1	1.070	11.250	-7.201	1.00	0.00	O
ATOM	26	C1'	DA	A	1	1.466	9.887	-7.222	1.00	0.00	C
ATOM	27	C3'	DA	A	1	-0.528	10.006	-5.970	1.00	0.00	C
ATOM	28	H2''	DA	A	1	-0.363	8.835	-7.783	1.00	0.00	H
ATOM	29	H3'	DA	A	1	-0.190	9.916	-4.939	1.00	0.00	H
ATOM	30	O3'	DA	A	1	-1.940	9.772	-6.028	1.00	0.00	O
ATOM	31	P	DC	A	2	-2.515	8.287	-5.809	1.00	0.00	P
ATOM	32	O1P	DC	A	2	-2.054	7.818	-4.478	1.00	0.00	O
ATOM	33	O2P	DC	A	2	-3.970	8.319	-6.111	1.00	0.00	O
ATOM	34	O5'	DC	A	2	-1.779	7.423	-6.929	1.00	0.00	O
ATOM	35	H5'	DC	A	2	-2.087	6.526	-8.759	1.00	0.00	H
ATOM	36	H5''	DC	A	2	-3.554	6.840	-7.811	1.00	0.00	H
ATOM	37	H4'	DC	A	2	-2.434	4.433	-8.043	1.00	0.00	H
ATOM	38	H1'	DC	A	2	-1.241	2.977	-6.036	1.00	0.00	H
ATOM	39	N1	DC	A	2	-0.667	4.021	-4.314	1.00	0.00	N
ATOM	40	C6	DC	A	2	-0.902	4.991	-3.378	1.00	0.00	C
ATOM	41	H6	DC	A	2	-1.742	5.671	-3.505	1.00	0.00	H
ATOM	42	C2	DC	A	2	0.419	3.150	-4.169	1.00	0.00	C
ATOM	43	O2	DC	A	2	0.604	2.269	-5.022	1.00	0.00	O

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ATOM	44	N3	DC	A	2	1.240	3.289	-3.104	1.00	0.00	N
ATOM	45	C4	DC	A	2	1.004	4.242	-2.201	1.00	0.00	C
ATOM	46	N4	DC	A	2	1.846	4.349	-1.173	1.00	0.00	N
ATOM	47	H41	DC	A	2	1.696	5.064	-0.475	1.00	0.00	H
ATOM	48	H42	DC	A	2	2.630	3.716	-1.094	1.00	0.00	H
ATOM	49	C5	DC	A	2	-0.103	5.132	-2.313	1.00	0.00	C
ATOM	50	H5	DC	A	2	-0.292	5.897	-1.561	1.00	0.00	H
ATOM	51	H2'	DC	A	2	-3.276	4.282	-4.237	1.00	0.00	H
ATOM	52	C2'	DC	A	2	-3.037	3.878	-5.220	1.00	0.00	C
ATOM	53	C5'	DC	A	2	-2.513	6.524	-7.756	1.00	0.00	C
ATOM	54	C4'	DC	A	2	-2.445	5.123	-7.196	1.00	0.00	C
ATOM	55	O4'	DC	A	2	-1.300	4.983	-6.336	1.00	0.00	O
ATOM	56	C1'	DC	A	2	-1.537	3.877	-5.495	1.00	0.00	C
ATOM	57	C3'	DC	A	2	-3.641	4.731	-6.333	1.00	0.00	C
ATOM	58	H2''	DC	A	2	-3.414	2.856	-5.255	1.00	0.00	C
ATOM	59	H3'	DC	A	2	-4.135	5.619	-5.939	1.00	0.00	H
ATOM	60	O3'	DC	A	2	-4.581	3.978	-7.108	1.00	0.00	O
ATOM	61	P	DG	A	3	-5.937	3.443	-6.427	1.00	0.00	P
ATOM	62	O1P	DG	A	3	-7.020	3.585	-7.430	1.00	0.00	O
ATOM	63	O2P	DG	A	3	-6.087	4.079	-5.096	1.00	0.00	O
ATOM	64	O5'	DG	A	3	-5.664	1.888	-6.211	1.00	0.00	O
ATOM	65	H5'	DG	A	3	-3.925	1.691	-7.312	1.00	0.00	H
ATOM	66	H5''	DG	A	3	-5.388	1.033	-8.074	1.00	0.00	H
ATOM	67	H4'	DG	A	3	-4.390	-0.888	-7.416	1.00	0.00	H
ATOM	68	H1'	DG	A	3	-3.197	-1.572	-4.327	1.00	0.00	H
ATOM	69	N9	DG	A	3	-2.947	0.310	-3.481	1.00	0.00	N
ATOM	70	C4	DG	A	3	-1.712	0.103	-2.916	1.00	0.00	C
ATOM	71	N3	DG	A	3	-0.911	-0.960	-3.133	1.00	0.00	N
ATOM	72	C2	DG	A	3	0.214	-0.878	-2.446	1.00	0.00	C
ATOM	73	N2	DG	A	3	1.123	-1.852	-2.544	1.00	0.00	N
ATOM	74	H21	DG	A	3	0.945	-2.646	-3.141	1.00	0.00	H
ATOM	75	H22	DG	A	3	1.987	-1.796	-2.020	1.00	0.00	H
