The Oxidization Potential of AA steps in single strand DNA Oligomers

– Electronic Supplementary Information –

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TABLE S1. Sum of the Mulliken spin densities[(a)] (PCM/M06-2X/6-31G**) for the singly ionized trimers (H model).

	5′-CCA-3′	5′-ACC-3′	5′-CAA-3′	5′-AAC-3′
5′-B_1	0.00	0.94	0.05	0.08
B_2	0.02	0.06	0.87	0.85
B_3-3′	0.98	0.00	0.08	0.07

[(a)]The sum has been carried out only for the atoms belonging to each nucleobase B_i, (i = 1,2,3) without including ribose and phosphate atoms.

TABLE S2. Sum of the Mulliken spin densities[(a)] (PCM/M06-2X/6-31G**) for the singly ionized trimers (PO- model).

	5′-CCA-3′	5′-ACC-3′	5′-CAA-3′	5′-AAC-3′
5′-B_1	0.00	0.94	0.05	0.07
B_2	0.03	0.05	0.93	0.91
B_3-3′	0.97	0.00	0.01	0.02

[(a)]The sum has been carried out only for the atoms belonging to each nucleobase B_i.

TABLE S3. Sum of the Mulliken spin densities[(a)] (PCM/B3LYP-D/6-31G**) for the singly ionized trimers (H model).

	5′-CCA-3′	5′-ACC-3′	5′-CAA-3′	5′-AAC-3′
5′-B_1	0.00	0.81	0.02	0.37
B_2	0.36	0.18	0.55	0.56
B_3-3′	0.63	0.00	0.43	0.07

[(a)]The sum has been carried out only for the atoms belonging to each nucleobase B_i.

TABLE S4. Sum of the Mulliken spin densities[(a)] (PCM/B3LYP-D/6-31G**) for the singly ionized trimers (PO- model).

	5′-CCA-3′	5′-ACC-3′	5′-CAA-3′	5′-AAC-3′
5′-B_1	0.03	0.79	0.16	0.36
B_2	0.39	0.19	0.76	0.56
B_3-3′	0.57	0.02	0.07	0.08

[(a)]The sum has been carried out only for the atoms belonging to each nucleobase B_i.

TABLE S5. Mulliken charges of neutral and singly ionized 5′-ACC-3′ single strand evaluated by using the M06-2X functional. See scheme SI for the definition of the fragments.

	A1	dR1	P12	(H/Na)12	dR2	C2	P23	(H/Na)13	dR3	C3
H model										
neut.	-0.27	0.01	-0.48	0.40	0.33	-0.24	-0.47	0.40	0.60	-0.28
sing. ion.	0.53	0.09	-0.47	0.40	0.34	-0.16	-0.47	0.40	0.61	-0.27
Na model										
neut.	-0.28	-0.05	-0.67	0.72	0.21	-0.26	-0.66	0.72	0.54	-0.27
sing. ion.	0.51	0.02	-0.67	0.73	0.23	-0.16	-0.65	0.72	0.54	-0.27
PO- model										
neut.	-0.28	-0.10	-0.84	–	0.15	-0.29	-0.84	–	0.51	-0.30
sing. ion.	0.53	0.00	-0.84	–	0.17	-0.21	-0.84	–	0.49	-0.29

TABLE S6. Mulliken charges of neutral and singly ionized 5′-AAC-3′ single strand evaluated by using the M06-2X functional. See scheme SI for the definition of the fragments.

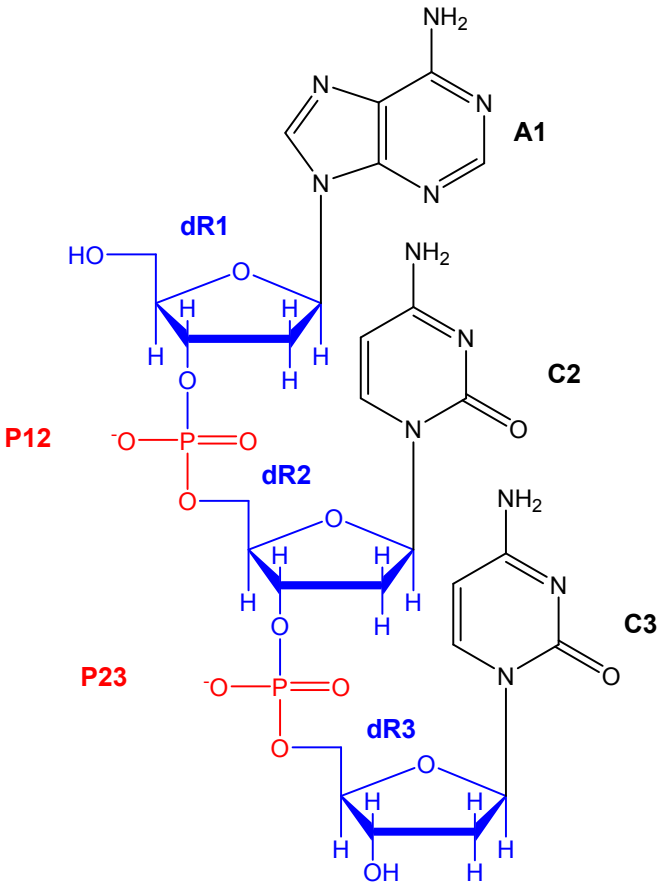
	A1	dR1	P12	(H/Na)12	dR2	A2	P23	(H/Na)13	dR3	C3
H model										
neut.	-0.28	0.02	-0.48	0.40	0.35	-0.27	-0.48	0.40	0.61	-0.28
sing. ion.	-0.20	0.04	-0.47	0.40	0.40	0.44	-0.47	0.40	0.63	-0.18
Na model										
neut.	-0.28	-0.03	-0.67	0.72	0.23	-0.30	-0.65	0.72	0.55	-0.27
sing. ion.	-0.20	-0.03	-0.67	0.73	0.29	0.44	-0.65	0.72	0.58	-0.20
PO- model										
neut.	-0.28	-0.08	-0.85	–	0.17	-0.30	-0.83	–	0.49	-0.31
sing. ion.	-0.22	-0.07	-0.83	–	0.24	0.44	-0.81	–	0.52	-0.26

TABLE S7. Mulliken charges of neutral and singly ionized 5′-ACC-3′ single strand evaluated by using the B3LYP-D functional. See scheme SI for the definition of the fragments.

	A1	dR1	P12	(H/Na)12	dR2	C2	P23	(H/Na)13	dR3	C3
H model										
neut.	-0.26	0.02	-0.45	0.37	0.32	-0.24	-0.44	0.37	0.57	-0.27
sing. ion.	0.42	0.09	-0.44	0.37	0.34	-0.05	-0.44	0.37	0.58	-0.25
Na model										
neut.	-0.27	-0.04	-0.63	0.70	0.20	-0.27	-0.64	0.71	0.50	-0.28
sing. ion.	0.41	0.02	-0.62	0.71	0.22	-0.07	-0.64	0.71	0.51	-0.26
PO- model										
neut.	-0.27	-0.09	-0.82	–	0.12	-0.29	-0.83	–	0.47	-0.29
sing. ion.	0.40	-0.02	-0.81	–	0.16	-0.09	-0.82	–	0.46	-0.27

TABLE S8. Mulliken charges of neutral and singly ionized 5′-AAC-3′ single strand evaluated by using the B3LYP-D functional. See scheme SI for the definition of the fragments.

	A1	dR1	P12	(H/Na)12	dR2	A2	P23	(H/Na)13	dR3	C3
H model										
neut.	-0.27	0.03	-0.45	0.37	0.35	-0.26	-0.45	0.37	0.58	-0.28
sing. ion.	0.06	0.07	-0.45	0.37	0.37	0.20	-0.44	0.37	0.61	-0.17
Na model										
neut.	-0.26	-0.03	-0.63	0.70	0.22	-0.30	-0.62	0.70	0.52	-0.30
sing. ion.	-0.01	0.00	-0.63	0.70	0.26	0.21	-0.62	0.70	0.55	-0.19
PO- model										
neut.	-0.26	-0.08	-0.83	–	0.16	-0.30	-0.81	–	0.44	-0.31
sing. ion.	0.04	-0.05	-0.81	–	0.21	0.17	-0.81	–	0.48	-0.22



SCHEME SI

Optimized Geometries: local base, helical step and conformational parameters

5′-ACC-3′ (H model) neutral / B3LYP-D

step overlap area (Å^2)
1 A/C 3.88
2 C/C 4.37

Local base step parameters

step	Shift	Slide	Rise	Tilt	Roll	Twist
1 A/C	0.49	0.26	2.44	13.93	-0.28	34.11
2 C/C	0.32	0.46	2.83	6.43	-2.31	36.88
ave.	0.41	0.36	2.63	10.18	-1.29	35.50
s.d.	0.12	0.14	0.27	5.30	1.44	1.96

Local base helical parameters

step	X-disp	Y-disp	h-Rise	Incl.	Tip	h-Twist
1 A/C	0.45	0.70	2.45	-0.45	-22.62	36.77
2 C/C	0.98	0.23	2.81	-3.61	-10.06	37.49
ave.	0.71	0.46	2.63	-2.03	-16.34	37.13
s.d.	0.38	0.33	0.25	2.23	8.88	0.51

Sugar conformational parameters:
Note: v0: C4'-O4'-C1'-C2'; v1: O4'-C1'-C2'-C3'; v2: C1'-C2'-C3'-C4'
v3: C2'-C3'-C4'-O4'; v4: C3'-C4'-O4'-C1'
tm: the amplitude of pucker; P: the phase angle of pseudorotation

base	v0	v1	v2	v3	v4	tm	P	Puckering
1 A	-10.6	30.1	-36.9	31.8	-13.3	37.0	182.2	C3'-exo
2 C	-44.3	46.6	-31.5	6.5	23.4	47.1	132.0	C1'-exo
3 C	-45.0	44.6	-27.4	1.9	26.7	46.2	126.4	C1'-exo

5′-ACC-3′ (H model) singly ionized / B3LYP-D

step overlap area (Å^2)
1 A/C 3.53
2 C/C 5.19

Local base step parameters

step	Shift	Slide	Rise	Tilt	Roll	Twist
1 A/C	1.69	1.30	1.63	30.05	-4.22	43.98
2 C/C	0.65	0.72	3.31	-1.38	-1.69	37.79
ave.	1.17	1.01	2.47	14.34	-2.95	40.89
s.d.	0.74	0.40	1.19	22.23	1.79	4.38

Local base helical parameters

step	X-disp	Y-disp	h-Rise	Incl.	Tip	h-Twist
1 A/C	1.63	-0.65	2.18	-4.99	-35.57	53.01
2 C/C	1.33	-1.18	3.25	-2.60	2.13	37.85
ave.	1.48	-0.91	2.72	-3.79	-16.72	45.43
s.d.	0.21	0.38	0.76	1.69	26.66	10.72

Sugar conformational parameters:

base	v0	v1	v2	v3	v4	tm	P	Puckering
1 A	-9.9	27.1	-32.7	28.0	-11.5	32.7	181.4	C3'-exo
2 C	-44.1	46.7	-32.0	7.3	22.7	47.1	132.8	C1'-exo
3 C	-44.9	45.2	-28.3	2.8	26.0	46.4	127.5	C1'-exo

5'-AAC-3' (H model) neutral / B3LYP-D

step overlap area (Å^2)
1 A/A 5.51
2 A/C 4.14

Local base step parameters

step	Shift	Slide	Rise	Tilt	Roll	Twist
1 A/A	2.86	1.96	2.92	17.20	-11.77	50.54
2 A/C	0.62	0.01	2.79	5.64	3.87	35.79
ave.	1.74	0.98	2.86	11.42	-3.95	43.17
s.d.	1.58	1.38	0.09	8.17	11.06	10.43

Local base helical parameters

step	X-disp	Y-disp	h-Rise	Incl.	Tip	h-Twist
1 A/A	2.84	-2.11	3.18	-13.17	-19.24	54.41
2 A/C	-0.45	-0.32	2.84	6.22	-9.08	36.42
ave.	1.19	-1.21	3.01	-3.47	-14.16	45.42
s.d.	2.33	1.27	0.24	13.71	7.18	12.72

Sugar conformational parameters:

base	v0	v1	v2	v3	v4	tm	P	Puckering
1 A	-10.1	27.1	-32.6	27.6	-11.1	32.6	180.9	C3'-exo
2 A	-40.9	45.8	-33.5	10.7	18.7	45.5	137.5	C1'-exo
3 C	-45.1	45.3	-28.2	2.6	26.2	46.6	127.3	C1'-exo

5′-AAC-3′ (H model) singly ionized / B3LYP-D

step overlap area (Å^2)
1 A/A 5.27
2 A/C 5.05

Local base step parameters

step	Shift	Slide	Rise	Tilt	Roll	Twist
1 A/A	1.07	1.86	2.85	6.17	-2.67	40.93
2 A/C	1.72	0.88	2.67	8.30	-2.31	44.97
ave.	1.39	1.37	2.76	7.24	-2.49	42.95
s.d.	0.46	0.69	0.13	1.51	0.25	2.86

Local base helical parameters

step	X-disp	Y-disp	h-Rise	Incl.	Tip	h-Twist
1 A/A	2.87	-0.94	2.85	-3.78	-8.76	41.45
2 A/C	1.30	-1.59	2.88	-2.99	-10.74	45.74
ave.	2.09	-1.26	2.86	-3.39	-9.75	43.60
s.d.	1.11	0.46	0.02	0.56	1.40	3.03

Sugar conformational parameters:

base	v0	v1	v2	v3	v4	tm	P	Puckering
1 A	-3.2	25.0	-35.9	35.1	-20.1	37.0	193.7	C3'-exo
2 A	-39.4	45.8	-34.7	12.9	16.3	45.1	140.3	C1'-exo
3 C	-45.1	44.7	-27.4	1.8	26.8	46.3	126.3	C1'-exo

5'-CCA-3' (H model) neutral / B3LYP-D

step overlap area (Å^2)
1 C/C 4.86
2 C/A 4.60

Local base step parameters

step		Shift	Slide	Rise	Tilt	Roll	Twist
1	C/C	0.21	0.80	2.15	20.91	-6.05	32.84
2	C/A	0.70	1.09	3.02	3.98	2.25	38.79
	ave.	0.45	0.95	2.59	12.44	-1.90	35.81
	s.d.	0.34	0.21	0.62	11.97	5.87	4.21

Local base helical parameters

step		X-disp	Y-disp	h-Rise	Incl.	Tip	h-Twist
1	C/C	1.67	1.34	1.80	-9.52	-32.87	39.23
2	C/A	1.38	-0.59	3.13	3.38	-5.97	39.05
	ave.	1.52	0.38	2.47	-3.07	-19.42	39.14
	s.d.	0.21	1.36	0.94	9.12	19.03	0.13

Sugar conformational parameters:

base		v0	v1	v2	v3	v4	tm	P	Puckering
1	C	-16.0	31.9	-35.0	26.6	-6.7	35.3	172.3	C2'-endo
2	C	-43.8	46.3	-31.7	7.1	22.7	46.8	132.8	C1'-exo
3	A	-42.4	44.2	-29.3	5.4	22.8	44.7	130.9	C1'-exo

5'-CCA-3' (H model) singly ionized / B3LYP-D

step overlap area (Å^2)
1 C/C 4.55
2 C/A 5.98

Local base step parameters

step		Shift	Slide	Rise	Tilt	Roll	Twist
1	C/C	0.37	0.97	1.97	23.98	-6.34	36.58
2	C/A	1.06	2.01	2.75	7.25	0.07	41.60
	ave.	0.72	1.49	2.36	15.61	-3.14	39.09
	s.d.	0.49	0.74	0.55	11.83	4.53	3.55

Local base helical parameters

step		X-disp	Y-disp	h-Rise	Incl.	Tip	h-Twist
1	C/C	1.67	0.92	1.71	-8.95	-33.85	43.96
2	C/A	2.79	-0.83	2.89	0.10	-10.12	42.20
	ave.	2.23	0.04	2.30	-4.43	-21.98	43.08
	s.d.	0.80	1.24	0.83	6.40	16.78	1.24

Sugar conformational parameters:

base		v0	v1	v2	v3	v4	tm	P	Puckering
1	C	-15.8	31.7	-34.8	26.5	-6.8	35.1	172.4	C2'-endo
2	C	-43.5	45.7	-30.8	6.5	22.8	46.1	131.9	C1'-exo
3	A	-41.5	44.3	-30.1	7.1	21.1	44.2	132.8	C1'-exo

5'-CAA-3' (H model) neutral / B3LYP-D

step overlap area (Å^2)
1 C/A 4.13
2 A/A 5.34

Local base step parameters

step	Shift	Slide	Rise	Tilt	Roll	Twist
1 C/A	3.16	3.13	2.63	19.95	-7.07	56.81
2 A/A	0.43	0.88	3.17	-0.35	8.66	32.85
ave.	1.80	2.00	2.90	9.80	0.80	44.83
s.d.	1.93	1.60	0.38	14.36	11.13	16.94

Local base helical parameters

step	X-disp	Y-disp	h-Rise	Incl.	Tip	h-Twist
1 C/A	3.43	-2.26	3.11	-7.17	-20.21	60.31
2 A/A	0.11	-0.80	3.28	15.00	0.61	33.95
ave.	1.77	-1.53	3.20	3.91	-9.80	47.13
s.d.	2.35	1.03	0.12	15.67	14.72	18.64

Sugar conformational parameters:

base	v0	v1	v2	v3	v4	tm	P	Puckering
1 C	-13.8	29.1	-32.7	25.4	-7.3	32.8	174.3	C2'-endo
2 A	-37.8	43.9	-33.6	12.5	15.6	43.4	140.6	C1'-exo
3 A	-42.4	45.2	-30.6	6.8	22.0	45.3	132.5	C1'-exo

5'-CAA-3' (H model) singly ionized / B3LYP-D

step overlap area (Å^2)
1 C/A 4.20
2 A/A 5.81

Local base step parameters

step	Shift	Slide	Rise	Tilt	Roll	Twist
1 C/A	3.38	3.14	2.53	23.06	-7.64	62.39
2 A/A	1.23	1.60	2.91	2.93	1.43	40.32
ave.	2.30	2.37	2.72	13.00	-3.10	51.36
s.d.	1.52	1.09	0.27	14.24	6.42	15.60

Local base helical parameters

step	X-disp	Y-disp	h-Rise	Incl.	Tip	h-Twist
1 C/A	3.14	-2.25	3.12	-7.10	-21.42	66.50
2 A/A	2.17	-1.48	3.04	2.07	-4.24	40.45
ave.	2.65	-1.87	3.08	-2.51	-12.83	53.48
s.d.	0.69	0.54	0.05	6.48	12.15	18.42

Sugar conformational parameters:

base	v0	v1	v2	v3	v4	tm	P	Puckering
1 C	-14.5	30.3	-33.7	26.1	-7.4	33.9	173.8	C2'-endo
2 A	-37.9	44.2	-33.9	13.0	15.3	43.6	141.0	C1'-exo
3 A	-40.8	45.0	-31.7	9.1	19.5	44.5	135.4	C1'-exo

5'-ACC-3' (Na model) neutral / B3LYP-D

step overlap area (Å^2)
1 A/C 4.01
2 C/C 2.81

Local base step parameters

step	Shift	Slide	Rise	Tilt	Roll	Twist
1 A/C	0.54	-0.06	2.77	6.57	0.85	35.83
2 C/C	0.77	-0.42	3.71	-8.75	9.60	45.82
ave.	0.66	-0.24	3.24	-1.09	5.22	40.82
s.d.	0.16	0.26	0.66	10.84	6.19	7.06

Local base helical parameters

step	X-disp	Y-disp	h-Rise	Incl.	Tip	h-Twist
1 A/C	-0.20	-0.08	2.82	1.36	-10.57	36.41
2 C/C	-1.38	-1.74	3.37	12.04	10.99	47.53
ave.	-0.79	-0.91	3.10	6.70	0.21	41.97
s.d.	0.83	1.17	0.38	7.55	15.24	7.86

Sugar conformational parameters:

base	v0	v1	v2	v3	v4	tm	P	Puckering
1 A	-12.8	32.8	-39.0	32.8	-12.7	39.0	180.0	C2'-endo
2 C	-42.5	43.6	-28.2	4.1	23.9	44.5	129.4	C1'-exo
3 C	-18.9	33.7	-34.8	24.8	-3.8	35.7	167.4	C2'-endo

5'-ACC-3' (Na model) singly ionized / B3LYP-D

step overlap area (Å^2)
1 A/C 1.68
2 C/C 2.64

Local base step parameters

step	Shift	Slide	Rise	Tilt	Roll	Twist
1 A/C	-1.15	-0.22	2.68	9.69	-19.23	25.28
2 C/C	1.43	-0.78	4.02	-13.95	9.67	50.88
ave.	0.14	-0.50	3.35	-2.13	-4.78	38.08
s.d.	1.82	0.39	0.94	16.71	20.44	18.11

Local base helical parameters

step	X-disp	Y-disp	h-Rise	Incl.	Tip	h-Twist
1 A/C	2.19	3.32	1.86	-36.60	-18.44	33.09
2 C/C	-1.57	-2.61	3.36	10.92	15.74	53.46
ave.	0.31	0.36	2.61	-12.84	-1.35	43.27
s.d.	2.66	4.19	1.06	33.60	24.17	14.40

Sugar conformational parameters:

base	v0	v1	v2	v3	v4	tm	P	Puckering
1 A	-10.6	30.2	-37.0	32.1	-13.6	37.1	182.4	C3'-exo
2 C	-41.6	45.9	-32.4	9.2	19.9	45.5	135.4	C1'-exo
3 C	-17.0	32.4	-34.7	25.8	-5.7	35.1	170.5	C2'-endo

5'-AAC-3' (Na model) neutral / B3LYP-D

step overlap area (Å^2)
1 A/A 5.01
2 A/C 4.23

Local base step parameters

step	Shift	Slide	Rise	Tilt	Roll	Twist
1 A/A	0.12	1.14	3.01	2.04	11.77	27.42
2 A/C	0.68	-0.17	2.83	5.06	5.23	37.43
ave.	0.40	0.48	2.92	3.55	8.50	32.43
s.d.	0.40	0.93	0.13	2.13	4.63	7.08

Local base helical parameters

step	X-disp	Y-disp	h-Rise	Incl.	Tip	h-Twist
1 A/A	-0.23	0.19	3.22	23.47	-4.07	29.87
2 A/C	-0.85	-0.48	2.84	8.05	-7.79	38.11
ave.	-0.54	-0.15	3.03	15.76	-5.93	33.99
s.d.	0.44	0.47	0.27	10.90	2.64	5.83

Sugar conformational parameters:

base	v0	v1	v2	v3	v4	tm	P	Puckering
1 A	-25.4	38.9	-36.9	23.3	1.1	39.4	159.7	C2'-endo
2 A	-34.8	44.8	-37.4	18.4	10.0	44.0	148.2	C2'-endo
3 C	-43.4	44.6	-28.7	4.2	24.2	45.3	129.3	C1'-exo

5'-AAC-3' (Na model) singly ionized / B3LYP-D

step overlap area (Å^2)
1 A/A 5.30
2 A/C 5.17

Local base step parameters

step	Shift	Slide	Rise	Tilt	Roll	Twist
1 A/A	1.09	1.81	2.88	5.36	-2.31	41.34
2 A/C	1.60	0.72	2.73	7.06	-1.79	44.24
ave.	1.34	1.26	2.81	6.21	-2.05	42.79
s.d.	0.36	0.77	0.10	1.20	0.37	2.05

Local base helical parameters

step	X-disp	Y-disp	h-Rise	Incl.	Tip	h-Twist
1 A/A	2.75	-1.02	2.89	-3.25	-7.55	41.74
2 A/C	1.08	-1.54	2.91	-2.35	-9.30	44.80
ave.	1.92	-1.28	2.90	-2.80	-8.43	43.27
s.d.	1.18	0.37	0.02	0.63	1.24	2.17

Sugar conformational parameters:

base	v0	v1	v2	v3	v4	tm	P	Puckering
1 A	-5.9	27.6	-37.5	35.3	-18.5	38.1	190.0	C3'-exo
2 A	-35.4	45.8	-38.3	19.1	9.8	44.9	148.6	C2'-endo
3 C	-42.8	44.7	-29.5	5.5	23.1	45.2	130.9	C1'-exo

5'-CCA-3' (Na model) neutral / B3LYP-D

step overlap area (Å^2)
1 C/C 2.92
2 C/A 2.33

Local base step parameters

step		Shift	Slide	Rise	Tilt	Roll	Twist
1	C/C	-0.44	-0.05	2.57	11.10	-12.14	30.81
2	C/A	0.79	0.76	3.03	2.40	0.94	49.79
	ave.	0.18	0.35	2.80	6.75	-5.60	40.30
	s.d.	0.87	0.57	0.33	6.15	9.25	13.42

Local base helical parameters

step		X-disp	Y-disp	h-Rise	Incl.	Tip	h-Twist
1	C/C	1.34	2.03	2.16	-21.07	-19.27	34.84
2	C/A	0.83	-0.77	3.07	1.12	-2.85	49.85
	ave.	1.09	0.63	2.62	-9.97	-11.06	42.35
	s.d.	0.36	1.98	0.65	15.69	11.61	10.62

Sugar conformational parameters:

base		v0	v1	v2	v3	v4	tm	P	Puckering
1	C	-17.1	34.5	-37.8	29.0	-7.5	38.2	172.6	C2'-endo
2	C	-40.0	45.8	-34.0	11.6	17.5	45.2	138.8	C1'-exo
3	A	-12.2	29.3	-34.2	28.1	-10.2	34.2	178.3	C2'-endo

5'-CCA-3' (Na model) singly ionized / B3LYP-D

step overlap area (Å^2)
1 C/C 2.74
2 C/A 4.56

Local base step parameters

step		Shift	Slide	Rise	Tilt	Roll	Twist
1	C/C	-0.37	-0.11	2.69	8.74	-17.63	32.32
2	C/A	1.72	1.15	2.81	8.49	7.40	57.84
	ave.	0.68	0.52	2.75	8.62	-5.12	45.08
	s.d.	1.48	0.89	0.08	0.17	17.70	18.05

Local base helical parameters

step		X-disp	Y-disp	h-Rise	Incl.	Tip	h-Twist
1	C/C	1.71	1.50	2.28	-28.61	-14.18	37.70
2	C/A	0.82	-1.35	3.12	7.57	-8.69	58.84
	ave.	1.26	0.08	2.70	-10.52	-11.43	48.27
	s.d.	0.63	2.02	0.59	25.58	3.88	14.95

Sugar conformational parameters:

base		v0	v1	v2	v3	v4	tm	P	Puckering
1	C	-17.9	35.4	-38.5	29.2	-7.2	38.9	171.9	C2'-endo
2	C	-41.1	47.0	-34.2	11.4	18.3	46.1	138.0	C1'-exo
3	A	10.1	10.9	-26.0	32.5	-27.1	32.3	216.3	C4'-endo

5'-CAA-3' (Na model) neutral / B3LYP-D

step overlap area (Å^2)
1 C/A 2.17
2 A/A 5.06

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Local base step parameters

step		Shift	Slide	Rise	Tilt	Roll	Twist
1	C/A	-0.02	0.71	2.68	11.37	-9.89	35.44
2	A/A	1.08	0.06	3.23	-3.52	8.22	49.20
	ave.	0.53	0.38	2.96	3.93	-0.83	42.32
	s.d.	0.78	0.46	0.39	10.53	12.81	9.73

****

Local base helical parameters

step		X-disp	Y-disp	h-Rise	Incl.	Tip	h-Twist
1	C/A	2.06	1.15	2.30	-15.42	-17.73	38.42
2	A/A	-0.52	-1.53	3.12	9.78	4.18	49.96
	ave.	0.77	-0.19	2.71	-2.82	-6.77	44.19
	s.d.	1.82	1.90	0.58	17.82	15.49	8.16

****

Sugar conformational parameters:

base		v0	v1	v2	v3	v4	tm	P	Puckering
1	C	-17.3	34.5	-37.8	28.8	-7.3	38.1	172.3	C2'-endo
2	A	-34.0	43.4	-35.8	16.9	10.6	42.6	147.2	C2'-endo
3	A	-12.2	29.6	-34.5	28.4	-10.4	34.5	178.4	C2'-endo

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5'-CAA-3' (Na model) singly ionized / B3LYP-D

step overlap area (Å^2)
1 C/A 0.03
2 A/A 5.71

****

Local base step parameters

step		Shift	Slide	Rise	Tilt	Roll	Twist
1	C/A	-1.79	0.30	2.24	16.43	-27.56	21.40
2	A/A	1.66	-0.12	3.03	-0.17	8.60	55.09
	ave.	-0.07	0.09	2.64	8.13	-9.48	38.25
	s.d.	2.44	0.29	0.56	11.74	25.56	23.82

****

Local base helical parameters

step		X-disp	Y-disp	h-Rise	Incl.	Tip	h-Twist
1	C/A	2.20	3.77	0.29	-49.08	-29.26	38.41
2	A/A	-0.58	-1.78	2.98	9.23	0.18	55.71
	ave.	0.81	0.99	1.64	-19.93	-14.54	47.06
	s.d.	1.97	3.92	1.90	41.23	20.82	12.23

****

Sugar conformational parameters:

base		v0	v1	v2	v3	v4	tm	P	Puckering
1	C	-15.6	32.2	-35.7	27.7	-7.7	35.9	173.6	C2'-endo
2	A	-36.2	46.1	-37.3	17.6	11.3	44.7	146.5	C2'-endo
3	A	1.8	18.1	-29.6	31.4	-21.1	31.8	201.7	C3'-exo

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5'-ACC-3' (PO- model) neutral / B3LYP-D

step overlap area (Å^2)
1 A/C 4.04
2 C/C 2.09

Local base step parameters

step	Shift	Slide	Rise	Tilt	Roll	Twist
1 A/C	0.53	-0.07	2.80	5.69	2.10	35.44
2 C/C	1.11	-0.82	4.22	-16.78	13.85	49.31
ave.	0.82	-0.44	3.51	-5.54	7.97	42.38
s.d.	0.41	0.53	1.00	15.89	8.31	9.81

Local base helical parameters

step	X-disp	Y-disp	h-Rise	Incl.	Tip	h-Twist
1 A/C	-0.37	-0.16	2.84	3.41	-9.27	35.94
2 C/C	-1.97	-2.52	3.38	15.74	19.08	53.62
ave.	-1.17	-1.34	3.11	9.58	4.90	44.78
s.d.	1.13	1.67	0.38	8.72	20.05	12.50

Sugar conformational parameters:

base	v0	v1	v2	v3	v4	tm	P	Puckering
1 A	-17.2	35.7	-39.4	30.7	-8.6	39.6	173.6	C2'-endo
2 C	-40.8	44.7	-31.2	8.3	20.2	44.5	134.6	C1'-exo
3 C	-14.2	30.8	-34.6	27.3	-8.4	34.8	175.0	C2'-endo

5'-ACC-3' (PO- model) singly ionized / B3LYP-D

step overlap area (Å^2)
1 A/C 1.72
2 C/C 0.78

Local base step parameters

step	Shift	Slide	Rise	Tilt	Roll	Twist
1 A/C	-1.14	-0.25	2.71	8.85	-18.76	25.44
2 C/C	1.18	-1.28	4.78	-26.30	16.67	49.27
ave.	0.02	-0.77	3.75	-8.73	-1.05	37.35
s.d.	1.64	0.73	1.46	24.86	25.05	16.85

Local base helical parameters

step	X-disp	Y-disp	h-Rise	Incl.	Tip	h-Twist
1 A/C	2.18	3.27	1.96	-35.94	-16.96	32.72
2 C/C	-2.54	-3.13	3.28	18.07	28.52	57.76
ave.	-0.18	0.07	2.62	-8.93	5.78	45.24
s.d.	3.34	4.53	0.93	38.19	32.16	17.71

Sugar conformational parameters:

base	v0	v1	v2	v3	v4	tm	P	Puckering
1 A	-11.1	30.7	-37.2	32.0	-13.3	37.3	181.7	C3'-exo
2 C	-39.3	47.0	-35.9	14.2	15.4	45.8	141.6	C1'-exo
3 C	-10.3	27.7	-33.5	28.5	-11.7	33.5	181.2	C3'-exo

5'-AAC-3' (PO- model) neutral / B3LYP-D

step overlap area (Å^2)
1 A/A 5.73
2 A/C 4.91

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Local base step parameters

step	Shift	Slide	Rise	Tilt	Roll	Twist
1 A/A	0.63	0.59	3.22	-1.29	8.42	35.27
2 A/C	1.16	-1.33	4.06	-16.27	23.24	49.71
ave.	0.90	-0.37	3.64	-8.78	15.83	42.49
s.d.	0.38	1.35	0.60	10.60	10.48	10.21

****

Local base helical parameters

step	X-disp	Y-disp	h-Rise	Incl.	Tip	h-Twist
1 A/A	-0.24	-1.19	3.24	13.65	2.09	36.26
2 A/C	-2.86	-2.25	2.77	25.41	17.79	56.79
ave.	-1.55	-1.72	3.01	19.53	9.94	46.52
s.d.	1.85	0.74	0.33	8.31	11.10	14.52

****

Sugar conformational parameters:

base	v0	v1	v2	v3	v4	tm	P	Puckering
1 A	-29.6	42.7	-38.8	23.0	3.8	42.5	156.0	C2'-endo
2 A	-33.5	45.0	-38.3	19.9	8.2	44.0	150.4	C2'-endo
3 C	-8.4	26.1	-32.9	29.0	-13.2	33.0	184.3	C3'-exo

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5'-AAC-3' (PO- model) singly ionized / B3LYP-D

step overlap area (Å^2)
1 A/A 7.39
2 A/C 5.14

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Local base step parameters

step	Shift	Slide	Rise	Tilt	Roll	Twist
1 A/A	1.39	0.31	3.05	-0.53	5.07	37.53
2 A/C	1.72	-1.55	3.60	-11.45	12.82	54.63
ave.	1.56	-0.62	3.33	-5.99	8.94	46.08
s.d.	0.23	1.31	0.39	7.72	5.48	12.09

****

Local base helical parameters

step	X-disp	Y-disp	h-Rise	Incl.	Tip	h-Twist
1 A/A	-0.14	-2.21	3.05	7.83	0.82	37.87
2 A/C	-2.33	-2.44	2.82	13.59	12.14	57.07
ave.	-1.23	-2.32	2.94	10.71	6.48	47.47
s.d.	1.55	0.16	0.16	4.08	8.00	13.58

****

Sugar conformational parameters:

base	v0	v1	v2	v3	v4	tm	P	Puckering
1 A	-30.6	44.6	-40.6	24.5	3.4	44.2	156.6	C2'-endo
2 A	-37.4	47.0	-37.3	17.1	12.3	45.4	145.3	C2'-endo
3 C	-9.8	27.0	-33.0	28.2	-11.8	33.0	181.8	C3'-exo

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5'-CCA-3' (PO- model) neutral / B3LYP-D

step overlap area (Å^2)
1 C/C 2.60
2 C/A 2.42

Local base step parameters

step		Shift	Slide	Rise	Tilt	Roll	Twist
1	C/C	-0.73	0.02	2.57	11.17	-11.76	29.18
2	C/A	0.84	0.73	3.05	1.82	1.33	49.93
	ave.	0.06	0.37	2.81	6.49	-5.21	39.56
	s.d.	1.11	0.50	0.33	6.61	9.25	14.67

Local base helical parameters

step		X-disp	Y-disp	h-Rise	Incl.	Tip	h-Twist
1	C/C	1.50	2.67	2.02	-21.38	-20.31	33.30
2	C/A	0.77	-0.87	3.09	1.57	-2.15	49.98
	ave.	1.14	0.90	2.56	-9.90	-11.23	41.64
	s.d.	0.52	2.50	0.76	16.23	12.84	11.80

Sugar conformational parameters:

base		v0	v1	v2	v3	v4	tm	P	Puckering
1	C	-17.2	34.3	-37.4	28.5	-7.2	37.7	172.2	C2'-endo
2	C	-37.0	45.2	-35.9	15.2	13.4	44.4	143.9	C1'-exo
3	A	-10.2	28.1	-34.1	29.2	-12.1	34.1	181.7	C3'-exo

5'-CCA-3' (PO- model) singly ionized / B3LYP-D

step overlap area (Å^2)
1 C/C 2.73
2 C/A 4.52

Local base step parameters

step		Shift	Slide	Rise	Tilt	Roll	Twist
1	C/C	-0.38	-0.08	2.72	8.22	-17.58	32.61
2	C/A	1.70	1.14	2.83	8.14	7.74	57.77
	ave.	0.66	0.53	2.77	8.18	-4.92	45.19
	s.d.	1.47	0.86	0.08	0.05	17.90	17.79

Local base helical parameters

step		X-disp	Y-disp	h-Rise	Incl.	Tip	h-Twist
1	C/C	1.76	1.47	2.31	-28.38	-13.27	37.81
2	C/A	0.80	-1.35	3.14	7.93	-8.34	58.76
	ave.	1.28	0.06	2.72	-10.23	-10.80	48.29
	s.d.	0.68	1.99	0.59	25.68	3.49	14.81

Sugar conformational parameters:

base		v0	v1	v2	v3	v4	tm	P	Puckering
1	C	-18.2	35.7	-38.7	29.3	-7.1	39.2	171.6	C2'-endo
2	C	-38.5	46.9	-36.4	15.1	14.4	45.7	142.9	C1'-exo
3	A	11.2	9.7	-25.2	32.2	-27.6	32.1	218.4	C4'-endo

5'-CAA-3' (PO- model) neutral / B3LYP-D

step overlap area (Å^2)
1 C/A 1.94
2 A/A 4.91

Local base step parameters

step	Shift	Slide	Rise	Tilt	Roll	Twist
1 C/A	-0.07	0.70	2.68	11.14	-9.67	35.73
2 A/A	0.99	0.10	3.25	-3.66	8.81	48.46
ave.	0.46	0.40	2.97	3.74	-0.43	42.10
s.d.	0.75	0.42	0.40	10.47	13.07	9.00

Local base helical parameters

step	X-disp	Y-disp	h-Rise	Incl.	Tip	h-Twist
1 C/A	2.01	1.20	2.30	-15.00	-17.28	38.57
2 A/A	-0.53	-1.45	3.15	10.62	4.41	49.34
ave.	0.74	-0.13	2.72	-2.19	-6.44	43.95
s.d.	1.80	1.87	0.60	18.11	15.34	7.62

Sugar conformational parameters:

base	v0	v1	v2	v3	v4	tm	P	Puckering
1 C	-17.6	34.9	-38.0	28.9	-7.2	38.3	172.1	C2'-endo
2 A	-30.8	42.4	-37.3	20.2	6.4	42.0	152.6	C2'-endo
3 A	-10.2	28.1	-34.2	29.3	-12.2	34.2	181.7	C3'-exo

5'-CAA-3' (PO- model) singly ionized / B3LYP-D

step overlap area (Å^2)
1 C/A 0.00
2 A/A 5.75

Local base step parameters

step	Shift	Slide	Rise	Tilt	Roll	Twist
1 C/A	-1.83	0.38	2.28	15.65	-28.18	21.60
2 A/A	1.67	-0.12	3.03	-0.20	9.14	54.97
ave.	-0.08	0.13	2.66	7.72	-9.52	38.28
s.d.	2.48	0.35	0.53	11.21	26.39	23.60