ATOM	76	N1	DG	A	3	0.532	0.164	-1.613	1.00	0.00	N
ATOM	77	H1	DG	A	3	1.423	0.127	-1.137	1.00	0.00	H
ATOM	78	C6	DG	A	3	-0.278	1.269	-1.373	1.00	0.00	C
ATOM	79	O6	DG	A	3	0.102	2.153	-0.598	1.00	0.00	O
ATOM	80	C5	DG	A	3	-1.492	1.196	-2.105	1.00	0.00	C
ATOM	81	N7	DG	A	3	-2.567	2.074	-2.159	1.00	0.00	N
ATOM	82	C8	DG	A	3	-3.403	1.506	-2.984	1.00	0.00	C
ATOM	83	H8	DG	A	3	-4.360	1.931	-3.246	1.00	0.00	H
ATOM	84	H2'	DG	A	3	-5.537	0.301	-3.853	1.00	0.00	H
ATOM	85	C2'	DG	A	3	-5.135	-0.617	-4.280	1.00	0.00	C
ATOM	86	C5'	DG	A	3	-4.855	1.152	-7.130	1.00	0.00	C
ATOM	87	C4'	DG	A	3	-4.533	-0.214	-6.570	1.00	0.00	C
ATOM	88	O4'	DG	A	3	-3.357	-0.102	-5.730	1.00	0.00	O
ATOM	89	C1'	DG	A	3	-3.626	-0.575	-4.422	1.00	0.00	C
ATOM	90	C3'	DG	A	3	-5.628	-0.834	-5.700	1.00	0.00	C

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ATOM	91	H2"	DG	A	3	-5.428	-1.440	-3.628	1.00	0.00	H
ATOM	92	H3'	DG	A	3	-6.587	-0.346	-5.874	1.00	0.00	H
ATOM	93	O3'	DG	A	3	-5.756	-2.231	-5.994	1.00	0.00	O
ATOM	94	P	DC	A	4	-6.710	-3.159	-5.088	1.00	0.00	P
ATOM	95	O1P	DC	A	4	-7.343	-4.152	-5.989	1.00	0.00	O
ATOM	96	O2P	DC	A	4	-7.566	-2.293	-4.241	1.00	0.00	O
ATOM	97	O5'	DC	A	4	-5.693	-3.935	-4.139	1.00	0.00	O
ATOM	98	H5'	DC	A	4	-3.721	-3.329	-4.242	1.00	0.00	H
ATOM	99	H5"	DC	A	4	-4.303	-4.261	-5.633	1.00	0.00	H
ATOM	100	H4'	DC	A	4	-3.460	-6.079	-4.726	1.00	0.00	H
ATOM	101	H1'	DC	A	4	-2.579	-5.500	-1.008	1.00	0.00	H
ATOM	102	N1	DC	A	4	-3.393	-3.599	-1.290	1.00	0.00	N
ATOM	103	C6	DC	A	4	-4.483	-2.852	-1.638	1.00	0.00	C
ATOM	104	H6	DC	A	4	-5.289	-3.310	-2.212	1.00	0.00	H
ATOM	105	C2	DC	A	4	-2.351	-3.024	-0.557	1.00	0.00	C
ATOM	106	O2	DC	A	4	-1.373	-3.723	-0.254	1.00	0.00	O
ATOM	107	N3	DC	A	4	-2.434	-1.724	-0.196	1.00	0.00	N
ATOM	108	C4	DC	A	4	-3.502	-1.004	-0.543	1.00	0.00	C
ATOM	109	N4	DC	A	4	-3.538	0.276	-0.177	1.00	0.00	N
ATOM	110	H41	DC	A	4	-4.333	0.842	-0.432	1.00	0.00	H
ATOM	111	H42	DC	A	4	-2.773	0.678	0.346	1.00	0.00	H
ATOM	112	C5	DC	A	4	-4.580	-1.564	-1.287	1.00	0.00	C
ATOM	113	H5	DC	A	4	-5.452	-0.968	-1.556	1.00	0.00	H
ATOM	114	H2'	DC	A	4	-5.449	-5.148	-1.350	1.00	0.00	H
ATOM	115	C2'	DC	A	4	-4.621	-5.769	-1.683	1.00	0.00	C
ATOM	116	C5'	DC	A	4	-4.344	-4.167	-4.549	1.00	0.00	C
ATOM	117	C4'	DC	A	4	-3.810	-5.432	-3.919	1.00	0.00	C
ATOM	118	O4'	DC	A	4	-2.767	-5.077	-2.988	1.00	0.00	O
ATOM	119	C1'	DC	A	4	-3.293	-5.017	-1.674	1.00	0.00	C
ATOM	120	C3'	DC	A	4	-4.820	-6.248	-3.113	1.00	0.00	C
ATOM	121	H2"	DC	A	4	-4.541	-6.608	-0.995	1.00	0.00	H
ATOM	122	H3'	DC	A	4	-5.836	-6.067	-3.463	1.00	0.00	H
ATOM	123	O3'	DC	A	4	-4.533	-7.648	-3.215	1.00	0.00	O
ATOM	124	P	DG	A	5	-5.435	-8.712	-2.411	1.00	0.00	P
ATOM	125	O1P	DG	A	5	-5.265	-10.029	-3.072	1.00	0.00	O