Local base helical parameters

step	X-disp	Y-disp	h-Rise	Incl.	Tip	h-Twist
1 C/A	2.36	3.76	0.29	-49.87	-27.69	38.64
2 A/A	-0.62	-1.80	2.97	9.82	0.22	55.67
ave.	0.87	0.98	1.63	-20.02	-13.74	47.15
s.d.	2.11	3.93	1.90	42.21	19.73	12.04

Sugar conformational parameters:

base	v0	v1	v2	v3	v4	tm	P	Puckering
1 C	-15.6	32.4	-35.9	27.9	-7.9	36.2	173.7	C2'-endo
2 A	-33.3	45.7	-39.3	21.4	7.0	44.6	151.9	C2'-endo
3 A	2.9	17.2	-29.2	31.7	-22.0	31.9	203.7	C3'-exo

5'-ACC-3' (H model) neutral / M06-2X

step overlap area (Å^2)
1 A/C 3.90
2 C/C 3.56

Local base step parameters

step		Shift	Slide	Rise	Tilt	Roll	Twist
1	A/C	0.47	0.18	2.52	11.60	-0.45	33.60
2	C/C	0.06	0.02	2.71	7.22	-7.19	34.92
	ave.	0.26	0.10	2.62	9.41	-3.82	34.26
	s.d.	0.28	0.12	0.14	3.10	4.77	0.93

Local base helical parameters

step		X-disp	Y-disp	h-Rise	Incl.	Tip	h-Twist
1	A/C	0.35	0.59	2.54	-0.75	-19.36	35.50
2	C/C	0.87	0.74	2.62	-11.67	-11.73	36.33
	ave.	0.61	0.66	2.58	-6.21	-15.54	35.92
	s.d.	0.36	0.11	0.06	7.73	5.40	0.59

Sugar conformational parameters:

base		v0	v1	v2	v3	v4	tm	P	Puckering
1	A	-15.2	33.4	-37.9	30.3	-9.5	38.0	175.7	C2'-endo
2	C	-45.0	47.4	-32.3	7.2	23.4	47.9	132.5	C1'-exo
3	C	-46.7	44.5	-25.5	-1.0	29.6	47.1	122.8	C1'-exo

5'-ACC-3' singly ionized H model / M06-2X

step overlap area (Å^2)
1 A/C 3.06
2 C/C 4.60

Local base step parameters

step		Shift	Slide	Rise	Tilt	Roll	Twist
1	A/C	1.65	1.43	1.52	32.67	-5.82	43.81
2	C/C	0.23	0.63	3.26	-0.92	-2.20	34.51
	ave.	0.94	1.03	2.39	15.88	-4.01	39.16
	s.d.	1.00	0.56	1.22	23.75	2.56	6.57

Local base helical parameters

step		X-disp	Y-disp	h-Rise	Incl.	Tip	h-Twist
1	A/C	1.78	-0.58	2.04	-6.77	-38.02	54.46
2	C/C	1.40	-0.52	3.20	-3.70	1.54	34.59
	ave.	1.59	-0.55	2.62	-5.23	-18.24	44.53
	s.d.	0.27	0.04	0.82	2.17	27.97	14.05

Sugar conformational parameters:

base		v0	v1	v2	v3	v4	tm	P	Puckering
1	A	-12.2	28.1	-32.1	26.1	-8.8	32.1	176.9	C2'-endo
2	C	-44.2	46.9	-32.3	7.7	22.5	47.2	133.2	C1'-exo
3	C	-46.1	45.3	-27.5	1.4	27.7	47.1	125.7	C1'-exo

5'-AAC-3' neutral H model / M06-2X

step overlap area (Å^2)
1 A/A 5.40
2 A/C 4.17

Local base step parameters

step		Shift	Slide	Rise	Tilt	Roll	Twist
1	A/A	2.78	2.10	3.01	17.61	-15.86	51.36
2	A/C	0.61	0.01	2.73	6.72	2.99	35.08
	ave.	1.70	1.05	2.87	12.16	-6.44	43.22
	s.d.	1.53	1.48	0.20	7.70	13.33	11.51

Local base helical parameters

step		X-disp	Y-disp	h-Rise	Incl.	Tip	h-Twist
1	A/A	3.11	-1.97	3.02	-17.29	-19.20	56.22
2	A/C	-0.35	-0.17	2.79	4.90	-11.00	35.82
	ave.	1.38	-1.07	2.91	-6.20	-15.10	46.02
	s.d.	2.45	1.27	0.17	15.69	5.80	14.43

Sugar conformational parameters:

base		v0	v1	v2	v3	v4	tm	P	Puckering
1	A	-12.8	29.7	-34.3	27.9	-9.6	34.4	177.3	C2'-endo
2	A	-42.1	46.6	-33.8	10.5	19.5	46.3	136.8	C1'-exo
3	C	-46.9	45.6	-27.0	0.4	28.7	47.6	124.5	C1'-exo

5'-AAC-3' singly ionized H model / M06-2X

step overlap area (Å^2)
1 A/A 4.98
2 A/C 5.00

Local base step parameters

step		Shift	Slide	Rise	Tilt	Roll	Twist
1	A/A	0.82	1.84	2.85	6.70	-1.43	37.23
2	A/C	1.66	0.88	2.42	12.15	-3.39	43.49
	ave.	1.24	1.36	2.63	9.43	-2.41	40.36
	s.d.	0.59	0.68	0.30	3.85	1.39	4.42

Local base helical parameters

step		X-disp	Y-disp	h-Rise	Incl.	Tip	h-Twist
1	A/A	3.00	-0.51	2.88	-2.22	-10.39	37.84
2	A/C	1.39	-1.29	2.69	-4.47	-16.00	45.20
	ave.	2.20	-0.90	2.79	-3.34	-13.19	41.52
	s.d.	1.14	0.55	0.13	1.59	3.97	5.20

Sugar conformational parameters:

base		v0	v1	v2	v3	v4	tm	P	Puckering
1	A	-4.0	25.2	-35.5	34.3	-19.1	36.3	192.5	C3'-exo
2	A	-40.6	46.4	-34.6	12.6	17.2	45.7	139.3	C1'-exo
3	C	-47.1	44.3	-24.9	-1.8	30.3	47.2	121.8	C1'-exo

5'-CCA-3' neutral / H model / M06-2X

step overlap area (Å^2)
1 C/C 4.98
2 C/A 6.87

Local base step parameters

step	Shift	Slide	Rise	Tilt	Roll	Twist
1 C/C	0.04	0.95	2.56	10.36	2.00	29.72
2 C/A	1.84	0.99	2.78	8.85	-2.97	44.93
ave.	0.94	0.97	2.67	9.60	-0.49	37.32
s.d.	1.27	0.03	0.16	1.07	3.52	10.76

Local base helical parameters

step	X-disp	Y-disp	h-Rise	Incl.	Tip	h-Twist
1 C/C	1.44	1.47	2.49	3.75	-19.44	31.49
2 C/A	1.50	-1.67	3.00	-3.84	-11.43	45.84
ave.	1.47	-0.10	2.75	-0.04	-15.44	38.67
s.d.	0.04	2.22	0.36	5.37	5.66	10.15

Sugar conformational parameters:

base	v0	v1	v2	v3	v4	tm	P	Puckering
1 C	-34.0	42.6	-35.3	16.6	10.7	42.1	146.9	C2'-endo
2 C	-43.2	47.6	-34.3	10.3	20.3	47.5	136.3	C1'-exo
3 A	-44.9	45.0	-28.1	2.9	26.0	46.2	127.4	C1'-exo

5'-CCA-3' singly ionized / H model / M06-2X

step overlap area (Å^2)
1 C/C 4.90
2 C/A 1.41

Local base step parameters

step	Shift	Slide	Rise	Tilt	Roll	Twist
1 C/C	0.22	0.43	2.77	6.55	-1.44	32.14
2 C/A	0.30	0.10	2.30	13.69	-11.09	38.66
ave.	0.26	0.26	2.53	10.12	-6.26	35.40
s.d.	0.05	0.23	0.33	5.05	6.83	4.61

Local base helical parameters

step	X-disp	Y-disp	h-Rise	Incl.	Tip	h-Twist
1 C/C	0.97	0.56	2.74	-2.56	-11.68	32.82
2 C/A	0.95	0.59	2.18	-15.79	-19.49	42.35
ave.	0.96	0.58	2.46	-9.18	-15.58	37.58
s.d.	0.01	0.02	0.40	9.36	5.53	6.74

Sugar conformational parameters:

base	v0	v1	v2	v3	v4	tm	P	Puckering
1 C	-35.2	43.6	-35.7	16.4	11.6	43.0	146.1	C2'-endo
2 C	-45.3	48.3	-33.2	8.1	23.0	48.5	133.3	C1'-exo
3 A	-43.9	45.6	-29.6	5.3	23.7	45.9	130.2	C1'-exo

5'-CAA-3' neutral / H model / M06-2X

step overlap area (Å^2)
1 C/A 1.45
2 A/A 4.68

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Local base step parameters

step	Shift	Slide	Rise	Tilt	Roll	Twist
1 C/A	-0.59	0.49	2.48	17.64	-19.41	27.27
2 A/A	1.01	0.07	3.17	-2.30	5.94	51.11
ave.	0.21	0.28	2.83	7.67	-6.73	39.19
s.d.	1.13	0.30	0.49	14.10	17.93	16.86

****

Local base helical parameters

step	X-disp	Y-disp	h-Rise	Incl.	Tip	h-Twist
1 C/A	2.47	2.47	1.29	-33.05	-30.04	37.66
2 A/A	-0.31	-1.32	3.11	6.86	2.66	51.48
ave.	1.08	0.58	2.20	-13.10	-13.69	44.57
s.d.	1.97	2.68	1.29	28.22	23.12	9.77

****

Sugar conformational parameters:

base	v0	v1	v2	v3	v4	tm	P	Puckering
1 C	-18.7	33.6	-35.1	25.3	-4.2	35.9	168.1	C2'-endo
2 A	-42.3	46.5	-33.2	9.7	20.1	46.2	135.8	C1'-exo
3 A	-17.3	32.5	-34.5	25.6	-5.4	35.1	170.0	C2'-endo

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5'-CAA-3' singly ionized H model / M06-2X

step overlap area (Å^2)
1 C/A 0.00
2 A/A 3.83

****

Local base step parameters

step	Shift	Slide	Rise	Tilt	Roll	Twist
1 C/A	-1.63	0.61	1.82	29.17	-30.96	25.91
2 A/A	1.35	2.11	2.85	5.87	-0.18	55.91
ave.	-0.14	1.36	2.33	17.52	-15.57	40.91
s.d.	2.10	1.06	0.73	16.47	21.76	21.22

****

Local base helical parameters

step	X-disp	Y-disp	h-Rise	Incl.	Tip	h-Twist
1 C/A	1.43	2.61	-0.34	-43.71	-41.19	49.49
2 A/A	2.25	-1.14	2.96	-0.19	-6.24	56.19
ave.	1.84	0.73	1.31	-21.95	-23.72	52.84
s.d.	0.58	2.65	2.33	30.77	24.71	4.74

****

Sugar conformational parameters:

base	v0	v1	v2	v3	v4	tm	P	Puckering
1 C	-18.6	33.3	-34.9	25.1	-4.2	35.6	168.1	C2'-endo
2 A	-39.3	46.3	-35.8	14.6	15.1	45.4	141.9	C1'-exo
3 A	-17.7	32.7	-34.4	25.3	-4.9	35.0	169.2	C2'-endo

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5'-ACC-3' (Na model) neutral / M06-2X

step overlap area (Å^2)
1 A/C 3.78
2 C/C 2.86

Local base step parameters

step		Shift	Slide	Rise	Tilt	Roll	Twist
1	A/C	0.43	0.07	2.65	9.57	-0.47	34.64
2	C/C	0.15	0.27	2.92	3.43	-7.12	42.91
	ave.	0.29	0.17	2.78	6.50	-3.80	38.78
	s.d.	0.20	0.14	0.20	4.34	4.71	5.85

Local base helical parameters

step		X-disp	Y-disp	h-Rise	Incl.	Tip	h-Twist
1	A/C	0.16	0.44	2.67	-0.77	-15.70	35.90
2	C/C	0.97	0.09	2.85	-9.64	-4.64	43.60
	ave.	0.57	0.26	2.76	-5.20	-10.17	39.75
	s.d.	0.57	0.24	0.13	6.27	7.82	5.45

Sugar conformational parameters:

base		v0	v1	v2	v3	v4	tm	P	Puckering
1	A	-14.2	33.6	-39.0	32.1	-11.4	39.1	178.0	C2'-endo
2	C	-42.4	48.1	-35.5	12.0	18.8	47.5	138.3	C1'-exo
3	C	-24.0	36.5	-34.5	21.7	1.3	36.9	159.3	C2'-endo

5'-ACC-3' (Na model) singly ionized / M06-2X

step overlap area (Å^2)
1 A/C 4.51
2 C/C 3.32

Local base step parameters

step		Shift	Slide	Rise	Tilt	Roll	Twist
1	A/C	1.44	0.98	2.16	17.73	-3.77	42.02
2	C/C	0.27	0.59	3.04	1.87	-4.68	43.08
	ave.	0.86	0.78	2.60	9.80	-4.22	42.55
	s.d.	0.83	0.28	0.63	11.22	0.65	0.75

Local base helical parameters

step		X-disp	Y-disp	h-Rise	Incl.	Tip	h-Twist
1	A/C	1.51	-0.71	2.45	-4.98	-23.46	45.60
2	C/C	1.21	-0.20	2.98	-6.35	-2.54	43.36
	ave.	1.36	-0.46	2.71	-5.67	-13.00	44.48
	s.d.	0.21	0.36	0.37	0.96	14.80	1.58

Sugar conformational parameters:

base		v0	v1	v2	v3	v4	tm	P	Puckering
1	A	-8.7	30.2	-38.8	35.3	-16.7	39.0	186.3	C3'-exo
2	C	-41.0	48.1	-37.0	14.6	16.2	47.3	141.5	C1'-exo
3	C	-24.2	36.7	-34.7	21.8	1.4	37.1	159.2	C2'-endo

5'-AAC-3' (Na model) neutral / M06-2X

step overlap area (Å^2)
1 A/A 5.05
2 A/C 3.60

Local base step parameters

step		Shift	Slide	Rise	Tilt	Roll	Twist
1	A/A	0.20	1.31	2.94	3.61	10.45	26.42
2	A/C	0.82	0.12	2.76	6.87	1.01	44.68
	ave.	0.51	0.72	2.85	5.24	5.73	35.55
	s.d.	0.44	0.84	0.13	2.30	6.68	12.91

Local base helical parameters

step		X-disp	Y-disp	h-Rise	Incl.	Tip	h-Twist
1	A/A	0.33	0.39	3.22	21.70	-7.50	28.61
2	A/C	0.08	-0.54	2.85	1.32	-8.97	45.19
	ave.	0.20	-0.07	3.03	11.51	-8.23	36.90
	s.d.	0.18	0.66	0.26	14.41	1.04	11.72

Sugar conformational parameters:

base		v0	v1	v2	v3	v4	tm	P	Puckering
1	A	-27.3	39.7	-36.6	22.1	3.0	39.8	157.0	C2'-endo
2	A	-36.3	45.6	-37.2	17.6	11.5	44.7	146.5	C2'-endo
3	C	-25.6	37.6	-34.7	21.0	2.7	37.7	157.3	C2'-endo

5′-AAC-3′ (Na model) singly ionized / M06-2X

step overlap area (Å^2)
1 A/A 5.43
2 A/C 5.31

Local base step parameters

step		Shift	Slide	Rise	Tilt	Roll	Twist
1	A/A	0.86	1.58	2.88	4.85	2.12	35.70
2	A/C	1.53	0.55	2.44	12.07	-2.15	42.49
	ave.	1.20	1.06	2.66	8.46	-0.02	39.10
	s.d.	0.48	0.72	0.31	5.11	3.02	4.80

Sugar conformational parameters:

base		v0	v1	v2	v3	v4	tm	P	Puckering
1	A	-21.8	37.5	-38.2	27.0	-3.5	39.4	166.2	C2'-endo
2	A	-37.7	47.0	-38.0	17.8	12.0	45.8	146.0	C2'-endo
3	C	-45.2	45.7	-28.8	3.6	25.7	46.7	128.1	C1'-exo

5'-CCA-3' (Na model) neutral / M06-2X

step overlap area (Å^2)
1 C/C 1.89
2 C/A 1.50

Local base step parameters

step		Shift	Slide	Rise	Tilt	Roll	Twist
1	C/C	-0.84	-0.37	2.33	13.77	-16.10	26.71
2	C/A	0.68	0.54	2.95	1.98	-3.62	50.16
	ave.	-0.08	0.08	2.64	7.87	-9.86	38.43
	s.d.	1.07	0.65	0.44	8.34	8.82	16.58

Local base helical parameters

step		X-disp	Y-disp	h-Rise	Incl.	Tip	h-Twist
1	C/C	1.14	2.97	1.68	-29.63	-25.34	33.97
2	C/A	0.87	-0.67	2.93	-4.26	-2.33	50.31
	ave.	1.01	1.15	2.30	-16.95	-13.84	42.14
	s.d.	0.19	2.57	0.88	17.94	16.27	11.56

Sugar conformational parameters:

base		v0	v1	v2	v3	v4	tm	P	Puckering
1	C	-19.8	36.2	-38.0	27.7	-5.0	38.8	168.8	C2'-endo
2	C	-42.4	48.4	-35.8	12.4	18.5	47.7	138.7	C1'-exo
3	A	-14.7	31.0	-34.5	27.0	-7.9	34.7	174.2	C2'-endo

5'-CCA-3' (Na model) singly ionized / M06-2X

step overlap area (Å^2)
1 C/C 1.38
2 C/A 1.64

Local base step parameters

step		Shift	Slide	Rise	Tilt	Roll	Twist
1	C/C	-1.10	-0.54	2.62	9.87	-20.35	24.52
2	C/A	1.07	0.36	2.41	11.26	-11.19	54.34
	ave.	-0.01	-0.09	2.51	10.56	-15.77	39.43
	s.d.	1.53	0.64	0.15	0.98	6.47	21.08

Local base helical parameters

step		X-disp	Y-disp	h-Rise	Incl.	Tip	h-Twist
1	C/C	1.81	3.26	1.95	-38.94	-18.88	33.24
2	C/A	0.86	-0.65	2.46	-11.97	-12.04	56.44
	ave.	1.34	1.30	2.21	-25.45	-15.46	44.84
	s.d.	0.67	2.76	0.36	19.07	4.84	16.41

Sugar conformational parameters:

base		v0	v1	v2	v3	v4	tm	P	Puckering
1	C	-20.1	36.2	-37.8	27.3	-4.6	38.7	168.1	C2'-endo
2	C	-42.8	47.7	-34.2	10.4	20.0	47.2	136.4	C1'-exo
3	A	-10.7	28.1	-33.6	28.5	-11.4	33.6	180.6	C3'-exo

5'-CAA-3' (Na model) neutral / M06-2X

step overlap area (Å^2)
1 C/A 0.87
2 A/A 4.79

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Local base step parameters

	step	Shift	Slide	Rise	Tilt	Roll	Twist
1	C/A	-0.72	0.11	2.46	13.44	-15.83	28.77
2	A/A	1.10	-0.03	3.17	-2.44	4.59	51.63
	ave.	0.19	0.04	2.81	5.50	-5.62	40.20
	s.d.	1.28	0.10	0.50	11.23	14.44	16.16

****

Local base helical parameters

	step	X-disp	Y-disp	h-Rise	Incl.	Tip	h-Twist
1	C/A	1.83	2.58	1.69	-27.76	-23.57	35.35
2	A/A	-0.33	-1.41	3.10	5.25	2.80	51.87
	ave.	0.75	0.59	2.40	-11.25	-10.39	43.61
	s.d.	1.53	2.82	1.00	23.35	18.64	11.68

****

Sugar conformational parameters:

base		v0	v1	v2	v3	v4	tm	P	Puckering
1	C	-19.7	36.0	-37.8	27.6	-5.0	38.5	168.7	C2'-endo
2	A	-35.9	45.1	-36.8	17.1	11.6	44.2	146.4	C2'-endo
3	A	-14.1	30.7	-34.5	27.4	-8.5	34.7	175.2	C2'-endo

****

5'-CAA-3' (Na model) singly ionized / M06-2X

step overlap area (Å^2)
1 C/A 0.00
2 A/A 5.61

****

Local base step parameters

	step	Shift	Slide	Rise	Tilt	Roll	Twist
1	C/A	-1.72	0.64	2.17	18.97	-31.63	25.46
2	A/A	1.38	-0.12	3.04	-0.69	5.24	50.27
	ave.	-0.17	0.26	2.60	9.14	-13.20	37.86
	s.d.	2.19	0.54	0.62	13.91	26.07	17.55

****

Local base helical parameters

	step	X-disp	Y-disp	h-Rise	Incl.	Tip	h-Twist
1	C/A	2.16	3.05	0.09	-48.49	-29.09	44.56
2	A/A	-0.48	-1.66	3.00	6.14	0.81	50.53
	ave.	0.84	0.70	1.54	-21.17	-14.14	47.55
	s.d.	1.87	3.33	2.06	38.64	21.14	4.22

****

Sugar conformational parameters:

base		v0	v1	v2	v3	v4	tm	P	Puckering
1	C	-19.8	34.9	-36.2	25.9	-3.9	37.1	167.4	C2'-endo
2	A	-30.2	42.1	-37.2	21.0	5.5	41.5	153.6	C2'-endo
3	A	-15.2	31.3	-34.5	26.8	-7.5	34.7	173.4	C2'-endo

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5'-ACC-3' (PO- model) neutral / M06-2X

step overlap area (Å^2)
1 A/C 4.22
2 C/C 1.07

Local base step parameters

step	Shift	Slide	Rise	Tilt	Roll	Twist
1 A/C	0.59	-0.08	2.76	6.37	1.70	34.48
2 C/C	1.08	-1.15	4.34	-19.31	14.17	48.66
ave.	0.83	-0.61	3.55	-6.47	7.93	41.57
s.d.	0.35	0.76	1.12	18.16	8.82	10.03

Local base helical parameters

step	X-disp	Y-disp	h-Rise	Incl.	Tip	h-Twist
1 A/C	-0.35	-0.15	2.81	2.84	-10.63	35.08
2 C/C	-2.36	-2.68	3.30	16.11	21.96	53.92
ave.	-1.35	-1.41	3.06	9.47	5.66	44.50
s.d.	1.43	1.79	0.35	9.39	23.05	13.32

Sugar conformational parameters:

base	v0	v1	v2	v3	v4	tm	P	Puckering
1 A	-26.1	40.9	-39.4	25.7	-0.0	41.6	161.2	C2'-endo
2 C	-43.0	45.8	-30.8	6.7	22.5	45.9	132.2	C1'-exo
3 C	-16.8	32.3	-34.7	25.9	-5.9	35.1	170.7	C2'-endo

5'-ACC-3' (PO- model) singly ionized / M06-2X

step overlap area (Å^2)
1 A/C 1.74
2 C/C 0.19

Local base step parameters

step	Shift	Slide	Rise	Tilt	Roll	Twist
1 A/C	-1.15	-0.30	2.81	7.85	-19.51	25.54
2 C/C	1.06	-1.52	5.11	-31.63	17.04	47.84
ave.	-0.04	-0.91	3.96	-11.89	-1.24	36.69
s.d.	1.56	0.87	1.63	27.92	25.85	15.77

Local base helical parameters

step	X-disp	Y-disp	h-Rise	Incl.	Tip	h-Twist
1 A/C	2.29	3.16	2.09	-37.13	-14.94	32.98
2 C/C	-2.80	-3.41	3.25	18.33	34.02	59.19
ave.	-0.25	-0.12	2.67	-9.40	9.54	46.08
s.d.	3.60	4.65	0.82	39.21	34.62	18.53

Sugar conformational parameters:

base	v0	v1	v2	v3	v4	tm	P	Puckering
1 A	-12.9	32.1	-37.9	31.8	-12.0	37.9	179.4	C2'-endo
2 C	-41.1	47.8	-35.5	12.8	17.4	46.7	139.5	C1'-exo
3 C	-14.1	30.3	-34.1	27.0	-8.3	34.3	175.1	C2'-endo

5'-AAC-3' (PO- model) neutral / M06-2X

step overlap area (Å^2)
1 A/A 5.78
2 A/C 4.92

****

Local base step parameters

step		Shift	Slide	Rise	Tilt	Roll	Twist
1	A/A	0.74	0.49	3.19	-0.68	7.64	37.10
2	A/C	1.17	-1.38	4.05	-16.08	20.29	49.33
	ave.	0.95	-0.44	3.62	-8.38	13.96	43.22
	s.d.	0.31	1.32	0.61	10.89	8.94	8.65

****

Local base helical parameters

step		X-disp	Y-disp	h-Rise	Incl.	Tip	h-Twist
1	A/A	-0.21	-1.23	3.22	11.85	1.06	37.86
2	A/C	-2.83	-2.33	2.85	22.60	17.92	55.34
	ave.	-1.52	-1.78	3.03	17.23	9.49	46.60
	s.d.	1.85	0.78	0.26	7.60	11.92	12.36

****

Sugar conformational parameters:

base		v0	v1	v2	v3	v4	tm	P	Puckering
1	A	-31.7	44.1	-39.2	22.4	5.5	43.7	154.0	C2'-endo
2	A	-34.1	45.1	-38.0	19.5	8.9	44.1	149.6	C2'-endo
3	C	-12.8	29.0	-33.3	26.9	-9.1	33.4	176.8	C2'-endo

****

5'-AAC-3' (PO- model) singly ionized / M06-2X

step overlap area (Å^2)
1 A/A 7.04
2 A/C 4.97

****

Local base step parameters

step		Shift	Slide	Rise	Tilt	Roll	Twist
1	A/A	1.53	0.34	3.05	0.20	4.99	41.93
2	A/C	1.81	0.05	2.62	10.82	1.32	55.74
	ave.	1.67	0.19	2.83	5.51	3.15	48.84
	s.d.	0.20	0.20	0.30	7.51	2.59	9.77

****

Local base helical parameters

step		X-disp	Y-disp	h-Rise	Incl.	Tip	h-Twist
1	A/A	-0.01	-2.10	3.07	6.94	-0.28	42.21
2	A/C	-0.01	-1.39	2.90	1.40	-11.45	56.72
	ave.	-0.01	-1.75	2.99	4.17	-5.87	49.46
	s.d.	0.00	0.50	0.12	3.92	7.90	10.25

****

Sugar conformational parameters:

base		v0	v1	v2	v3	v4	tm	P	Puckering
1	A	-32.1	45.5	-40.9	24.0	4.7	45.1	155.2	C2'-endo
2	A	-39.2	47.4	-36.3	15.1	14.6	45.9	142.4	C1'-exo
3	C	2.4	18.0	-30.1	32.5	-22.2	32.7	202.9	C3'-exo

****

5'-CCA-3' (PO- model) neutral / M06-2X

step overlap area (Å^2)
1 C/C 1.86
2 C/A 1.85

****

Local base step parameters

	step	Shift	Slide	Rise	Tilt	Roll	Twist
1	C/C	-0.84	-0.30	2.42	12.27	-15.92	28.06
2	C/A	0.78	0.59	2.98	2.19	-0.86	50.39
	ave.	-0.03	0.14	2.70	7.23	-8.39	39.22
	s.d.	1.14	0.63	0.39	7.13	10.65	15.79

****

Local base helical parameters

	step	X-disp	Y-disp	h-Rise	Incl.	Tip	h-Twist
1	C/C	1.28	2.80	1.83	-28.65	-22.08	34.40
2	C/A	0.74	-0.77	3.00	-1.01	-2.57	50.44
	ave.	1.01	1.01	2.41	-14.83	-12.33	42.42
	s.d.	0.38	2.53	0.82	19.54	13.79	11.34

****

Sugar conformational parameters:

base		v0	v1	v2	v3	v4	tm	P	Puckering
1	C	-20.8	37.0	-38.4	27.6	-4.4	39.3	167.7	C2'-endo
2	C	-38.7	47.1	-37.4	16.1	13.9	46.2	144.0	C2'-endo
3	A	-11.8	29.2	-34.4	28.6	-10.8	34.5	179.1	C2'-endo

****

5'-CCA-3' (PO- model) singly ionized / M06-2X

step overlap area (Å^2)
1 C/C 1.37
2 C/A 2.05

****

Local base step parameters

	step	Shift	Slide	Rise	Tilt	Roll	Twist
1	C/C	-1.07	-0.54	2.72	7.56	-18.21	25.19
2	C/A	1.22	0.42	2.43	11.90	-6.02	55.41
	ave.	0.08	-0.06	2.58	9.73	-12.11	40.30
	s.d.	1.62	0.68	0.20	3.07	8.62	21.37

****

Local base helical parameters

	step	X-disp	Y-disp	h-Rise	Incl.	Tip	h-Twist
1	C/C	1.83	3.11	2.21	-35.60	-14.78	31.89
2	C/A	0.70	-0.77	2.57	-6.37	-12.59	56.87
	ave.	1.27	1.17	2.39	-20.98	-13.68	44.38
	s.d.	0.80	2.75	0.25	20.67	1.54	17.66

****

Sugar conformational parameters:

base		v0	v1	v2	v3	v4	tm	P	Puckering
1	C	-20.4	36.6	-38.1	27.4	-4.5	38.9	167.9	C2'-endo
2	C	-42.9	47.5	-33.4	9.5	20.6	46.9	135.3	C1'-exo
3	A	10.1	11.6	-27.0	33.5	-27.7	33.2	215.7	C3'-exo

****

5'-CAA-3' (PO- model) neutral / M06-2X

step overlap area (Å^2)
1 C/A 0.72
2 A/A 4.81

Local base step parameters

step	Shift	Slide	Rise	Tilt	Roll	Twist
1 C/A	-0.78	0.18	2.45	13.79	-17.19	29.34
2 A/A	1.08	0.00	3.18	-2.47	5.98	50.96
ave.	0.15	0.09	2.82	5.66	-5.60	40.15
s.d.	1.32	0.13	0.51	11.50	16.38	15.29

Local base helical parameters

step	X-disp	Y-disp	h-Rise	Incl.	Tip	h-Twist
1 C/A	1.93	2.57	1.61	-29.29	-23.50	36.55
2 A/A	-0.40	-1.40	3.11	6.92	2.86	51.34
ave.	0.77	0.58	2.36	-11.19	-10.32	43.94
s.d.	1.64	2.81	1.06	25.60	18.64	10.46

Sugar conformational parameters:

base	v0	v1	v2	v3	v4	tm	P	Puckering
1 C	-20.6	36.8	-38.2	27.5	-4.4	39.1	167.7	C2'-endo
2 A	-33.1	44.4	-38.2	20.1	8.0	43.7	150.9	C2'-endo
3 A	-12.7	29.9	-34.6	28.4	-10.0	34.7	177.8	C2'-endo

5'-CAA-3' (PO- model) singly ionized / M06-2X

step overlap area (Å^2)
1 C/A 0.00
2 A/A 5.16

Local base step parameters

step	Shift	Slide	Rise	Tilt	Roll	Twist
1 C/A	-1.85	0.68	2.38	15.49	-35.03	25.04
2 A/A	1.31	-0.15	2.97	1.72	4.33	52.90
ave.	-0.27	0.27	2.67	8.61	-15.35	38.97
s.d.	2.23	0.59	0.42	9.74	27.83	19.70

Local base helical parameters

step	X-disp	Y-disp	h-Rise	Incl.	Tip	h-Twist
1 C/A	2.50	3.10	0.20	-53.07	-23.47	45.50
2 A/A	-0.42	-1.37	2.99	4.85	-1.92	53.09
ave.	1.04	0.87	1.59	-24.11	-12.70	49.30
s.d.	2.06	3.16	1.97	40.95	15.24	5.37

Sugar conformational parameters:

base	v0	v1	v2	v3	v4	tm	P	Puckering
1 C	-20.2	35.6	-36.8	26.3	-3.9	37.7	167.3	C2'-endo
2 A	-22.7	39.6	-40.0	28.4	-3.9	41.2	166.2	C2'-endo
3 A	1.3	18.5	-29.7	31.3	-20.7	31.8	200.8	C3'-exo