ATOM	126	O2P	DG	A	5	-6.797	-8.148	-2.249	1.00	0.00	O
ATOM	127	O5'	DG	A	5	-4.753	-8.787	-0.972	1.00	0.00	O
ATOM	128	H5'	DG	A	5	-2.799	-8.136	-1.137	1.00	0.00	H
ATOM	129	H5"	DG	A	5	-3.060	-9.856	-1.471	1.00	0.00	H
ATOM	130	H4'	DG	A	5	-2.221	-10.118	0.571	1.00	0.00	H
ATOM	131	H1'	DG	A	5	-2.980	-7.867	3.248	1.00	0.00	H
ATOM	132	N9	DG	A	5	-3.888	-6.400	2.092	1.00	0.00	N
ATOM	133	C4	DG	A	5	-3.301	-5.291	2.655	1.00	0.00	C
ATOM	134	N3	DG	A	5	-2.254	-5.292	3.507	1.00	0.00	N
ATOM	135	C2	DG	A	5	-1.922	-4.068	3.883	1.00	0.00	C
ATOM	136	N2	DG	A	5	-0.899	-3.881	4.726	1.00	0.00	N
ATOM	137	H21	DG	A	5	-0.384	-4.677	5.072	1.00	0.00	H

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ATOM	138	H22	DG	A	5	-0.643	-2.946	5.014	1.00	0.00	H
ATOM	139	N1	DG	A	5	-2.566	-2.933	3.459	1.00	0.00	N
ATOM	140	H1	DG	A	5	-2.234	-2.052	3.822	1.00	0.00	H
ATOM	141	C6	DG	A	5	-3.640	-2.907	2.577	1.00	0.00	C
ATOM	142	O6	DG	A	5	-4.143	-1.824	2.252	1.00	0.00	O
ATOM	143	C5	DG	A	5	-4.010	-4.214	2.165	1.00	0.00	C
ATOM	144	N7	DG	A	5	-5.020	-4.637	1.311	1.00	0.00	N
ATOM	145	C8	DG	A	5	-4.909	-5.937	1.303	1.00	0.00	C
ATOM	146	H8	DG	A	5	-5.560	-6.588	0.739	1.00	0.00	H
ATOM	147	H2'	DG	A	5	-5.551	-8.334	1.782	1.00	0.00	H
ATOM	148	C2'	DG	A	5	-4.664	-8.773	2.233	1.00	0.00	C
ATOM	149	C5'	DG	A	5	-3.351	-9.024	-0.836	1.00	0.00	C
ATOM	150	C4'	DG	A	5	-3.005	-9.358	0.596	1.00	0.00	C
ATOM	151	O4'	DG	A	5	-2.594	-8.145	1.268	1.00	0.00	O
ATOM	152	C1'	DG	A	5	-3.503	-7.792	2.296	1.00	0.00	C
ATOM	153	C3'	DG	A	5	-4.150	-9.946	1.419	1.00	0.00	C
ATOM	154	H2"	DG	A	5	-4.930	-9.083	3.241	1.00	0.00	H
ATOM	155	H3'	DG	A	5	-4.924	-10.353	0.772	1.00	0.00	H
ATOM	156	O3'	DG	A	5	-3.663	-10.986	2.275	1.00	0.00	O
ATOM	157	P	2AU	A	6	-4.704	-11.938	3.049	1.00	0.00	P
ATOM	158	O1P	2AU	A	6	-5.998	-11.887	2.324	1.00	0.00	O
ATOM	159	O2P	2AU	A	6	-4.048	-13.249	3.275	1.00	0.00	O
ATOM	160	O5'	2AU	A	6	-4.888	-11.224	4.461	1.00	0.00	O
ATOM	161	C5'	2AU	A	6	-6.092	-10.533	4.792	1.00	0.00	C
ATOM	162	H5'	2AU	A	6	-6.879	-11.254	5.013	1.00	0.00	H
ATOM	163	H5"	2AU	A	6	-6.408	-9.914	3.953	1.00	0.00	H
ATOM	164	C4'	2AU	A	6	-5.874	-9.650	6.002	1.00	0.00	C
ATOM	165	H4'	2AU	A	6	-6.598	-9.955	6.751	1.00	0.00	H
ATOM	166	O4'	2AU	A	6	-4.494	-9.789	6.445	1.00	0.00	O
ATOM	167	C1'	2AU	A	6	-3.829	-8.547	6.345	1.00	0.00	C
ATOM	168	H1'	2AU	A	6	-3.727	-8.155	7.358	1.00	0.00	H
ATOM	169	N1	2AU	A	6	-2.481	-8.784	5.809	1.00	0.00	N
ATOM	170	C6	2AU	A	6	-2.291	-9.537	4.672	1.00	0.00	C
ATOM	171	H6	2AU	A	6	-3.162	-9.951	4.163	1.00	0.00	H
ATOM	172	C2	2AU	A	6	-1.411	-8.225	6.482	1.00	0.00	C
ATOM	173	O2	2AU	A	6	-1.541	-7.549	7.488	1.00	0.00	O
ATOM	174	N3	2AU	A	6	-0.182	-8.485	5.932	1.00	0.00	N
ATOM	175	H3	2AU	A	6	0.617	-8.089	6.404	1.00	0.00	H