Optimized Geometries. Cartesian coordinates (Å), PDB format

```
COMPND    ACC / M06-2X / H MODEL / NEUTRAL
ATOM      1  O5'  DA A   1       0.000   0.000   0.000  1.00  0.00           O
ATOM      2  C5'  DA A   1       0.000   0.000   1.415  1.00  0.00           C
ATOM      3  C4'  DA A   1       1.436   0.000   1.905  1.00  0.00           C
ATOM      4  O4'  DA A   1       2.090  -1.207   1.507  1.00  0.00           O
ATOM      5  C3'  DA A   1       2.295   1.128   1.326  1.00  0.00           C
ATOM      6  O3'  DA A   1       3.346   1.362   2.298  1.00  0.00           O
ATOM      7  C2'  DA A   1       2.872   0.494   0.076  1.00  0.00           C
ATOM      8  C1'  DA A   1       3.122  -0.927   0.571  1.00  0.00           C
ATOM      9  N9   DA A   1       3.128  -1.919  -0.479  1.00  0.00           N
ATOM     10  C8   DA A   1       2.477  -1.914  -1.693  1.00  0.00           C
ATOM     11  N7   DA A   1       2.798  -2.920  -2.466  1.00  0.00           N
ATOM     12  C5   DA A   1       3.703  -3.643  -1.713  1.00  0.00           C
ATOM     13  C6   DA A   1       4.483  -4.782  -1.986  1.00  0.00           C
ATOM     14  N6   DA A   1       4.502  -5.355  -3.214  1.00  0.00           N
ATOM     15  N1   DA A   1       5.280  -5.265  -1.024  1.00  0.00           N
ATOM     16  C2   DA A   1       5.358  -4.595   0.135  1.00  0.00           C
ATOM     17  N3   DA A   1       4.730  -3.479   0.493  1.00  0.00           N
ATOM     18  C4   DA A   1       3.915  -3.046  -0.475  1.00  0.00           C
ATOM     19  P    DC A   2       4.449   2.494   2.078  1.00  0.00           P
ATOM     20  OP1  DC A   2       3.747   3.891   2.384  1.00  0.00           O
ATOM     21  OP2  DC A   2       5.104   2.544   0.755  1.00  0.00           O
ATOM     22  O5'  DC A   2       5.388   2.268   3.338  1.00  0.00           O
ATOM     23  C5'  DC A   2       5.607   1.010   4.001  1.00  0.00           C
ATOM     24  C4'  DC A   2       6.725   0.219   3.361  1.00  0.00           C
ATOM     25  O4'  DC A   2       6.268  -0.392   2.157  1.00  0.00           O
ATOM     26  C3'  DC A   2       7.968   1.059   2.970  1.00  0.00           C
ATOM     27  O3'  DC A   2       9.104   0.373   3.539  1.00  0.00           O
ATOM     28  C2'  DC A   2       7.983   0.966   1.449  1.00  0.00           C
ATOM     29  C1'  DC A   2       7.401  -0.435   1.282  1.00  0.00           C
ATOM     30  N1   DC A   2       6.977  -0.850  -0.031  1.00  0.00           N
ATOM     31  C2   DC A   2       7.334  -2.158  -0.472  1.00  0.00           C
ATOM     32  O2   DC A   2       8.010  -2.873   0.259  1.00  0.00           O
ATOM     33  N3   DC A   2       6.897  -2.550  -1.700  1.00  0.00           N
ATOM     34  C4   DC A   2       6.163  -1.745  -2.444  1.00  0.00           C
ATOM     35  N4   DC A   2       5.790  -2.190  -3.666  1.00  0.00           N
ATOM     36  C5   DC A   2       5.786  -0.422  -2.029  1.00  0.00           C
ATOM     37  C6   DC A   2       6.219  -0.027  -0.808  1.00  0.00           C
ATOM     38  P    DC A   3      10.570   1.002   3.484  1.00  0.00           P
ATOM     39  OP1  DC A   3      10.521   2.344   4.344  1.00  0.00           O
ATOM     40  OP2  DC A   3      11.130   1.288   2.148  1.00  0.00           O
ATOM     41  O5'  DC A   3      11.377  -0.008   4.406  1.00  0.00           O
ATOM     42  C5'  DC A   3      11.026  -1.388   4.610  1.00  0.00           C
ATOM     43  C4'  DC A   3      11.498  -2.267   3.478  1.00  0.00           C
ATOM     44  O4'  DC A   3      10.720  -2.022   2.309  1.00  0.00           O
ATOM     45  C3'  DC A   3      12.984  -2.084   3.073  1.00  0.00           C
ATOM     46  O3'  DC A   3      13.618  -3.328   3.312  1.00  0.00           O
ATOM     47  C2'  DC A   3      12.889  -1.749   1.582  1.00  0.00           C
ATOM     48  C1'  DC A   3      11.563  -2.411   1.224  1.00  0.00           C
ATOM     49  N1   DC A   3      10.963  -2.021  -0.031  1.00  0.00           N
ATOM     50  C2   DC A   3      10.721  -3.008  -1.022  1.00  0.00           C
ATOM     51  O2   DC A   3      11.086  -4.163  -0.819  1.00  0.00           O
ATOM     52  N3   DC A   3      10.116  -2.613  -2.177  1.00  0.00           N
ATOM     53  C4   DC A   3       9.735  -1.358  -2.337  1.00  0.00           C
ATOM     54  N4   DC A   3       9.128  -1.028  -3.498  1.00  0.00           N
ATOM     55  C5   DC A   3       9.969  -0.337  -1.356  1.00  0.00           C
ATOM     56  C6   DC A   3      10.589  -0.728  -0.217  1.00  0.00           C
END

COMPND    ACC / M06-2X / H MODEL / SINGLY IONIZED
ATOM      1  O5'  DA A   1       0.000   0.000   0.000  1.00  0.00           O
ATOM      2  C5'  DA A   1       0.000   0.000   1.418  1.00  0.00           C
ATOM      3  C4'  DA A   1       1.441   0.000   1.890  1.00  0.00           C
ATOM      4  O4'  DA A   1       2.067  -1.240   1.524  1.00  0.00           O
ATOM      5  C3'  DA A   1       2.285   1.102   1.242  1.00  0.00           C
ATOM      6  O3'  DA A   1       3.317   1.478   2.184  1.00  0.00           O
ATOM      7  C2'  DA A   1       2.913   0.402   0.054  1.00  0.00           C
ATOM      8  C1'  DA A   1       3.072  -1.025   0.568  1.00  0.00           C
ATOM      9  N9   DA A   1       2.943  -1.997  -0.521  1.00  0.00           N
ATOM     10  C8   DA A   1       1.930  -2.114  -1.407  1.00  0.00           C
ATOM     11  N7   DA A   1       2.165  -3.001  -2.391  1.00  0.00           N
ATOM     12  C5   DA A   1       3.388  -3.462  -2.120  1.00  0.00           C
ATOM     13  C6   DA A   1       4.254  -4.396  -2.781  1.00  0.00           C
ATOM     14  N6   DA A   1       3.898  -5.004  -3.889  1.00  0.00           N
ATOM     15  N1   DA A   1       5.470  -4.652  -2.239  1.00  0.00           N
ATOM     16  C2   DA A   1       5.808  -4.033  -1.132  1.00  0.00           C
ATOM     17  N3   DA A   1       5.075  -3.136  -0.389  1.00  0.00           N
ATOM     18  C4   DA A   1       3.926  -2.878  -0.933  1.00  0.00           C
ATOM     19  P    DC A   2       4.239   2.745   1.849  1.00  0.00           P
ATOM     20  OP1  DC A   2       3.611   3.992   2.611  1.00  0.00           O
ATOM     21  OP2  DC A   2       4.403   3.051   0.415  1.00  0.00           O
ATOM     22  O5'  DC A   2       5.547   2.441   2.701  1.00  0.00           O
ATOM     23  C5'  DC A   2       6.086   1.134   2.957  1.00  0.00           C
ATOM     24  C4'  DC A   2       6.984   0.658   1.839  1.00  0.00           C
ATOM     25  O4'  DC A   2       6.196   0.254   0.723  1.00  0.00           O
ATOM     26  C3'  DC A   2       7.973   1.723   1.300  1.00  0.00           C
ATOM     27  O3'  DC A   2       9.268   1.092   1.314  1.00  0.00           O
ATOM     28  C2'  DC A   2       7.488   1.963  -0.127  1.00  0.00           C
ATOM     29  C1'  DC A   2       6.967   0.568  -0.445  1.00  0.00           C
ATOM     30  N1   DC A   2       6.133   0.373  -1.607  1.00  0.00           N
ATOM     31  C2   DC A   2       6.150  -0.921  -2.200  1.00  0.00           C
ATOM     32  O2   DC A   2       7.004  -1.727  -1.843  1.00  0.00           O
ATOM     33  N3   DC A   2       5.182  -1.221  -3.109  1.00  0.00           N
ATOM     34  C4   DC A   2       4.346  -0.274  -3.526  1.00  0.00           C
ATOM     35  N4   DC A   2       3.394  -0.631  -4.397  1.00  0.00           N
ATOM     36  C5   DC A   2       4.420   1.086  -3.072  1.00  0.00           C
ATOM     37  C6   DC A   2       5.305   1.346  -2.083  1.00  0.00           C
ATOM     38  P    DC A   3      10.600   1.887   0.942  1.00  0.00           P
ATOM     39  OP1  DC A   3      10.754   3.043   2.031  1.00  0.00           O
ATOM     40  OP2  DC A   3      10.681   2.469  -0.413  1.00  0.00           O
ATOM     41  O5'  DC A   3      11.719   0.832   1.333  1.00  0.00           O
ATOM     42  C5'  DC A   3      11.509  -0.587   1.456  1.00  0.00           C
ATOM     43  C4'  DC A   3      11.576  -1.275   0.115  1.00  0.00           C
ATOM     44  O4'  DC A   3      10.436  -0.925  -0.665  1.00  0.00           O
ATOM     45  C3'  DC A   3      12.824  -0.924  -0.737  1.00  0.00           C
ATOM     46  O3'  DC A   3      13.497  -2.146  -0.984  1.00  0.00           O
ATOM     47  C2'  DC A   3      12.210  -0.330  -2.007  1.00  0.00           C
ATOM     48  C1'  DC A   3      10.863  -1.044  -2.022  1.00  0.00           C
ATOM     49  N1   DC A   3       9.847  -0.518  -2.904  1.00  0.00           N
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ATOM     50  C2   DC A   3       9.219  -1.392  -3.834  1.00  0.00           C
ATOM     51  O2   DC A   3       9.577  -2.563  -3.893  1.00  0.00           O
ATOM     52  N3   DC A   3       8.257  -0.868  -4.643  1.00  0.00           N
ATOM     53  C4   DC A   3       7.906   0.402  -4.533  1.00  0.00           C
ATOM     54  N4   DC A   3       6.938   0.854  -5.352  1.00  0.00           N
ATOM     55  C5   DC A   3       8.514   1.307  -3.598  1.00  0.00           C
ATOM     56  C6   DC A   3       9.481   0.790  -2.805  1.00  0.00           C
END

COMPND    AAC / M06-2X / H MODEL / NEUTRAL
ATOM      1  O5'  DA A   1       0.000   0.000   0.000  1.00  0.00           O
ATOM      2  C5'  DA A   1       0.000   0.000   1.416  1.00  0.00           C
ATOM      3  C4'  DA A   1       1.437   0.000   1.902  1.00  0.00           C
ATOM      4  O4'  DA A   1       2.071  -1.237   1.568  1.00  0.00           O
ATOM      5  C3'  DA A   1       2.297   1.090   1.257  1.00  0.00           C
ATOM      6  O3'  DA A   1       3.333   1.423   2.217  1.00  0.00           O
ATOM      7  C2'  DA A   1       2.913   0.380   0.067  1.00  0.00           C
ATOM      8  C1'  DA A   1       3.098  -1.035   0.609  1.00  0.00           C
ATOM      9  N9   DA A   1       3.019  -2.051  -0.417  1.00  0.00           N
ATOM     10  C8   DA A   1       2.054  -2.195  -1.389  1.00  0.00           C
ATOM     11  N7   DA A   1       2.277  -3.195  -2.203  1.00  0.00           N
ATOM     12  C5   DA A   1       3.452  -3.750  -1.736  1.00  0.00           C
ATOM     13  C6   DA A   1       4.243  -4.830  -2.176  1.00  0.00           C
ATOM     14  N6   DA A   1       3.911  -5.571  -3.252  1.00  0.00           N
ATOM     15  N1   DA A   1       5.353  -5.137  -1.487  1.00  0.00           N
ATOM     16  C2   DA A   1       5.665  -4.395  -0.412  1.00  0.00           C
ATOM     17  N3   DA A   1       5.020  -3.351   0.094  1.00  0.00           N
ATOM     18  C4   DA A   1       3.923  -3.066  -0.619  1.00  0.00           C
ATOM     19  P    DA A   2       4.256   2.702   1.966  1.00  0.00           P
ATOM     20  OP1  DA A   2       3.596   3.918   2.756  1.00  0.00           O
ATOM     21  OP2  DA A   2       4.470   3.074   0.554  1.00  0.00           O
ATOM     22  O5'  DA A   2       5.539   2.372   2.849  1.00  0.00           O
ATOM     23  C5'  DA A   2       6.015   1.050   3.147  1.00  0.00           C
ATOM     24  C4'  DA A   2       6.918   0.525   2.055  1.00  0.00           C
ATOM     25  O4'  DA A   2       6.131   0.224   0.904  1.00  0.00           O
ATOM     26  C3'  DA A   2       8.006   1.518   1.580  1.00  0.00           C
ATOM     27  O3'  DA A   2       9.228   0.755   1.520  1.00  0.00           O
ATOM     28  C2'  DA A   2       7.543   1.895   0.179  1.00  0.00           C
ATOM     29  C1'  DA A   2       6.919   0.570  -0.238  1.00  0.00           C
ATOM     30  N9   DA A   2       6.099   0.590  -1.412  1.00  0.00           N
ATOM     31  C8   DA A   2       5.382   1.633  -1.964  1.00  0.00           C
ATOM     32  N7   DA A   2       4.776   1.315  -3.078  1.00  0.00           N
ATOM     33  C5   DA A   2       5.113  -0.011  -3.280  1.00  0.00           C
ATOM     34  C6   DA A   2       4.862  -0.910  -4.335  1.00  0.00           C
ATOM     35  N6   DA A   2       4.184  -0.532  -5.446  1.00  0.00           N
ATOM     36  N1   DA A   2       5.372  -2.146  -4.266  1.00  0.00           N
ATOM     37  C2   DA A   2       6.166  -2.450  -3.228  1.00  0.00           C
ATOM     38  N3   DA A   2       6.514  -1.686  -2.196  1.00  0.00           N
ATOM     39  C4   DA A   2       5.943  -0.479  -2.269  1.00  0.00           C
ATOM     40  P    DC A   3      10.622   1.416   1.124  1.00  0.00           P
ATOM     41  OP2  DC A   3      10.713   2.092  -0.189  1.00  0.00           O
ATOM     42  OP1  DC A   3      10.944   2.394   2.345  1.00  0.00           O
ATOM     43  O5'  DC A   3      11.614   0.205   1.369  1.00  0.00           O
ATOM     44  C5'  DC A   3      11.241  -1.182   1.287  1.00  0.00           C
ATOM     45  C4'  DC A   3      11.233  -1.679  -0.137  1.00  0.00           C
ATOM     46  O4'  DC A   3      10.133  -1.119  -0.852  1.00  0.00           O
ATOM     47  C3'  DC A   3      12.511  -1.346  -0.950  1.00  0.00           C
ATOM     48  O3'  DC A   3      13.071  -2.587  -1.340  1.00  0.00           O
ATOM     49  C2'  DC A   3      11.959  -0.555  -2.139  1.00  0.00           C
ATOM     50  C1'  DC A   3      10.550  -1.130  -2.218  1.00  0.00           C
ATOM     51  N1   DC A   3       9.595  -0.419  -3.038  1.00  0.00           N
ATOM     52  C2   DC A   3       8.961  -1.110  -4.107  1.00  0.00           C
ATOM     53  O2   DC A   3       9.236  -2.288  -4.310  1.00  0.00           O
ATOM     54  N3   DC A   3       8.075  -0.413  -4.872  1.00  0.00           N
ATOM     55  C4   DC A   3       7.801   0.850  -4.602  1.00  0.00           C
ATOM     56  N4   DC A   3       6.918   1.484  -5.408  1.00  0.00           N
ATOM     57  C5   DC A   3       8.418   1.572  -3.524  1.00  0.00           C
ATOM     58  C6   DC A   3       9.314   0.888  -2.774  1.00  0.00           C
END

COMPND    AAC / M06-2X / H MODEL / SINGLY IONIZED
ATOM      1  O5'  DA A   1       0.000   0.000   0.000  1.00  0.00           O
ATOM      2  C5'  DA A   1       0.000   0.000   1.415  1.00  0.00           C
ATOM      3  C4'  DA A   1       1.436   0.000   1.909  1.00  0.00           C
ATOM      4  O4'  DA A   1       2.114  -1.187   1.491  1.00  0.00           O
ATOM      5  C3'  DA A   1       2.298   1.138   1.363  1.00  0.00           C
ATOM      6  O3'  DA A   1       3.383   1.295   2.311  1.00  0.00           O
ATOM      7  C2'  DA A   1       2.818   0.564   0.056  1.00  0.00           C
ATOM      8  C1'  DA A   1       3.001  -0.909   0.424  1.00  0.00           C
ATOM      9  N9   DA A   1       2.750  -1.826  -0.678  1.00  0.00           N
ATOM     10  C8   DA A   1       2.043  -1.653  -1.844  1.00  0.00           C
ATOM     11  N7   DA A   1       1.958  -2.739  -2.576  1.00  0.00           N
ATOM     12  C5   DA A   1       2.622  -3.692  -1.839  1.00  0.00           C
ATOM     13  C6   DA A   1       2.900  -5.060  -2.068  1.00  0.00           C
ATOM     14  N6   DA A   1       2.529  -5.680  -3.195  1.00  0.00           N
ATOM     15  N1   DA A   1       3.570  -5.742  -1.125  1.00  0.00           N
ATOM     16  C2   DA A   1       3.974  -5.089  -0.029  1.00  0.00           C
ATOM     17  N3   DA A   1       3.808  -3.803   0.290  1.00  0.00           N
ATOM     18  C4   DA A   1       3.121  -3.155  -0.655  1.00  0.00           C
ATOM     19  P    DA A   2       4.486   2.433   2.133  1.00  0.00           P
ATOM     20  OP1  DA A   2       3.801   3.813   2.532  1.00  0.00           O
ATOM     21  OP2  DA A   2       5.109   2.554   0.799  1.00  0.00           O
ATOM     22  O5'  DA A   2       5.471   2.124   3.341  1.00  0.00           O
ATOM     23  C5'  DA A   2       5.625   0.851   3.991  1.00  0.00           C
ATOM     24  C4'  DA A   2       6.649  -0.010   3.288  1.00  0.00           C
ATOM     25  O4'  DA A   2       6.102  -0.481   2.051  1.00  0.00           O
ATOM     26  C3'  DA A   2       7.966   0.715   2.918  1.00  0.00           C
ATOM     27  O3'  DA A   2       9.018  -0.200   3.277  1.00  0.00           O
ATOM     28  C2'  DA A   2       7.874   0.852   1.402  1.00  0.00           C
ATOM     29  C1'  DA A   2       7.151  -0.451   1.095  1.00  0.00           C
ATOM     30  N9   DA A   2       6.563  -0.578  -0.221  1.00  0.00           N
ATOM     31  C8   DA A   2       6.019   0.371  -1.023  1.00  0.00           C
ATOM     32  N7   DA A   2       5.462  -0.118  -2.139  1.00  0.00           N
ATOM     33  C5   DA A   2       5.670  -1.439  -2.054  1.00  0.00           C
ATOM     34  C6   DA A   2       5.366  -2.534  -2.927  1.00  0.00           C
ATOM     35  N6   DA A   2       4.719  -2.358  -4.057  1.00  0.00           N
ATOM     36  N1   DA A   2       5.755  -3.782  -2.563  1.00  0.00           N
ATOM     37  C2   DA A   2       6.389  -3.937  -1.422  1.00  0.00           C
ATOM     38  N3   DA A   2       6.717  -2.985  -0.486  1.00  0.00           N
ATOM     39  C4   DA A   2       6.354  -1.792  -0.858  1.00  0.00           C
ATOM     40  P    DC A   3      10.567   0.141   3.102  1.00  0.00           P
ATOM     41  OP1  DC A   3      10.866   1.187   4.269  1.00  0.00           O
ATOM     42  OP2  DC A   3      11.020   0.614   1.775  1.00  0.00           O
ATOM     43  O5'  DC A   3      11.226  -1.192   3.653  1.00  0.00           O
ATOM     44  C5'  DC A   3      10.606  -2.487   3.565  1.00  0.00           C
ATOM     45  C4'  DC A   3      10.730  -3.090   2.187  1.00  0.00           C
ATOM     46  O4'  DC A   3       9.922  -2.368   1.258  1.00  0.00           O
ATOM     47  C3'  DC A   3      12.165  -3.114   1.600  1.00  0.00           C
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ATOM     48  O3'  DC A   3      12.504  -4.478   1.435  1.00  0.00           O
ATOM     49  C2'  DC A   3      12.004  -2.379   0.264  1.00  0.00           C
ATOM     50  C1'  DC A   3      10.524  -2.620  -0.011  1.00  0.00           C
ATOM     51  N1   DC A   3       9.895  -1.800  -1.026  1.00  0.00           N
ATOM     52  C2   DC A   3       9.152  -2.435  -2.055  1.00  0.00           C
ATOM     53  O2   DC A   3       9.071  -3.660  -2.075  1.00  0.00           O
ATOM     54  N3   DC A   3       8.525  -1.646  -2.972  1.00  0.00           N
ATOM     55  C4   DC A   3       8.674  -0.324  -2.935  1.00  0.00           C
ATOM     56  N4   DC A   3       8.051   0.392  -3.877  1.00  0.00           N
ATOM     57  C5   DC A   3       9.444   0.343  -1.925  1.00  0.00           C
ATOM     58  C6   DC A   3      10.028  -0.443  -0.991  1.00  0.00           C
END

COMPND    CCA / M06-2X / H MODEL / NEUTRAL
ATOM      1  O5'  DC A   1       0.000   0.000   0.000  1.00  0.00           O
ATOM      2  C5'  DC A   1       0.000   0.000   1.414  1.00  0.00           C
ATOM      3  C4'  DC A   1       1.422   0.000   1.951  1.00  0.00           C
ATOM      4  O4'  DC A   1       2.072  -1.165   1.435  1.00  0.00           O
ATOM      5  C3'  DC A   1       2.261   1.197   1.468  1.00  0.00           C
ATOM      6  O3'  DC A   1       3.085   1.588   2.589  1.00  0.00           O
ATOM      7  C2'  DC A   1       3.106   0.606   0.348  1.00  0.00           C
ATOM      8  C1'  DC A   1       3.345  -0.789   0.908  1.00  0.00           C
ATOM      9  N1   DC A   1       3.779  -1.816  -0.015  1.00  0.00           N
ATOM     10  C2   DC A   1       4.344  -2.987   0.570  1.00  0.00           C
ATOM     11  O2   DC A   1       4.461  -3.031   1.789  1.00  0.00           O
ATOM     12  N3   DC A   1       4.722  -3.997  -0.261  1.00  0.00           N
ATOM     13  C4   DC A   1       4.540  -3.892  -1.565  1.00  0.00           C
ATOM     14  N4   DC A   1       4.990  -4.894  -2.341  1.00  0.00           N
ATOM     15  C5   DC A   1       3.918  -2.754  -2.183  1.00  0.00           C
ATOM     16  C6   DC A   1       3.561  -1.745  -1.359  1.00  0.00           C
ATOM     17  P    DC A   2       3.978   2.907   2.521  1.00  0.00           P
ATOM     18  OP1  DC A   2       2.968   4.134   2.390  1.00  0.00           O
ATOM     19  OP2  DC A   2       4.988   2.975   1.446  1.00  0.00           O
ATOM     20  O5'  DC A   2       4.527   3.005   4.008  1.00  0.00           O
ATOM     21  C5'  DC A   2       4.542   1.934   4.970  1.00  0.00           C
ATOM     22  C4'  DC A   2       5.816   1.129   4.856  1.00  0.00           C
ATOM     23  O4'  DC A   2       5.777   0.332   3.677  1.00  0.00           O
ATOM     24  C3'  DC A   2       7.090   2.002   4.742  1.00  0.00           C
ATOM     25  O3'  DC A   2       8.039   1.441   5.675  1.00  0.00           O
ATOM     26  C2'  DC A   2       7.536   1.771   3.305  1.00  0.00           C
ATOM     27  C1'  DC A   2       7.114   0.314   3.155  1.00  0.00           C
ATOM     28  N1   DC A   2       7.110  -0.272   1.839  1.00  0.00           N
ATOM     29  C2   DC A   2       7.395  -1.668   1.744  1.00  0.00           C
ATOM     30  O2   DC A   2       7.650  -2.293   2.766  1.00  0.00           O
ATOM     31  N3   DC A   2       7.390  -2.233   0.505  1.00  0.00           N
ATOM     32  C4   DC A   2       7.073  -1.515  -0.557  1.00  0.00           C
ATOM     33  N4   DC A   2       7.125  -2.119  -1.758  1.00  0.00           N
ATOM     34  C5   DC A   2       6.706  -0.127  -0.486  1.00  0.00           C
ATOM     35  C6   DC A   2       6.743   0.446   0.739  1.00  0.00           C
ATOM     36  P    DA A   3       9.462   2.107   5.943  1.00  0.00           P
ATOM     37  OP1  DA A   3       9.189   3.440   6.777  1.00  0.00           O
ATOM     38  OP2  DA A   3      10.300   2.424   4.770  1.00  0.00           O
ATOM     39  O5'  DA A   3      10.072   1.110   7.019  1.00  0.00           O
ATOM     40  C5'  DA A   3       9.701  -0.275   7.144  1.00  0.00           C
ATOM     41  C4'  DA A   3      10.417  -1.137   6.134  1.00  0.00           C
ATOM     42  O4'  DA A   3       9.929  -0.845   4.824  1.00  0.00           O
ATOM     43  C3'  DA A   3      11.956  -0.952   6.089  1.00  0.00           C
ATOM     44  O3'  DA A   3      12.519  -2.230   6.324  1.00  0.00           O
ATOM     45  C2'  DA A   3      12.197  -0.468   4.657  1.00  0.00           C
ATOM     46  C1'  DA A   3      11.015  -1.116   3.945  1.00  0.00           C
ATOM     47  N9   DA A   3      10.721  -0.629   2.625  1.00  0.00           N
ATOM     48  C8   DA A   3      10.562   0.678   2.216  1.00  0.00           C
ATOM     49  N7   DA A   3      10.300   0.798   0.939  1.00  0.00           N
ATOM     50  C5   DA A   3      10.306  -0.503   0.471  1.00  0.00           C
ATOM     51  C6   DA A   3      10.124  -1.060  -0.810  1.00  0.00           C
ATOM     52  N6   DA A   3       9.873  -0.291  -1.898  1.00  0.00           N
ATOM     53  N1   DA A   3      10.240  -2.386  -0.959  1.00  0.00           N
ATOM     54  C2   DA A   3      10.499  -3.128   0.128  1.00  0.00           C
ATOM     55  N3   DA A   3      10.679  -2.733   1.384  1.00  0.00           N
ATOM     56  C4   DA A   3      10.568  -1.405   1.498  1.00  0.00           C
END

COMPND    CCA / M06-2X / H MODEL / SINGLY IONIZED
ATOM      1  O5'  DC A   1       0.000   0.000   0.000  1.00  0.00           O
ATOM      2  C5'  DC A   1       0.000   0.000   1.414  1.00  0.00           C
ATOM      3  C4'  DC A   1       1.421   0.000   1.953  1.00  0.00           C
ATOM      4  O4'  DC A   1       2.071  -1.170   1.446  1.00  0.00           O
ATOM      5  C3'  DC A   1       2.264   1.194   1.465  1.00  0.00           C
ATOM      6  O3'  DC A   1       3.082   1.590   2.590  1.00  0.00           O
ATOM      7  C2'  DC A   1       3.114   0.593   0.356  1.00  0.00           C
ATOM      8  C1'  DC A   1       3.353  -0.794   0.941  1.00  0.00           C
ATOM      9  N1   DC A   1       3.825  -1.829   0.047  1.00  0.00           N
ATOM     10  C2   DC A   1       4.528  -2.917   0.642  1.00  0.00           C
ATOM     11  O2   DC A   1       4.712  -2.905   1.854  1.00  0.00           O
ATOM     12  N3   DC A   1       4.965  -3.916  -0.172  1.00  0.00           N
ATOM     13  C4   DC A   1       4.745  -3.865  -1.473  1.00  0.00           C
ATOM     14  N4   DC A   1       5.259  -4.849  -2.233  1.00  0.00           N
ATOM     15  C5   DC A   1       4.019  -2.797  -2.104  1.00  0.00           C
ATOM     16  C6   DC A   1       3.577  -1.812  -1.293  1.00  0.00           C
ATOM     17  P    DC A   2       4.037   2.864   2.525  1.00  0.00           P
ATOM     18  OP1  DC A   2       3.095   4.137   2.348  1.00  0.00           O
ATOM     19  OP2  DC A   2       5.082   2.871   1.481  1.00  0.00           O
ATOM     20  O5'  DC A   2       4.552   2.955   4.026  1.00  0.00           O
ATOM     21  C5'  DC A   2       4.493   1.887   4.987  1.00  0.00           C
ATOM     22  C4'  DC A   2       5.703   0.991   4.878  1.00  0.00           C
ATOM     23  O4'  DC A   2       5.650   0.245   3.663  1.00  0.00           O
ATOM     24  C3'  DC A   2       7.057   1.746   4.858  1.00  0.00           C
ATOM     25  O3'  DC A   2       7.880   1.087   5.846  1.00  0.00           O
ATOM     26  C2'  DC A   2       7.576   1.479   3.450  1.00  0.00           C
ATOM     27  C1'  DC A   2       7.008   0.078   3.252  1.00  0.00           C
ATOM     28  N1   DC A   2       7.060  -0.486   1.925  1.00  0.00           N
ATOM     29  C2   DC A   2       7.583  -1.795   1.770  1.00  0.00           C
ATOM     30  O2   DC A   2       7.991  -2.402   2.758  1.00  0.00           O
ATOM     31  N3   DC A   2       7.672  -2.301   0.511  1.00  0.00           N
ATOM     32  C4   DC A   2       7.233  -1.605  -0.526  1.00  0.00           C
ATOM     33  N4   DC A   2       7.362  -2.161  -1.744  1.00  0.00           N
ATOM     34  C5   DC A   2       6.679  -0.287  -0.401  1.00  0.00           C
ATOM     35  C6   DC A   2       6.619   0.228   0.849  1.00  0.00           C
ATOM     36  P    DA A   3       9.349   1.584   6.216  1.00  0.00           P
ATOM     37  OP1  DA A   3       9.199   3.018   6.891  1.00  0.00           O
ATOM     38  OP2  DA A   3      10.325   1.655   5.108  1.00  0.00           O
ATOM     39  O5'  DA A   3       9.711   0.621   7.425  1.00  0.00           O
ATOM     40  C5'  DA A   3       9.128  -0.673   7.657  1.00  0.00           C
ATOM     41  C4'  DA A   3       9.873  -1.753   6.911  1.00  0.00           C
ATOM     42  O4'  DA A   3       9.620  -1.624   5.506  1.00  0.00           O
ATOM     43  C3'  DA A   3      11.412  -1.731   7.089  1.00  0.00           C
ATOM     44  O3'  DA A   3      11.782  -3.025   7.526  1.00  0.00           O
ATOM     45  C2'  DA A   3      11.913  -1.442   5.671  1.00  0.00           C
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ATOM     46  C1'  DA A   3      10.793  -2.083   4.864  1.00  0.00           C
ATOM     47  N9   DA A   3      10.733  -1.712   3.463  1.00  0.00           N
ATOM     48  C8   DA A   3      10.555  -0.476   2.958  1.00  0.00           C
ATOM     49  N7   DA A   3      10.442  -0.446   1.614  1.00  0.00           N
ATOM     50  C5   DA A   3      10.554  -1.724   1.256  1.00  0.00           C
ATOM     51  C6   DA A   3      10.522  -2.387  -0.016  1.00  0.00           C
ATOM     52  N6   DA A   3      10.409  -1.722  -1.141  1.00  0.00           N
ATOM     53  N1   DA A   3      10.639  -3.741  -0.048  1.00  0.00           N
ATOM     54  C2   DA A   3      10.786  -4.381   1.088  1.00  0.00           C
ATOM     55  N3   DA A   3      10.853  -3.873   2.364  1.00  0.00           N
ATOM     56  C4   DA A   3      10.720  -2.582   2.387  1.00  0.00           C
END

COMPND    CAA / M06-2X / H MODEL / NEUTRAL
ATOM      1  O5'  DC A   1       0.000   0.000   0.000  1.00  0.00           O
ATOM      2  C5'  DC A   1       0.000   0.000   1.417  1.00  0.00           C
ATOM      3  C4'  DC A   1       1.439   0.000   1.896  1.00  0.00           C
ATOM      4  O4'  DC A   1       2.059  -1.243   1.567  1.00  0.00           O
ATOM      5  C3'  DC A   1       2.295   1.083   1.229  1.00  0.00           C
ATOM      6  O3'  DC A   1       3.297   1.475   2.200  1.00  0.00           O
ATOM      7  C2'  DC A   1       2.945   0.342   0.075  1.00  0.00           C
ATOM      8  C1'  DC A   1       3.158  -1.043   0.684  1.00  0.00           C
ATOM      9  N1   DC A   1       3.192  -2.123  -0.285  1.00  0.00           N
ATOM     10  C2   DC A   1       4.216  -3.101  -0.200  1.00  0.00           C
ATOM     11  O2   DC A   1       5.002  -3.068   0.742  1.00  0.00           O
ATOM     12  N3   DC A   1       4.281  -4.032  -1.192  1.00  0.00           N
ATOM     13  C4   DC A   1       3.341  -4.085  -2.121  1.00  0.00           C
ATOM     14  N4   DC A   1       3.482  -4.995  -3.099  1.00  0.00           N
ATOM     15  C5   DC A   1       2.190  -3.224  -2.122  1.00  0.00           C
ATOM     16  C6   DC A   1       2.168  -2.257  -1.179  1.00  0.00           C
ATOM     17  P    DA A   2       4.203   2.751   1.914  1.00  0.00           P
ATOM     18  OP2  DA A   2       4.920   2.803   0.620  1.00  0.00           O
ATOM     19  OP1  DA A   2       3.203   3.980   2.111  1.00  0.00           O
ATOM     20  O5'  DA A   2       5.110   2.814   3.214  1.00  0.00           O
ATOM     21  C5'  DA A   2       5.401   1.711   4.087  1.00  0.00           C
ATOM     22  C4'  DA A   2       6.606   0.937   3.606  1.00  0.00           C
ATOM     23  O4'  DA A   2       6.250   0.186   2.445  1.00  0.00           O
ATOM     24  C3'  DA A   2       7.813   1.818   3.195  1.00  0.00           C
ATOM     25  O3'  DA A   2       8.963   1.219   3.838  1.00  0.00           O
ATOM     26  C2'  DA A   2       7.871   1.633   1.684  1.00  0.00           C
ATOM     27  C1'  DA A   2       7.390   0.193   1.587  1.00  0.00           C
ATOM     28  N9   DA A   2       7.025  -0.286   0.290  1.00  0.00           N
ATOM     29  C8   DA A   2       6.337   0.357  -0.713  1.00  0.00           C
ATOM     30  N7   DA A   2       6.174  -0.377  -1.786  1.00  0.00           N
ATOM     31  C5   DA A   2       6.805  -1.570  -1.477  1.00  0.00           C
ATOM     32  C6   DA A   2       7.019  -2.757  -2.200  1.00  0.00           C
ATOM     33  N6   DA A   2       6.572  -2.915  -3.472  1.00  0.00           N
ATOM     34  N1   DA A   2       7.748  -3.730  -1.637  1.00  0.00           N
ATOM     35  C2   DA A   2       8.231  -3.533  -0.402  1.00  0.00           C
ATOM     36  N3   DA A   2       8.082  -2.476   0.391  1.00  0.00           N
ATOM     37  C4   DA A   2       7.351  -1.529  -0.200  1.00  0.00           C
ATOM     38  P    DA A   3      10.430   1.819   3.668  1.00  0.00           P
ATOM     39  OP2  DA A   3      10.610   2.860   2.642  1.00  0.00           O
ATOM     40  OP1  DA A   3      10.748   2.212   5.181  1.00  0.00           O
ATOM     41  O5'  DA A   3      11.321   0.535   3.344  1.00  0.00           O
ATOM     42  C5'  DA A   3      11.244  -0.648   4.160  1.00  0.00           C
ATOM     43  C4'  DA A   3      11.968  -1.764   3.436  1.00  0.00           C
ATOM     44  O4'  DA A   3      11.265  -2.078   2.233  1.00  0.00           O
ATOM     45  C3'  DA A   3      13.408  -1.439   3.019  1.00  0.00           C
ATOM     46  O3'  DA A   3      14.117  -2.663   3.086  1.00  0.00           O
ATOM     47  C2'  DA A   3      13.238  -0.974   1.577  1.00  0.00           C
ATOM     48  C1'  DA A   3      12.089  -1.861   1.098  1.00  0.00           C
ATOM     49  N9   DA A   3      11.288  -1.269   0.048  1.00  0.00           N
ATOM     50  C8   DA A   3      10.600  -0.080   0.108  1.00  0.00           C
ATOM     51  N7   DA A   3       9.889   0.175  -0.960  1.00  0.00           N
ATOM     52  C5   DA A   3      10.118  -0.916  -1.778  1.00  0.00           C
ATOM     53  C6   DA A   3       9.635  -1.279  -3.051  1.00  0.00           C
ATOM     54  N6   DA A   3       8.779  -0.496  -3.757  1.00  0.00           N
ATOM     55  N1   DA A   3      10.059  -2.429  -3.596  1.00  0.00           N
ATOM     56  C2   DA A   3      10.892  -3.204  -2.887  1.00  0.00           C
ATOM     57  N3   DA A   3      11.393  -2.995  -1.673  1.00  0.00           N
ATOM     58  C4   DA A   3      10.975  -1.829  -1.167  1.00  0.00           C
END

COMPND    CAA / M06-2X / H MODEL / SINGLY IONIZED
ATOM      1  O5'  DC A   1       0.000   0.000   0.000  1.00  0.00           O
ATOM      2  C5'  DC A   1       0.000   0.000   1.417  1.00  0.00           C
ATOM      3  C4'  DC A   1       1.439   0.000   1.894  1.00  0.00           C
ATOM      4  O4'  DC A   1       2.063  -1.244   1.569  1.00  0.00           O
ATOM      5  C3'  DC A   1       2.302   1.081   1.235  1.00  0.00           C
ATOM      6  O3'  DC A   1       3.291   1.462   2.223  1.00  0.00           O
ATOM      7  C2'  DC A   1       2.966   0.340   0.088  1.00  0.00           C
ATOM      8  C1'  DC A   1       3.166  -1.046   0.699  1.00  0.00           C
ATOM      9  N1   DC A   1       3.175  -2.127  -0.280  1.00  0.00           N
ATOM     10  C2   DC A   1       4.323  -2.929  -0.427  1.00  0.00           C
ATOM     11  O2   DC A   1       5.313  -2.691   0.274  1.00  0.00           O
ATOM     12  N3   DC A   1       4.297  -3.927  -1.345  1.00  0.00           N
ATOM     13  C4   DC A   1       3.202  -4.142  -2.066  1.00  0.00           C
ATOM     14  N4   DC A   1       3.241  -5.131  -2.969  1.00  0.00           N
ATOM     15  C5   DC A   1       2.002  -3.371  -1.909  1.00  0.00           C
ATOM     16  C6   DC A   1       2.042  -2.374  -0.997  1.00  0.00           C
ATOM     17  P    DA A   2       4.191   2.751   1.981  1.00  0.00           P
ATOM     18  OP1  DA A   2       3.167   3.969   2.083  1.00  0.00           O
ATOM     19  OP2  DA A   2       4.998   2.783   0.741  1.00  0.00           O
ATOM     20  O5'  DA A   2       4.996   2.848   3.344  1.00  0.00           O
ATOM     21  C5'  DA A   2       5.277   1.754   4.234  1.00  0.00           C
ATOM     22  C4'  DA A   2       6.615   1.127   3.913  1.00  0.00           C
ATOM     23  O4'  DA A   2       6.506   0.355   2.712  1.00  0.00           O
ATOM     24  C3'  DA A   2       7.741   2.150   3.653  1.00  0.00           C
ATOM     25  O3'  DA A   2       8.919   1.616   4.292  1.00  0.00           O
ATOM     26  C2'  DA A   2       7.929   2.090   2.141  1.00  0.00           C
ATOM     27  C1'  DA A   2       7.676   0.601   1.946  1.00  0.00           C
ATOM     28  N9   DA A   2       7.437   0.118   0.603  1.00  0.00           N
ATOM     29  C8   DA A   2       6.775   0.697  -0.430  1.00  0.00           C
ATOM     30  N7   DA A   2       6.590  -0.119  -1.479  1.00  0.00           N
ATOM     31  C5   DA A   2       7.155  -1.268  -1.100  1.00  0.00           C
ATOM     32  C6   DA A   2       7.260  -2.558  -1.719  1.00  0.00           C
ATOM     33  N6   DA A   2       6.757  -2.792  -2.909  1.00  0.00           N
ATOM     34  N1   DA A   2       7.884  -3.555  -1.046  1.00  0.00           N
ATOM     35  C2   DA A   2       8.330  -3.306   0.166  1.00  0.00           C
ATOM     36  N3   DA A   2       8.273  -2.141   0.883  1.00  0.00           N
ATOM     37  C4   DA A   2       7.698  -1.185   0.214  1.00  0.00           C
ATOM     38  P    DA A   3      10.136   2.566   4.687  1.00  0.00           P
ATOM     39  OP1  DA A   3       9.631   3.139   6.088  1.00  0.00           O
ATOM     40  OP2  DA A   3      10.559   3.570   3.694  1.00  0.00           O
ATOM     41  O5'  DA A   3      11.283   1.506   4.986  1.00  0.00           O
ATOM     42  C5'  DA A   3      11.033   0.320   5.767  1.00  0.00           C
ATOM     43  C4'  DA A   3      11.729  -0.848   5.097  1.00  0.00           C
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ATOM     44  O4'  DA A   3      11.206  -1.007   3.777  1.00  0.00           O
ATOM     45  C3'  DA A   3      13.249  -0.709   4.944  1.00  0.00           C
ATOM     46  O3'  DA A   3      13.774  -2.020   5.053  1.00  0.00           O
ATOM     47  C2'  DA A   3      13.395  -0.169   3.525  1.00  0.00           C
ATOM     48  C1'  DA A   3      12.240  -0.867   2.812  1.00  0.00           C
ATOM     49  N9   DA A   3      11.716  -0.132   1.679  1.00  0.00           N
ATOM     50  C8   DA A   3      11.387   1.202   1.634  1.00  0.00           C
ATOM     51  N7   DA A   3      10.766   1.554   0.535  1.00  0.00           N
ATOM     52  C5   DA A   3      10.670   0.382  -0.181  1.00  0.00           C
ATOM     53  C6   DA A   3      10.074   0.074  -1.424  1.00  0.00           C
ATOM     54  N6   DA A   3       9.428   0.999  -2.146  1.00  0.00           N
ATOM     55  N1   DA A   3      10.125  -1.198  -1.861  1.00  0.00           N
ATOM     56  C2   DA A   3      10.763  -2.107  -1.105  1.00  0.00           C
ATOM     57  N3   DA A   3      11.336  -1.948   0.085  1.00  0.00           N
ATOM     58  C4   DA A   3      11.249  -0.680   0.506  1.00  0.00           C
END
COMPND    ACC / M06-2X / NA MODEL / NEUTRAL
ATOM      1  O5'  DA A   1       7.107   0.774  -0.532  1.00  0.00           O
ATOM      2  C5'  DA A   1       6.770   1.663  -1.581  1.00  0.00           C
ATOM      3  C4'  DA A   1       5.261   1.822  -1.641  1.00  0.00           C
ATOM      4  O4'  DA A   1       4.650   0.568  -1.961  1.00  0.00           O
ATOM      5  C3'  DA A   1       4.607   2.257  -0.326  1.00  0.00           C
ATOM      6  O3'  DA A   1       3.372   2.891  -0.685  1.00  0.00           O
ATOM      7  C2'  DA A   1       4.335   0.923   0.349  1.00  0.00           C
ATOM      8  C1'  DA A   1       3.900   0.090  -0.852  1.00  0.00           C
ATOM      9  N9   DA A   1       4.108  -1.333  -0.684  1.00  0.00           N
ATOM     10  C8   DA A   1       5.063  -1.990   0.057  1.00  0.00           C
ATOM     11  N7   DA A   1       4.888  -3.286   0.115  1.00  0.00           N
ATOM     12  C5   DA A   1       3.755  -3.501  -0.646  1.00  0.00           C
ATOM     13  C6   DA A   1       2.995  -4.652  -0.929  1.00  0.00           C
ATOM     14  N6   DA A   1       3.273  -5.848  -0.356  1.00  0.00           N
ATOM     15  N1   DA A   1       1.930  -4.541  -1.733  1.00  0.00           N
ATOM     16  C2   DA A   1       1.590  -3.322  -2.175  1.00  0.00           C
ATOM     17  N3   DA A   1       2.179  -2.155  -1.932  1.00  0.00           N
ATOM     18  C4   DA A   1       3.260  -2.306  -1.159  1.00  0.00           C
ATOM     19  P    DC A   2       2.464   3.610   0.456  1.00  0.00           P
ATOM     20  OP1  DC A   2       3.094   4.898   0.918  1.00  0.00           O
ATOM     21  OP2  DC A   2       2.127   2.659   1.585  1.00  0.00           O
ATOM     22  O5'  DC A   2       1.159   3.958  -0.431  1.00  0.00           O
ATOM     23  C5'  DC A   2       0.772   3.348  -1.662  1.00  0.00           C
ATOM     24  C4'  DC A   2      -0.236   2.234  -1.468  1.00  0.00           C
ATOM     25  O4'  DC A   2       0.424   1.036  -1.052  1.00  0.00           O
ATOM     26  C3'  DC A   2      -1.306   2.532  -0.390  1.00  0.00           C
ATOM     27  O3'  DC A   2      -2.576   2.160  -0.938  1.00  0.00           O
ATOM     28  C2'  DC A   2      -0.922   1.577   0.732  1.00  0.00           C
ATOM     29  C1'  DC A   2      -0.442   0.401  -0.110  1.00  0.00           C
ATOM     30  N1   DC A   2       0.272  -0.668   0.553  1.00  0.00           N
ATOM     31  C2   DC A   2      -0.053  -2.015   0.224  1.00  0.00           C
ATOM     32  O2   DC A   2      -0.956  -2.241  -0.574  1.00  0.00           O
ATOM     33  N3   DC A   2       0.666  -3.004   0.828  1.00  0.00           N
ATOM     34  C4   DC A   2       1.655  -2.710   1.650  1.00  0.00           C
ATOM     35  N4   DC A   2       2.315  -3.742   2.228  1.00  0.00           N
ATOM     36  C5   DC A   2       2.024  -1.363   1.981  1.00  0.00           C
ATOM     37  C6   DC A   2       1.298  -0.377   1.398  1.00  0.00           C
ATOM     38  P    DC A   3      -3.939   2.689  -0.210  1.00  0.00           P
ATOM     39  OP1  DC A   3      -4.372   3.999  -0.814  1.00  0.00           O
ATOM     40  OP2  DC A   3      -3.805   2.663   1.290  1.00  0.00           O
ATOM     41  O5'  DC A   3      -4.933   1.476  -0.627  1.00  0.00           O
ATOM     42  C5'  DC A   3      -5.043   1.084  -1.995  1.00  0.00           C
ATOM     43  C4'  DC A   3      -5.432  -0.379  -2.032  1.00  0.00           C
ATOM     44  O4'  DC A   3      -4.391  -1.144  -1.420  1.00  0.00           O
ATOM     45  C3'  DC A   3      -6.726  -0.717  -1.276  1.00  0.00           C
ATOM     46  O3'  DC A   3      -7.368  -1.738  -2.021  1.00  0.00           O
ATOM     47  C2'  DC A   3      -6.207  -1.241   0.058  1.00  0.00           C
ATOM     48  C1'  DC A   3      -4.925  -1.947  -0.376  1.00  0.00           C
ATOM     49  N1   DC A   3      -3.926  -2.089   0.672  1.00  0.00           N
ATOM     50  C2   DC A   3      -3.428  -3.380   0.987  1.00  0.00           C
ATOM     51  O2   DC A   3      -3.868  -4.357   0.387  1.00  0.00           O
ATOM     52  N3   DC A   3      -2.487  -3.479   1.968  1.00  0.00           N
ATOM     53  C4   DC A   3      -2.038  -2.396   2.572  1.00  0.00           C
ATOM     54  N4   DC A   3      -1.091  -2.550   3.524  1.00  0.00           N
ATOM     55  C5   DC A   3      -2.523  -1.077   2.281  1.00  0.00           C
ATOM     56  C6   DC A   3      -3.449  -0.979   1.299  1.00  0.00           C
END

COMPND    ACC / M06-2X / NA MODEL / SINGLY IONIZED
ATOM      1  O5'  DA A   1       6.783   0.071  -0.671  1.00  0.00           O
ATOM      2  C5'  DA A   1       6.629   1.032  -1.702  1.00  0.00           C
ATOM      3  C4'  DA A   1       5.176   1.466  -1.774  1.00  0.00           C
ATOM      4  O4'  DA A   1       4.339   0.336  -2.059  1.00  0.00           O
ATOM      5  C3'  DA A   1       4.595   2.049  -0.483  1.00  0.00           C
ATOM      6  O3'  DA A   1       3.452   2.815  -0.881  1.00  0.00           O
ATOM      7  C2'  DA A   1       4.148   0.799   0.257  1.00  0.00           C
ATOM      8  C1'  DA A   1       3.605  -0.022  -0.909  1.00  0.00           C
ATOM      9  N9   DA A   1       3.699  -1.470  -0.694  1.00  0.00           N
ATOM     10  C8   DA A   1       4.606  -2.192  -0.003  1.00  0.00           C
ATOM     11  N7   DA A   1       4.349  -3.512   0.028  1.00  0.00           N
ATOM     12  C5   DA A   1       3.229  -3.636  -0.685  1.00  0.00           C
ATOM     13  C6   DA A   1       2.392  -4.755  -1.016  1.00  0.00           C
ATOM     14  N6   DA A   1       2.660  -5.968  -0.588  1.00  0.00           N
ATOM     15  N1   DA A   1       1.303  -4.544  -1.794  1.00  0.00           N
ATOM     16  C2   DA A   1       1.049  -3.321  -2.203  1.00  0.00           C
ATOM     17  N3   DA A   1       1.757  -2.169  -1.962  1.00  0.00           N
ATOM     18  C4   DA A   1       2.785  -2.380  -1.196  1.00  0.00           C
ATOM     19  P    DC A   2       2.578   3.662   0.202  1.00  0.00           P
ATOM     20  OP1  DC A   2       3.226   4.987   0.507  1.00  0.00           O
ATOM     21  OP2  DC A   2       2.262   2.840   1.432  1.00  0.00           O
ATOM     22  O5'  DC A   2       1.254   3.934  -0.685  1.00  0.00           O
ATOM     23  C5'  DC A   2       0.820   3.203  -1.831  1.00  0.00           C
ATOM     24  C4'  DC A   2      -0.205   2.139  -1.493  1.00  0.00           C
ATOM     25  O4'  DC A   2       0.450   0.987  -0.956  1.00  0.00           O
ATOM     26  C3'  DC A   2      -1.251   2.563  -0.437  1.00  0.00           C
ATOM     27  O3'  DC A   2      -2.519   2.082  -0.893  1.00  0.00           O
ATOM     28  C2'  DC A   2      -0.814   1.782   0.799  1.00  0.00           C
ATOM     29  C1'  DC A   2      -0.370   0.500   0.107  1.00  0.00           C
ATOM     30  N1   DC A   2       0.381  -0.480   0.866  1.00  0.00           N
ATOM     31  C2   DC A   2       0.217  -1.850   0.524  1.00  0.00           C
ATOM     32  O2   DC A   2      -0.597  -2.158  -0.344  1.00  0.00           O
ATOM     33  N3   DC A   2       1.002  -2.768   1.152  1.00  0.00           N
ATOM     34  C4   DC A   2       1.851  -2.385   2.103  1.00  0.00           C
ATOM     35  N4   DC A   2       2.572  -3.339   2.704  1.00  0.00           N
ATOM     36  C5   DC A   2       2.029  -1.014   2.478  1.00  0.00           C
ATOM     37  C6   DC A   2       1.278  -0.100   1.817  1.00  0.00           C
ATOM     38  P    DC A   3      -3.887   2.637  -0.200  1.00  0.00           P
ATOM     39  OP1  DC A   3      -4.233   3.996  -0.752  1.00  0.00           O
ATOM     40  OP2  DC A   3      -3.830   2.536   1.303  1.00  0.00           O
ATOM     41  O5'  DC A   3      -4.901   1.482  -0.717  1.00  0.00           O
ATOM     42  C5'  DC A   3      -4.900   1.057  -2.081  1.00  0.00           C
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ATOM     43  C4'  DC A   3      -5.154  -0.436  -2.112  1.00  0.00           C
ATOM     44  O4'  DC A   3      -4.100  -1.101  -1.412  1.00  0.00           O
ATOM     45  C3'  DC A   3      -6.468  -0.877  -1.447  1.00  0.00           C
ATOM     46  O3'  DC A   3      -6.961  -1.960  -2.218  1.00  0.00           O
ATOM     47  C2'  DC A   3      -6.006  -1.336  -0.069  1.00  0.00           C
ATOM     48  C1'  DC A   3      -4.642  -1.937  -0.396  1.00  0.00           C
ATOM     49  N1   DC A   3      -3.714  -1.984   0.723  1.00  0.00           N
ATOM     50  C2   DC A   3      -3.133  -3.224   1.097  1.00  0.00           C
ATOM     51  O2   DC A   3      -3.447  -4.242   0.488  1.00  0.00           O
ATOM     52  N3   DC A   3      -2.260  -3.228   2.143  1.00  0.00           N
ATOM     53  C4   DC A   3      -1.945  -2.099   2.753  1.00  0.00           C
ATOM     54  N4   DC A   3      -1.038  -2.154   3.745  1.00  0.00           N
ATOM     55  C5   DC A   3      -2.517  -0.830   2.402  1.00  0.00           C
ATOM     56  C6   DC A   3      -3.384  -0.829   1.364  1.00  0.00           C
END

COMPND    AAC / M06-2X / NA MODEL / NEUTRAL
ATOM      1  O5'  DA A   1       6.648   2.170  -1.018  1.00  0.00           O
ATOM      2  C5'  DA A   1       5.907   2.540  -2.164  1.00  0.00           C
ATOM      3  C4'  DA A   1       4.447   2.223  -1.912  1.00  0.00           C
ATOM      4  O4'  DA A   1       4.271   0.803  -1.857  1.00  0.00           O
ATOM      5  C3'  DA A   1       3.929   2.765  -0.572  1.00  0.00           C
ATOM      6  O3'  DA A   1       2.561   3.139  -0.762  1.00  0.00           O
ATOM      7  C2'  DA A   1       4.019   1.547   0.339  1.00  0.00           C
ATOM      8  C1'  DA A   1       3.634   0.449  -0.642  1.00  0.00           C
ATOM      9  N9   DA A   1       4.078  -0.874  -0.252  1.00  0.00           N
ATOM     10  C8   DA A   1       4.741  -1.260   0.889  1.00  0.00           C
ATOM     11  N7   DA A   1       4.926  -2.551   0.984  1.00  0.00           N
ATOM     12  C5   DA A   1       4.349  -3.053  -0.166  1.00  0.00           C
ATOM     13  C6   DA A   1       4.142  -4.364  -0.634  1.00  0.00           C
ATOM     14  N6   DA A   1       4.507  -5.447   0.096  1.00  0.00           N
ATOM     15  N1   DA A   1       3.509  -4.540  -1.800  1.00  0.00           N
ATOM     16  C2   DA A   1       3.040  -3.457  -2.438  1.00  0.00           C
ATOM     17  N3   DA A   1       3.125  -2.177  -2.085  1.00  0.00           N
ATOM     18  C4   DA A   1       3.802  -2.033  -0.939  1.00  0.00           C
ATOM     19  P    DA A   2       1.852   4.040   0.390  1.00  0.00           P
ATOM     20  OP1  DA A   2       2.619   5.321   0.597  1.00  0.00           O
ATOM     21  OP2  DA A   2       1.618   3.255   1.662  1.00  0.00           O
ATOM     22  O5'  DA A   2       0.431   4.335  -0.324  1.00  0.00           O
ATOM     23  C5'  DA A   2       0.016   3.886  -1.613  1.00  0.00           C
ATOM     24  C4'  DA A   2      -0.848   2.646  -1.504  1.00  0.00           C
ATOM     25  O4'  DA A   2      -0.032   1.517  -1.176  1.00  0.00           O
ATOM     26  C3'  DA A   2      -1.922   2.732  -0.399  1.00  0.00           C
ATOM     27  O3'  DA A   2      -3.096   2.099  -0.919  1.00  0.00           O
ATOM     28  C2'  DA A   2      -1.326   1.875   0.709  1.00  0.00           C
ATOM     29  C1'  DA A   2      -0.689   0.790  -0.145  1.00  0.00           C
ATOM     30  N9   DA A   2       0.247  -0.071   0.526  1.00  0.00           N
ATOM     31  C8   DA A   2       1.051   0.206   1.612  1.00  0.00           C
ATOM     32  N7   DA A   2       1.706  -0.839   2.055  1.00  0.00           N
ATOM     33  C5   DA A   2       1.309  -1.867   1.219  1.00  0.00           C
ATOM     34  C6   DA A   2       1.576  -3.250   1.199  1.00  0.00           C
ATOM     35  N6   DA A   2       2.328  -3.858   2.158  1.00  0.00           N
ATOM     36  N1   DA A   2       1.025  -4.000   0.238  1.00  0.00           N
ATOM     37  C2   DA A   2       0.196  -3.413  -0.637  1.00  0.00           C
ATOM     38  N3   DA A   2      -0.182  -2.139  -0.695  1.00  0.00           N
ATOM     39  C4   DA A   2       0.410  -1.412   0.259  1.00  0.00           C
ATOM     40  P    DC A   3      -4.520   2.219  -0.131  1.00  0.00           P
ATOM     41  OP1  DC A   3      -5.258   3.453  -0.581  1.00  0.00           O
ATOM     42  OP2  DC A   3      -4.349   2.066   1.358  1.00  0.00           O
ATOM     43  O5'  DC A   3      -5.215   0.857  -0.673  1.00  0.00           O
ATOM     44  C5'  DC A   3      -5.155   0.490  -2.051  1.00  0.00           C
ATOM     45  C4'  DC A   3      -5.119  -1.022  -2.128  1.00  0.00           C
ATOM     46  O4'  DC A   3      -3.938  -1.489  -1.470  1.00  0.00           O
ATOM     47  C3'  DC A   3      -6.307  -1.723  -1.447  1.00  0.00           C
ATOM     48  O3'  DC A   3      -6.615  -2.854  -2.247  1.00  0.00           O
ATOM     49  C2'  DC A   3      -5.724  -2.134  -0.101  1.00  0.00           C
ATOM     50  C1'  DC A   3      -4.285  -2.458  -0.490  1.00  0.00           C
ATOM     51  N1   DC A   3      -3.330  -2.389   0.606  1.00  0.00           N
ATOM     52  C2   DC A   3      -2.548  -3.532   0.912  1.00  0.00           C
ATOM     53  O2   DC A   3      -2.686  -4.555   0.247  1.00  0.00           O
ATOM     54  N3   DC A   3      -1.673  -3.443   1.954  1.00  0.00           N
ATOM     55  C4   DC A   3      -1.545  -2.315   2.627  1.00  0.00           C
ATOM     56  N4   DC A   3      -0.670  -2.298   3.659  1.00  0.00           N
ATOM     57  C5   DC A   3      -2.306  -1.134   2.328  1.00  0.00           C
ATOM     58  C6   DC A   3      -3.179  -1.225   1.296  1.00  0.00           C
END

COMPND    AAC / M06-2X / NA MODEL / SINGLY IONIZED
ATOM      1  O5'  DA A   1       6.511   2.148  -0.495  1.00  0.00           O
ATOM      2  C5'  DA A   1       5.955   2.736  -1.656  1.00  0.00           C
ATOM      3  C4'  DA A   1       4.456   2.512  -1.643  1.00  0.00           C
ATOM      4  O4'  DA A   1       4.173   1.114  -1.785  1.00  0.00           O
ATOM      5  C3'  DA A   1       3.772   2.938  -0.338  1.00  0.00           C
ATOM      6  O3'  DA A   1       2.439   3.329  -0.681  1.00  0.00           O
ATOM      7  C2'  DA A   1       3.752   1.641   0.460  1.00  0.00           C
ATOM      8  C1'  DA A   1       3.456   0.647  -0.655  1.00  0.00           C
ATOM      9  N9   DA A   1       3.872  -0.714  -0.370  1.00  0.00           N
ATOM     10  C8   DA A   1       4.723  -1.186   0.601  1.00  0.00           C
ATOM     11  N7   DA A   1       4.953  -2.476   0.521  1.00  0.00           N
ATOM     12  C5   DA A   1       4.227  -2.875  -0.577  1.00  0.00           C
ATOM     13  C6   DA A   1       4.035  -4.135  -1.190  1.00  0.00           C
ATOM     14  N6   DA A   1       4.587  -5.252  -0.695  1.00  0.00           N
ATOM     15  N1   DA A   1       3.256  -4.203  -2.280  1.00  0.00           N
ATOM     16  C2   DA A   1       2.663  -3.082  -2.713  1.00  0.00           C
ATOM     17  N3   DA A   1       2.738  -1.847  -2.214  1.00  0.00           N
ATOM     18  C4   DA A   1       3.542  -1.804  -1.146  1.00  0.00           C
ATOM     19  P    DA A   2       1.522   4.064   0.441  1.00  0.00           P
ATOM     20  OP1  DA A   2       2.119   5.389   0.838  1.00  0.00           O
ATOM     21  OP2  DA A   2       1.238   3.150   1.615  1.00  0.00           O
ATOM     22  O5'  DA A   2       0.176   4.296  -0.423  1.00  0.00           O
ATOM     23  C5'  DA A   2      -0.095   3.769  -1.721  1.00  0.00           C
ATOM     24  C4'  DA A   2      -0.902   2.489  -1.648  1.00  0.00           C
ATOM     25  O4'  DA A   2      -0.069   1.408  -1.199  1.00  0.00           O
ATOM     26  C3'  DA A   2      -2.085   2.548  -0.658  1.00  0.00           C
ATOM     27  O3'  DA A   2      -3.162   1.845  -1.277  1.00  0.00           O
ATOM     28  C2'  DA A   2      -1.560   1.758   0.536  1.00  0.00           C
ATOM     29  C1'  DA A   2      -0.806   0.682  -0.230  1.00  0.00           C
ATOM     30  N9   DA A   2       0.120  -0.125   0.544  1.00  0.00           N
ATOM     31  C8   DA A   2       0.845   0.217   1.636  1.00  0.00           C
ATOM     32  N7   DA A   2       1.608  -0.781   2.114  1.00  0.00           N
ATOM     33  C5   DA A   2       1.351  -1.806   1.293  1.00  0.00           C
ATOM     34  C6   DA A   2       1.774  -3.176   1.279  1.00  0.00           C
ATOM     35  N6   DA A   2       2.592  -3.656   2.188  1.00  0.00           N
ATOM     36  N1   DA A   2       1.316  -3.987   0.294  1.00  0.00           N
ATOM     37  C2   DA A   2       0.481  -3.492  -0.593  1.00  0.00           C
ATOM     38  N3   DA A   2      -0.026  -2.218  -0.678  1.00  0.00           N
ATOM     39  C4   DA A   2       0.426  -1.448   0.271  1.00  0.00           C
ATOM     40  P    DC A   3      -4.652   1.865  -0.622  1.00  0.00           P
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ATOM     41  OP1  DC A   3      -5.230   3.256  -0.653  1.00  0.00           O
ATOM     42  OP2  DC A   3      -4.679   1.223   0.748  1.00  0.00           O
ATOM     43  O5'  DC A   3      -5.411   0.953  -1.720  1.00  0.00           O
ATOM     44  C5'  DC A   3      -4.775   0.042  -2.616  1.00  0.00           C
ATOM     45  C4'  DC A   3      -4.550  -1.324  -2.010  1.00  0.00           C
ATOM     46  O4'  DC A   3      -3.500  -1.282  -1.042  1.00  0.00           O
ATOM     47  C3'  DC A   3      -5.785  -1.932  -1.299  1.00  0.00           C
ATOM     48  O3'  DC A   3      -6.047  -3.173  -1.934  1.00  0.00           O
ATOM     49  C2'  DC A   3      -5.297  -2.110   0.140  1.00  0.00           C
ATOM     50  C1'  DC A   3      -3.807  -2.311  -0.109  1.00  0.00           C
ATOM     51  N1   DC A   3      -2.928  -2.205   1.040  1.00  0.00           N
ATOM     52  C2   DC A   3      -1.997  -3.243   1.289  1.00  0.00           C
ATOM     53  O2   DC A   3      -1.944  -4.206   0.527  1.00  0.00           O
ATOM     54  N3   DC A   3      -1.168  -3.115   2.363  1.00  0.00           N
ATOM     55  C4   DC A   3      -1.267  -2.058   3.166  1.00  0.00           C
ATOM     56  N4   DC A   3      -0.447  -2.013   4.223  1.00  0.00           N
ATOM     57  C5   DC A   3      -2.182  -0.983   2.923  1.00  0.00           C
ATOM     58  C6   DC A   3      -2.992  -1.107   1.842  1.00  0.00           C
END

COMPND    CCA / M06-2X / NA MODEL / NEUTRAL
ATOM      1  O5'  DC A   1      -7.314  -0.919  -0.443  1.00  0.00           O
ATOM      2  C5'  DC A   1      -6.920  -1.858  -1.430  1.00  0.00           C
ATOM      3  C4'  DC A   1      -5.405  -1.906  -1.487  1.00  0.00           C
ATOM      4  O4'  DC A   1      -4.898  -0.663  -1.975  1.00  0.00           O
ATOM      5  C3'  DC A   1      -4.730  -2.120  -0.125  1.00  0.00           C
ATOM      6  O3'  DC A   1      -3.492  -2.794  -0.388  1.00  0.00           O
ATOM      7  C2'  DC A   1      -4.461  -0.695   0.332  1.00  0.00           C
ATOM      8  C1'  DC A   1      -4.071  -0.044  -0.993  1.00  0.00           C
ATOM      9  N1   DC A   1      -4.276   1.392  -1.040  1.00  0.00           N
ATOM     10  C2   DC A   1      -3.224   2.227  -1.496  1.00  0.00           C
ATOM     11  O2   DC A   1      -2.210   1.715  -1.960  1.00  0.00           O
ATOM     12  N3   DC A   1      -3.397   3.574  -1.382  1.00  0.00           N
ATOM     13  C4   DC A   1      -4.552   4.065  -0.965  1.00  0.00           C
ATOM     14  N4   DC A   1      -4.644   5.399  -0.817  1.00  0.00           N
ATOM     15  C5   DC A   1      -5.692   3.245  -0.664  1.00  0.00           C
ATOM     16  C6   DC A   1      -5.494   1.908  -0.714  1.00  0.00           C
ATOM     17  P    DC A   2      -2.622  -3.369   0.860  1.00  0.00           P
ATOM     18  OP1  DC A   2      -3.337  -4.512   1.534  1.00  0.00           O
ATOM     19  OP2  DC A   2      -2.210  -2.266   1.811  1.00  0.00           O
ATOM     20  O5'  DC A   2      -1.351  -3.950   0.048  1.00  0.00           O
ATOM     21  C5'  DC A   2      -0.948  -3.598  -1.276  1.00  0.00           C
ATOM     22  C4'  DC A   2       0.111  -2.515  -1.298  1.00  0.00           C
ATOM     23  O4'  DC A   2      -0.485  -1.233  -1.092  1.00  0.00           O
ATOM     24  C3'  DC A   2       1.200  -2.668  -0.209  1.00  0.00           C
ATOM     25  O3'  DC A   2       2.462  -2.456  -0.859  1.00  0.00           O
ATOM     26  C2'  DC A   2       0.884  -1.515   0.736  1.00  0.00           C
ATOM     27  C1'  DC A   2       0.436  -0.485  -0.293  1.00  0.00           C
ATOM     28  N1   DC A   2      -0.208   0.717   0.181  1.00  0.00           N
ATOM     29  C2   DC A   2       0.232   1.971  -0.318  1.00  0.00           C
ATOM     30  O2   DC A   2       1.160   2.012  -1.119  1.00  0.00           O
ATOM     31  N3   DC A   2      -0.387   3.093   0.151  1.00  0.00           N
ATOM     32  C4   DC A   2      -1.402   2.994   0.984  1.00  0.00           C
ATOM     33  N4   DC A   2      -1.939   4.150   1.458  1.00  0.00           N
ATOM     34  C5   DC A   2      -1.911   1.740   1.457  1.00  0.00           C
ATOM     35  C6   DC A   2      -1.269   0.626   1.023  1.00  0.00           C
ATOM     36  P    DA A   3       3.848  -2.871  -0.107  1.00  0.00           P
ATOM     37  OP1  DA A   3       4.350  -4.189  -0.636  1.00  0.00           O
ATOM     38  OP2  DA A   3       3.712  -2.756   1.387  1.00  0.00           O
ATOM     39  O5'  DA A   3       4.794  -1.644  -0.601  1.00  0.00           O
ATOM     40  C5'  DA A   3       4.959  -1.405  -1.999  1.00  0.00           C
ATOM     41  C4'  DA A   3       5.519  -0.010  -2.187  1.00  0.00           C
ATOM     42  O4'  DA A   3       4.565   0.953  -1.729  1.00  0.00           O
ATOM     43  C3'  DA A   3       6.813   0.278  -1.419  1.00  0.00           C
ATOM     44  O3'  DA A   3       7.539   1.210  -2.203  1.00  0.00           O
ATOM     45  C2'  DA A   3       6.299   0.915  -0.134  1.00  0.00           C
ATOM     46  C1'  DA A   3       5.077   1.689  -0.632  1.00  0.00           C
ATOM     47  N9   DA A   3       4.043   1.839   0.370  1.00  0.00           N
ATOM     48  C8   DA A   3       3.407   0.830   1.053  1.00  0.00           C
ATOM     49  N7   DA A   3       2.479   1.253   1.875  1.00  0.00           N
ATOM     50  C5   DA A   3       2.498   2.624   1.718  1.00  0.00           C
ATOM     51  C6   DA A   3       1.715   3.654   2.269  1.00  0.00           C
ATOM     52  N6   DA A   3       0.757   3.408   3.201  1.00  0.00           N
ATOM     53  N1   DA A   3       1.949   4.917   1.886  1.00  0.00           N
ATOM     54  C2   DA A   3       2.911   5.137   0.977  1.00  0.00           C
ATOM     55  N3   DA A   3       3.704   4.258   0.370  1.00  0.00           N
ATOM     56  C4   DA A   3       3.448   3.009   0.775  1.00  0.00           C
END

COMPND    CCA / M06-2X / NA MODEL / SINGLY IONIZED
ATOM      1  O5'  DC A   1      -7.306  -0.737  -0.602  1.00  0.00           O
ATOM      2  C5'  DC A   1      -6.900  -1.695  -1.565  1.00  0.00           C
ATOM      3  C4'  DC A   1      -5.387  -1.790  -1.557  1.00  0.00           C
ATOM      4  O4'  DC A   1      -4.823  -0.565  -2.034  1.00  0.00           O
ATOM      5  C3'  DC A   1      -4.779  -2.012  -0.166  1.00  0.00           C
ATOM      6  O3'  DC A   1      -3.556  -2.734  -0.365  1.00  0.00           O
ATOM      7  C2'  DC A   1      -4.479  -0.592   0.288  1.00  0.00           C
ATOM      8  C1'  DC A   1      -4.014   0.033  -1.026  1.00  0.00           C
ATOM      9  N1   DC A   1      -4.172   1.476  -1.090  1.00  0.00           N
ATOM     10  C2   DC A   1      -3.073   2.284  -1.480  1.00  0.00           C
ATOM     11  O2   DC A   1      -2.045   1.749  -1.885  1.00  0.00           O
ATOM     12  N3   DC A   1      -3.217   3.635  -1.371  1.00  0.00           N
ATOM     13  C4   DC A   1      -4.386   4.157  -1.036  1.00  0.00           C
ATOM     14  N4   DC A   1      -4.456   5.492  -0.908  1.00  0.00           N
ATOM     15  C5   DC A   1      -5.565   3.365  -0.814  1.00  0.00           C
ATOM     16  C6   DC A   1      -5.396   2.024  -0.847  1.00  0.00           C
ATOM     17  P    DC A   2      -2.769  -3.334   0.925  1.00  0.00           P
ATOM     18  OP1  DC A   2      -3.588  -4.401   1.606  1.00  0.00           O
ATOM     19  OP2  DC A   2      -2.303  -2.237   1.860  1.00  0.00           O
ATOM     20  O5'  DC A   2      -1.515  -4.023   0.174  1.00  0.00           O
ATOM     21  C5'  DC A   2      -1.081  -3.764  -1.159  1.00  0.00           C
ATOM     22  C4'  DC A   2       0.012  -2.719  -1.222  1.00  0.00           C
ATOM     23  O4'  DC A   2      -0.541  -1.412  -1.043  1.00  0.00           O
ATOM     24  C3'  DC A   2       1.121  -2.876  -0.149  1.00  0.00           C
ATOM     25  O3'  DC A   2       2.366  -2.803  -0.859  1.00  0.00           O
ATOM     26  C2'  DC A   2       0.891  -1.659   0.737  1.00  0.00           C
ATOM     27  C1'  DC A   2       0.431  -0.664  -0.319  1.00  0.00           C
ATOM     28  N1   DC A   2      -0.150   0.570   0.162  1.00  0.00           N
ATOM     29  C2   DC A   2       0.434   1.797  -0.225  1.00  0.00           C
ATOM     30  O2   DC A   2       1.423   1.795  -0.956  1.00  0.00           O
ATOM     31  N3   DC A   2      -0.078   2.944   0.303  1.00  0.00           N
ATOM     32  C4   DC A   2      -1.148   2.899   1.083  1.00  0.00           C
ATOM     33  N4   DC A   2      -1.564   4.065   1.620  1.00  0.00           N
ATOM     34  C5   DC A   2      -1.800   1.676   1.442  1.00  0.00           C
ATOM     35  C6   DC A   2      -1.243   0.533   0.969  1.00  0.00           C
ATOM     36  P    DA A   3       3.816  -2.876  -0.123  1.00  0.00           P
ATOM     37  OP1  DA A   3       4.570  -4.080  -0.616  1.00  0.00           O
ATOM     38  OP2  DA A   3       3.709  -2.699   1.367  1.00  0.00           O
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ATOM     39  O5'  DA A   3       4.493  -1.504  -0.693  1.00  0.00           O
ATOM     40  C5'  DA A   3       4.608  -1.313  -2.100  1.00  0.00           C
ATOM     41  C4'  DA A   3       5.227   0.048  -2.344  1.00  0.00           C
ATOM     42  O4'  DA A   3       4.369   1.065  -1.810  1.00  0.00           O
ATOM     43  C3'  DA A   3       6.592   0.275  -1.689  1.00  0.00           C
ATOM     44  O3'  DA A   3       7.275   1.196  -2.521  1.00  0.00           O
ATOM     45  C2'  DA A   3       6.222   0.908  -0.351  1.00  0.00           C
ATOM     46  C1'  DA A   3       4.977   1.716  -0.724  1.00  0.00           C
ATOM     47  N9   DA A   3       4.015   1.817   0.381  1.00  0.00           N
ATOM     48  C8   DA A   3       3.489   0.813   1.110  1.00  0.00           C
ATOM     49  N7   DA A   3       2.566   1.209   2.010  1.00  0.00           N
ATOM     50  C5   DA A   3       2.489   2.525   1.826  1.00  0.00           C
ATOM     51  C6   DA A   3       1.701   3.553   2.445  1.00  0.00           C
ATOM     52  N6   DA A   3       0.876   3.291   3.431  1.00  0.00           N
ATOM     53  N1   DA A   3       1.831   4.831   2.003  1.00  0.00           N
ATOM     54  C2   DA A   3       2.678   5.068   1.029  1.00  0.00           C
ATOM     55  N3   DA A   3       3.502   4.190   0.366  1.00  0.00           N
ATOM     56  C4   DA A   3       3.364   2.968   0.785  1.00  0.00           C
END

COMPND    CAA / M06-2X / NA MODEL / NEUTRAL
ATOM      1  O5'  DC A   1      -7.276  -0.856  -0.308  1.00  0.00           O
ATOM      2  C5'  DC A   1      -6.931  -1.817  -1.290  1.00  0.00           C
ATOM      3  C4'  DC A   1      -5.419  -1.909  -1.379  1.00  0.00           C
ATOM      4  O4'  DC A   1      -4.891  -0.684  -1.892  1.00  0.00           O
ATOM      5  C3'  DC A   1      -4.725  -2.124  -0.028  1.00  0.00           C
ATOM      6  O3'  DC A   1      -3.510  -2.838  -0.296  1.00  0.00           O
ATOM      7  C2'  DC A   1      -4.408  -0.702   0.407  1.00  0.00           C
ATOM      8  C1'  DC A   1      -4.031  -0.076  -0.933  1.00  0.00           C
ATOM      9  N1   DC A   1      -4.193   1.366  -0.993  1.00  0.00           N
ATOM     10  C2   DC A   1      -3.164   2.150  -1.576  1.00  0.00           C
ATOM     11  O2   DC A   1      -2.228   1.592  -2.139  1.00  0.00           O
ATOM     12  N3   DC A   1      -3.267   3.505  -1.465  1.00  0.00           N
ATOM     13  C4   DC A   1      -4.362   4.049  -0.963  1.00  0.00           C
ATOM     14  N4   DC A   1      -4.386   5.388  -0.826  1.00  0.00           N
ATOM     15  C5   DC A   1      -5.507   3.281  -0.557  1.00  0.00           C
ATOM     16  C6   DC A   1      -5.362   1.937  -0.588  1.00  0.00           C
ATOM     17  P    DA A   2      -2.703  -3.486   0.957  1.00  0.00           P
ATOM     18  OP1  DA A   2      -3.507  -4.590   1.597  1.00  0.00           O
ATOM     19  OP2  DA A   2      -2.242  -2.427   1.935  1.00  0.00           O
ATOM     20  O5'  DA A   2      -1.431  -4.107   0.179  1.00  0.00           O
ATOM     21  C5'  DA A   2      -1.086  -3.951  -1.196  1.00  0.00           C
ATOM     22  C4'  DA A   2       0.058  -2.973  -1.373  1.00  0.00           C
ATOM     23  O4'  DA A   2      -0.421  -1.627  -1.267  1.00  0.00           O
ATOM     24  C3'  DA A   2       1.171  -3.120  -0.311  1.00  0.00           C
ATOM     25  O3'  DA A   2       2.414  -2.999  -1.014  1.00  0.00           O
ATOM     26  C2'  DA A   2       0.907  -1.927   0.598  1.00  0.00           C
ATOM     27  C1'  DA A   2       0.480  -0.899  -0.439  1.00  0.00           C
ATOM     28  N9   DA A   2      -0.177   0.275   0.065  1.00  0.00           N
ATOM     29  C8   DA A   2      -1.150   0.340   1.032  1.00  0.00           C
ATOM     30  N7   DA A   2      -1.534   1.565   1.307  1.00  0.00           N
ATOM     31  C5   DA A   2      -0.755   2.352   0.478  1.00  0.00           C
ATOM     32  C6   DA A   2      -0.663   3.741   0.292  1.00  0.00           C
ATOM     33  N6   DA A   2      -1.414   4.617   1.014  1.00  0.00           N