ATOM	176	C4	2AU	A	6	0.081	-9.229	4.803	1.00	0.00	C
ATOM	177	O4	2AU	A	6	1.247	-9.376	4.434	1.00	0.00	O
ATOM	178	C5	2AU	A	6	-1.077	-9.770	4.164	1.00	0.00	C
ATOM	179	H5	2AU	A	6	-0.971	-10.369	3.260	1.00	0.00	H
ATOM	180	C2'	2AU	A	6	-4.686	-7.647	5.460	1.00	0.00	C
ATOM	181	H2'	2AU	A	6	-4.462	-7.793	4.405	1.00	0.00	H
ATOM	182	H3'	2AU	A	6	-6.793	-7.966	4.976	1.00	0.00	H
ATOM	183	C3'	2AU	A	6	-6.087	-8.155	5.784	1.00	0.00	C
ATOM	184	O3'	2AU	A	6	-6.646	-7.529	6.943	1.00	0.00	O

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ATOM	185	H3T 2AU A	6	-7.511	-7.193	6.696	1.00	0.00	H
ATOM	186	C4A AQC A	7	-4.483	-1.183	6.610	1.00	0.00	C
ATOM	187	C1A AQC A	7	-5.385	-1.485	5.565	1.00	0.00	C
ATOM	188	C9 AQC A	7	-6.148	-0.403	4.866	1.00	0.00	C
ATOM	189	C8A AQC A	7	-5.911	1.003	5.320	1.00	0.00	C
ATOM	190	C5A AQC A	7	-5.007	1.296	6.363	1.00	0.00	C
ATOM	191	C10 AQC A	7	-4.251	0.220	7.061	1.00	0.00	C
ATOM	192	C4 AQC A	7	-3.786	-2.216	7.241	1.00	0.00	C
ATOM	193	C3 AQC A	7	-3.979	-3.537	6.840	1.00	0.00	C
ATOM	194	C2 AQC A	7	-4.877	-3.847	5.798	1.00	0.00	C
ATOM	195	C1 AQC A	7	-5.572	-2.812	5.172	1.00	0.00	C
ATOM	196	C8 AQC A	7	-6.600	2.047	4.694	1.00	0.00	C
ATOM	197	C5 AQC A	7	-4.813	2.624	6.755	1.00	0.00	C
ATOM	198	C7 AQC A	7	-6.395	3.365	5.097	1.00	0.00	C
ATOM	199	C6 AQC A	7	-5.500	3.651	6.128	1.00	0.00	C
ATOM	200	C1L AQC A	7	-5.155	-5.241	5.291	1.00	0.00	C
ATOM	201	H4 AQC A	7	-3.100	-1.961	8.040	1.00	0.00	H
ATOM	202	H3 AQC A	7	-3.421	-4.309	7.350	1.00	0.00	H
ATOM	203	H1 AQC A	7	-6.261	-3.045	4.372	1.00	0.00	H
ATOM	204	H8 AQC A	7	-7.285	1.804	3.903	1.00	0.00	H
ATOM	205	H5 AQC A	7	-4.118	2.828	7.553	1.00	0.00	H
ATOM	206	H7 AQC A	7	-6.928	4.166	4.611	1.00	0.00	H
ATOM	207	H6 AQC A	7	-5.340	4.672	6.440	1.00	0.00	H
ATOM	208	N2' AQC A	7	-4.490	-6.269	5.883	1.00	0.00	N
ATOM	209	O9 AQC A	7	-6.927	-0.658	3.964	1.00	0.00	O
ATOM	210	O10 AQC A	7	-3.473	0.469	7.961	1.00	0.00	O
ATOM	211	O1L AQC A	7	-5.946	-5.435	4.383	1.00	0.00	O
ATOM	212	H2'N AQC A	7	-3.785	-6.052	6.697	1.00	0.00	H
TER									
ATOM	213	H5T DA B	1	-8.091	4.978	11.516	1.00	0.00	H
ATOM	214	O5' DA B	1	-8.051	5.821	11.056	1.00	0.00	O
ATOM	215	H5' DA B	1	-6.340	6.782	10.408	1.00	0.00	H
ATOM	216	H5'' DA B	1	-7.078	5.672	9.238	1.00	0.00	H
ATOM	217	H4' DA B	1	-5.340	5.104	11.593	1.00	0.00	H
ATOM	218	H1' DA B	1	-6.107	1.600	11.166	1.00	0.00	H
ATOM	219	N9 DA B	1	-7.032	2.017	9.342	1.00	0.00	N
ATOM	220	C4 DA B	1	-7.251	0.749	8.855	1.00	0.00	C
ATOM	221	N3 DA B	1	-6.689	-0.398	9.274	1.00	0.00	N
ATOM	222	C2 DA B	1	-7.142	-1.429	8.562	1.00	0.00	C
ATOM	223	H2 DA B	1	-6.729	-2.400	8.830	1.00	0.00	H
ATOM	224	N1 DA B	1	-8.027	-1.444	7.559	1.00	0.00	N
ATOM	225	C6 DA B	1	-8.572	-0.276	7.163	1.00	0.00	C