ATOM     34  N1   DA A   2       0.244   4.217  -0.574  1.00  0.00           N
ATOM     35  C2   DA A   2       1.014   3.340  -1.235  1.00  0.00           C
ATOM     36  N3   DA A   2       1.007   2.011  -1.170  1.00  0.00           N
ATOM     37  C4   DA A   2       0.096   1.571  -0.298  1.00  0.00           C
ATOM     38  P    DA A   3       3.848  -3.102  -0.242  1.00  0.00           P
ATOM     39  OP1  DA A   3       4.667  -4.193  -0.876  1.00  0.00           O
ATOM     40  OP2  DA A   3       3.669  -3.158   1.249  1.00  0.00           O
ATOM     41  O5'  DA A   3       4.479  -1.640  -0.601  1.00  0.00           O
ATOM     42  C5'  DA A   3       4.670  -1.316  -1.978  1.00  0.00           C
ATOM     43  C4'  DA A   3       5.278   0.067  -2.083  1.00  0.00           C
ATOM     44  O4'  DA A   3       4.363   1.039  -1.570  1.00  0.00           O
ATOM     45  C3'  DA A   3       6.582   0.261  -1.300  1.00  0.00           C
ATOM     46  O3'  DA A   3       7.340   1.214  -2.026  1.00  0.00           O
ATOM     47  C2'  DA A   3       6.089   0.834   0.023  1.00  0.00           C
ATOM     48  C1'  DA A   3       4.896   1.681  -0.425  1.00  0.00           C
ATOM     49  N9   DA A   3       3.857   1.793   0.578  1.00  0.00           N
ATOM     50  C8   DA A   3       3.153   0.757   1.145  1.00  0.00           C
ATOM     51  N7   DA A   3       2.199   1.147   1.953  1.00  0.00           N
ATOM     52  C5   DA A   3       2.273   2.526   1.911  1.00  0.00           C
ATOM     53  C6   DA A   3       1.501   3.544   2.502  1.00  0.00           C
ATOM     54  N6   DA A   3       0.445   3.277   3.317  1.00  0.00           N
ATOM     55  N1   DA A   3       1.831   4.822   2.264  1.00  0.00           N
ATOM     56  C2   DA A   3       2.851   5.075   1.432  1.00  0.00           C
ATOM     57  N3   DA A   3       3.625   4.214   0.777  1.00  0.00           N
ATOM     58  C4   DA A   3       3.291   2.948   1.056  1.00  0.00           C
END

COMPND    CAA / M06-2X / NA MODEL / SINGLY IONIZED
ATOM      1  O5'  DC A   1      -6.984  -1.619  -0.498  1.00  0.00           O
ATOM      2  C5'  DC A   1      -6.409  -2.463  -1.482  1.00  0.00           C
ATOM      3  C4'  DC A   1      -4.906  -2.262  -1.469  1.00  0.00           C
ATOM      4  O4'  DC A   1      -4.593  -0.945  -1.932  1.00  0.00           O
ATOM      5  C3'  DC A   1      -4.279  -2.372  -0.074  1.00  0.00           C
ATOM      6  O3'  DC A   1      -2.942  -2.860  -0.244  1.00  0.00           O
ATOM      7  C2'  DC A   1      -4.232  -0.924   0.389  1.00  0.00           C
ATOM      8  C1'  DC A   1      -3.916  -0.209  -0.925  1.00  0.00           C
ATOM      9  N1   DC A   1      -4.376   1.173  -0.980  1.00  0.00           N
ATOM     10  C2   DC A   1      -3.476   2.205  -1.312  1.00  0.00           C
ATOM     11  O2   DC A   1      -2.305   1.919  -1.592  1.00  0.00           O
ATOM     12  N3   DC A   1      -3.924   3.484  -1.289  1.00  0.00           N
ATOM     13  C4   DC A   1      -5.208   3.735  -1.054  1.00  0.00           C
ATOM     14  N4   DC A   1      -5.593   5.017  -1.030  1.00  0.00           N
ATOM     15  C5   DC A   1      -6.176   2.698  -0.842  1.00  0.00           C
ATOM     16  C6   DC A   1      -5.705   1.431  -0.812  1.00  0.00           C
ATOM     17  P    DA A   2      -2.271  -3.653   1.007  1.00  0.00           P
ATOM     18  OP1  DA A   2      -3.148  -4.800   1.432  1.00  0.00           O
ATOM     19  OP2  DA A   2      -1.902  -2.705   2.129  1.00  0.00           O
ATOM     20  O5'  DA A   2      -0.903  -4.159   0.317  1.00  0.00           O
ATOM     21  C5'  DA A   2      -0.593  -4.167  -1.075  1.00  0.00           C
ATOM     22  C4'  DA A   2       0.519  -3.173  -1.352  1.00  0.00           C
ATOM     23  O4'  DA A   2      -0.003  -1.835  -1.306  1.00  0.00           O
ATOM     24  C3'  DA A   2       1.660  -3.220  -0.316  1.00  0.00           C
ATOM     25  O3'  DA A   2       2.868  -3.022  -1.054  1.00  0.00           O
ATOM     26  C2'  DA A   2       1.319  -2.043   0.592  1.00  0.00           C
ATOM     27  C1'  DA A   2       0.797  -1.057  -0.440  1.00  0.00           C
ATOM     28  N9   DA A   2      -0.015   0.017   0.106  1.00  0.00           N
ATOM     29  C8   DA A   2      -0.916  -0.049   1.117  1.00  0.00           C
ATOM     30  N7   DA A   2      -1.466   1.135   1.433  1.00  0.00           N
ATOM     31  C5   DA A   2      -0.882   1.993   0.595  1.00  0.00           C
ATOM     32  C6   DA A   2      -1.036   3.401   0.375  1.00  0.00           C
ATOM     33  N6   DA A   2      -1.895   4.106   1.073  1.00  0.00           N
ATOM     34  N1   DA A   2      -0.273   4.004  -0.569  1.00  0.00           N
ATOM     35  C2   DA A   2       0.556   3.257  -1.267  1.00  0.00           C
ATOM     36  N3   DA A   2       0.775   1.907  -1.191  1.00  0.00           N
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ATOM     37  C4   DA A   2       0.049   1.343  -0.272  1.00  0.00           C
ATOM     38  P    DA A   3       4.304  -2.733  -0.332  1.00  0.00           P
ATOM     39  OP1  DA A   3       5.354  -3.538  -1.046  1.00  0.00           O
ATOM     40  OP2  DA A   3       4.217  -2.874   1.161  1.00  0.00           O
ATOM     41  O5'  DA A   3       4.489  -1.142  -0.658  1.00  0.00           O
ATOM     42  C5'  DA A   3       4.605  -0.768  -2.033  1.00  0.00           C
ATOM     43  C4'  DA A   3       5.027   0.683  -2.119  1.00  0.00           C
ATOM     44  O4'  DA A   3       4.011   1.515  -1.552  1.00  0.00           O
ATOM     45  C3'  DA A   3       6.320   1.021  -1.369  1.00  0.00           C
ATOM     46  O3'  DA A   3       6.934   2.071  -2.095  1.00  0.00           O
ATOM     47  C2'  DA A   3       5.802   1.506  -0.020  1.00  0.00           C
ATOM     48  C1'  DA A   3       4.503   2.206  -0.419  1.00  0.00           C
ATOM     49  N9   DA A   3       3.490   2.182   0.620  1.00  0.00           N
ATOM     50  C8   DA A   3       2.990   1.069   1.253  1.00  0.00           C
ATOM     51  N7   DA A   3       2.015   1.331   2.088  1.00  0.00           N
ATOM     52  C5   DA A   3       1.860   2.703   1.996  1.00  0.00           C
ATOM     53  C6   DA A   3       0.988   3.617   2.625  1.00  0.00           C
ATOM     54  N6   DA A   3       0.028   3.221   3.485  1.00  0.00           N
ATOM     55  N1   DA A   3       1.077   4.917   2.301  1.00  0.00           N
ATOM     56  C2   DA A   3       1.992   5.291   1.396  1.00  0.00           C
ATOM     57  N3   DA A   3       2.870   4.538   0.738  1.00  0.00           N
ATOM     58  C4   DA A   3       2.761   3.249   1.081  1.00  0.00           C
END
COMPND    ACC / M06-2X / PO- MODEL / NEUTRAL
ATOM      1  O5'  DA A   1      -7.345  -0.356   0.238  1.00  0.00           O
ATOM      2  C5'  DA A   1      -7.088  -1.316  -0.770  1.00  0.00           C
ATOM      3  C4'  DA A   1      -5.591  -1.521  -0.882  1.00  0.00           C
ATOM      4  O4'  DA A   1      -4.979  -0.326  -1.384  1.00  0.00           O
ATOM      5  C3'  DA A   1      -4.893  -1.817   0.455  1.00  0.00           C
ATOM      6  O3'  DA A   1      -3.776  -2.649   0.159  1.00  0.00           O
ATOM      7  C2'  DA A   1      -4.423  -0.433   0.884  1.00  0.00           C
ATOM      8  C1'  DA A   1      -3.985   0.111  -0.467  1.00  0.00           C
ATOM      9  N9   DA A   1      -3.863   1.550  -0.533  1.00  0.00           N
ATOM     10  C8   DA A   1      -4.436   2.509   0.270  1.00  0.00           C
ATOM     11  N7   DA A   1      -4.003   3.722   0.039  1.00  0.00           N
ATOM     12  C5   DA A   1      -3.089   3.557  -0.984  1.00  0.00           C
ATOM     13  C6   DA A   1      -2.215   4.447  -1.636  1.00  0.00           C
ATOM     14  N6   DA A   1      -2.114   5.748  -1.266  1.00  0.00           N
ATOM     15  N1   DA A   1      -1.414   3.976  -2.600  1.00  0.00           N
ATOM     16  C2   DA A   1      -1.435   2.660  -2.857  1.00  0.00           C
ATOM     17  N3   DA A   1      -2.170   1.711  -2.284  1.00  0.00           N
ATOM     18  C4   DA A   1      -2.984   2.220  -1.352  1.00  0.00           C
ATOM     19  P    DC A   2      -2.907  -3.279   1.407  1.00  0.00           P
ATOM     20  OP2  DC A   2      -2.163  -2.194   2.139  1.00  0.00           O
ATOM     21  OP1  DC A   2      -3.772  -4.217   2.191  1.00  0.00           O
ATOM     22  O5'  DC A   2      -1.864  -4.171   0.520  1.00  0.00           O
ATOM     23  C5'  DC A   2      -1.548  -3.963  -0.848  1.00  0.00           C
ATOM     24  C4'  DC A   2      -0.401  -2.999  -1.074  1.00  0.00           C
ATOM     25  O4'  DC A   2      -0.834  -1.645  -0.910  1.00  0.00           O
ATOM     26  C3'  DC A   2       0.810  -3.199  -0.128  1.00  0.00           C
ATOM     27  O3'  DC A   2       1.955  -3.386  -0.958  1.00  0.00           O
ATOM     28  C2'  DC A   2       0.841  -1.887   0.651  1.00  0.00           C
ATOM     29  C1'  DC A   2       0.286  -0.933  -0.399  1.00  0.00           C
ATOM     30  N1   DC A   2      -0.134   0.372   0.073  1.00  0.00           N
ATOM     31  C2   DC A   2       0.426   1.534  -0.522  1.00  0.00           C
ATOM     32  O2   DC A   2       1.206   1.417  -1.461  1.00  0.00           O
ATOM     33  N3   DC A   2       0.071   2.746  -0.003  1.00  0.00           N
ATOM     34  C4   DC A   2      -0.794   2.822   0.992  1.00  0.00           C
ATOM     35  N4   DC A   2      -1.108   4.054   1.460  1.00  0.00           N
ATOM     36  C5   DC A   2      -1.377   1.666   1.611  1.00  0.00           C
ATOM     37  C6   DC A   2      -1.016   0.458   1.105  1.00  0.00           C
ATOM     38  P    DC A   3       3.451  -3.493  -0.278  1.00  0.00           P
ATOM     39  OP1  DC A   3       4.264  -4.375  -1.171  1.00  0.00           O
ATOM     40  OP2  DC A   3       3.333  -3.710   1.195  1.00  0.00           O
ATOM     41  O5'  DC A   3       3.962  -1.930  -0.469  1.00  0.00           O
ATOM     42  C5'  DC A   3       4.229  -1.489  -1.795  1.00  0.00           C
ATOM     43  C4'  DC A   3       5.240  -0.361  -1.771  1.00  0.00           C
ATOM     44  O4'  DC A   3       4.649   0.825  -1.233  1.00  0.00           O
ATOM     45  C3'  DC A   3       6.477  -0.646  -0.912  1.00  0.00           C
ATOM     46  O3'  DC A   3       7.566   0.012  -1.539  1.00  0.00           O
ATOM     47  C2'  DC A   3       6.115   0.015   0.414  1.00  0.00           C
ATOM     48  C1'  DC A   3       5.311   1.232  -0.049  1.00  0.00           C
ATOM     49  N1   DC A   3       4.298   1.675   0.906  1.00  0.00           N
ATOM     50  C2   DC A   3       4.373   2.969   1.470  1.00  0.00           C
ATOM     51  O2   DC A   3       5.332   3.688   1.202  1.00  0.00           O
ATOM     52  N3   DC A   3       3.359   3.359   2.295  1.00  0.00           N
ATOM     53  C4   DC A   3       2.372   2.526   2.579  1.00  0.00           C
ATOM     54  N4   DC A   3       1.410   2.954   3.422  1.00  0.00           N
ATOM     55  C5   DC A   3       2.291   1.194   2.054  1.00  0.00           C
ATOM     56  C6   DC A   3       3.269   0.832   1.192  1.00  0.00           C
END

COMPND    ACC / M06-2X / PO- MODEL / SINGLY IONIZED
ATOM      1  O5'  DA A   1      -7.125  -0.479   0.519  1.00  0.00           O
ATOM      2  C5'  DA A   1      -7.010  -1.611  -0.327  1.00  0.00           C
ATOM      3  C4'  DA A   1      -5.543  -1.918  -0.560  1.00  0.00           C
ATOM      4  O4'  DA A   1      -4.924  -0.838  -1.279  1.00  0.00           O
ATOM      5  C3'  DA A   1      -4.697  -2.083   0.705  1.00  0.00           C
ATOM      6  O3'  DA A   1      -3.590  -2.901   0.345  1.00  0.00           O
ATOM      7  C2'  DA A   1      -4.229  -0.658   0.969  1.00  0.00           C
ATOM      8  C1'  DA A   1      -3.989  -0.178  -0.460  1.00  0.00           C
ATOM      9  N9   DA A   1      -4.181   1.269  -0.610  1.00  0.00           N
ATOM     10  C8   DA A   1      -5.242   1.998  -0.210  1.00  0.00           C
ATOM     11  N7   DA A   1      -5.130   3.316  -0.464  1.00  0.00           N
ATOM     12  C5   DA A   1      -3.945   3.424  -1.066  1.00  0.00           C
ATOM     13  C6   DA A   1      -3.218   4.540  -1.603  1.00  0.00           C
ATOM     14  N6   DA A   1      -3.677   5.766  -1.527  1.00  0.00           N
ATOM     15  N1   DA A   1      -2.025   4.310  -2.210  1.00  0.00           N
ATOM     16  C2   DA A   1      -1.581   3.076  -2.277  1.00  0.00           C
ATOM     17  N3   DA A   1      -2.176   1.922  -1.811  1.00  0.00           N
ATOM     18  C4   DA A   1      -3.306   2.155  -1.212  1.00  0.00           C
ATOM     19  P    DC A   2      -2.583  -3.437   1.535  1.00  0.00           P
ATOM     20  OP2  DC A   2      -1.894  -2.271   2.193  1.00  0.00           O
ATOM     21  OP1  DC A   2      -3.304  -4.427   2.392  1.00  0.00           O
ATOM     22  O5'  DC A   2      -1.527  -4.248   0.592  1.00  0.00           O
ATOM     23  C5'  DC A   2      -1.340  -4.077  -0.807  1.00  0.00           C
ATOM     24  C4'  DC A   2      -0.206  -3.132  -1.153  1.00  0.00           C
ATOM     25  O4'  DC A   2      -0.629  -1.766  -1.024  1.00  0.00           O
ATOM     26  C3'  DC A   2       1.061  -3.290  -0.273  1.00  0.00           C
ATOM     27  O3'  DC A   2       2.171  -3.389  -1.167  1.00  0.00           O
ATOM     28  C2'  DC A   2       1.036  -2.002   0.548  1.00  0.00           C
ATOM     29  C1'  DC A   2       0.483  -1.048  -0.500  1.00  0.00           C
ATOM     30  N1   DC A   2       0.039   0.249  -0.027  1.00  0.00           N
ATOM     31  C2   DC A   2       0.530   1.422  -0.651  1.00  0.00           C
ATOM     32  O2   DC A   2       1.296   1.338  -1.604  1.00  0.00           O
ATOM     33  N3   DC A   2       0.104   2.628  -0.164  1.00  0.00           N
ATOM     34  C4   DC A   2      -0.812   2.678   0.790  1.00  0.00           C
ATOM     35  N4   DC A   2      -1.321   3.893   1.086  1.00  0.00           N
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ATOM     36  C5   DC A   2      -1.330   1.509   1.436  1.00  0.00           C
ATOM     37  C6   DC A   2      -0.870   0.315   0.982  1.00  0.00           C
ATOM     38  P    DC A   3       3.705  -3.051  -0.675  1.00  0.00           P
ATOM     39  OP1  DC A   3       4.614  -3.636  -1.707  1.00  0.00           O
ATOM     40  OP2  DC A   3       3.853  -3.320   0.789  1.00  0.00           O
ATOM     41  O5'  DC A   3       3.701  -1.407  -0.829  1.00  0.00           O
ATOM     42  C5'  DC A   3       4.054  -0.795  -2.065  1.00  0.00           C
ATOM     43  C4'  DC A   3       5.224   0.147  -1.846  1.00  0.00           C
ATOM     44  O4'  DC A   3       4.801   1.298  -1.109  1.00  0.00           O
ATOM     45  C3'  DC A   3       6.366  -0.475  -1.035  1.00  0.00           C
ATOM     46  O3'  DC A   3       7.568   0.119  -1.502  1.00  0.00           O
ATOM     47  C2'  DC A   3       6.041  -0.032   0.390  1.00  0.00           C
ATOM     48  C1'  DC A   3       5.426   1.352   0.162  1.00  0.00           C
ATOM     49  N1   DC A   3       4.416   1.739   1.146  1.00  0.00           N
ATOM     50  C2   DC A   3       4.555   2.950   1.866  1.00  0.00           C
ATOM     51  O2   DC A   3       5.595   3.596   1.763  1.00  0.00           O
ATOM     52  N3   DC A   3       3.510   3.347   2.649  1.00  0.00           N
ATOM     53  C4   DC A   3       2.428   2.594   2.749  1.00  0.00           C
ATOM     54  N4   DC A   3       1.407   3.051   3.496  1.00  0.00           N
ATOM     55  C5   DC A   3       2.284   1.334   2.080  1.00  0.00           C
ATOM     56  C6   DC A   3       3.294   0.975   1.257  1.00  0.00           C
END

COMPND    AAC / M06-2X / PO- MODEL / NEUTRAL
ATOM      1  O5'  DA A   1      -7.349  -0.395   0.191  1.00  0.00           O
ATOM      2  C5'  DA A   1      -6.992  -1.252  -0.877  1.00  0.00           C
ATOM      3  C4'  DA A   1      -5.484  -1.388  -0.903  1.00  0.00           C
ATOM      4  O4'  DA A   1      -4.898  -0.137  -1.290  1.00  0.00           O
ATOM      5  C3'  DA A   1      -4.867  -1.737   0.464  1.00  0.00           C
ATOM      6  O3'  DA A   1      -3.733  -2.562   0.213  1.00  0.00           O
ATOM      7  C2'  DA A   1      -4.416  -0.371   0.973  1.00  0.00           C
ATOM      8  C1'  DA A   1      -3.904   0.208  -0.336  1.00  0.00           C
ATOM      9  N9   DA A   1      -3.705   1.638  -0.348  1.00  0.00           N
ATOM     10  C8   DA A   1      -4.064   2.583   0.584  1.00  0.00           C
ATOM     11  N7   DA A   1      -3.620   3.785   0.317  1.00  0.00           N
ATOM     12  C5   DA A   1      -2.921   3.626  -0.865  1.00  0.00           C
ATOM     13  C6   DA A   1      -2.148   4.506  -1.647  1.00  0.00           C
ATOM     14  N6   DA A   1      -1.970   5.804  -1.309  1.00  0.00           N
ATOM     15  N1   DA A   1      -1.523   4.022  -2.730  1.00  0.00           N
ATOM     16  C2   DA A   1      -1.638   2.714  -3.005  1.00  0.00           C
ATOM     17  N3   DA A   1      -2.325   1.782  -2.350  1.00  0.00           N
ATOM     18  C4   DA A   1      -2.950   2.301  -1.286  1.00  0.00           C
ATOM     19  P    DA A   2      -3.046  -3.340   1.489  1.00  0.00           P
ATOM     20  OP1  DA A   2      -4.031  -4.316   2.053  1.00  0.00           O
ATOM     21  OP2  DA A   2      -2.378  -2.354   2.411  1.00  0.00           O
ATOM     22  O5'  DA A   2      -1.864  -4.129   0.684  1.00  0.00           O
ATOM     23  C5'  DA A   2      -1.701  -4.209  -0.724  1.00  0.00           C
ATOM     24  C4'  DA A   2      -0.498  -3.399  -1.169  1.00  0.00           C
ATOM     25  O4'  DA A   2      -0.804  -1.996  -1.113  1.00  0.00           O
ATOM     26  C3'  DA A   2       0.751  -3.608  -0.283  1.00  0.00           C
ATOM     27  O3'  DA A   2       1.875  -3.673  -1.163  1.00  0.00           O
ATOM     28  C2'  DA A   2       0.728  -2.352   0.582  1.00  0.00           C
ATOM     29  C1'  DA A   2       0.264  -1.338  -0.449  1.00  0.00           C
ATOM     30  N9   DA A   2      -0.190  -0.081   0.094  1.00  0.00           N
ATOM     31  C8   DA A   2      -1.016   0.115   1.178  1.00  0.00           C
ATOM     32  N7   DA A   2      -1.140   1.379   1.513  1.00  0.00           N
ATOM     33  C5   DA A   2      -0.338   2.049   0.607  1.00  0.00           C
ATOM     34  C6   DA A   2      -0.001   3.407   0.449  1.00  0.00           C
ATOM     35  N6   DA A   2      -0.531   4.379   1.237  1.00  0.00           N
ATOM     36  N1   DA A   2       0.899   3.740  -0.487  1.00  0.00           N
ATOM     37  C2   DA A   2       1.408   2.768  -1.260  1.00  0.00           C
ATOM     38  N3   DA A   2       1.141   1.466  -1.241  1.00  0.00           N
ATOM     39  C4   DA A   2       0.266   1.161  -0.278  1.00  0.00           C
ATOM     40  P    DC A   3       3.409  -3.364  -0.650  1.00  0.00           P
ATOM     41  OP1  DC A   3       4.319  -3.958  -1.676  1.00  0.00           O
ATOM     42  OP2  DC A   3       3.537  -3.641   0.814  1.00  0.00           O
ATOM     43  O5'  DC A   3       3.438  -1.720  -0.789  1.00  0.00           O
ATOM     44  C5'  DC A   3       3.834  -1.096  -2.005  1.00  0.00           C
ATOM     45  C4'  DC A   3       5.033  -0.201  -1.745  1.00  0.00           C
ATOM     46  O4'  DC A   3       4.639   0.926  -0.959  1.00  0.00           O
ATOM     47  C3'  DC A   3       6.157  -0.889  -0.964  1.00  0.00           C
ATOM     48  O3'  DC A   3       7.373  -0.307  -1.407  1.00  0.00           O
ATOM     49  C2'  DC A   3       5.847  -0.503   0.483  1.00  0.00           C
ATOM     50  C1'  DC A   3       5.250   0.898   0.322  1.00  0.00           C
ATOM     51  N1   DC A   3       4.240   1.260   1.315  1.00  0.00           N
ATOM     52  C2   DC A   3       4.273   2.550   1.903  1.00  0.00           C
ATOM     53  O2   DC A   3       5.255   3.266   1.731  1.00  0.00           O
ATOM     54  N3   DC A   3       3.187   2.946   2.631  1.00  0.00           N
ATOM     55  C4   DC A   3       2.163   2.128   2.803  1.00  0.00           C
ATOM     56  N4   DC A   3       1.097   2.578   3.505  1.00  0.00           N
ATOM     57  C5   DC A   3       2.135   0.792   2.285  1.00  0.00           C
ATOM     58  C6   DC A   3       3.173   0.433   1.499  1.00  0.00           C
END

COMPND    AAC / M06-2X / PO- MODEL / SINGLY IONIZED
ATOM      1  O5'  DA A   1      -7.282   0.442  -0.256  1.00  0.00           O
ATOM      2  C5'  DA A   1      -7.004  -0.491  -1.283  1.00  0.00           C
ATOM      3  C4'  DA A   1      -5.549  -0.901  -1.192  1.00  0.00           C
ATOM      4  O4'  DA A   1      -4.712   0.211  -1.548  1.00  0.00           O
ATOM      5  C3'  DA A   1      -5.099  -1.324   0.219  1.00  0.00           C
ATOM      6  O3'  DA A   1      -4.098  -2.321   0.037  1.00  0.00           O
ATOM      7  C2'  DA A   1      -4.475  -0.036   0.748  1.00  0.00           C
ATOM      8  C1'  DA A   1      -3.753   0.394  -0.518  1.00  0.00           C
ATOM      9  N9   DA A   1      -3.279   1.760  -0.529  1.00  0.00           N
ATOM     10  C8   DA A   1      -3.599   2.806   0.307  1.00  0.00           C
ATOM     11  N7   DA A   1      -2.922   3.902   0.066  1.00  0.00           N
ATOM     12  C5   DA A   1      -2.108   3.561  -0.991  1.00  0.00           C
ATOM     13  C6   DA A   1      -1.122   4.274  -1.710  1.00  0.00           C
ATOM     14  N6   DA A   1      -0.825   5.552  -1.423  1.00  0.00           N
ATOM     15  N1   DA A   1      -0.440   3.630  -2.671  1.00  0.00           N
ATOM     16  C2   DA A   1      -0.735   2.344  -2.916  1.00  0.00           C
ATOM     17  N3   DA A   1      -1.646   1.569  -2.330  1.00  0.00           N
ATOM     18  C4   DA A   1      -2.304   2.233  -1.372  1.00  0.00           C
ATOM     19  P    DA A   2      -3.403  -3.058   1.329  1.00  0.00           P
ATOM     20  OP1  DA A   2      -4.411  -3.905   2.037  1.00  0.00           O
ATOM     21  OP2  DA A   2      -2.599  -2.068   2.134  1.00  0.00           O
ATOM     22  O5'  DA A   2      -2.379  -4.031   0.504  1.00  0.00           O
ATOM     23  C5'  DA A   2      -2.059  -3.920  -0.875  1.00  0.00           C
ATOM     24  C4'  DA A   2      -0.795  -3.124  -1.126  1.00  0.00           C
ATOM     25  O4'  DA A   2      -1.037  -1.720  -0.905  1.00  0.00           O
ATOM     26  C3'  DA A   2       0.405  -3.511  -0.225  1.00  0.00           C
ATOM     27  O3'  DA A   2       1.541  -3.644  -1.082  1.00  0.00           O
ATOM     28  C2'  DA A   2       0.481  -2.321   0.723  1.00  0.00           C
ATOM     29  C1'  DA A   2       0.104  -1.215  -0.244  1.00  0.00           C
ATOM     30  N9   DA A   2      -0.204   0.065   0.376  1.00  0.00           N
ATOM     31  C8   DA A   2      -1.089   0.328   1.362  1.00  0.00           C
ATOM     32  N7   DA A   2      -1.091   1.620   1.755  1.00  0.00           N
ATOM     33  C5   DA A   2      -0.145   2.189   1.002  1.00  0.00           C
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ATOM     34  C6   DA A   2       0.373   3.525   0.909  1.00  0.00           C
ATOM     35  N6   DA A   2      -0.157   4.517   1.588  1.00  0.00           N
ATOM     36  N1   DA A   2       1.411   3.769   0.071  1.00  0.00           N
ATOM     37  C2   DA A   2       1.879   2.779  -0.655  1.00  0.00           C
ATOM     38  N3   DA A   2       1.441   1.477  -0.711  1.00  0.00           N
ATOM     39  C4   DA A   2       0.465   1.248   0.120  1.00  0.00           C
ATOM     40  P    DC A   3       3.091  -3.314  -0.637  1.00  0.00           P
ATOM     41  OP1  DC A   3       3.954  -3.928  -1.690  1.00  0.00           O
ATOM     42  OP2  DC A   3       3.295  -3.559   0.828  1.00  0.00           O
ATOM     43  O5'  DC A   3       3.113  -1.674  -0.790  1.00  0.00           O
ATOM     44  C5'  DC A   3       3.443  -1.068  -2.034  1.00  0.00           C
ATOM     45  C4'  DC A   3       4.712  -0.254  -1.874  1.00  0.00           C
ATOM     46  O4'  DC A   3       4.509   0.832  -0.969  1.00  0.00           O
ATOM     47  C3'  DC A   3       5.887  -1.039  -1.294  1.00  0.00           C
ATOM     48  O3'  DC A   3       7.066  -0.409  -1.770  1.00  0.00           O
ATOM     49  C2'  DC A   3       5.714  -0.846   0.217  1.00  0.00           C
ATOM     50  C1'  DC A   3       5.048   0.534   0.306  1.00  0.00           C
ATOM     51  N1   DC A   3       4.002   0.687   1.332  1.00  0.00           N
ATOM     52  C2   DC A   3       3.675   2.032   1.660  1.00  0.00           C
ATOM     53  O2   DC A   3       4.292   2.940   1.110  1.00  0.00           O
ATOM     54  N3   DC A   3       2.678   2.260   2.561  1.00  0.00           N
ATOM     55  C4   DC A   3       2.047   1.238   3.128  1.00  0.00           C
ATOM     56  N4   DC A   3       1.113   1.523   4.050  1.00  0.00           N
ATOM     57  C5   DC A   3       2.317  -0.123   2.783  1.00  0.00           C
ATOM     58  C6   DC A   3       3.298  -0.342   1.870  1.00  0.00           C
END

COMPND    CCA / M06-2X / PO- MODEL / NEUTRAL
ATOM      1  O5'  DC A   1      -7.342  -0.870   0.004  1.00  0.00           O
ATOM      2  C5'  DC A   1      -7.024  -1.924  -0.888  1.00  0.00           C
ATOM      3  C4'  DC A   1      -5.516  -2.029  -1.013  1.00  0.00           C
ATOM      4  O4'  DC A   1      -5.005  -0.856  -1.652  1.00  0.00           O
ATOM      5  C3'  DC A   1      -4.772  -2.129   0.326  1.00  0.00           C
ATOM      6  O3'  DC A   1      -3.577  -2.871   0.082  1.00  0.00           O
ATOM      7  C2'  DC A   1      -4.439  -0.673   0.619  1.00  0.00           C
ATOM      8  C1'  DC A   1      -4.098  -0.180  -0.784  1.00  0.00           C
ATOM      9  N1   DC A   1      -4.246   1.252  -0.979  1.00  0.00           N
ATOM     10  C2   DC A   1      -3.180   1.987  -1.559  1.00  0.00           C
ATOM     11  O2   DC A   1      -2.197   1.389  -1.982  1.00  0.00           O
ATOM     12  N3   DC A   1      -3.306   3.345  -1.606  1.00  0.00           N
ATOM     13  C4   DC A   1      -4.428   3.925  -1.217  1.00  0.00           C
ATOM     14  N4   DC A   1      -4.473   5.269  -1.236  1.00  0.00           N
ATOM     15  C5   DC A   1      -5.582   3.190  -0.776  1.00  0.00           C
ATOM     16  C6   DC A   1      -5.430   1.850  -0.673  1.00  0.00           C
ATOM     17  P    DC A   2      -2.699  -3.370   1.382  1.00  0.00           P
ATOM     18  OP1  DC A   2      -3.437  -4.460   2.096  1.00  0.00           O
ATOM     19  OP2  DC A   2      -2.216  -2.184   2.172  1.00  0.00           O
ATOM     20  O5'  DC A   2      -1.449  -4.045   0.576  1.00  0.00           O
ATOM     21  C5'  DC A   2      -1.102  -3.858  -0.789  1.00  0.00           C
ATOM     22  C4'  DC A   2       0.042  -2.878  -0.983  1.00  0.00           C
ATOM     23  O4'  DC A   2      -0.439  -1.531  -0.952  1.00  0.00           O
ATOM     24  C3'  DC A   2       1.145  -2.971   0.096  1.00  0.00           C
ATOM     25  O3'  DC A   2       2.399  -2.899  -0.586  1.00  0.00           O
ATOM     26  C2'  DC A   2       0.886  -1.718   0.926  1.00  0.00           C
ATOM     27  C1'  DC A   2       0.496  -0.763  -0.193  1.00  0.00           C
ATOM     28  N1   DC A   2      -0.116   0.496   0.175  1.00  0.00           N
ATOM     29  C2   DC A   2       0.337   1.687  -0.448  1.00  0.00           C
ATOM     30  O2   DC A   2       1.240   1.633  -1.277  1.00  0.00           O
ATOM     31  N3   DC A   2      -0.242   2.863  -0.068  1.00  0.00           N
ATOM     32  C4   DC A   2      -1.242   2.866   0.787  1.00  0.00           C
ATOM     33  N4   DC A   2      -1.742   4.076   1.166  1.00  0.00           N
ATOM     34  C5   DC A   2      -1.770   1.674   1.379  1.00  0.00           C
ATOM     35  C6   DC A   2      -1.163   0.509   1.037  1.00  0.00           C
ATOM     36  P    DA A   3       3.798  -3.229   0.223  1.00  0.00           P
ATOM     37  OP1  DA A   3       4.359  -4.512  -0.303  1.00  0.00           O
ATOM     38  OP2  DA A   3       3.619  -2.974   1.686  1.00  0.00           O
ATOM     39  O5'  DA A   3       4.701  -1.971  -0.336  1.00  0.00           O
ATOM     40  C5'  DA A   3       4.915  -1.854  -1.733  1.00  0.00           C
ATOM     41  C4'  DA A   3       5.583  -0.521  -2.009  1.00  0.00           C
ATOM     42  O4'  DA A   3       4.701   0.545  -1.643  1.00  0.00           O
ATOM     43  C3'  DA A   3       6.877  -0.275  -1.229  1.00  0.00           C
ATOM     44  O3'  DA A   3       7.675   0.573  -2.040  1.00  0.00           O
ATOM     45  C2'  DA A   3       6.380   0.455   0.014  1.00  0.00           C
ATOM     46  C1'  DA A   3       5.217   1.276  -0.545  1.00  0.00           C
ATOM     47  N9   DA A   3       4.164   1.515   0.422  1.00  0.00           N
ATOM     48  C8   DA A   3       3.489   0.575   1.169  1.00  0.00           C
ATOM     49  N7   DA A   3       2.545   1.085   1.921  1.00  0.00           N
ATOM     50  C5   DA A   3       2.592   2.436   1.648  1.00  0.00           C
ATOM     51  C6   DA A   3       1.817   3.523   2.090  1.00  0.00           C
ATOM     52  N6   DA A   3       0.835   3.375   3.018  1.00  0.00           N
ATOM     53  N1   DA A   3       2.085   4.745   1.608  1.00  0.00           N
ATOM     54  C2   DA A   3       3.073   4.870   0.709  1.00  0.00           C
ATOM     55  N3   DA A   3       3.865   3.930   0.202  1.00  0.00           N
ATOM     56  C4   DA A   3       3.576   2.723   0.706  1.00  0.00           C
END

COMPND    CCA / M06-2X / PO- MODEL / SINGLY IONIZED
ATOM      1  O5'  DC A   1      -7.286  -0.330  -0.186  1.00  0.00           O
ATOM      2  C5'  DC A   1      -7.026  -1.451  -1.014  1.00  0.00           C
ATOM      3  C4'  DC A   1      -5.532  -1.709  -1.042  1.00  0.00           C
ATOM      4  O4'  DC A   1      -4.868  -0.630  -1.706  1.00  0.00           O
ATOM      5  C3'  DC A   1      -4.880  -1.809   0.344  1.00  0.00           C
ATOM      6  O3'  DC A   1      -3.763  -2.684   0.211  1.00  0.00           O
ATOM      7  C2'  DC A   1      -4.411  -0.380   0.582  1.00  0.00           C
ATOM      8  C1'  DC A   1      -3.947   0.003  -0.822  1.00  0.00           C
ATOM      9  N1   DC A   1      -3.954   1.433  -1.088  1.00  0.00           N
ATOM     10  C2   DC A   1      -2.796   2.055  -1.621  1.00  0.00           C
ATOM     11  O2   DC A   1      -1.841   1.365  -1.964  1.00  0.00           O
ATOM     12  N3   DC A   1      -2.801   3.416  -1.716  1.00  0.00           N
ATOM     13  C4   DC A   1      -3.893   4.102  -1.422  1.00  0.00           C
ATOM     14  N4   DC A   1      -3.822   5.443  -1.494  1.00  0.00           N
ATOM     15  C5   DC A   1      -5.131   3.482  -1.038  1.00  0.00           C
ATOM     16  C6   DC A   1      -5.100   2.140  -0.881  1.00  0.00           C
ATOM     17  P    DC A   2      -2.985  -3.179   1.574  1.00  0.00           P
ATOM     18  OP2  DC A   2      -2.325  -2.013   2.262  1.00  0.00           O
ATOM     19  OP1  DC A   2      -3.889  -4.068   2.370  1.00  0.00           O
ATOM     20  O5'  DC A   2      -1.850  -4.116   0.862  1.00  0.00           O
ATOM     21  C5'  DC A   2      -1.448  -4.051  -0.498  1.00  0.00           C
ATOM     22  C4'  DC A   2      -0.267  -3.134  -0.740  1.00  0.00           C
ATOM     23  O4'  DC A   2      -0.679  -1.763  -0.713  1.00  0.00           O
ATOM     24  C3'  DC A   2       0.894  -3.275   0.286  1.00  0.00           C
ATOM     25  O3'  DC A   2       2.083  -3.532  -0.470  1.00  0.00           O
ATOM     26  C2'  DC A   2       0.853  -1.924   0.990  1.00  0.00           C
ATOM     27  C1'  DC A   2       0.413  -1.037  -0.163  1.00  0.00           C
ATOM     28  N1   DC A   2      -0.013   0.303   0.190  1.00  0.00           N
ATOM     29  C2   DC A   2       0.723   1.400  -0.304  1.00  0.00           C
ATOM     30  O2   DC A   2       1.742   1.201  -0.965  1.00  0.00           O
ATOM     31  N3   DC A   2       0.302   2.654   0.030  1.00  0.00           N
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ATOM     32  C4   DC A   2      -0.777   2.816   0.780  1.00  0.00           C
ATOM     33  N4   DC A   2      -1.107   4.085   1.117  1.00  0.00           N
ATOM     34  C5   DC A   2      -1.524   1.722   1.317  1.00  0.00           C
ATOM     35  C6   DC A   2      -1.090   0.476   0.995  1.00  0.00           C
ATOM     36  P    DA A   3       3.585  -2.975  -0.136  1.00  0.00           P
ATOM     37  OP1  DA A   3       4.506  -3.753  -1.019  1.00  0.00           O
ATOM     38  OP2  DA A   3       3.815  -2.830   1.342  1.00  0.00           O
ATOM     39  O5'  DA A   3       3.484  -1.419  -0.667  1.00  0.00           O
ATOM     40  C5'  DA A   3       3.685  -1.104  -2.038  1.00  0.00           C
ATOM     41  C4'  DA A   3       4.959  -0.296  -2.197  1.00  0.00           C
ATOM     42  O4'  DA A   3       4.840   0.997  -1.587  1.00  0.00           O
ATOM     43  C3'  DA A   3       6.187  -0.917  -1.532  1.00  0.00           C
ATOM     44  O3'  DA A   3       7.316  -0.430  -2.238  1.00  0.00           O
ATOM     45  C2'  DA A   3       6.130  -0.346  -0.106  1.00  0.00           C
ATOM     46  C1'  DA A   3       5.381   0.982  -0.298  1.00  0.00           C
ATOM     47  N9   DA A   3       4.305   1.202   0.696  1.00  0.00           N
ATOM     48  C8   DA A   3       3.639   0.337   1.485  1.00  0.00           C