ATOM	226	N6 DA B	1	-9.451	-0.292	6.160	1.00	0.00	N
ATOM	227	H61 DA B	1	-9.872	0.570	5.844	1.00	0.00	H
ATOM	228	H62 DA B	1	-9.696	-1.167	5.718	1.00	0.00	H
ATOM	229	C5 DA B	1	-8.175	0.893	7.835	1.00	0.00	C
ATOM	230	N7 DA B	1	-8.532	2.224	7.680	1.00	0.00	N

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ATOM	231	C8	DA B	1	-7.829	2.847	8.592	1.00	0.00	C
ATOM	232	H8	DA B	1	-7.868	3.914	8.738	1.00	0.00	H
ATOM	233	H2'	DA B	1	-4.408	2.234	9.126	1.00	0.00	H
ATOM	234	C2'	DA B	1	-4.736	2.790	10.003	1.00	0.00	C
ATOM	235	C5'	DA B	1	-6.842	5.822	10.291	1.00	0.00	C
ATOM	236	C4'	DA B	1	-5.912	4.723	10.746	1.00	0.00	C
ATOM	237	O4'	DA B	1	-6.693	3.547	11.067	1.00	0.00	O
ATOM	238	C1'	DA B	1	-6.137	2.403	10.435	1.00	0.00	C
ATOM	239	C3'	DA B	1	-4.896	4.268	9.700	1.00	0.00	C
ATOM	240	H2"	DA B	1	-3.992	2.625	10.780	1.00	0.00	H
ATOM	241	H3'	DA B	1	-5.266	4.441	8.690	1.00	0.00	H
ATOM	242	O3'	DA B	1	-3.664	4.976	9.881	1.00	0.00	O
ATOM	243	P	DC B	2	-2.331	4.466	9.142	1.00	0.00	P
ATOM	244	O1P	DC B	2	-2.605	4.443	7.683	1.00	0.00	O
ATOM	245	O2P	DC B	2	-1.193	5.268	9.661	1.00	0.00	O
ATOM	246	O5'	DC B	2	-2.167	2.962	9.645	1.00	0.00	O
ATOM	247	H5'	DC B	2	-1.072	1.786	10.936	1.00	0.00	H
ATOM	248	H5"	DC B	2	-0.306	3.316	10.468	1.00	0.00	H
ATOM	249	H4'	DC B	2	0.387	0.949	9.458	1.00	0.00	H
ATOM	250	H1'	DC B	2	0.063	0.116	6.856	1.00	0.00	H
ATOM	251	N1	DC B	2	-1.309	1.175	5.680	1.00	0.00	N
ATOM	252	C6	DC B	2	-1.891	2.355	5.304	1.00	0.00	C
ATOM	253	H6	DC B	2	-1.656	3.270	5.846	1.00	0.00	H
ATOM	254	C2	DC B	2	-1.615	-0.009	5.001	1.00	0.00	C
ATOM	255	O2	DC B	2	-1.065	-1.065	5.350	1.00	0.00	O
ATOM	256	N3	DC B	2	-2.501	0.024	3.981	1.00	0.00	N
ATOM	257	C4	DC B	2	-3.066	1.179	3.626	1.00	0.00	C
ATOM	258	N4	DC B	2	-3.943	1.163	2.621	1.00	0.00	N
ATOM	259	H41	DC B	2	-4.390	2.022	2.333	1.00	0.00	H
ATOM	260	H42	DC B	2	-4.156	0.293	2.152	1.00	0.00	H
ATOM	261	C5	DC B	2	-2.762	2.403	4.289	1.00	0.00	C
ATOM	262	H5	DC B	2	-3.220	3.343	3.980	1.00	0.00	H
ATOM	263	H2'	DC B	2	0.503	3.012	6.149	1.00	0.00	H
ATOM	264	C2'	DC B	2	0.734	2.178	6.810	1.00	0.00	C
ATOM	265	C5'	DC B	2	-0.910	2.482	10.114	1.00	0.00	C
ATOM	266	C4'	DC B	2	-0.175	1.768	9.004	1.00	0.00	C
ATOM	267	O4'	DC B	2	-1.100	1.329	7.993	1.00	0.00	O
ATOM	268	C1'	DC B	2	-0.364	1.119	6.810	1.00	0.00	C
ATOM	269	C3'	DC B	2	0.841	2.634	8.264	1.00	0.00	C
ATOM	270	H2"	DC B	2	1.668	1.734	6.465	1.00	0.00	H
ATOM	271	H3'	DC B	2	0.596	3.690	8.375	1.00	0.00	H
ATOM	272	O3'	DC B	2	2.155	2.401	8.783	1.00	0.00	O
ATOM	273	P	DG B	3	3.413	3.195	8.169	1.00	0.00	P
ATOM	274	O1P	DG B	3	2.891	4.260	7.277	1.00	0.00	O
ATOM	275	O2P	DG B	3	4.321	3.558	9.284	1.00	0.00	O
ATOM	276	O5'	DG B	3	4.144	2.107	7.264	1.00	0.00	O
ATOM	277	H5'	DG B	3	3.124	0.415	7.875	1.00	0.00	H

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ATOM	278	H5"	DG B	3	4.776	0.579	8.506	1.00	0.00	H
ATOM	279	H4'	DG B	3	5.111	-1.015	6.935	1.00	0.00	H
ATOM	280	H1'	DG B	3	4.126	-0.882	3.703	1.00	0.00	H
ATOM	281	N9	DG B	3	2.618	0.550	3.719	1.00	0.00	N
ATOM	282	C4	DG B	3	1.715	-0.116	2.927	1.00	0.00	C
ATOM	283	N3	DG B	3	1.806	-1.403	2.532	1.00	0.00	N
ATOM	284	C2	DG B	3	0.785	-1.760	1.774	1.00	0.00	C
ATOM	285	N2	DG B	3	0.719	-3.005	1.294	1.00	0.00	N
ATOM	286	H21	DG B	3	1.450	-3.666	1.512	1.00	0.00	H
ATOM	287	H22	DG B	3	-0.060	-3.285	0.712	1.00	0.00	H
ATOM	288	N1	DG B	3	-0.246	-0.923	1.430	1.00	0.00	N
ATOM	289	H1	DG B	3	-0.979	-1.301	0.846	1.00	0.00	H
ATOM	290	C6	DG B	3	-0.360	0.406	1.823	1.00	0.00	C
ATOM	291	O6	DG B	3	-1.330	1.075	1.452	1.00	0.00	O
ATOM	292	C5	DG B	3	0.730	0.805	2.640	1.00	0.00	C
ATOM	293	N7	DG B	3	1.007	2.026	3.240	1.00	0.00	N
ATOM	294	C8	DG B	3	2.135	1.827	3.866	1.00	0.00	C
ATOM	295	H8	DG B	3	2.641	2.591	4.437	1.00	0.00	H
ATOM	296	H2'	DG B	3	4.659	2.006	4.467	1.00	0.00	H
ATOM	297	C2'	DG B	3	4.997	0.974	4.386	1.00	0.00	C
ATOM	298	C5'	DG B	3	4.140	0.726	7.633	1.00	0.00	C
ATOM	299	C4'	DG B	3	4.659	-0.123	6.496	1.00	0.00	C
ATOM	300	O4'	DG B	3	3.556	-0.427	5.607	1.00	0.00	O
ATOM	301	C1'	DG B	3	3.844	-0.005	4.286	1.00	0.00	C
ATOM	302	C3'	DG B	3	5.741	0.533	5.635	1.00	0.00	C
ATOM	303	H2"	DG B	3	5.629	0.902	3.502	1.00	0.00	H
ATOM	304	H3'	DG B	3	6.193	1.377	6.155	1.00	0.00	H
ATOM	305	O3'	DG B	3	6.762	-0.422	5.319	1.00	0.00	O
ATOM	306	P	DC B	4	7.923	-0.040	4.271	1.00	0.00	P
ATOM	307	O1P	DC B	4	7.872	1.424	4.035	1.00	0.00	O
ATOM	308	O2P	DC B	4	9.187	-0.659	4.737	1.00	0.00	O
ATOM	309	O5'	DC B	4	7.477	-0.772	2.929	1.00	0.00	O
ATOM	310	H5'	DC B	4	5.612	-1.659	2.958	1.00	0.00	H
ATOM	311	H5"	DC B	4	6.867	-2.498	3.888	1.00	0.00	H
ATOM	312	H4'	DC B	4	7.217	-3.817	2.164	1.00	0.00	H
ATOM	313	H1'	DC B	4	5.576	-2.397	-1.033	1.00	0.00	H
ATOM	314	N1	DC B	4	5.050	-0.772	0.167	1.00	0.00	N
ATOM	315	C6	DC B	4	5.470	0.248	0.975	1.00	0.00	C
ATOM	316	H6	DC B	4	6.464	0.209	1.418	1.00	0.00	H
ATOM	317	C2	DC B	4	3.776	-0.736	-0.407	1.00	0.00	C
ATOM	318	O2	DC B	4	3.420	-1.674	-1.136	1.00	0.00	O
ATOM	319	N3	DC B	4	2.966	0.316	-0.156	1.00	0.00	N
ATOM	320	C4	DC B	4	3.385	1.305	0.636	1.00	0.00	C
ATOM	321	N4	DC B	4	2.551	2.317	0.866	1.00	0.00	N
ATOM	322	H41	DC B	4	2.844	3.073	1.465	1.00	0.00	H
ATOM	323	H42	DC B	4	1.631	2.323	0.449	1.00	0.00	H
ATOM	324	C5	DC B	4	4.679	1.297	1.232	1.00	0.00	C

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ATOM	325	H5	DC B	4	5.014	2.115	1.868	1.00	0.00	H
ATOM	326	H2'	DC B	4	7.598	-0.515	-0.111	1.00	0.00	H