ATOM     49  N7   DA A   3       2.661   0.910   2.227  1.00  0.00           N
ATOM     50  C5   DA A   3       2.698   2.190   1.871  1.00  0.00           C
ATOM     51  C6   DA A   3       1.948   3.340   2.284  1.00  0.00           C
ATOM     52  N6   DA A   3       1.025   3.264   3.215  1.00  0.00           N
ATOM     53  N1   DA A   3       2.222   4.539   1.708  1.00  0.00           N
ATOM     54  C2   DA A   3       3.173   4.590   0.805  1.00  0.00           C
ATOM     55  N3   DA A   3       3.983   3.582   0.341  1.00  0.00           N
ATOM     56  C4   DA A   3       3.706   2.434   0.886  1.00  0.00           C
END

COMPND    CAA / M06-2X / PO- MODEL / NEUTRAL
ATOM      1  O5'  DC A   1      -7.289  -0.728   0.077  1.00  0.00           O
ATOM      2  C5'  DC A   1      -7.020  -1.785  -0.828  1.00  0.00           C
ATOM      3  C4'  DC A   1      -5.518  -1.942  -0.971  1.00  0.00           C
ATOM      4  O4'  DC A   1      -4.974  -0.783  -1.609  1.00  0.00           O
ATOM      5  C3'  DC A   1      -4.767  -2.075   0.360  1.00  0.00           C
ATOM      6  O3'  DC A   1      -3.599  -2.857   0.110  1.00  0.00           O
ATOM      7  C2'  DC A   1      -4.379  -0.634   0.658  1.00  0.00           C
ATOM      8  C1'  DC A   1      -4.038  -0.144  -0.746  1.00  0.00           C
ATOM      9  N1   DC A   1      -4.136   1.294  -0.929  1.00  0.00           N
ATOM     10  C2   DC A   1      -3.077   1.985  -1.570  1.00  0.00           C
ATOM     11  O2   DC A   1      -2.156   1.349  -2.070  1.00  0.00           O
ATOM     12  N3   DC A   1      -3.137   3.348  -1.587  1.00  0.00           N
ATOM     13  C4   DC A   1      -4.214   3.973  -1.143  1.00  0.00           C
ATOM     14  N4   DC A   1      -4.196   5.319  -1.140  1.00  0.00           N
ATOM     15  C5   DC A   1      -5.382   3.284  -0.669  1.00  0.00           C
ATOM     16  C6   DC A   1      -5.283   1.939  -0.577  1.00  0.00           C
ATOM     17  P    DA A   2      -2.818  -3.471   1.422  1.00  0.00           P
ATOM     18  OP1  DA A   2      -3.672  -4.525   2.057  1.00  0.00           O
ATOM     19  OP2  DA A   2      -2.281  -2.356   2.278  1.00  0.00           O
ATOM     20  O5'  DA A   2      -1.567  -4.187   0.655  1.00  0.00           O
ATOM     21  C5'  DA A   2      -1.261  -4.158  -0.731  1.00  0.00           C
ATOM     22  C4'  DA A   2      -0.046  -3.294  -1.024  1.00  0.00           C
ATOM     23  O4'  DA A   2      -0.415  -1.908  -1.056  1.00  0.00           O
ATOM     24  C3'  DA A   2       1.073  -3.416   0.031  1.00  0.00           C
ATOM     25  O3'  DA A   2       2.306  -3.408  -0.687  1.00  0.00           O
ATOM     26  C2'  DA A   2       0.869  -2.150   0.852  1.00  0.00           C
ATOM     27  C1'  DA A   2       0.506  -1.176  -0.256  1.00  0.00           C
ATOM     28  N9   DA A   2      -0.104   0.058   0.166  1.00  0.00           N
ATOM     29  C8   DA A   2      -1.057   0.230   1.140  1.00  0.00           C
ATOM     30  N7   DA A   2      -1.393   1.486   1.325  1.00  0.00           N
ATOM     31  C5   DA A   2      -0.605   2.180   0.426  1.00  0.00           C
ATOM     32  C6   DA A   2      -0.476   3.544   0.127  1.00  0.00           C
ATOM     33  N6   DA A   2      -1.183   4.499   0.794  1.00  0.00           N
ATOM     34  N1   DA A   2       0.421   3.921  -0.796  1.00  0.00           N
ATOM     35  C2   DA A   2       1.148   2.970  -1.400  1.00  0.00           C
ATOM     36  N3   DA A   2       1.105   1.652  -1.226  1.00  0.00           N
ATOM     37  C4   DA A   2       0.204   1.311  -0.301  1.00  0.00           C
ATOM     38  P    DA A   3       3.756  -3.513   0.092  1.00  0.00           P
ATOM     39  OP1  DA A   3       4.530  -4.619  -0.551  1.00  0.00           O
ATOM     40  OP2  DA A   3       3.562  -3.414   1.570  1.00  0.00           O
ATOM     41  O5'  DA A   3       4.403  -2.068  -0.374  1.00  0.00           O
ATOM     42  C5'  DA A   3       4.617  -1.865  -1.762  1.00  0.00           C
ATOM     43  C4'  DA A   3       5.322  -0.539  -1.966  1.00  0.00           C
ATOM     44  O4'  DA A   3       4.479   0.533  -1.531  1.00  0.00           O
ATOM     45  C3'  DA A   3       6.630  -0.383  -1.185  1.00  0.00           C
ATOM     46  O3'  DA A   3       7.456   0.476  -1.955  1.00  0.00           O
ATOM     47  C2'  DA A   3       6.168   0.296   0.099  1.00  0.00           C
ATOM     48  C1'  DA A   3       5.036   1.191  -0.408  1.00  0.00           C
ATOM     49  N9   DA A   3       3.997   1.422   0.574  1.00  0.00           N
ATOM     50  C8   DA A   3       3.248   0.466   1.222  1.00  0.00           C
ATOM     51  N7   DA A   3       2.308   0.963   1.987  1.00  0.00           N
ATOM     52  C5   DA A   3       2.438   2.330   1.828  1.00  0.00           C
ATOM     53  C6   DA A   3       1.711   3.426   2.330  1.00  0.00           C
ATOM     54  N6   DA A   3       0.650   3.271   3.167  1.00  0.00           N
ATOM     55  N1   DA A   3       2.093   4.664   1.986  1.00  0.00           N
ATOM     56  C2   DA A   3       3.122   4.803   1.139  1.00  0.00           C
ATOM     57  N3   DA A   3       3.861   3.859   0.564  1.00  0.00           N
ATOM     58  C4   DA A   3       3.475   2.635   0.948  1.00  0.00           C
END

COMPND    CAA / M06-2X / PO- MODEL / SINGLY IONIZED
ATOM      1  O5'  DC A   1      -7.072  -0.991  -0.518  1.00  0.00           O
ATOM      2  C5'  DC A   1      -6.518  -2.012  -1.332  1.00  0.00           C
ATOM      3  C4'  DC A   1      -5.009  -1.979  -1.191  1.00  0.00           C
ATOM      4  O4'  DC A   1      -4.504  -0.766  -1.761  1.00  0.00           O
ATOM      5  C3'  DC A   1      -4.512  -1.995   0.261  1.00  0.00           C
ATOM      6  O3'  DC A   1      -3.235  -2.631   0.278  1.00  0.00           O
ATOM      7  C2'  DC A   1      -4.340  -0.515   0.569  1.00  0.00           C
ATOM      8  C1'  DC A   1      -3.827  -0.001  -0.776  1.00  0.00           C
ATOM      9  N1   DC A   1      -4.100   1.410  -1.024  1.00  0.00           N
ATOM     10  C2   DC A   1      -3.056   2.281  -1.395  1.00  0.00           C
ATOM     11  O2   DC A   1      -1.920   1.822  -1.571  1.00  0.00           O
ATOM     12  N3   DC A   1      -3.336   3.601  -1.529  1.00  0.00           N
ATOM     13  C4   DC A   1      -4.590   4.028  -1.427  1.00  0.00           C
ATOM     14  N4   DC A   1      -4.807   5.344  -1.560  1.00  0.00           N
ATOM     15  C5   DC A   1      -5.696   3.144  -1.197  1.00  0.00           C
ATOM     16  C6   DC A   1      -5.393   1.842  -0.997  1.00  0.00           C
ATOM     17  P    DA A   2      -2.826  -3.383   1.688  1.00  0.00           P
ATOM     18  OP1  DA A   2      -3.735  -4.551   1.895  1.00  0.00           O
ATOM     19  OP2  DA A   2      -2.627  -2.350   2.762  1.00  0.00           O
ATOM     20  O5'  DA A   2      -1.322  -3.852   1.258  1.00  0.00           O
ATOM     21  C5'  DA A   2      -1.056  -4.469   0.008  1.00  0.00           C
ATOM     22  C4'  DA A   2       0.113  -3.757  -0.652  1.00  0.00           C
ATOM     23  O4'  DA A   2      -0.249  -2.384  -0.879  1.00  0.00           O
ATOM     24  C3'  DA A   2       1.408  -3.711   0.182  1.00  0.00           C
ATOM     25  O3'  DA A   2       2.487  -3.695  -0.756  1.00  0.00           O
ATOM     26  C2'  DA A   2       1.243  -2.393   0.924  1.00  0.00           C
ATOM     27  C1'  DA A   2       0.653  -1.546  -0.188  1.00  0.00           C
ATOM     28  N9   DA A   2      -0.034  -0.355   0.288  1.00  0.00           N
ATOM     29  C8   DA A   2      -0.966  -0.232   1.262  1.00  0.00           C
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ATOM     30  N7   DA A   2      -1.320   1.045   1.511  1.00  0.00           N
ATOM     31  C5   DA A   2      -0.566   1.758   0.674  1.00  0.00           C
ATOM     32  C6   DA A   2      -0.477   3.160   0.379  1.00  0.00           C
ATOM     33  N6   DA A   2      -1.252   4.033   0.978  1.00  0.00           N
ATOM     34  N1   DA A   2       0.434   3.581  -0.533  1.00  0.00           N
ATOM     35  C2   DA A   2       1.169   2.675  -1.143  1.00  0.00           C
ATOM     36  N3   DA A   2       1.136   1.312  -1.018  1.00  0.00           N
ATOM     37  C4   DA A   2       0.277   0.923  -0.122  1.00  0.00           C
ATOM     38  P    DA A   3       3.955  -2.997  -0.474  1.00  0.00           P
ATOM     39  OP1  DA A   3       4.890  -3.589  -1.477  1.00  0.00           O
ATOM     40  OP2  DA A   3       4.247  -2.958   0.996  1.00  0.00           O
ATOM     41  O5'  DA A   3       3.642  -1.431  -0.876  1.00  0.00           O
ATOM     42  C5'  DA A   3       3.796  -0.963  -2.208  1.00  0.00           C
ATOM     43  C4'  DA A   3       4.837   0.141  -2.235  1.00  0.00           C
ATOM     44  O4'  DA A   3       4.382   1.297  -1.525  1.00  0.00           O
ATOM     45  C3'  DA A   3       6.156  -0.247  -1.566  1.00  0.00           C
ATOM     46  O3'  DA A   3       7.170   0.516  -2.198  1.00  0.00           O
ATOM     47  C2'  DA A   3       5.945   0.190  -0.114  1.00  0.00           C
ATOM     48  C1'  DA A   3       4.985   1.379  -0.250  1.00  0.00           C
ATOM     49  N9   DA A   3       3.958   1.431   0.785  1.00  0.00           N
ATOM     50  C8   DA A   3       3.317   0.406   1.444  1.00  0.00           C
ATOM     51  N7   DA A   3       2.340   0.808   2.222  1.00  0.00           N
ATOM     52  C5   DA A   3       2.332   2.181   2.065  1.00  0.00           C
ATOM     53  C6   DA A   3       1.550   3.210   2.631  1.00  0.00           C
ATOM     54  N6   DA A   3       0.528   2.957   3.474  1.00  0.00           N
ATOM     55  N1   DA A   3       1.795   4.479   2.267  1.00  0.00           N
ATOM     56  C2   DA A   3       2.774   4.712   1.381  1.00  0.00           C
ATOM     57  N3   DA A   3       3.583   3.841   0.783  1.00  0.00           N
ATOM     58  C4   DA A   3       3.322   2.586   1.172  1.00  0.00           C
END
COMPND    ACC / D-B3LYP / H MODEL / NEUTRAL
ATOM      1  O5'  DA A   1      -6.945  -1.095   0.101  1.00  0.00           O
ATOM      2  C5'  DA A   1      -6.699  -2.134  -0.844  1.00  0.00           C
ATOM      3  C4'  DA A   1      -5.200  -2.316  -1.042  1.00  0.00           C
ATOM      4  O4'  DA A   1      -4.620  -1.144  -1.642  1.00  0.00           O
ATOM      5  C3'  DA A   1      -4.415  -2.534   0.257  1.00  0.00           C
ATOM      6  O3'  DA A   1      -3.215  -3.281  -0.114  1.00  0.00           O
ATOM      7  C2'  DA A   1      -4.058  -1.117   0.663  1.00  0.00           C
ATOM      8  C1'  DA A   1      -3.786  -0.466  -0.696  1.00  0.00           C
ATOM      9  N9   DA A   1      -4.048   0.958  -0.713  1.00  0.00           N
ATOM     10  C8   DA A   1      -5.012   1.667  -0.019  1.00  0.00           C
ATOM     11  N7   DA A   1      -4.897   2.970  -0.140  1.00  0.00           N
ATOM     12  C5   DA A   1      -3.806   3.132  -0.976  1.00  0.00           C
ATOM     13  C6   DA A   1      -3.108   4.268  -1.427  1.00  0.00           C
ATOM     14  N6   DA A   1      -3.398   5.516  -0.962  1.00  0.00           N
ATOM     15  N1   DA A   1      -2.076   4.106  -2.275  1.00  0.00           N
ATOM     16  C2   DA A   1      -1.707   2.854  -2.591  1.00  0.00           C
ATOM     17  N3   DA A   1      -2.230   1.697  -2.171  1.00  0.00           N
ATOM     18  C4   DA A   1      -3.275   1.899  -1.360  1.00  0.00           C
ATOM     19  P    DC A   2      -2.125  -3.735   0.975  1.00  0.00           P
ATOM     20  OP1  DC A   2      -2.664  -5.092   1.645  1.00  0.00           O
ATOM     21  OP2  DC A   2      -1.781  -2.757   2.038  1.00  0.00           O
ATOM     22  O5'  DC A   2      -0.940  -4.256   0.037  1.00  0.00           O
ATOM     23  C5'  DC A   2      -0.570  -3.698  -1.249  1.00  0.00           C
ATOM     24  C4'  DC A   2       0.375  -2.518  -1.133  1.00  0.00           C
ATOM     25  O4'  DC A   2      -0.350  -1.328  -0.803  1.00  0.00           O
ATOM     26  C3'  DC A   2       1.477  -2.671  -0.047  1.00  0.00           C
ATOM     27  O3'  DC A   2       2.743  -2.417  -0.718  1.00  0.00           O
ATOM     28  C2'  DC A   2       1.144  -1.561   0.946  1.00  0.00           C
ATOM     29  C1'  DC A   2       0.550  -0.526  -0.008  1.00  0.00           C
ATOM     30  N1   DC A   2      -0.173   0.592   0.548  1.00  0.00           N
ATOM     31  C2   DC A   2       0.023   1.893  -0.034  1.00  0.00           C
ATOM     32  O2   DC A   2       0.863   2.033  -0.921  1.00  0.00           O
ATOM     33  N3   DC A   2      -0.741   2.915   0.439  1.00  0.00           N
ATOM     34  C4   DC A   2      -1.642   2.708   1.387  1.00  0.00           C
ATOM     35  N4   DC A   2      -2.357   3.780   1.816  1.00  0.00           N
ATOM     36  C5   DC A   2      -1.856   1.425   1.995  1.00  0.00           C
ATOM     37  C6   DC A   2      -1.098   0.398   1.533  1.00  0.00           C
ATOM     38  P    DC A   3       4.146  -2.641   0.033  1.00  0.00           P
ATOM     39  OP1  DC A   3       4.298  -4.225   0.263  1.00  0.00           O
ATOM     40  OP2  DC A   3       4.348  -1.932   1.322  1.00  0.00           O
ATOM     41  O5'  DC A   3       5.185  -2.341  -1.142  1.00  0.00           O
ATOM     42  C5'  DC A   3       4.970  -1.402  -2.229  1.00  0.00           C
ATOM     43  C4'  DC A   3       5.214   0.036  -1.828  1.00  0.00           C
ATOM     44  O4'  DC A   3       4.131   0.514  -1.020  1.00  0.00           O
ATOM     45  C3'  DC A   3       6.523   0.296  -1.029  1.00  0.00           C
ATOM     46  O3'  DC A   3       7.294   1.220  -1.795  1.00  0.00           O
ATOM     47  C2'  DC A   3       6.008   0.906   0.283  1.00  0.00           C
ATOM     48  C1'  DC A   3       4.703   1.544  -0.194  1.00  0.00           C
ATOM     49  N1   DC A   3       3.748   1.946   0.815  1.00  0.00           N
ATOM     50  C2   DC A   3       3.200   3.270   0.773  1.00  0.00           C
ATOM     51  O2   DC A   3       3.631   4.076  -0.054  1.00  0.00           O
ATOM     52  N3   DC A   3       2.227   3.583   1.677  1.00  0.00           N
ATOM     53  C4   DC A   3       1.794   2.675   2.542  1.00  0.00           C
ATOM     54  N4   DC A   3       0.799   3.037   3.391  1.00  0.00           N
ATOM     55  C5   DC A   3       2.347   1.355   2.632  1.00  0.00           C
ATOM     56  C6   DC A   3       3.316   1.037   1.736  1.00  0.00           C
END

COMPND    ACC / D-B3LYP / H MODEL / SINGLY IONIZED
ATOM      1  O5'  DA A   1      -6.571  -0.378   0.321  1.00  0.00           O
ATOM      2  C5'  DA A   1      -6.680  -1.456  -0.609  1.00  0.00           C
ATOM      3  C4'  DA A   1      -5.288  -1.904  -1.030  1.00  0.00           C
ATOM      4  O4'  DA A   1      -4.649  -0.877  -1.821  1.00  0.00           O
ATOM      5  C3'  DA A   1      -4.346  -2.169   0.152  1.00  0.00           C
ATOM      6  O3'  DA A   1      -3.398  -3.197  -0.262  1.00  0.00           O
ATOM      7  C2'  DA A   1      -3.637  -0.839   0.324  1.00  0.00           C
ATOM      8  C1'  DA A   1      -3.563  -0.313  -1.111  1.00  0.00           C
ATOM      9  N9   DA A   1      -3.631   1.152  -1.149  1.00  0.00           N
ATOM     10  C8   DA A   1      -4.548   1.958  -0.548  1.00  0.00           C
ATOM     11  N7   DA A   1      -4.256   3.266  -0.626  1.00  0.00           N
ATOM     12  C5   DA A   1      -3.093   3.297  -1.303  1.00  0.00           C
ATOM     13  C6   DA A   1      -2.234   4.366  -1.719  1.00  0.00           C
ATOM     14  N6   DA A   1      -2.511   5.630  -1.438  1.00  0.00           N
ATOM     15  N1   DA A   1      -1.115   4.070  -2.424  1.00  0.00           N
ATOM     16  C2   DA A   1      -0.861   2.800  -2.694  1.00  0.00           C
ATOM     17  N3   DA A   1      -1.604   1.688  -2.382  1.00  0.00           N
ATOM     18  C4   DA A   1      -2.666   1.990  -1.679  1.00  0.00           C
ATOM     19  P    DC A   2      -2.333  -3.788   0.795  1.00  0.00           P
ATOM     20  OP1  DC A   2      -2.924  -5.178   1.335  1.00  0.00           O
ATOM     21  OP2  DC A   2      -1.986  -2.902   1.934  1.00  0.00           O
ATOM     22  O5'  DC A   2      -1.149  -4.277  -0.166  1.00  0.00           O
ATOM     23  C5'  DC A   2      -0.731  -3.609  -1.381  1.00  0.00           C
ATOM     24  C4'  DC A   2       0.249  -2.481  -1.132  1.00  0.00           C
ATOM     25  O4'  DC A   2      -0.438  -1.320  -0.647  1.00  0.00           O
ATOM     26  C3'  DC A   2       1.361  -2.790  -0.091  1.00  0.00           C
ATOM     27  O3'  DC A   2       2.612  -2.476  -0.756  1.00  0.00           O
ATOM     28  C2'  DC A   2       1.063  -1.811   1.045  1.00  0.00           C
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ATOM     29  C1'  DC A   2       0.489  -0.652   0.235  1.00  0.00           C
ATOM     30  N1   DC A   2      -0.219   0.407   0.925  1.00  0.00           N
ATOM     31  C2   DC A   2      -0.206   1.707   0.331  1.00  0.00           C
ATOM     32  O2   DC A   2       0.567   1.930  -0.606  1.00  0.00           O
ATOM     33  N3   DC A   2      -1.076   2.642   0.798  1.00  0.00           N
ATOM     34  C4   DC A   2      -1.851   2.371   1.855  1.00  0.00           C
ATOM     35  N4   DC A   2      -2.718   3.317   2.244  1.00  0.00           N
ATOM     36  C5   DC A   2      -1.779   1.127   2.560  1.00  0.00           C
ATOM     37  C6   DC A   2      -0.979   0.165   2.033  1.00  0.00           C
ATOM     38  P    DC A   3       4.051  -2.696  -0.078  1.00  0.00           P
ATOM     39  OP1  DC A   3       4.272  -4.284   0.040  1.00  0.00           O
ATOM     40  OP2  DC A   3       4.283  -2.065   1.246  1.00  0.00           O
ATOM     41  O5'  DC A   3       5.020  -2.269  -1.273  1.00  0.00           O
ATOM     42  C5'  DC A   3       4.685  -1.320  -2.319  1.00  0.00           C
ATOM     43  C4'  DC A   3       4.851   0.118  -1.880  1.00  0.00           C
ATOM     44  O4'  DC A   3       3.800   0.487  -0.975  1.00  0.00           O
ATOM     45  C3'  DC A   3       6.195   0.438  -1.167  1.00  0.00           C
ATOM     46  O3'  DC A   3       6.832   1.460  -1.931  1.00  0.00           O
ATOM     47  C2'  DC A   3       5.739   0.935   0.212  1.00  0.00           C
ATOM     48  C1'  DC A   3       4.367   1.510  -0.138  1.00  0.00           C
ATOM     49  N1   DC A   3       3.471   1.801   0.959  1.00  0.00           N
ATOM     50  C2   DC A   3       2.878   3.105   1.049  1.00  0.00           C
ATOM     51  O2   DC A   3       3.185   3.968   0.225  1.00  0.00           O
ATOM     52  N3   DC A   3       2.005   3.331   2.073  1.00  0.00           N
ATOM     53  C4   DC A   3       1.722   2.370   2.944  1.00  0.00           C
ATOM     54  N4   DC A   3       0.847   2.660   3.932  1.00  0.00           N
ATOM     55  C5   DC A   3       2.307   1.061   2.885  1.00  0.00           C
ATOM     56  C6   DC A   3       3.175   0.827   1.868  1.00  0.00           C
END

COMPND    AAC / D-B3LYP / H MODEL / NEUTRAL
ATOM      1  O5'  DA A   1       0.000   0.000   0.000  1.00  0.00           O
ATOM      2  C5'  DA A   1       0.000   0.000   1.426  1.00  0.00           C
ATOM      3  C4'  DA A   1       1.435   0.000   1.936  1.00  0.00           C
ATOM      4  O4'  DA A   1       2.072  -1.260   1.660  1.00  0.00           O
ATOM      5  C3'  DA A   1       2.312   1.071   1.276  1.00  0.00           C
ATOM      6  O3'  DA A   1       3.319   1.469   2.260  1.00  0.00           O
ATOM      7  C2'  DA A   1       2.961   0.320   0.128  1.00  0.00           C
ATOM      8  C1'  DA A   1       3.105  -1.097   0.687  1.00  0.00           C
ATOM      9  N9   DA A   1       2.999  -2.118  -0.337  1.00  0.00           N
ATOM     10  C8   DA A   1       2.041  -2.225  -1.328  1.00  0.00           C
ATOM     11  N7   DA A   1       2.246  -3.229  -2.151  1.00  0.00           N
ATOM     12  C5   DA A   1       3.402  -3.823  -1.672  1.00  0.00           C
ATOM     13  C6   DA A   1       4.174  -4.911  -2.124  1.00  0.00           C
ATOM     14  N6   DA A   1       3.832  -5.633  -3.221  1.00  0.00           N
ATOM     15  N1   DA A   1       5.280  -5.254  -1.432  1.00  0.00           N
ATOM     16  C2   DA A   1       5.599  -4.531  -0.343  1.00  0.00           C
ATOM     17  N3   DA A   1       4.969  -3.474   0.175  1.00  0.00           N
ATOM     18  C4   DA A   1       3.880  -3.158  -0.539  1.00  0.00           C
ATOM     19  P    DA A   2       4.296   2.709   1.956  1.00  0.00           P
ATOM     20  OP1  DA A   2       3.732   3.967   2.780  1.00  0.00           O
ATOM     21  OP2  DA A   2       4.462   3.072   0.527  1.00  0.00           O
ATOM     22  O5'  DA A   2       5.612   2.329   2.789  1.00  0.00           O
ATOM     23  C5'  DA A   2       6.084   0.985   3.047  1.00  0.00           C
ATOM     24  C4'  DA A   2       6.957   0.447   1.931  1.00  0.00           C
ATOM     25  O4'  DA A   2       6.140   0.078   0.811  1.00  0.00           O
ATOM     26  C3'  DA A   2       8.014   1.444   1.387  1.00  0.00           C
ATOM     27  O3'  DA A   2       9.260   0.702   1.334  1.00  0.00           O
ATOM     28  C2'  DA A   2       7.503   1.758  -0.016  1.00  0.00           C
ATOM     29  C1'  DA A   2       6.884   0.411  -0.375  1.00  0.00           C
ATOM     30  N9   DA A   2       6.015   0.395  -1.515  1.00  0.00           N
ATOM     31  C8   DA A   2       5.246   1.419  -2.042  1.00  0.00           C
ATOM     32  N7   DA A   2       4.587   1.073  -3.123  1.00  0.00           N
ATOM     33  C5   DA A   2       4.942  -0.252  -3.326  1.00  0.00           C
ATOM     34  C6   DA A   2       4.664  -1.166  -4.361  1.00  0.00           C
ATOM     35  N6   DA A   2       3.935  -0.810  -5.452  1.00  0.00           N
ATOM     36  N1   DA A   2       5.201  -2.397  -4.303  1.00  0.00           N
ATOM     37  C2   DA A   2       6.041  -2.677  -3.292  1.00  0.00           C
ATOM     38  N3   DA A   2       6.423  -1.890  -2.282  1.00  0.00           N
ATOM     39  C4   DA A   2       5.833  -0.691  -2.348  1.00  0.00           C
ATOM     40  P    DC A   3      10.644   1.342   0.843  1.00  0.00           P
ATOM     41  OP1  DC A   3      11.057   2.350   2.029  1.00  0.00           O
ATOM     42  OP2  DC A   3      10.671   1.990  -0.497  1.00  0.00           O
ATOM     43  O5'  DC A   3      11.641   0.119   1.073  1.00  0.00           O
ATOM     44  C5'  DC A   3      11.269  -1.282   0.994  1.00  0.00           C
ATOM     45  C4'  DC A   3      11.238  -1.803  -0.426  1.00  0.00           C
ATOM     46  O4'  DC A   3      10.082  -1.310  -1.121  1.00  0.00           O
ATOM     47  C3'  DC A   3      12.478  -1.431  -1.289  1.00  0.00           C
ATOM     48  O3'  DC A   3      13.064  -2.660  -1.714  1.00  0.00           O
ATOM     49  C2'  DC A   3      11.859  -0.645  -2.452  1.00  0.00           C
ATOM     50  C1'  DC A   3      10.469  -1.275  -2.506  1.00  0.00           C
ATOM     51  N1   DC A   3       9.465  -0.582  -3.285  1.00  0.00           N
ATOM     52  C2   DC A   3       8.801  -1.280  -4.346  1.00  0.00           C
ATOM     53  O2   DC A   3       9.100  -2.453  -4.580  1.00  0.00           O
ATOM     54  N3   DC A   3       7.861  -0.598  -5.059  1.00  0.00           N
ATOM     55  C4   DC A   3       7.559   0.658  -4.754  1.00  0.00           C
ATOM     56  N4   DC A   3       6.602   1.273  -5.500  1.00  0.00           N
ATOM     57  C5   DC A   3       8.211   1.384  -3.703  1.00  0.00           C
ATOM     58  C6   DC A   3       9.160   0.718  -2.996  1.00  0.00           C
END

COMPND    AAC / D-B3LYP / H MODEL / SINGLY IONIZED
ATOM      1  O5'  DA A   1      -6.362  -1.479  -0.024  1.00  0.00           O
ATOM      2  C5'  DA A   1      -6.067  -2.473  -1.001  1.00  0.00           C
ATOM      3  C4'  DA A   1      -4.559  -2.646  -1.129  1.00  0.00           C
ATOM      4  O4'  DA A   1      -3.935  -1.434  -1.589  1.00  0.00           O
ATOM      5  C3'  DA A   1      -3.833  -2.975   0.177  1.00  0.00           C
ATOM      6  O3'  DA A   1      -2.589  -3.629  -0.219  1.00  0.00           O
ATOM      7  C2'  DA A   1      -3.559  -1.595   0.756  1.00  0.00           C
ATOM      8  C1'  DA A   1      -3.274  -0.779  -0.510  1.00  0.00           C
ATOM      9  N9   DA A   1      -3.722   0.610  -0.439  1.00  0.00           N
ATOM     10  C8   DA A   1      -4.718   1.187   0.304  1.00  0.00           C
ATOM     11  N7   DA A   1      -4.931   2.466   0.015  1.00  0.00           N
ATOM     12  C5   DA A   1      -4.047   2.730  -0.990  1.00  0.00           C
ATOM     13  C6   DA A   1      -3.783   3.897  -1.758  1.00  0.00           C
ATOM     14  N6   DA A   1      -4.424   5.047  -1.539  1.00  0.00           N
ATOM     15  N1   DA A   1      -2.855   3.827  -2.741  1.00  0.00           N
ATOM     16  C2   DA A   1      -2.210   2.674  -2.922  1.00  0.00           C
ATOM     17  N3   DA A   1      -2.355   1.504  -2.255  1.00  0.00           N
ATOM     18  C4   DA A   1      -3.279   1.596  -1.307  1.00  0.00           C
ATOM     19  P    DA A   2      -1.501  -4.152   0.837  1.00  0.00           P
ATOM     20  OP1  DA A   2      -2.009  -5.574   1.381  1.00  0.00           O
ATOM     21  OP2  DA A   2      -1.193  -3.264   1.987  1.00  0.00           O
ATOM     22  O5'  DA A   2      -0.276  -4.535  -0.118  1.00  0.00           O
ATOM     23  C5'  DA A   2       0.008  -3.960  -1.417  1.00  0.00           C
ATOM     24  C4'  DA A   2       0.861  -2.710  -1.326  1.00  0.00           C
ATOM     25  O4'  DA A   2       0.058  -1.604  -0.873  1.00  0.00           O
ATOM     26  C3'  DA A   2       2.056  -2.803  -0.341  1.00  0.00           C
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ATOM     27  O3'  DA A   2       3.190  -2.244  -1.056  1.00  0.00           O
ATOM     28  C2'  DA A   2       1.628  -1.898   0.809  1.00  0.00           C
ATOM     29  C1'  DA A   2       0.870  -0.835   0.024  1.00  0.00           C
ATOM     30  N9   DA A   2       0.006   0.037   0.782  1.00  0.00           N
ATOM     31  C8   DA A   2      -0.730  -0.243   1.903  1.00  0.00           C
ATOM     32  N7   DA A   2      -1.526   0.752   2.281  1.00  0.00           N
ATOM     33  C5   DA A   2      -1.290   1.728   1.365  1.00  0.00           C
ATOM     34  C6   DA A   2      -1.812   3.042   1.197  1.00  0.00           C
ATOM     35  N6   DA A   2      -2.753   3.527   1.999  1.00  0.00           N
ATOM     36  N1   DA A   2      -1.346   3.804   0.176  1.00  0.00           N
ATOM     37  C2   DA A   2      -0.423   3.287  -0.627  1.00  0.00           C
ATOM     38  N3   DA A   2       0.123   2.041  -0.599  1.00  0.00           N
ATOM     39  C4   DA A   2      -0.338   1.324   0.407  1.00  0.00           C
ATOM     40  P    DC A   3       4.668  -2.095  -0.445  1.00  0.00           P
ATOM     41  OP1  DC A   3       5.345  -3.551  -0.496  1.00  0.00           O
ATOM     42  OP2  DC A   3       4.789  -1.542   0.927  1.00  0.00           O
ATOM     43  O5'  DC A   3       5.403  -1.309  -1.627  1.00  0.00           O
ATOM     44  C5'  DC A   3       4.754  -0.372  -2.526  1.00  0.00           C
ATOM     45  C4'  DC A   3       4.584   1.004  -1.922  1.00  0.00           C
ATOM     46  O4'  DC A   3       3.570   0.984  -0.906  1.00  0.00           O
ATOM     47  C3'  DC A   3       5.860   1.607  -1.270  1.00  0.00           C
ATOM     48  O3'  DC A   3       6.140   2.819  -1.966  1.00  0.00           O
ATOM     49  C2'  DC A   3       5.423   1.851   0.183  1.00  0.00           C
ATOM     50  C1'  DC A   3       3.920   2.048  -0.005  1.00  0.00           C
ATOM     51  N1   DC A   3       3.086   1.981   1.178  1.00  0.00           N
ATOM     52  C2   DC A   3       2.146   3.031   1.429  1.00  0.00           C
ATOM     53  O2   DC A   3       2.099   3.998   0.663  1.00  0.00           O
ATOM     54  N3   DC A   3       1.321   2.905   2.506  1.00  0.00           N
ATOM     55  C4   DC A   3       1.433   1.858   3.325  1.00  0.00           C
ATOM     56  N4   DC A   3       0.604   1.808   4.384  1.00  0.00           N
ATOM     57  C5   DC A   3       2.386   0.808   3.116  1.00  0.00           C
ATOM     58  C6   DC A   3       3.184   0.912   2.023  1.00  0.00           C
END

COMPND    CCA / D-B3LYP / H MODEL / NEUTRAL
ATOM      1  O5'  DC A   1      -6.945  -1.204   0.390  1.00  0.00           O
ATOM      2  C5'  DC A   1      -6.738  -2.253  -0.555  1.00  0.00           C
ATOM      3  C4'  DC A   1      -5.255  -2.356  -0.884  1.00  0.00           C
ATOM      4  O4'  DC A   1      -4.829  -1.211  -1.639  1.00  0.00           O
ATOM      5  C3'  DC A   1      -4.356  -2.400   0.360  1.00  0.00           C
ATOM      6  O3'  DC A   1      -3.188  -3.207   0.012  1.00  0.00           O
ATOM      7  C2'  DC A   1      -3.962  -0.946   0.547  1.00  0.00           C
ATOM      8  C1'  DC A   1      -3.857  -0.457  -0.901  1.00  0.00           C
ATOM      9  N1   DC A   1      -4.113   0.967  -1.076  1.00  0.00           N
ATOM     10  C2   DC A   1      -3.258   1.734  -1.931  1.00  0.00           C
ATOM     11  O2   DC A   1      -2.380   1.162  -2.578  1.00  0.00           O
ATOM     12  N3   DC A   1      -3.460   3.083  -1.972  1.00  0.00           N
ATOM     13  C4   DC A   1      -4.469   3.631  -1.312  1.00  0.00           C
ATOM     14  N4   DC A   1      -4.532   4.986  -1.278  1.00  0.00           N
ATOM     15  C5   DC A   1      -5.458   2.863  -0.610  1.00  0.00           C
ATOM     16  C6   DC A   1      -5.233   1.528  -0.526  1.00  0.00           C
ATOM     17  P    DC A   2      -2.130  -3.616   1.150  1.00  0.00           P
ATOM     18  OP1  DC A   2      -2.734  -4.896   1.912  1.00  0.00           O
ATOM     19  OP2  DC A   2      -1.775  -2.570   2.142  1.00  0.00           O
ATOM     20  O5'  DC A   2      -0.949  -4.257   0.283  1.00  0.00           O
ATOM     21  C5'  DC A   2      -0.543  -3.832  -1.043  1.00  0.00           C
ATOM     22  C4'  DC A   2       0.416  -2.658  -1.019  1.00  0.00           C
ATOM     23  O4'  DC A   2      -0.304  -1.442  -0.796  1.00  0.00           O
ATOM     24  C3'  DC A   2       1.505  -2.728   0.088  1.00  0.00           C
ATOM     25  O3'  DC A   2       2.780  -2.527  -0.585  1.00  0.00           O
ATOM     26  C2'  DC A   2       1.162  -1.547   0.993  1.00  0.00           C
ATOM     27  C1'  DC A   2       0.584  -0.585  -0.044  1.00  0.00           C
ATOM     28  N1   DC A   2      -0.153   0.571   0.404  1.00  0.00           N
ATOM     29  C2   DC A   2      -0.092   1.759  -0.408  1.00  0.00           C
ATOM     30  O2   DC A   2       0.693   1.798  -1.353  1.00  0.00           O
ATOM     31  N3   DC A   2      -0.913   2.794  -0.076  1.00  0.00           N
ATOM     32  C4   DC A   2      -1.724   2.707   0.966  1.00  0.00           C
ATOM     33  N4   DC A   2      -2.512   3.779   1.242  1.00  0.00           N
ATOM     34  C5   DC A   2      -1.770   1.561   1.827  1.00  0.00           C
ATOM     35  C6   DC A   2      -0.979   0.511   1.488  1.00  0.00           C
ATOM     36  P    DA A   3       4.173  -2.694   0.197  1.00  0.00           P
ATOM     37  OP1  DA A   3       4.320  -4.258   0.544  1.00  0.00           O
ATOM     38  OP2  DA A   3       4.362  -1.894   1.433  1.00  0.00           O
ATOM     39  O5'  DA A   3       5.230  -2.476  -0.982  1.00  0.00           O
ATOM     40  C5'  DA A   3       5.014  -1.669  -2.168  1.00  0.00           C
ATOM     41  C4'  DA A   3       5.243  -0.193  -1.924  1.00  0.00           C
ATOM     42  O4'  DA A   3       4.151   0.347  -1.164  1.00  0.00           O
ATOM     43  C3'  DA A   3       6.545   0.157  -1.152  1.00  0.00           C
ATOM     44  O3'  DA A   3       7.263   1.086  -1.962  1.00  0.00           O
ATOM     45  C2'  DA A   3       6.017   0.799   0.138  1.00  0.00           C
ATOM     46  C1'  DA A   3       4.706   1.399  -0.362  1.00  0.00           C
ATOM     47  N9   DA A   3       3.752   1.790   0.639  1.00  0.00           N
ATOM     48  C8   DA A   3       3.307   1.048   1.718  1.00  0.00           C
ATOM     49  N7   DA A   3       2.344   1.631   2.394  1.00  0.00           N
ATOM     50  C5   DA A   3       2.143   2.831   1.729  1.00  0.00           C
ATOM     51  C6   DA A   3       1.242   3.895   1.928  1.00  0.00           C
ATOM     52  N6   DA A   3       0.335   3.898   2.945  1.00  0.00           N
ATOM     53  N1   DA A   3       1.299   4.956   1.100  1.00  0.00           N
ATOM     54  C2   DA A   3       2.196   4.935   0.100  1.00  0.00           C
ATOM     55  N3   DA A   3       3.080   3.981  -0.215  1.00  0.00           N
ATOM     56  C4   DA A   3       3.003   2.950   0.634  1.00  0.00           C
END

COMPND    CCA / D-B3LYP / H MODEL / SINGLY IONIZED
ATOM      1  O5'  DC A   1      -6.867  -1.394   0.467  1.00  0.00           O
ATOM      2  C5'  DC A   1      -6.637  -2.474  -0.436  1.00  0.00           C
ATOM      3  C4'  DC A   1      -5.159  -2.535  -0.793  1.00  0.00           C
ATOM      4  O4'  DC A   1      -4.794  -1.415  -1.617  1.00  0.00           O
ATOM      5  C3'  DC A   1      -4.233  -2.479   0.430  1.00  0.00           C
ATOM      6  O3'  DC A   1      -3.044  -3.257   0.090  1.00  0.00           O
ATOM      7  C2'  DC A   1      -3.891  -1.002   0.529  1.00  0.00           C