ATOM	327	C2'	DC B	4	7.410	-1.582	-0.217	1.00	0.00	C
ATOM	328	C5'	DC B	4	6.663	-1.944	2.973	1.00	0.00	C
ATOM	329	C4'	DC B	4	6.946	-2.831	1.782	1.00	0.00	C
ATOM	330	O4'	DC B	4	5.777	-2.854	0.938	1.00	0.00	O
ATOM	331	C1'	DC B	4	5.926	-1.921	-0.118	1.00	0.00	C
ATOM	332	C3'	DC B	4	8.095	-2.382	0.881	1.00	0.00	C
ATOM	333	H2"	DC B	4	7.763	-1.882	-1.201	1.00	0.00	H
ATOM	334	H3'	DC B	4	8.813	-1.777	1.435	1.00	0.00	H
ATOM	335	O3'	DC B	4	8.772	-3.517	0.324	1.00	0.00	O
ATOM	336	P	DG B	5	9.994	-3.297	-0.701	1.00	0.00	P
ATOM	337	O1P	DG B	5	10.629	-1.998	-0.373	1.00	0.00	O
ATOM	338	O2P	DG B	5	10.819	-4.530	-0.712	1.00	0.00	O
ATOM	339	O5'	DG B	5	9.286	-3.154	-2.122	1.00	0.00	O
ATOM	340	H5'	DG B	5	7.416	-4.028	-2.015	1.00	0.00	H
ATOM	341	H5"	DG B	5	8.748	-5.125	-2.415	1.00	0.00	H
ATOM	342	H4'	DG B	5	7.940	-4.944	-4.478	1.00	0.00	H
ATOM	343	H1'	DG B	5	6.671	-1.855	-5.765	1.00	0.00	H
ATOM	344	N9	DG B	5	6.631	-0.829	-3.960	1.00	0.00	N
ATOM	345	C4	DG B	5	5.396	-0.234	-4.079	1.00	0.00	C
ATOM	346	N3	DG B	5	4.460	-0.525	-5.007	1.00	0.00	N
ATOM	347	C2	DG B	5	3.379	0.223	-4.869	1.00	0.00	C
ATOM	348	N2	DG B	5	2.346	0.066	-5.705	1.00	0.00	N
ATOM	349	H21	DG B	5	2.396	-0.626	-6.438	1.00	0.00	H
ATOM	350	H22	DG B	5	1.517	0.636	-5.601	1.00	0.00	H
ATOM	351	N1	DG B	5	3.228	1.183	-3.901	1.00	0.00	N
ATOM	352	H1	DG B	5	2.363	1.704	-3.898	1.00	0.00	H
ATOM	353	C6	DG B	5	4.174	1.495	-2.930	1.00	0.00	C
ATOM	354	O6	DG B	5	3.931	2.374	-2.095	1.00	0.00	O
ATOM	355	C5	DG B	5	5.342	0.700	-3.065	1.00	0.00	C
ATOM	356	N7	DG B	5	6.516	0.691	-2.324	1.00	0.00	N
ATOM	357	C8	DG B	5	7.247	-0.227	-2.894	1.00	0.00	C
ATOM	358	H8	DG B	5	8.243	-0.485	-2.566	1.00	0.00	H
ATOM	359	H2'	DG B	5	9.162	-1.177	-4.243	1.00	0.00	H
ATOM	360	C2'	DG B	5	8.687	-1.824	-4.977	1.00	0.00	C
ATOM	361	C5'	DG B	5	8.344	-4.129	-2.573	1.00	0.00	C
ATOM	362	C4'	DG B	5	8.057	-3.948	-4.045	1.00	0.00	C
ATOM	363	O4'	DG B	5	6.874	-3.128	-4.188	1.00	0.00	O
ATOM	364	C1'	DG B	5	7.177	-1.888	-4.801	1.00	0.00	C
ATOM	365	C3'	DG B	5	9.163	-3.259	-4.842	1.00	0.00	C
ATOM	366	H2"	DG B	5	8.920	-1.426	-5.962	1.00	0.00	H
ATOM	367	H3'	DG B	5	10.114	-3.316	-4.315	1.00	0.00	H
ATOM	368	O3'	DG B	5	9.305	-3.872	-6.128	1.00	0.00	O
ATOM	369	P	2AU B	6	10.570	-3.507	-7.054	1.00	0.00	P
ATOM	370	O1P 2AU B	6	10.829	-4.679	-7.924	1.00	0.00	O	
ATOM	371	O2P 2AU B	6	11.658	-2.982	-6.193	1.00	0.00	O	

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ATOM	372	O5'	2AU	B	6	10.032	-2.321	-7.973	1.00	0.00	O
ATOM	373	C5'	2AU	B	6	10.461	-0.974	-7.772	1.00	0.00	C
ATOM	374	H5'	2AU	B	6	11.478	-0.854	-8.150	1.00	0.00	H
ATOM	375	H5"	2AU	B	6	10.450	-0.735	-6.710	1.00	0.00	H
ATOM	376	C4'	2AU	B	6	9.544	-0.018	-8.504	1.00	0.00	C
ATOM	377	H4'	2AU	B	6	10.164	0.559	-9.182	1.00	0.00	H
ATOM	378	O4'	2AU	B	6	8.508	-0.784	-9.182	1.00	0.00	O
ATOM	379	C1'	2AU	B	6	7.239	-0.436	-8.668	1.00	0.00	C
ATOM	380	H1'	2AU	B	6	6.751	0.190	-9.417	1.00	0.00	H
ATOM	381	N1	2AU	B	6	6.448	-1.665	-8.514	1.00	0.00	N
ATOM	382	C6	2AU	B	6	6.960	-2.762	-7.859	1.00	0.00	C
ATOM	383	H6	2AU	B	6	7.966	-2.704	-7.443	1.00	0.00	H
ATOM	384	C2	2AU	B	6	5.172	-1.683	-9.046	1.00	0.00	C
ATOM	385	O2	2AU	B	6	4.683	-0.730	-9.628	1.00	0.00	O
ATOM	386	N3	2AU	B	6	4.488	-2.859	-8.870	1.00	0.00	N
ATOM	387	H3	2AU	B	6	3.554	-2.899	-9.249	1.00	0.00	H
ATOM	388	C4	2AU	B	6	4.938	-3.992	-8.230	1.00	0.00	C
ATOM	389	O4	2AU	B	6	4.203	-4.977	-8.155	1.00	0.00	O
ATOM	390	C5	2AU	B	6	6.264	-3.892	-7.705	1.00	0.00	C
ATOM	391	H5	2AU	B	6	6.707	-4.737	-7.177	1.00	0.00	H
ATOM	392	C2'	2AU	B	6	7.472	0.307	-7.356	1.00	0.00	C
ATOM	393	H2'	2AU	B	6	7.565	-0.381	-6.518	1.00	0.00	H
ATOM	394	H3'	2AU	B	6	9.356	1.212	-6.720	1.00	0.00	H
ATOM	395	C3'	2AU	B	6	8.805	0.994	-7.634	1.00	0.00	C
ATOM	396	O3'	2AU	B	6	8.649	2.249	-8.303	1.00	0.00	O
ATOM	397	H3T	2AU	B	6	9.138	2.903	-7.799	1.00	0.00	H
ATOM	398	C4A	AQC	B	7	3.078	4.876	-5.634	1.00	0.00	C
ATOM	399	C1A	AQC	B	7	4.125	4.796	-4.689	1.00	0.00	C
ATOM	400	C9	AQC	B	7	4.142	5.677	-3.479	1.00	0.00	C
ATOM	401	C8A	AQC	B	7	3.007	6.638	-3.317	1.00	0.00	C
ATOM	402	C5A	AQC	B	7	1.964	6.710	-4.265	1.00	0.00	C
ATOM	403	C10	AQC	B	7	1.948	5.836	-5.470	1.00	0.00	C
ATOM	404	C4	AQC	B	7	3.092	4.038	-6.752	1.00	0.00	C
ATOM	405	C3	AQC	B	7	4.132	3.128	-6.932	1.00	0.00	C
ATOM	406	C2	AQC	B	7	5.181	3.042	-5.993	1.00	0.00	C
ATOM	407	C1	AQC	B	7	5.163	3.882	-4.879	1.00	0.00	C
ATOM	408	C8	AQC	B	7	2.980	7.480	-2.200	1.00	0.00	C
ATOM	409	C5	AQC	B	7	0.920	7.621	-4.075	1.00	0.00	C
ATOM	410	C7	AQC	B	7	1.932	8.381	-2.026	1.00	0.00	C
ATOM	411	C6	AQC	B	7	0.902	8.449	-2.964	1.00	0.00	C
ATOM	412	C1L	AQC	B	7	6.349	2.092	-6.096	1.00	0.00	C
ATOM	413	H4	AQC	B	7	2.278	4.118	-7.464	1.00	0.00	H
ATOM	414	H3	AQC	B	7	4.107	2.495	-7.808	1.00	0.00	H
ATOM	415	H1	AQC	B	7	5.965	3.818	-4.156	1.00	0.00	H
ATOM	416	H8	AQC	B	7	3.782	7.411	-1.490	1.00	0.00	H
ATOM	417	H5	AQC	B	7	0.132	7.660	-4.810	1.00	0.00	H
ATOM	418	H7	AQC	B	7	1.915	9.027	-1.163	1.00	0.00	H

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ATOM	419	H6	AQC	B	7	0.089	9.147	-2.829	1.00	0.00	H
ATOM	420	N2'	AQC	B	7	6.390	1.261	-7.172	1.00	0.00	N
ATOM	421	O9	AQC	B	7	5.043	5.613	-2.660	1.00	0.00	O
ATOM	422	O10	AQC	B	7	1.053	5.897	-6.290	1.00	0.00	O
ATOM	423	O1L	AQC	B	7	7.221	2.072	-5.244	1.00	0.00	O
ATOM	424	H2'N	AQC	B	7	5.584	1.310	-7.918	1.00	0.00	H

END

13. References

References for Supporting Information

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