ATOM      8  C1'  DC A   1      -3.839  -0.585  -0.944  1.00  0.00           C
ATOM      9  N1   DC A   1      -4.169   0.817  -1.173  1.00  0.00           N
ATOM     10  C2   DC A   1      -3.320   1.620  -1.999  1.00  0.00           C
ATOM     11  O2   DC A   1      -2.365   1.097  -2.576  1.00  0.00           O
ATOM     12  N3   DC A   1      -3.606   2.951  -2.083  1.00  0.00           N
ATOM     13  C4   DC A   1      -4.679   3.447  -1.482  1.00  0.00           C
ATOM     14  N4   DC A   1      -4.823   4.796  -1.476  1.00  0.00           N
ATOM     15  C5   DC A   1      -5.648   2.633  -0.805  1.00  0.00           C
ATOM     16  C6   DC A   1      -5.342   1.318  -0.678  1.00  0.00           C
ATOM     17  P    DC A   2      -1.906  -3.548   1.185  1.00  0.00           P
ATOM     18  OP1  DC A   2      -2.361  -4.842   2.018  1.00  0.00           O
ATOM     19  OP2  DC A   2      -1.581  -2.442   2.120  1.00  0.00           O
ATOM     20  O5'  DC A   2      -0.729  -4.124   0.267  1.00  0.00           O
ATOM     21  C5'  DC A   2      -0.408  -3.664  -1.069  1.00  0.00           C
ATOM     22  C4'  DC A   2       0.517  -2.463  -1.067  1.00  0.00           C
ATOM     23  O4'  DC A   2      -0.228  -1.266  -0.793  1.00  0.00           O
ATOM     24  C3'  DC A   2       1.648  -2.520  -0.006  1.00  0.00           C
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ATOM     25  O3'  DC A   2       2.890  -2.297  -0.722  1.00  0.00           O
ATOM     26  C2'  DC A   2       1.320  -1.353   0.927  1.00  0.00           C
ATOM     27  C1'  DC A   2       0.661  -0.403  -0.070  1.00  0.00           C
ATOM     28  N1   DC A   2      -0.125   0.715   0.440  1.00  0.00           N
ATOM     29  C2   DC A   2      -0.221   1.907  -0.390  1.00  0.00           C
ATOM     30  O2   DC A   2       0.584   2.045  -1.306  1.00  0.00           O
ATOM     31  N3   DC A   2      -1.172   2.823  -0.088  1.00  0.00           N
ATOM     32  C4   DC A   2      -1.975   2.658   0.956  1.00  0.00           C
ATOM     33  N4   DC A   2      -2.916   3.587   1.187  1.00  0.00           N
ATOM     34  C5   DC A   2      -1.834   1.544   1.855  1.00  0.00           C
ATOM     35  C6   DC A   2      -0.934   0.568   1.512  1.00  0.00           C
ATOM     36  P    DA A   3       4.311  -2.507  -0.001  1.00  0.00           P
ATOM     37  OP1  DA A   3       4.476  -4.085   0.246  1.00  0.00           O
ATOM     38  OP2  DA A   3       4.528  -1.782   1.276  1.00  0.00           O
ATOM     39  O5'  DA A   3       5.324  -2.206  -1.198  1.00  0.00           O
ATOM     40  C5'  DA A   3       5.050  -1.337  -2.327  1.00  0.00           C
ATOM     41  C4'  DA A   3       5.239   0.126  -1.991  1.00  0.00           C
ATOM     42  O4'  DA A   3       4.167   0.561  -1.132  1.00  0.00           O
ATOM     43  C3'  DA A   3       6.565   0.472  -1.261  1.00  0.00           C
ATOM     44  O3'  DA A   3       7.181   1.517  -2.008  1.00  0.00           O
ATOM     45  C2'  DA A   3       6.088   0.952   0.119  1.00  0.00           C
ATOM     46  C1'  DA A   3       4.732   1.537  -0.256  1.00  0.00           C
ATOM     47  N9   DA A   3       3.800   1.774   0.824  1.00  0.00           N
ATOM     48  C8   DA A   3       3.566   1.019   1.943  1.00  0.00           C
ATOM     49  N7   DA A   3       2.533   1.439   2.668  1.00  0.00           N
ATOM     50  C5   DA A   3       2.070   2.521   1.983  1.00  0.00           C
ATOM     51  C6   DA A   3       0.994   3.423   2.196  1.00  0.00           C
ATOM     52  N6   DA A   3       0.120   3.261   3.192  1.00  0.00           N
ATOM     53  N1   DA A   3       0.810   4.455   1.333  1.00  0.00           N
ATOM     54  C2   DA A   3       1.623   4.551   0.289  1.00  0.00           C
ATOM     55  N3   DA A   3       2.664   3.742  -0.045  1.00  0.00           N
ATOM     56  C4   DA A   3       2.840   2.767   0.824  1.00  0.00           C
END

COMPND    CAA / D-B3LYP / H MODEL / NEUTRAL
ATOM      1  O5'  DC A   1      -6.236  -0.662   0.768  1.00  0.00           O
ATOM      2  C5'  DC A   1      -6.430  -1.860   0.018  1.00  0.00           C
ATOM      3  C4'  DC A   1      -5.099  -2.314  -0.565  1.00  0.00           C
ATOM      4  O4'  DC A   1      -4.686  -1.441  -1.628  1.00  0.00           O
ATOM      5  C3'  DC A   1      -3.958  -2.303   0.461  1.00  0.00           C
ATOM      6  O3'  DC A   1      -3.054  -3.398   0.102  1.00  0.00           O
ATOM      7  C2'  DC A   1      -3.283  -0.963   0.223  1.00  0.00           C
ATOM      8  C1'  DC A   1      -3.473  -0.756  -1.282  1.00  0.00           C
ATOM      9  N1   DC A   1      -3.586   0.640  -1.691  1.00  0.00           N
ATOM     10  C2   DC A   1      -2.790   1.130  -2.772  1.00  0.00           C
ATOM     11  O2   DC A   1      -2.000   0.371  -3.339  1.00  0.00           O
ATOM     12  N3   DC A   1      -2.939   2.441  -3.122  1.00  0.00           N
ATOM     13  C4   DC A   1      -3.842   3.203  -2.512  1.00  0.00           C
ATOM     14  N4   DC A   1      -3.932   4.494  -2.896  1.00  0.00           N
ATOM     15  C5   DC A   1      -4.729   2.708  -1.499  1.00  0.00           C
ATOM     16  C6   DC A   1      -4.562   1.416  -1.127  1.00  0.00           C
ATOM     17  P    DA A   2      -1.953  -3.890   1.164  1.00  0.00           P
ATOM     18  OP1  DA A   2      -2.497  -5.256   1.813  1.00  0.00           O
ATOM     19  OP2  DA A   2      -1.613  -2.918   2.231  1.00  0.00           O
ATOM     20  O5'  DA A   2      -0.767  -4.425   0.227  1.00  0.00           O
ATOM     21  C5'  DA A   2      -0.428  -3.914  -1.084  1.00  0.00           C
ATOM     22  C4'  DA A   2       0.532  -2.742  -1.022  1.00  0.00           C
ATOM     23  O4'  DA A   2      -0.176  -1.563  -0.613  1.00  0.00           O
ATOM     24  C3'  DA A   2       1.702  -2.911  -0.021  1.00  0.00           C
ATOM     25  O3'  DA A   2       2.894  -2.491  -0.738  1.00  0.00           O
ATOM     26  C2'  DA A   2       1.351  -1.933   1.097  1.00  0.00           C
ATOM     27  C1'  DA A   2       0.672  -0.833   0.291  1.00  0.00           C
ATOM     28  N9   DA A   2      -0.141   0.087   1.037  1.00  0.00           N
ATOM     29  C8   DA A   2      -0.684  -0.046   2.300  1.00  0.00           C
ATOM     30  N7   DA A   2      -1.473   0.946   2.639  1.00  0.00           N
ATOM     31  C5   DA A   2      -1.460   1.781   1.532  1.00  0.00           C
ATOM     32  C6   DA A   2      -2.058   3.027   1.267  1.00  0.00           C
ATOM     33  N6   DA A   2      -2.806   3.678   2.199  1.00  0.00           N
ATOM     34  N1   DA A   2      -1.826   3.618   0.081  1.00  0.00           N
ATOM     35  C2   DA A   2      -1.002   3.007  -0.786  1.00  0.00           C
ATOM     36  N3   DA A   2      -0.358   1.842  -0.648  1.00  0.00           N
ATOM     37  C4   DA A   2      -0.632   1.274   0.531  1.00  0.00           C
ATOM     38  P    DA A   3       4.364  -2.537  -0.095  1.00  0.00           P
ATOM     39  OP1  DA A   3       4.738  -4.089   0.096  1.00  0.00           O
ATOM     40  OP2  DA A   3       4.571  -1.818   1.187  1.00  0.00           O
ATOM     41  O5'  DA A   3       5.259  -2.083  -1.339  1.00  0.00           O
ATOM     42  C5'  DA A   3       4.802  -1.255  -2.441  1.00  0.00           C
ATOM     43  C4'  DA A   3       4.837   0.221  -2.111  1.00  0.00           C
ATOM     44  O4'  DA A   3       3.773   0.548  -1.201  1.00  0.00           O
ATOM     45  C3'  DA A   3       6.157   0.714  -1.456  1.00  0.00           C
ATOM     46  O3'  DA A   3       6.621   1.808  -2.245  1.00  0.00           O
ATOM     47  C2'  DA A   3       5.698   1.160  -0.062  1.00  0.00           C
ATOM     48  C1'  DA A   3       4.273   1.607  -0.374  1.00  0.00           C
ATOM     49  N9   DA A   3       3.394   1.798   0.747  1.00  0.00           N
ATOM     50  C8   DA A   3       3.163   0.945   1.811  1.00  0.00           C
ATOM     51  N7   DA A   3       2.260   1.393   2.653  1.00  0.00           N
ATOM     52  C5   DA A   3       1.876   2.615   2.123  1.00  0.00           C
ATOM     53  C6   DA A   3       0.930   3.584   2.520  1.00  0.00           C
ATOM     54  N6   DA A   3       0.158   3.447   3.633  1.00  0.00           N
ATOM     55  N1   DA A   3       0.797   4.699   1.773  1.00  0.00           N
ATOM     56  C2   DA A   3       1.547   4.825   0.667  1.00  0.00           C
ATOM     57  N3   DA A   3       2.447   3.972   0.166  1.00  0.00           N
ATOM     58  C4   DA A   3       2.567   2.885   0.937  1.00  0.00           C
END

COMPND    CAA / D-B3LYP / H MODEL / SINGLY IONIZED
ATOM      1  O5'  DC A   1       6.234   0.592   0.562  1.00  0.00           O
ATOM      2  C5'  DC A   1       6.392   1.838  -0.116  1.00  0.00           C
ATOM      3  C4'  DC A   1       5.038   2.319  -0.617  1.00  0.00           C
ATOM      4  O4'  DC A   1       4.576   1.498  -1.704  1.00  0.00           O
ATOM      5  C3'  DC A   1       3.938   2.261   0.452  1.00  0.00           C
ATOM      6  O3'  DC A   1       3.019   3.362   0.162  1.00  0.00           O
ATOM      7  C2'  DC A   1       3.264   0.926   0.181  1.00  0.00           C
ATOM      8  C1'  DC A   1       3.377   0.803  -1.341  1.00  0.00           C
ATOM      9  N1   DC A   1       3.459  -0.572  -1.821  1.00  0.00           N
ATOM     10  C2   DC A   1       2.546  -1.033  -2.821  1.00  0.00           C
ATOM     11  O2   DC A   1       1.708  -0.258  -3.284  1.00  0.00           O
ATOM     12  N3   DC A   1       2.641  -2.341  -3.204  1.00  0.00           N
ATOM     13  C4   DC A   1       3.611  -3.117  -2.724  1.00  0.00           C
ATOM     14  N4   DC A   1       3.631  -4.404  -3.120  1.00  0.00           N
ATOM     15  C5   DC A   1       4.611  -2.644  -1.810  1.00  0.00           C
ATOM     16  C6   DC A   1       4.487  -1.362  -1.387  1.00  0.00           C
ATOM     17  P    DA A   2       1.893   3.783   1.227  1.00  0.00           P
ATOM     18  OP1  DA A   2       2.387   5.132   1.940  1.00  0.00           O
ATOM     19  OP2  DA A   2       1.559   2.757   2.245  1.00  0.00           O
ATOM     20  O5'  DA A   2       0.709   4.320   0.287  1.00  0.00           O
ATOM     21  C5'  DA A   2       0.403   3.818  -1.035  1.00  0.00           C
ATOM     22  C4'  DA A   2      -0.552   2.643  -1.002  1.00  0.00           C
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ATOM     23  O4'  DA A   2       0.140   1.464  -0.557  1.00  0.00           O
ATOM     24  C3'  DA A   2      -1.761   2.812  -0.049  1.00  0.00           C
ATOM     25  O3'  DA A   2      -2.912   2.372  -0.812  1.00  0.00           O
ATOM     26  C2'  DA A   2      -1.448   1.848   1.093  1.00  0.00           C
ATOM     27  C1'  DA A   2      -0.738   0.746   0.316  1.00  0.00           C
ATOM     28  N9   DA A   2       0.068  -0.174   1.091  1.00  0.00           N
ATOM     29  C8   DA A   2       0.651  -0.000   2.317  1.00  0.00           C
ATOM     30  N7   DA A   2       1.517  -0.960   2.639  1.00  0.00           N
ATOM     31  C5   DA A   2       1.496  -1.798   1.571  1.00  0.00           C
ATOM     32  C6   DA A   2       2.221  -2.987   1.260  1.00  0.00           C
ATOM     33  N6   DA A   2       3.127  -3.491   2.090  1.00  0.00           N
ATOM     34  N1   DA A   2       1.975  -3.605   0.081  1.00  0.00           N
ATOM     35  C2   DA A   2       1.069  -3.076  -0.735  1.00  0.00           C
ATOM     36  N3   DA A   2       0.340  -1.936  -0.574  1.00  0.00           N
ATOM     37  C4   DA A   2       0.595  -1.352   0.580  1.00  0.00           C
ATOM     38  P    DA A   3      -4.422   2.417  -0.272  1.00  0.00           P
ATOM     39  OP1  DA A   3      -4.848   3.964  -0.204  1.00  0.00           O
ATOM     40  OP2  DA A   3      -4.696   1.772   1.037  1.00  0.00           O
ATOM     41  O5'  DA A   3      -5.215   1.846  -1.536  1.00  0.00           O
ATOM     42  C5'  DA A   3      -4.643   1.026  -2.587  1.00  0.00           C
ATOM     43  C4'  DA A   3      -4.605  -0.440  -2.216  1.00  0.00           C
ATOM     44  O4'  DA A   3      -3.606  -0.665  -1.201  1.00  0.00           O
ATOM     45  C3'  DA A   3      -5.940  -1.007  -1.661  1.00  0.00           C
ATOM     46  O3'  DA A   3      -6.226  -2.185  -2.409  1.00  0.00           O
ATOM     47  C2'  DA A   3      -5.594  -1.324  -0.200  1.00  0.00           C
ATOM     48  C1'  DA A   3      -4.122  -1.688  -0.347  1.00  0.00           C
ATOM     49  N9   DA A   3      -3.346  -1.721   0.871  1.00  0.00           N
ATOM     50  C8   DA A   3      -3.376  -0.838   1.924  1.00  0.00           C
ATOM     51  N7   DA A   3      -2.511  -1.131   2.885  1.00  0.00           N
ATOM     52  C5   DA A   3      -1.889  -2.263   2.436  1.00  0.00           C
ATOM     53  C6   DA A   3      -0.862  -3.076   2.981  1.00  0.00           C
ATOM     54  N6   DA A   3      -0.307  -2.816   4.164  1.00  0.00           N
ATOM     55  N1   DA A   3      -0.419  -4.140   2.260  1.00  0.00           N
ATOM     56  C2   DA A   3      -0.991  -4.389   1.083  1.00  0.00           C
ATOM     57  N3   DA A   3      -1.979  -3.701   0.465  1.00  0.00           N
ATOM     58  C4   DA A   3      -2.378  -2.656   1.180  1.00  0.00           C
END
COMPND    ACC / D-B3LYP / NA MODEL / NEUTRAL
ATOM      1  O5'  DA A   1       7.165   0.633   0.116  1.00  0.00           O
ATOM      2  C5'  DA A   1       6.985   1.644  -0.873  1.00  0.00           C
ATOM      3  C4'  DA A   1       5.501   1.892  -1.110  1.00  0.00           C
ATOM      4  O4'  DA A   1       4.874   0.718  -1.658  1.00  0.00           O
ATOM      5  C3'  DA A   1       4.691   2.229   0.150  1.00  0.00           C
ATOM      6  O3'  DA A   1       3.547   2.987  -0.296  1.00  0.00           O
ATOM      7  C2'  DA A   1       4.273   0.847   0.631  1.00  0.00           C
ATOM      8  C1'  DA A   1       3.968   0.158  -0.701  1.00  0.00           C
ATOM      9  N9   DA A   1       4.109  -1.284  -0.664  1.00  0.00           N
ATOM     10  C8   DA A   1       4.941  -2.053   0.125  1.00  0.00           C
ATOM     11  N7   DA A   1       4.717  -3.344   0.032  1.00  0.00           N
ATOM     12  C5   DA A   1       3.686  -3.436  -0.888  1.00  0.00           C
ATOM     13  C6   DA A   1       2.932  -4.522  -1.373  1.00  0.00           C
ATOM     14  N6   DA A   1       3.084  -5.780  -0.875  1.00  0.00           N
ATOM     15  N1   DA A   1       1.982  -4.294  -2.298  1.00  0.00           N
ATOM     16  C2   DA A   1       1.746  -3.023  -2.664  1.00  0.00           C
ATOM     17  N3   DA A   1       2.335  -1.904  -2.230  1.00  0.00           N
ATOM     18  C4   DA A   1       3.301  -2.173  -1.342  1.00  0.00           C
ATOM     19  P    DC A   2       2.448   3.587   0.763  1.00  0.00           P
ATOM     20  OP1  DC A   2       3.005   4.773   1.523  1.00  0.00           O
ATOM     21  OP2  DC A   2       1.857   2.497   1.646  1.00  0.00           O
ATOM     22  O5'  DC A   2       1.362   4.156  -0.310  1.00  0.00           O
ATOM     23  C5'  DC A   2       1.051   3.580  -1.588  1.00  0.00           C
ATOM     24  C4'  DC A   2       0.000   2.481  -1.552  1.00  0.00           C
ATOM     25  O4'  DC A   2       0.598   1.218  -1.217  1.00  0.00           O
ATOM     26  C3'  DC A   2      -1.162   2.706  -0.546  1.00  0.00           C
ATOM     27  O3'  DC A   2      -2.384   2.709  -1.312  1.00  0.00           O
ATOM     28  C2'  DC A   2      -1.039   1.506   0.394  1.00  0.00           C
ATOM     29  C1'  DC A   2      -0.411   0.466  -0.532  1.00  0.00           C
ATOM     30  N1   DC A   2       0.203  -0.685   0.103  1.00  0.00           N
ATOM     31  C2   DC A   2      -0.175  -2.002  -0.311  1.00  0.00           C
ATOM     32  O2   DC A   2      -1.039  -2.143  -1.177  1.00  0.00           O
ATOM     33  N3   DC A   2       0.456  -3.055   0.285  1.00  0.00           N
ATOM     34  C4   DC A   2       1.398  -2.853   1.193  1.00  0.00           C
ATOM     35  N4   DC A   2       1.995  -3.950   1.737  1.00  0.00           N
ATOM     36  C5   DC A   2       1.776  -1.547   1.648  1.00  0.00           C
ATOM     37  C6   DC A   2       1.149  -0.491   1.063  1.00  0.00           C
ATOM     38  P    DC A   3      -3.837   2.872  -0.554  1.00  0.00           P
ATOM     39  OP1  DC A   3      -4.713   3.742  -1.427  1.00  0.00           O
ATOM     40  OP2  DC A   3      -3.662   3.262   0.896  1.00  0.00           O
ATOM     41  O5'  DC A   3      -4.389   1.315  -0.571  1.00  0.00           O
ATOM     42  C5'  DC A   3      -4.651   0.739  -1.864  1.00  0.00           C
ATOM     43  C4'  DC A   3      -5.356  -0.596  -1.717  1.00  0.00           C
ATOM     44  O4'  DC A   3      -4.466  -1.567  -1.141  1.00  0.00           O
ATOM     45  C3'  DC A   3      -6.610  -0.570  -0.825  1.00  0.00           C
ATOM     46  O3'  DC A   3      -7.538  -1.494  -1.394  1.00  0.00           O
ATOM     47  C2'  DC A   3      -6.069  -1.065   0.516  1.00  0.00           C
ATOM     48  C1'  DC A   3      -5.011  -2.083   0.075  1.00  0.00           C
ATOM     49  N1   DC A   3      -3.917  -2.272   1.026  1.00  0.00           N
ATOM     50  C2   DC A   3      -3.593  -3.580   1.497  1.00  0.00           C
ATOM     51  O2   DC A   3      -4.295  -4.537   1.160  1.00  0.00           O
ATOM     52  N3   DC A   3      -2.506  -3.707   2.315  1.00  0.00           N
ATOM     53  C4   DC A   3      -1.790  -2.641   2.653  1.00  0.00           C
ATOM     54  N4   DC A   3      -0.734  -2.825   3.488  1.00  0.00           N
ATOM     55  C5   DC A   3      -2.095  -1.316   2.198  1.00  0.00           C
ATOM     56  C6   DC A   3      -3.154  -1.194   1.361  1.00  0.00           C
END

COMPND    ACC / D-B3LYP / NA MODEL / SINGLY IONIZED
ATOM      1  O5'  DA A   1      -7.099  -1.048   0.057  1.00  0.00           O
ATOM      2  C5'  DA A   1      -6.812  -2.024  -0.945  1.00  0.00           C
ATOM      3  C4'  DA A   1      -5.308  -2.158  -1.134  1.00  0.00           C
ATOM      4  O4'  DA A   1      -4.755  -0.953  -1.711  1.00  0.00           O
ATOM      5  C3'  DA A   1      -4.507  -2.386   0.155  1.00  0.00           C
ATOM      6  O3'  DA A   1      -3.307  -3.081  -0.228  1.00  0.00           O
ATOM      7  C2'  DA A   1      -4.187  -0.960   0.591  1.00  0.00           C
ATOM      8  C1'  DA A   1      -3.944  -0.282  -0.763  1.00  0.00           C
ATOM      9  N9   DA A   1      -4.304   1.139  -0.751  1.00  0.00           N
ATOM     10  C8   DA A   1      -5.469   1.689  -0.317  1.00  0.00           C
ATOM     11  N7   DA A   1      -5.501   3.029  -0.396  1.00  0.00           N
ATOM     12  C5   DA A   1      -4.299   3.350  -0.913  1.00  0.00           C
ATOM     13  C6   DA A   1      -3.690   4.598  -1.266  1.00  0.00           C
ATOM     14  N6   DA A   1      -4.306   5.753  -1.071  1.00  0.00           N
ATOM     15  N1   DA A   1      -2.450   4.590  -1.820  1.00  0.00           N
ATOM     16  C2   DA A   1      -1.854   3.426  -2.014  1.00  0.00           C
ATOM     17  N3   DA A   1      -2.334   2.163  -1.745  1.00  0.00           N
ATOM     18  C4   DA A   1      -3.517   2.191  -1.181  1.00  0.00           C
ATOM     19  P    DC A   2      -2.278  -3.640   0.922  1.00  0.00           P
ATOM     20  OP1  DC A   2      -2.909  -4.764   1.716  1.00  0.00           O
ATOM     21  OP2  DC A   2      -1.732  -2.501   1.776  1.00  0.00           O
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ATOM     22  O5'  DC A   2      -1.130  -4.268  -0.045  1.00  0.00           O
ATOM     23  C5'  DC A   2      -0.841  -3.874  -1.397  1.00  0.00           C
ATOM     24  C4'  DC A   2       0.186  -2.763  -1.509  1.00  0.00           C
ATOM     25  O4'  DC A   2      -0.420  -1.481  -1.249  1.00  0.00           O
ATOM     26  C3'  DC A   2       1.397  -2.887  -0.543  1.00  0.00           C
ATOM     27  O3'  DC A   2       2.583  -2.807  -1.360  1.00  0.00           O
ATOM     28  C2'  DC A   2       1.212  -1.681   0.380  1.00  0.00           C
ATOM     29  C1'  DC A   2       0.577  -0.693  -0.592  1.00  0.00           C
ATOM     30  N1   DC A   2      -0.050   0.481  -0.011  1.00  0.00           N
ATOM     31  C2   DC A   2       0.306   1.772  -0.495  1.00  0.00           C
ATOM     32  O2   DC A   2       1.104   1.889  -1.421  1.00  0.00           O
ATOM     33  N3   DC A   2      -0.282   2.861   0.098  1.00  0.00           N
ATOM     34  C4   DC A   2      -1.239   2.694   1.013  1.00  0.00           C
ATOM     35  N4   DC A   2      -1.888   3.804   1.414  1.00  0.00           N
ATOM     36  C5   DC A   2      -1.619   1.409   1.507  1.00  0.00           C
ATOM     37  C6   DC A   2      -0.989   0.330   0.962  1.00  0.00           C
ATOM     38  P    DC A   3       4.073  -2.683  -0.672  1.00  0.00           P
ATOM     39  OP1  DC A   3       5.056  -3.347  -1.608  1.00  0.00           O
ATOM     40  OP2  DC A   3       4.052  -3.117   0.775  1.00  0.00           O
ATOM     41  O5'  DC A   3       4.303  -1.047  -0.673  1.00  0.00           O
ATOM     42  C5'  DC A   3       4.468  -0.396  -1.947  1.00  0.00           C
ATOM     43  C4'  DC A   3       5.174   0.937  -1.773  1.00  0.00           C
ATOM     44  O4'  DC A   3       4.310   1.885  -1.123  1.00  0.00           O
ATOM     45  C3'  DC A   3       6.459   0.875  -0.931  1.00  0.00           C
ATOM     46  O3'  DC A   3       7.359   1.836  -1.482  1.00  0.00           O
ATOM     47  C2'  DC A   3       5.964   1.291   0.455  1.00  0.00           C
ATOM     48  C1'  DC A   3       4.879   2.319   0.111  1.00  0.00           C
ATOM     49  N1   DC A   3       3.805   2.418   1.101  1.00  0.00           N
ATOM     50  C2   DC A   3       3.494   3.676   1.704  1.00  0.00           C
ATOM     51  O2   DC A   3       4.198   4.657   1.452  1.00  0.00           O
ATOM     52  N3   DC A   3       2.416   3.727   2.541  1.00  0.00           N
ATOM     53  C4   DC A   3       1.705   2.634   2.792  1.00  0.00           C
ATOM     54  N4   DC A   3       0.656   2.744   3.639  1.00  0.00           N
ATOM     55  C5   DC A   3       2.007   1.354   2.218  1.00  0.00           C
ATOM     56  C6   DC A   3       3.054   1.310   1.356  1.00  0.00           C
END

COMPND    AAC / D-B3LYP / NA MODEL / NEUTRAL
ATOM      1  O5'  DA A   1       6.694   2.349  -0.633  1.00  0.00           O
ATOM      2  C5'  DA A   1       6.012   2.782  -1.806  1.00  0.00           C
ATOM      3  C4'  DA A   1       4.537   2.434  -1.689  1.00  0.00           C
ATOM      4  O4'  DA A   1       4.368   1.002  -1.751  1.00  0.00           O
ATOM      5  C3'  DA A   1       3.898   2.882  -0.362  1.00  0.00           C
ATOM      6  O3'  DA A   1       2.536   3.253  -0.644  1.00  0.00           O
ATOM      7  C2'  DA A   1       3.947   1.608   0.477  1.00  0.00           C
ATOM      8  C1'  DA A   1       3.663   0.558  -0.593  1.00  0.00           C
ATOM      9  N9   DA A   1       4.115  -0.777  -0.251  1.00  0.00           N
ATOM     10  C8   DA A   1       4.754  -1.204   0.895  1.00  0.00           C
ATOM     11  N7   DA A   1       4.950  -2.502   0.943  1.00  0.00           N
ATOM     12  C5   DA A   1       4.409  -2.963  -0.245  1.00  0.00           C
ATOM     13  C6   DA A   1       4.229  -4.257  -0.769  1.00  0.00           C
ATOM     14  N6   DA A   1       4.580  -5.369  -0.068  1.00  0.00           N
ATOM     15  N1   DA A   1       3.626  -4.395  -1.964  1.00  0.00           N
ATOM     16  C2   DA A   1       3.165  -3.289  -2.573  1.00  0.00           C
ATOM     17  N3   DA A   1       3.229  -2.017  -2.166  1.00  0.00           N
ATOM     18  C4   DA A   1       3.872  -1.912  -0.994  1.00  0.00           C
ATOM     19  P    DA A   2       1.697   4.055   0.513  1.00  0.00           P
ATOM     20  OP1  DA A   2       2.399   5.351   0.870  1.00  0.00           O
ATOM     21  OP2  DA A   2       1.391   3.161   1.708  1.00  0.00           O
ATOM     22  O5'  DA A   2       0.323   4.367  -0.303  1.00  0.00           O
ATOM     23  C5'  DA A   2      -0.024   3.930  -1.627  1.00  0.00           C
ATOM     24  C4'  DA A   2      -0.884   2.676  -1.617  1.00  0.00           C
ATOM     25  O4'  DA A   2      -0.075   1.515  -1.350  1.00  0.00           O
ATOM     26  C3'  DA A   2      -1.993   2.690  -0.539  1.00  0.00           C
ATOM     27  O3'  DA A   2      -3.169   2.114  -1.142  1.00  0.00           O
ATOM     28  C2'  DA A   2      -1.422   1.766   0.532  1.00  0.00           C
ATOM     29  C1'  DA A   2      -0.752   0.727  -0.361  1.00  0.00           C
ATOM     30  N9   DA A   2       0.189  -0.145   0.291  1.00  0.00           N
ATOM     31  C8   DA A   2       0.986   0.122   1.388  1.00  0.00           C
ATOM     32  N7   DA A   2       1.647  -0.930   1.822  1.00  0.00           N
ATOM     33  C5   DA A   2       1.262  -1.950   0.966  1.00  0.00           C
ATOM     34  C6   DA A   2       1.546  -3.328   0.927  1.00  0.00           C
ATOM     35  N6   DA A   2       2.318  -3.940   1.877  1.00  0.00           N
ATOM     36  N1   DA A   2       0.989  -4.078  -0.039  1.00  0.00           N
ATOM     37  C2   DA A   2       0.152  -3.486  -0.905  1.00  0.00           C
ATOM     38  N3   DA A   2      -0.230  -2.206  -0.953  1.00  0.00           N
ATOM     39  C4   DA A   2       0.359  -1.485   0.008  1.00  0.00           C
ATOM     40  P    DC A   3      -4.596   2.135  -0.334  1.00  0.00           P
ATOM     41  OP1  DC A   3      -5.080   3.557  -0.131  1.00  0.00           O
ATOM     42  OP2  DC A   3      -4.535   1.306   0.942  1.00  0.00           O
ATOM     43  O5'  DC A   3      -5.533   1.432  -1.466  1.00  0.00           O
ATOM     44  C5'  DC A   3      -5.095   0.485  -2.454  1.00  0.00           C
ATOM     45  C4'  DC A   3      -5.059  -0.953  -1.972  1.00  0.00           C
ATOM     46  O4'  DC A   3      -3.884  -1.198  -1.184  1.00  0.00           O
ATOM     47  C3'  DC A   3      -6.278  -1.399  -1.118  1.00  0.00           C
ATOM     48  O3'  DC A   3      -6.868  -2.515  -1.787  1.00  0.00           O
ATOM     49  C2'  DC A   3      -5.633  -1.791   0.216  1.00  0.00           C
ATOM     50  C1'  DC A   3      -4.247  -2.229  -0.256  1.00  0.00           C
ATOM     51  N1   DC A   3      -3.224  -2.346   0.768  1.00  0.00           N
ATOM     52  C2   DC A   3      -2.551  -3.595   0.951  1.00  0.00           C
ATOM     53  O2   DC A   3      -2.864  -4.562   0.252  1.00  0.00           O
ATOM     54  N3   DC A   3      -1.583  -3.655   1.910  1.00  0.00           N
ATOM     55  C4   DC A   3      -1.268  -2.581   2.622  1.00  0.00           C
ATOM     56  N4   DC A   3      -0.280  -2.709   3.552  1.00  0.00           N
ATOM     57  C5   DC A   3      -1.935  -1.322   2.468  1.00  0.00           C
ATOM     58  C6   DC A   3      -2.908  -1.254   1.521  1.00  0.00           C
END

COMPND    AAC / D-B3LYP / NA MODEL / SINGLY IONIZED
ATOM      1  O5'  DA A   1       6.440   1.524  -0.259  1.00  0.00           O
ATOM      2  C5'  DA A   1       6.103   2.379  -1.349  1.00  0.00           C
ATOM      3  C4'  DA A   1       4.591   2.461  -1.506  1.00  0.00           C
ATOM      4  O4'  DA A   1       4.038   1.169  -1.824  1.00  0.00           O
ATOM      5  C3'  DA A   1       3.823   2.910  -0.259  1.00  0.00           C
ATOM      6  O3'  DA A   1       2.564   3.432  -0.726  1.00  0.00           O
ATOM      7  C2'  DA A   1       3.615   1.593   0.480  1.00  0.00           C
ATOM      8  C1'  DA A   1       3.360   0.636  -0.689  1.00  0.00           C
ATOM      9  N9   DA A   1       3.824  -0.731  -0.457  1.00  0.00           N
ATOM     10  C8   DA A   1       4.820  -1.197   0.359  1.00  0.00           C
ATOM     11  N7   DA A   1       5.060  -2.497   0.225  1.00  0.00           N
ATOM     12  C5   DA A   1       4.192  -2.894  -0.751  1.00  0.00           C
ATOM     13  C6   DA A   1       3.958  -4.147  -1.378  1.00  0.00           C
ATOM     14  N6   DA A   1       4.616  -5.252  -1.017  1.00  0.00           N
ATOM     15  N1   DA A   1       3.043  -4.212  -2.372  1.00  0.00           N
ATOM     16  C2   DA A   1       2.380  -3.099  -2.695  1.00  0.00           C
ATOM     17  N3   DA A   1       2.495  -1.858  -2.171  1.00  0.00           N
ATOM     18  C4   DA A   1       3.409  -1.819  -1.208  1.00  0.00           C
ATOM     19  P    DA A   2       1.523   4.168   0.305  1.00  0.00           P
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ATOM     20  OP1  DA A   2       2.007   5.559   0.658  1.00  0.00           O
ATOM     21  OP2  DA A   2       1.213   3.290   1.510  1.00  0.00           O
ATOM     22  O5'  DA A   2       0.220   4.286  -0.668  1.00  0.00           O
ATOM     23  C5'  DA A   2       0.001   3.613  -1.917  1.00  0.00           C
ATOM     24  C4'  DA A   2      -0.849   2.361  -1.779  1.00  0.00           C
ATOM     25  O4'  DA A   2      -0.059   1.269  -1.261  1.00  0.00           O
ATOM     26  C3'  DA A   2      -2.057   2.505  -0.823  1.00  0.00           C
ATOM     27  O3'  DA A   2      -3.145   1.797  -1.440  1.00  0.00           O
ATOM     28  C2'  DA A   2      -1.573   1.779   0.431  1.00  0.00           C
ATOM     29  C1'  DA A   2      -0.825   0.630  -0.234  1.00  0.00           C
ATOM     30  N9   DA A   2       0.082  -0.119   0.609  1.00  0.00           N
ATOM     31  C8   DA A   2       0.807   0.320   1.680  1.00  0.00           C
ATOM     32  N7   DA A   2       1.617  -0.606   2.193  1.00  0.00           N
ATOM     33  C5   DA A   2       1.399  -1.697   1.417  1.00  0.00           C
ATOM     34  C6   DA A   2       1.943  -3.013   1.424  1.00  0.00           C
ATOM     35  N6   DA A   2       2.888  -3.370   2.288  1.00  0.00           N
ATOM     36  N1   DA A   2       1.498  -3.910   0.510  1.00  0.00           N
ATOM     37  C2   DA A   2       0.571  -3.519  -0.356  1.00  0.00           C
ATOM     38  N3   DA A   2       0.000  -2.291  -0.492  1.00  0.00           N
ATOM     39  C4   DA A   2       0.443  -1.438   0.410  1.00  0.00           C
ATOM     40  P    DC A   3      -4.655   1.797  -0.805  1.00  0.00           P
ATOM     41  OP1  DC A   3      -5.301   3.162  -0.938  1.00  0.00           O
ATOM     42  OP2  DC A   3      -4.680   1.232   0.609  1.00  0.00           O
ATOM     43  O5'  DC A   3      -5.364   0.782  -1.866  1.00  0.00           O
ATOM     44  C5'  DC A   3      -4.692  -0.219  -2.649  1.00  0.00           C
ATOM     45  C4'  DC A   3      -4.507  -1.545  -1.936  1.00  0.00           C
ATOM     46  O4'  DC A   3      -3.451  -1.462  -0.965  1.00  0.00           O
ATOM     47  C3'  DC A   3      -5.762  -2.075  -1.191  1.00  0.00           C
ATOM     48  O3'  DC A   3      -6.035  -3.375  -1.714  1.00  0.00           O
ATOM     49  C2'  DC A   3      -5.299  -2.121   0.270  1.00  0.00           C
ATOM     50  C1'  DC A   3      -3.804  -2.376   0.080  1.00  0.00           C
ATOM     51  N1   DC A   3      -2.947  -2.151   1.232  1.00  0.00           N
ATOM     52  C2   DC A   3      -2.003  -3.154   1.610  1.00  0.00           C
ATOM     53  O2   DC A   3      -1.947  -4.209   0.971  1.00  0.00           O
ATOM     54  N3   DC A   3      -1.180  -2.892   2.665  1.00  0.00           N
ATOM     55  C4   DC A   3      -1.286  -1.743   3.336  1.00  0.00           C
ATOM     56  N4   DC A   3      -0.466  -1.564   4.390  1.00  0.00           N
ATOM     57  C5   DC A   3      -2.220  -0.720   2.976  1.00  0.00           C
ATOM     58  C6   DC A   3      -3.024  -0.968   1.907  1.00  0.00           C
END

COMPND    CCA / D-B3LYP / NA MODEL / NEUTRAL
ATOM      1  O5'  DC A   1      -7.309  -0.916  -0.182  1.00  0.00           O
ATOM      2  C5'  DC A   1      -6.975  -1.875  -1.184  1.00  0.00           C
ATOM      3  C4'  DC A   1      -5.464  -1.965  -1.340  1.00  0.00           C
ATOM      4  O4'  DC A   1      -4.947  -0.750  -1.910  1.00  0.00           O
ATOM      5  C3'  DC A   1      -4.699  -2.166  -0.022  1.00  0.00           C
ATOM      6  O3'  DC A   1      -3.497  -2.894  -0.351  1.00  0.00           O
ATOM      7  C2'  DC A   1      -4.373  -0.734   0.384  1.00  0.00           C
ATOM      8  C1'  DC A   1      -4.066  -0.103  -0.977  1.00  0.00           C
ATOM      9  N1   DC A   1      -4.275   1.337  -1.046  1.00  0.00           N
ATOM     10  C2   DC A   1      -3.279   2.163  -1.657  1.00  0.00           C
ATOM     11  O2   DC A   1      -2.309   1.636  -2.204  1.00  0.00           O
ATOM     12  N3   DC A   1      -3.456   3.515  -1.591  1.00  0.00           N
ATOM     13  C4   DC A   1      -4.563   4.023  -1.064  1.00  0.00           C
ATOM     14  N4   DC A   1      -4.644   5.369  -0.957  1.00  0.00           N
ATOM     15  C5   DC A   1      -5.653   3.213  -0.597  1.00  0.00           C
ATOM     16  C6   DC A   1      -5.456   1.870  -0.614  1.00  0.00           C
ATOM     17  P    DC A   2      -2.520  -3.452   0.841  1.00  0.00           P
ATOM     18  OP1  DC A   2      -3.157  -4.615   1.574  1.00  0.00           O
ATOM     19  OP2  DC A   2      -2.054  -2.323   1.751  1.00  0.00           O
ATOM     20  O5'  DC A   2      -1.302  -4.032  -0.071  1.00  0.00           O
ATOM     21  C5'  DC A   2      -0.925  -3.602  -1.390  1.00  0.00           C
ATOM     22  C4'  DC A   2       0.143  -2.519  -1.411  1.00  0.00           C
ATOM     23  O4'  DC A   2      -0.445  -1.223  -1.217  1.00  0.00           O
ATOM     24  C3'  DC A   2       1.246  -2.672  -0.330  1.00  0.00           C
ATOM     25  O3'  DC A   2       2.513  -2.535  -1.009  1.00  0.00           O
ATOM     26  C2'  DC A   2       0.968  -1.494   0.599  1.00  0.00           C
ATOM     27  C1'  DC A   2       0.476  -0.464  -0.413  1.00  0.00           C
ATOM     28  N1   DC A   2      -0.200   0.710   0.100  1.00  0.00           N
ATOM     29  C2   DC A   2       0.147   2.000  -0.411  1.00  0.00           C
ATOM     30  O2   DC A   2       1.056   2.103  -1.236  1.00  0.00           O
ATOM     31  N3   DC A   2      -0.540   3.078   0.069  1.00  0.00           N
ATOM     32  C4   DC A   2      -1.525   2.913   0.936  1.00  0.00           C
ATOM     33  N4   DC A   2      -2.143   4.034   1.411  1.00  0.00           N
ATOM     34  C5   DC A   2      -1.920   1.633   1.439  1.00  0.00           C
ATOM     35  C6   DC A   2      -1.225   0.557   0.981  1.00  0.00           C
ATOM     36  P    DA A   3       3.925  -2.833  -0.219  1.00  0.00           P
ATOM     37  OP1  DA A   3       4.573  -4.071  -0.805  1.00  0.00           O
ATOM     38  OP2  DA A   3       3.742  -2.789   1.283  1.00  0.00           O
ATOM     39  O5'  DA A   3       4.770  -1.487  -0.629  1.00  0.00           O
ATOM     40  C5'  DA A   3       4.948  -1.155  -2.013  1.00  0.00           C
ATOM     41  C4'  DA A   3       5.529   0.244  -2.119  1.00  0.00           C
ATOM     42  O4'  DA A   3       4.584   1.207  -1.619  1.00  0.00           O
ATOM     43  C3'  DA A   3       6.825   0.469  -1.326  1.00  0.00           C
ATOM     44  O3'  DA A   3       7.582   1.441  -2.046  1.00  0.00           O
ATOM     45  C2'  DA A   3       6.308   1.026  -0.000  1.00  0.00           C
ATOM     46  C1'  DA A   3       5.087   1.841  -0.444  1.00  0.00           C
ATOM     47  N9   DA A   3       4.039   1.910   0.556  1.00  0.00           N
ATOM     48  C8   DA A   3       3.444   0.856   1.221  1.00  0.00           C
ATOM     49  N7   DA A   3       2.450   1.219   2.000  1.00  0.00           N
ATOM     50  C5   DA A   3       2.376   2.591   1.834  1.00  0.00           C
ATOM     51  C6   DA A   3       1.496   3.566   2.341  1.00  0.00           C
ATOM     52  N6   DA A   3       0.496   3.262   3.216  1.00  0.00           N
ATOM     53  N1   DA A   3       1.670   4.850   1.970  1.00  0.00           N
ATOM     54  C2   DA A   3       2.661   5.135   1.108  1.00  0.00           C
ATOM     55  N3   DA A   3       3.539   4.304   0.534  1.00  0.00           N
ATOM     56  C4   DA A   3       3.345   3.040   0.932  1.00  0.00           C
END

COMPND    CCA / D-B3LYP / NA MODEL / SINGLY IONIZED
ATOM      1  O5'  DC A   1      -7.286  -0.567  -0.118  1.00  0.00           O
ATOM      2  C5'  DC A   1      -7.029  -1.636  -1.028  1.00  0.00           C
ATOM      3  C4'  DC A   1      -5.530  -1.858  -1.164  1.00  0.00           C
ATOM      4  O4'  DC A   1      -4.916  -0.740  -1.832  1.00  0.00           O
ATOM      5  C3'  DC A   1      -4.781  -2.005   0.170  1.00  0.00           C
ATOM      6  O3'  DC A   1      -3.639  -2.846  -0.099  1.00  0.00           O
ATOM      7  C2'  DC A   1      -4.347  -0.573   0.452  1.00  0.00           C
ATOM      8  C1'  DC A   1      -3.980  -0.096  -0.956  1.00  0.00           C
ATOM      9  N1   DC A   1      -4.067   1.347  -1.151  1.00  0.00           N
ATOM     10  C2   DC A   1      -2.987   2.043  -1.780  1.00  0.00           C
ATOM     11  O2   DC A   1      -2.013   1.403  -2.187  1.00  0.00           O
ATOM     12  N3   DC A   1      -3.081   3.398  -1.880  1.00  0.00           N
ATOM     13  C4   DC A   1      -4.182   4.028  -1.483  1.00  0.00           C
ATOM     14  N4   DC A   1      -4.194   5.373  -1.556  1.00  0.00           N
ATOM     15  C5   DC A   1      -5.341   3.338  -0.986  1.00  0.00           C
ATOM     16  C6   DC A   1      -5.231   1.993  -0.845  1.00  0.00           C
ATOM     17  P    DC A   2      -2.643  -3.339   1.103  1.00  0.00           P
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ATOM     18  OP2  DC A   2      -2.057  -2.155   1.865  1.00  0.00           O
ATOM     19  OP1  DC A   2      -3.308  -4.372   1.988  1.00  0.00           O
ATOM     20  O5'  DC A   2      -1.508  -4.086   0.204  1.00  0.00           O
ATOM     21  C5'  DC A   2      -1.186  -3.812  -1.170  1.00  0.00           C
ATOM     22  C4'  DC A   2      -0.074  -2.794  -1.350  1.00  0.00           C
ATOM     23  O4'  DC A   2      -0.587  -1.454  -1.196  1.00  0.00           O
ATOM     24  C3'  DC A   2       1.114  -2.936  -0.357  1.00  0.00           C
ATOM     25  O3'  DC A   2       2.321  -2.997  -1.154  1.00  0.00           O
ATOM     26  C2'  DC A   2       0.966  -1.680   0.500  1.00  0.00           C
ATOM     27  C1'  DC A   2       0.442  -0.703  -0.548  1.00  0.00           C
ATOM     28  N1   DC A   2      -0.115   0.547  -0.043  1.00  0.00           N
ATOM     29  C2   DC A   2       0.349   1.805  -0.586  1.00  0.00           C
ATOM     30  O2   DC A   2       1.251   1.794  -1.417  1.00  0.00           O
ATOM     31  N3   DC A   2      -0.214   2.953  -0.120  1.00  0.00           N
ATOM     32  C4   DC A   2      -1.240   2.908   0.721  1.00  0.00           C
ATOM     33  N4   DC A   2      -1.787   4.068   1.126  1.00  0.00           N
ATOM     34  C5   DC A   2      -1.719   1.674   1.276  1.00  0.00           C
ATOM     35  C6   DC A   2      -1.117   0.511   0.850  1.00  0.00           C
ATOM     36  P    DA A   3       3.777  -2.409  -0.690  1.00  0.00           P
ATOM     37  OP1  DA A   3       4.803  -2.955  -1.657  1.00  0.00           O
ATOM     38  OP2  DA A   3       4.030  -2.599   0.795  1.00  0.00           O
ATOM     39  O5'  DA A   3       3.587  -0.790  -0.890  1.00  0.00           O
ATOM     40  C5'  DA A   3       3.888  -0.145  -2.140  1.00  0.00           C
ATOM     41  C4'  DA A   3       5.087   0.776  -1.972  1.00  0.00           C
ATOM     42  O4'  DA A   3       4.783   1.885  -1.105  1.00  0.00           O
ATOM     43  C3'  DA A   3       6.317   0.114  -1.343  1.00  0.00           C
ATOM     44  O3'  DA A   3       7.459   0.810  -1.838  1.00  0.00           O
ATOM     45  C2'  DA A   3       6.106   0.353   0.163  1.00  0.00           C
ATOM     46  C1'  DA A   3       5.232   1.622   0.208  1.00  0.00           C
ATOM     47  N9   DA A   3       4.066   1.518   1.113  1.00  0.00           N
ATOM     48  C8   DA A   3       3.501   0.431   1.725  1.00  0.00           C
ATOM     49  N7   DA A   3       2.380   0.705   2.391  1.00  0.00           N
ATOM     50  C5   DA A   3       2.195   2.036   2.186  1.00  0.00           C
ATOM     51  C6   DA A   3       1.202   2.951   2.615  1.00  0.00           C
ATOM     52  N6   DA A   3       0.146   2.554   3.335  1.00  0.00           N
ATOM     53  N1   DA A   3       1.306   4.256   2.265  1.00  0.00           N
ATOM     54  C2   DA A   3       2.340   4.619   1.514  1.00  0.00           C
ATOM     55  N3   DA A   3       3.349   3.849   1.029  1.00  0.00           N
ATOM     56  C4   DA A   3       3.233   2.583   1.393  1.00  0.00           C
END

COMPND    CAA / D-B3LYP / NA MODEL / NEUTRAL
ATOM      1  O5'  DC A   1      -7.176  -0.880  -0.067  1.00  0.00           O
ATOM      2  C5'  DC A   1      -6.902  -1.870  -1.058  1.00  0.00           C
ATOM      3  C4'  DC A   1      -5.399  -2.009  -1.254  1.00  0.00           C
ATOM      4  O4'  DC A   1      -4.864  -0.815  -1.851  1.00  0.00           O
ATOM      5  C3'  DC A   1      -4.609  -2.214   0.048  1.00  0.00           C
ATOM      6  O3'  DC A   1      -3.430  -2.979  -0.288  1.00  0.00           O
ATOM      7  C2'  DC A   1      -4.232  -0.788   0.428  1.00  0.00           C
ATOM      8  C1'  DC A   1      -3.942  -0.185  -0.950  1.00  0.00           C
ATOM      9  N1   DC A   1      -4.096   1.261  -1.045  1.00  0.00           N
ATOM     10  C2   DC A   1      -3.145   2.012  -1.807  1.00  0.00           C
ATOM     11  O2   DC A   1      -2.264   1.419  -2.430  1.00  0.00           O
ATOM     12  N3   DC A   1      -3.260   3.372  -1.793  1.00  0.00           N
ATOM     13  C4   DC A   1      -4.274   3.955  -1.169  1.00  0.00           C
ATOM     14  N4   DC A   1      -4.272   5.310  -1.106  1.00  0.00           N
ATOM     15  C5   DC A   1      -5.340   3.219  -0.553  1.00  0.00           C
ATOM     16  C6   DC A   1      -5.205   1.868  -0.528  1.00  0.00           C
ATOM     17  P    DA A   2      -2.551  -3.648   0.923  1.00  0.00           P
ATOM     18  OP1  DA A   2      -3.313  -4.786   1.573  1.00  0.00           O
ATOM     19  OP2  DA A   2      -2.053  -2.593   1.902  1.00  0.00           O
ATOM     20  O5'  DA A   2      -1.309  -4.256   0.064  1.00  0.00           O
ATOM     21  C5'  DA A   2      -0.959  -3.984  -1.302  1.00  0.00           C
ATOM     22  C4'  DA A   2       0.178  -2.983  -1.439  1.00  0.00           C
ATOM     23  O4'  DA A   2      -0.318  -1.637  -1.307  1.00  0.00           O
ATOM     24  C3'  DA A   2       1.302  -3.144  -0.386  1.00  0.00           C
ATOM     25  O3'  DA A   2       2.547  -3.036  -1.106  1.00  0.00           O
ATOM     26  C2'  DA A   2       1.041  -1.967   0.549  1.00  0.00           C
ATOM     27  C1'  DA A   2       0.573  -0.912  -0.446  1.00  0.00           C
ATOM     28  N9   DA A   2      -0.126   0.210   0.117  1.00  0.00           N
ATOM     29  C8   DA A   2      -1.057   0.187   1.131  1.00  0.00           C
ATOM     30  N7   DA A   2      -1.563   1.371   1.407  1.00  0.00           N
ATOM     31  C5   DA A   2      -0.915   2.223   0.528  1.00  0.00           C
ATOM     32  C6   DA A   2      -1.005   3.608   0.312  1.00  0.00           C
ATOM     33  N6   DA A   2      -1.862   4.392   1.031  1.00  0.00           N
ATOM     34  N1   DA A   2      -0.184   4.176  -0.590  1.00  0.00           N
ATOM     35  C2   DA A   2       0.664   3.381  -1.264  1.00  0.00           C
ATOM     36  N3   DA A   2       0.811   2.053  -1.186  1.00  0.00           N
ATOM     37  C4   DA A   2      -0.011   1.526  -0.274  1.00  0.00           C
ATOM     38  P    DA A   3       4.003  -3.003  -0.340  1.00  0.00           P
ATOM     39  OP1  DA A   3       4.938  -3.933  -1.081  1.00  0.00           O
ATOM     40  OP2  DA A   3       3.860  -3.184   1.154  1.00  0.00           O
ATOM     41  O5'  DA A   3       4.447  -1.436  -0.592  1.00  0.00           O
ATOM     42  C5'  DA A   3       4.642  -1.016  -1.953  1.00  0.00           C
ATOM     43  C4'  DA A   3       5.237   0.380  -1.984  1.00  0.00           C
ATOM     44  O4'  DA A   3       4.298   1.339  -1.467  1.00  0.00           O
ATOM     45  C3'  DA A   3       6.519   0.550  -1.157  1.00  0.00           C
ATOM     46  O3'  DA A   3       7.306   1.540  -1.818  1.00  0.00           O
ATOM     47  C2'  DA A   3       5.979   1.057   0.180  1.00  0.00           C
ATOM     48  C1'  DA A   3       4.785   1.914  -0.257  1.00  0.00           C
ATOM     49  N9   DA A   3       3.714   1.957   0.719  1.00  0.00           N
ATOM     50  C8   DA A   3       3.066   0.882   1.294  1.00  0.00           C
ATOM     51  N7   DA A   3       2.067   1.223   2.075  1.00  0.00           N
ATOM     52  C5   DA A   3       2.043   2.607   2.003  1.00  0.00           C
ATOM     53  C6   DA A   3       1.189   3.583   2.554  1.00  0.00           C
ATOM     54  N6   DA A   3       0.126   3.268   3.349  1.00  0.00           N
ATOM     55  N1   DA A   3       1.438   4.882   2.293  1.00  0.00           N
ATOM     56  C2   DA A   3       2.461   5.187   1.478  1.00  0.00           C
ATOM     57  N3   DA A   3       3.310   4.362   0.857  1.00  0.00           N
ATOM     58  C4   DA A   3       3.053   3.081   1.159  1.00  0.00           C
END

COMPND    CAA / D-B3LYP / NA MODEL / SINGLY IONIZED
ATOM      1  O5'  DC A   1      -7.152   0.834   0.489  1.00  0.00           O
ATOM      2  C5'  DC A   1      -6.710   1.786   1.457  1.00  0.00           C
ATOM      3  C4'  DC A   1      -5.192   1.879   1.432  1.00  0.00           C
ATOM      4  O4'  DC A   1      -4.606   0.670   1.955  1.00  0.00           O
ATOM      5  C3'  DC A   1      -4.595   2.061   0.029  1.00  0.00           C
ATOM      6  O3'  DC A   1      -3.380   2.821   0.178  1.00  0.00           O
ATOM      7  C2'  DC A   1      -4.283   0.626  -0.387  1.00  0.00           C
ATOM      8  C1'  DC A   1      -3.850   0.003   0.946  1.00  0.00           C
ATOM      9  N1   DC A   1      -4.113  -1.437   1.045  1.00  0.00           N
ATOM     10  C2   DC A   1      -3.092  -2.334   1.452  1.00  0.00           C
ATOM     11  O2   DC A   1      -1.979  -1.880   1.777  1.00  0.00           O
ATOM     12  N3   DC A   1      -3.357  -3.663   1.460  1.00  0.00           N
ATOM     13  C4   DC A   1      -4.588  -4.104   1.185  1.00  0.00           C
ATOM     14  N4   DC A   1      -4.783  -5.432   1.177  1.00  0.00           N
ATOM     15  C5   DC A   1      -5.680  -3.214   0.921  1.00  0.00           C
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ATOM     16  C6   DC A   1      -5.390  -1.887   0.861  1.00  0.00           C
ATOM     17  P    DA A   2      -2.715   3.493  -1.160  1.00  0.00           P
ATOM     18  OP2  DA A   2      -2.143   2.430  -2.091  1.00  0.00           O
ATOM     19  OP1  DA A   2      -3.698   4.433  -1.826  1.00  0.00           O
ATOM     20  O5'  DA A   2      -1.496   4.335  -0.484  1.00  0.00           O
ATOM     21  C5'  DA A   2      -1.110   4.343   0.899  1.00  0.00           C
ATOM     22  C4'  DA A   2       0.040   3.390   1.177  1.00  0.00           C
ATOM     23  O4'  DA A   2      -0.437   2.026   1.134  1.00  0.00           O
ATOM     24  C3'  DA A   2       1.212   3.482   0.160  1.00  0.00           C
ATOM     25  O3'  DA A   2       2.441   3.483   0.926  1.00  0.00           O
ATOM     26  C2'  DA A   2       0.984   2.236  -0.691  1.00  0.00           C
ATOM     27  C1'  DA A   2       0.516   1.273   0.390  1.00  0.00           C
ATOM     28  N9   DA A   2      -0.088   0.051  -0.087  1.00  0.00           N
ATOM     29  C8   DA A   2      -1.006  -0.110  -1.082  1.00  0.00           C
ATOM     30  N7   DA A   2      -1.332  -1.390  -1.310  1.00  0.00           N
ATOM     31  C5   DA A   2      -0.568  -2.078  -0.434  1.00  0.00           C
ATOM     32  C6   DA A   2      -0.454  -3.466  -0.118  1.00  0.00           C
ATOM     33  N6   DA A   2      -1.249  -4.365  -0.679  1.00  0.00           N
ATOM     34  N1   DA A   2       0.486  -3.859   0.775  1.00  0.00           N
ATOM     35  C2   DA A   2       1.221  -2.924   1.364  1.00  0.00           C
ATOM     36  N3   DA A   2       1.144  -1.569   1.233  1.00  0.00           N
ATOM     37  C4   DA A   2       0.253  -1.211   0.341  1.00  0.00           C
ATOM     38  P    DA A   3       3.835   2.712   0.536  1.00  0.00           P
ATOM     39  OP2  DA A   3       4.086   2.698  -0.960  1.00  0.00           O
ATOM     40  OP1  DA A   3       4.915   3.271   1.433  1.00  0.00           O
ATOM     41  O5'  DA A   3       3.509   1.151   0.925  1.00  0.00           O
ATOM     42  C5'  DA A   3       3.779   0.598   2.222  1.00  0.00           C
ATOM     43  C4'  DA A   3       4.850  -0.477   2.109  1.00  0.00           C
ATOM     44  O4'  DA A   3       4.369  -1.616   1.374  1.00  0.00           O
ATOM     45  C3'  DA A   3       6.117  -0.024   1.372  1.00  0.00           C
ATOM     46  O3'  DA A   3       7.199  -0.788   1.903  1.00  0.00           O
ATOM     47  C2'  DA A   3       5.815  -0.397  -0.087  1.00  0.00           C
ATOM     48  C1'  DA A   3       4.885  -1.615   0.048  1.00  0.00           C
ATOM     49  N9   DA A   3       3.786  -1.638  -0.917  1.00  0.00           N
ATOM     50  C8   DA A   3       3.083  -0.595  -1.491  1.00  0.00           C
ATOM     51  N7   DA A   3       2.054  -0.983  -2.214  1.00  0.00           N
ATOM     52  C5   DA A   3       2.067  -2.363  -2.103  1.00  0.00           C
ATOM     53  C6   DA A   3       1.263  -3.385  -2.657  1.00  0.00           C
ATOM     54  N6   DA A   3       0.209  -3.126  -3.464  1.00  0.00           N
ATOM     55  N1   DA A   3       1.562  -4.670  -2.371  1.00  0.00           N
ATOM     56  C2   DA A   3       2.610  -4.921  -1.572  1.00  0.00           C
ATOM     57  N3   DA A   3       3.448  -4.052  -0.990  1.00  0.00           N
ATOM     58  C4   DA A   3       3.134  -2.788  -1.300  1.00  0.00           C
END

COMPND    ACC / D-B3LYP / PO- MODEL / NEUTRAL
ATOM      1  O5'  DA A   1      -7.224  -0.279   0.355  1.00  0.00           O
ATOM      2  C5'  DA A   1      -7.076  -1.356  -0.567  1.00  0.00           C
ATOM      3  C4'  DA A   1      -5.601  -1.677  -0.764  1.00  0.00           C
ATOM      4  O4'  DA A   1      -4.928  -0.564  -1.384  1.00  0.00           O
ATOM      5  C3'  DA A   1      -4.822  -1.961   0.531  1.00  0.00           C
ATOM      6  O3'  DA A   1      -3.740  -2.832   0.180  1.00  0.00           O
ATOM      7  C2'  DA A   1      -4.312  -0.571   0.898  1.00  0.00           C
ATOM      8  C1'  DA A   1      -3.949  -0.034  -0.484  1.00  0.00           C
ATOM      9  N9   DA A   1      -3.925   1.413  -0.575  1.00  0.00           N
ATOM     10  C8   DA A   1      -4.587   2.342   0.203  1.00  0.00           C
ATOM     11  N7   DA A   1      -4.220   3.584  -0.022  1.00  0.00           N
ATOM     12  C5   DA A   1      -3.265   3.471  -1.019  1.00  0.00           C
ATOM     13  C6   DA A   1      -2.423   4.410  -1.645  1.00  0.00           C
ATOM     14  N6   DA A   1      -2.389   5.713  -1.254  1.00  0.00           N
ATOM     15  N1   DA A   1      -1.575   3.989  -2.600  1.00  0.00           N
ATOM     16  C2   DA A   1      -1.520   2.673  -2.864  1.00  0.00           C
ATOM     17  N3   DA A   1      -2.212   1.677  -2.301  1.00  0.00           N
ATOM     18  C4   DA A   1      -3.071   2.136  -1.381  1.00  0.00           C
ATOM     19  P    DC A   2      -2.733  -3.422   1.361  1.00  0.00           P
ATOM     20  OP2  DC A   2      -2.002  -2.291   2.054  1.00  0.00           O
ATOM     21  OP1  DC A   2      -3.468  -4.432   2.199  1.00  0.00           O
ATOM     22  O5'  DC A   2      -1.709  -4.253   0.374  1.00  0.00           O
ATOM     23  C5'  DC A   2      -1.410  -3.939  -0.988  1.00  0.00           C
ATOM     24  C4'  DC A   2      -0.260  -2.964  -1.188  1.00  0.00           C
ATOM     25  O4'  DC A   2      -0.705  -1.604  -1.030  1.00  0.00           O
ATOM     26  C3'  DC A   2       0.946  -3.156  -0.229  1.00  0.00           C
ATOM     27  O3'  DC A   2       2.114  -3.314  -1.049  1.00  0.00           O
ATOM     28  C2'  DC A   2       0.941  -1.857   0.579  1.00  0.00           C
ATOM     29  C1'  DC A   2       0.389  -0.880  -0.455  1.00  0.00           C
ATOM     30  N1   DC A   2      -0.091   0.395   0.049  1.00  0.00           N
ATOM     31  C2   DC A   2       0.414   1.609  -0.513  1.00  0.00           C
ATOM     32  O2   DC A   2       1.228   1.561  -1.437  1.00  0.00           O
ATOM     33  N3   DC A   2      -0.036   2.786   0.014  1.00  0.00           N
ATOM     34  C4   DC A   2      -0.950   2.789   0.974  1.00  0.00           C
ATOM     35  N4   DC A   2      -1.370   3.996   1.445  1.00  0.00           N
ATOM     36  C5   DC A   2      -1.472   1.587   1.555  1.00  0.00           C
ATOM     37  C6   DC A   2      -1.013   0.410   1.051  1.00  0.00           C
ATOM     38  P    DC A   3       3.613  -3.430  -0.340  1.00  0.00           P
ATOM     39  OP1  DC A   3       4.451  -4.272  -1.261  1.00  0.00           O
ATOM     40  OP2  DC A   3       3.479  -3.701   1.131  1.00  0.00           O
ATOM     41  O5'  DC A   3       4.110  -1.838  -0.459  1.00  0.00           O
ATOM     42  C5'  DC A   3       4.354  -1.319  -1.769  1.00  0.00           C
ATOM     43  C4'  DC A   3       5.305  -0.135  -1.711  1.00  0.00           C
ATOM     44  O4'  DC A   3       4.651   1.024  -1.160  1.00  0.00           O
ATOM     45  C3'  DC A   3       6.556  -0.367  -0.851  1.00  0.00           C
ATOM     46  O3'  DC A   3       7.621   0.367  -1.456  1.00  0.00           O
ATOM     47  C2'  DC A   3       6.144   0.235   0.494  1.00  0.00           C
ATOM     48  C1'  DC A   3       5.263   1.416   0.067  1.00  0.00           C
ATOM     49  N1   DC A   3       4.205   1.752   1.022  1.00  0.00           N
ATOM     50  C2   DC A   3       4.122   3.064   1.576  1.00  0.00           C
ATOM     51  O2   DC A   3       5.009   3.886   1.326  1.00  0.00           O
ATOM     52  N3   DC A   3       3.044   3.350   2.367  1.00  0.00           N
ATOM     53  C4   DC A   3       2.135   2.418   2.627  1.00  0.00           C
ATOM     54  N4   DC A   3       1.095   2.751   3.434  1.00  0.00           N
ATOM     55  C5   DC A   3       2.215   1.081   2.117  1.00  0.00           C
ATOM     56  C6   DC A   3       3.254   0.811   1.288  1.00  0.00           C
END

COMPND    ACC / D-B3LYP / PO- MODEL / SINGLY IONIZED
ATOM      1  O5'  DA A   1      -7.135   0.513  -0.429  1.00  0.00           O
ATOM      2  C5'  DA A   1      -6.977   1.615   0.463  1.00  0.00           C
ATOM      3  C4'  DA A   1      -5.502   1.922   0.668  1.00  0.00           C
ATOM      4  O4'  DA A   1      -4.854   0.840   1.378  1.00  0.00           O
ATOM      5  C3'  DA A   1      -4.684   2.106  -0.618  1.00  0.00           C
ATOM      6  O3'  DA A   1      -3.581   2.956  -0.289  1.00  0.00           O
ATOM      7  C2'  DA A   1      -4.210   0.682  -0.899  1.00  0.00           C
ATOM      8  C1'  DA A   1      -3.944   0.173   0.521  1.00  0.00           C
ATOM      9  N9   DA A   1      -4.147  -1.275   0.645  1.00  0.00           N
ATOM     10  C8   DA A   1      -5.219  -1.995   0.221  1.00  0.00           C
ATOM     11  N7   DA A   1      -5.104  -3.317   0.427  1.00  0.00           N
ATOM     12  C5   DA A   1      -3.900  -3.447   1.018  1.00  0.00           C
ATOM     13  C6   DA A   1      -3.173  -4.578   1.510  1.00  0.00           C
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ATOM     14  N6   DA A   1      -3.642  -5.810   1.397  1.00  0.00           N
ATOM     15  N1   DA A   1      -1.971  -4.376   2.110  1.00  0.00           N
ATOM     16  C2   DA A   1      -1.522  -3.136   2.217  1.00  0.00           C
ATOM     17  N3   DA A   1      -2.126  -1.968   1.809  1.00  0.00           N
ATOM     18  C4   DA A   1      -3.269  -2.184   1.204  1.00  0.00           C
ATOM     19  P    DC A   2      -2.575   3.488  -1.500  1.00  0.00           P
ATOM     20  OP1  DC A   2      -3.298   4.484  -2.364  1.00  0.00           O
ATOM     21  OP2  DC A   2      -1.887   2.311  -2.163  1.00  0.00           O
ATOM     22  O5'  DC A   2      -1.506   4.314  -0.561  1.00  0.00           O
ATOM     23  C5'  DC A   2      -1.271   4.129   0.838  1.00  0.00           C
ATOM     24  C4'  DC A   2      -0.125   3.184   1.162  1.00  0.00           C
ATOM     25  O4'  DC A   2      -0.557   1.807   1.077  1.00  0.00           O
ATOM     26  C3'  DC A   2       1.121   3.322   0.241  1.00  0.00           C
ATOM     27  O3'  DC A   2       2.269   3.433   1.102  1.00  0.00           O
ATOM     28  C2'  DC A   2       1.051   2.029  -0.575  1.00  0.00           C
ATOM     29  C1'  DC A   2       0.525   1.077   0.491  1.00  0.00           C
ATOM     30  N1   DC A   2       0.038  -0.211   0.019  1.00  0.00           N
ATOM     31  C2   DC A   2       0.522  -1.406   0.623  1.00  0.00           C
ATOM     32  O2   DC A   2       1.294  -1.357   1.578  1.00  0.00           O
ATOM     33  N3   DC A   2       0.081  -2.603   0.113  1.00  0.00           N
ATOM     34  C4   DC A   2      -0.853  -2.627  -0.840  1.00  0.00           C
ATOM     35  N4   DC A   2      -1.358  -3.835  -1.159  1.00  0.00           N
ATOM     36  C5   DC A   2      -1.359  -1.441  -1.452  1.00  0.00           C
ATOM     37  C6   DC A   2      -0.883  -0.253  -0.980  1.00  0.00           C
ATOM     38  P    DC A   3       3.793   2.975   0.630  1.00  0.00           P
ATOM     39  OP2  DC A   3       3.972   3.164  -0.852  1.00  0.00           O
ATOM     40  OP1  DC A   3       4.735   3.548   1.651  1.00  0.00           O
ATOM     41  O5'  DC A   3       3.671   1.330   0.848  1.00  0.00           O
ATOM     42  C5'  DC A   3       4.045   0.703   2.078  1.00  0.00           C
ATOM     43  C4'  DC A   3       5.218  -0.241   1.848  1.00  0.00           C
ATOM     44  O4'  DC A   3       4.796  -1.400   1.103  1.00  0.00           O
ATOM     45  C3'  DC A   3       6.365   0.385   1.044  1.00  0.00           C
ATOM     46  O3'  DC A   3       7.576  -0.223   1.498  1.00  0.00           O
ATOM     47  C2'  DC A   3       6.026  -0.024  -0.393  1.00  0.00           C
ATOM     48  C1'  DC A   3       5.376  -1.404  -0.201  1.00  0.00           C
ATOM     49  N1   DC A   3       4.327  -1.731  -1.174  1.00  0.00           N
ATOM     50  C2   DC A   3       4.346  -2.993  -1.846  1.00  0.00           C
ATOM     51  O2   DC A   3       5.321  -3.738  -1.710  1.00  0.00           O
ATOM     52  N3   DC A   3       3.265  -3.323  -2.616  1.00  0.00           N
ATOM     53  C4   DC A   3       2.251  -2.474  -2.746  1.00  0.00           C
ATOM     54  N4   DC A   3       1.203  -2.849  -3.513  1.00  0.00           N
ATOM     55  C5   DC A   3       2.220  -1.189  -2.112  1.00  0.00           C
ATOM     56  C6   DC A   3       3.269  -0.882  -1.307  1.00  0.00           C
END

COMPND    AAC / D-B3LYP / PO- MODEL / NEUTRAL
ATOM      1  O5'  DA A   1      -7.334  -0.465   0.195  1.00  0.00           O
ATOM      2  C5'  DA A   1      -6.960  -1.328  -0.874  1.00  0.00           C
ATOM      3  C4'  DA A   1      -5.448  -1.466  -0.908  1.00  0.00           C
ATOM      4  O4'  DA A   1      -4.854  -0.211  -1.305  1.00  0.00           O
ATOM      5  C3'  DA A   1      -4.819  -1.827   0.453  1.00  0.00           C
ATOM      6  O3'  DA A   1      -3.690  -2.669   0.192  1.00  0.00           O
ATOM      7  C2'  DA A   1      -4.363  -0.462   0.968  1.00  0.00           C
ATOM      8  C1'  DA A   1      -3.866   0.148  -0.336  1.00  0.00           C
ATOM      9  N9   DA A   1      -3.709   1.586  -0.322  1.00  0.00           N
ATOM     10  C8   DA A   1      -4.080   2.492   0.648  1.00  0.00           C
ATOM     11  N7   DA A   1      -3.687   3.723   0.407  1.00  0.00           N
ATOM     12  C5   DA A   1      -3.012   3.624  -0.799  1.00  0.00           C
ATOM     13  C6   DA A   1      -2.303   4.561  -1.576  1.00  0.00           C
ATOM     14  N6   DA A   1      -2.160   5.857  -1.193  1.00  0.00           N
ATOM     15  N1   DA A   1      -1.695   4.139  -2.702  1.00  0.00           N
ATOM     16  C2   DA A   1      -1.768   2.834  -3.016  1.00  0.00           C
ATOM     17  N3   DA A   1      -2.393   1.848  -2.363  1.00  0.00           N
ATOM     18  C4   DA A   1      -3.002   2.306  -1.261  1.00  0.00           C
ATOM     19  P    DA A   2      -2.967  -3.437   1.471  1.00  0.00           P
ATOM     20  OP1  DA A   2      -3.945  -4.399   2.091  1.00  0.00           O
ATOM     21  OP2  DA A   2      -2.258  -2.436   2.360  1.00  0.00           O
ATOM     22  O5'  DA A   2      -1.818  -4.275   0.639  1.00  0.00           O
ATOM     23  C5'  DA A   2      -1.611  -4.290  -0.774  1.00  0.00           C
ATOM     24  C4'  DA A   2      -0.421  -3.439  -1.191  1.00  0.00           C
ATOM     25  O4'  DA A   2      -0.767  -2.035  -1.151  1.00  0.00           O
ATOM     26  C3'  DA A   2       0.828  -3.613  -0.288  1.00  0.00           C
ATOM     27  O3'  DA A   2       1.972  -3.669  -1.161  1.00  0.00           O
ATOM     28  C2'  DA A   2       0.757  -2.355   0.575  1.00  0.00           C
ATOM     29  C1'  DA A   2       0.281  -1.349  -0.462  1.00  0.00           C
ATOM     30  N9   DA A   2      -0.206  -0.103   0.079  1.00  0.00           N
ATOM     31  C8   DA A   2      -1.014   0.072   1.183  1.00  0.00           C
ATOM     32  N7   DA A   2      -1.160   1.338   1.522  1.00  0.00           N
ATOM     33  C5   DA A   2      -0.388   2.028   0.602  1.00  0.00           C
ATOM     34  C6   DA A   2      -0.086   3.394   0.442  1.00  0.00           C
ATOM     35  N6   DA A   2      -0.632   4.359   1.235  1.00  0.00           N
ATOM     36  N1   DA A   2       0.795   3.752  -0.511  1.00  0.00           N
ATOM     37  C2   DA A   2       1.312   2.792  -1.297  1.00  0.00           C
ATOM     38  N3   DA A   2       1.070   1.478  -1.280  1.00  0.00           N
ATOM     39  C4   DA A   2       0.220   1.151  -0.298  1.00  0.00           C
ATOM     40  P    DC A   3       3.502  -3.239  -0.681  1.00  0.00           P
ATOM     41  OP1  DC A   3       4.434  -3.793  -1.724  1.00  0.00           O
ATOM     42  OP2  DC A   3       3.684  -3.478   0.794  1.00  0.00           O
ATOM     43  O5'  DC A   3       3.404  -1.587  -0.845  1.00  0.00           O
ATOM     44  C5'  DC A   3       3.835  -0.916  -2.031  1.00  0.00           C
ATOM     45  C4'  DC A   3       5.069  -0.070  -1.745  1.00  0.00           C
ATOM     46  O4'  DC A   3       4.728   1.064  -0.927  1.00  0.00           O
ATOM     47  C3'  DC A   3       6.173  -0.819  -0.987  1.00  0.00           C
ATOM     48  O3'  DC A   3       7.421  -0.254  -1.400  1.00  0.00           O
ATOM     49  C2'  DC A   3       5.859  -0.489   0.478  1.00  0.00           C
ATOM     50  C1'  DC A   3       5.281   0.932   0.384  1.00  0.00           C
ATOM     51  N1   DC A   3       4.237   1.258   1.362  1.00  0.00           N
ATOM     52  C2   DC A   3       4.225   2.560   1.956  1.00  0.00           C
ATOM     53  O2   DC A   3       5.204   3.299   1.816  1.00  0.00           O
ATOM     54  N3   DC A   3       3.108   2.938   2.649  1.00  0.00           N
ATOM     55  C4   DC A   3       2.088   2.098   2.791  1.00  0.00           C
ATOM     56  N4   DC A   3       0.992   2.531   3.468  1.00  0.00           N
ATOM     57  C5   DC A   3       2.100   0.766   2.266  1.00  0.00           C
ATOM     58  C6   DC A   3       3.173   0.416   1.515  1.00  0.00           C
END

COMPND    AAC / D-B3LYP / PO- MODEL / SINGLY IONIZED
ATOM      1  O5'  DA A   1      -7.277   0.884  -0.165  1.00  0.00           O
ATOM      2  C5'  DA A   1      -7.075  -0.129  -1.143  1.00  0.00           C
ATOM      3  C4'  DA A   1      -5.651  -0.650  -1.053  1.00  0.00           C
ATOM      4  O4'  DA A   1      -4.725   0.380  -1.479  1.00  0.00           O
ATOM      5  C3'  DA A   1      -5.209  -1.052   0.371  1.00  0.00           C
ATOM      6  O3'  DA A   1      -4.299  -2.149   0.224  1.00  0.00           O
ATOM      7  C2'  DA A   1      -4.477   0.206   0.838  1.00  0.00           C
ATOM      8  C1'  DA A   1      -3.748   0.542  -0.456  1.00  0.00           C
ATOM      9  N9   DA A   1      -3.199   1.887  -0.512  1.00  0.00           N
ATOM     10  C8   DA A   1      -3.359   2.918   0.384  1.00  0.00           C
ATOM     11  N7   DA A   1      -2.621   3.985   0.120  1.00  0.00           N
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ATOM     12  C5   DA A   1      -1.930   3.628  -1.002  1.00  0.00           C
ATOM     13  C6   DA A   1      -0.953   4.305  -1.783  1.00  0.00           C
ATOM     14  N6   DA A   1      -0.560   5.546  -1.481  1.00  0.00           N
ATOM     15  N1   DA A   1      -0.405   3.657  -2.832  1.00  0.00           N
ATOM     16  C2   DA A   1      -0.818   2.412  -3.099  1.00  0.00           C
ATOM     17  N3   DA A   1      -1.744   1.668  -2.460  1.00  0.00           N
ATOM     18  C4   DA A   1      -2.261   2.319  -1.424  1.00  0.00           C
ATOM     19  P    DA A   2      -3.608  -2.865   1.550  1.00  0.00           P
ATOM     20  OP2  DA A   2      -2.702  -1.886   2.272  1.00  0.00           O
ATOM     21  OP1  DA A   2      -4.654  -3.600   2.341  1.00  0.00           O
ATOM     22  O5'  DA A   2      -2.681  -3.971   0.753  1.00  0.00           O
ATOM     23  C5'  DA A   2      -2.385  -3.985  -0.645  1.00  0.00           C
ATOM     24  C4'  DA A   2      -1.082  -3.290  -1.000  1.00  0.00           C
ATOM     25  O4'  DA A   2      -1.243  -1.850  -0.935  1.00  0.00           O
ATOM     26  C3'  DA A   2       0.120  -3.645  -0.081  1.00  0.00           C
ATOM     27  O3'  DA A   2       1.242  -3.905  -0.944  1.00  0.00           O
ATOM     28  C2'  DA A   2       0.249  -2.376   0.761  1.00  0.00           C
ATOM     29  C1'  DA A   2      -0.078  -1.340  -0.302  1.00  0.00           C
ATOM     30  N9   DA A   2      -0.314  -0.002   0.210  1.00  0.00           N
ATOM     31  C8   DA A   2      -1.066   0.375   1.290  1.00  0.00           C
ATOM     32  N7   DA A   2      -0.900   1.656   1.631  1.00  0.00           N
ATOM     33  C5   DA A   2       0.015   2.122   0.736  1.00  0.00           C
ATOM     34  C6   DA A   2       0.723   3.352   0.617  1.00  0.00           C
ATOM     35  N6   DA A   2       0.418   4.412   1.360  1.00  0.00           N
ATOM     36  N1   DA A   2       1.727   3.446  -0.288  1.00  0.00           N
ATOM     37  C2   DA A   2       1.969   2.402  -1.075  1.00  0.00           C
ATOM     38  N3   DA A   2       1.340   1.199  -1.098  1.00  0.00           N
ATOM     39  C4   DA A   2       0.415   1.107  -0.165  1.00  0.00           C
ATOM     40  P    DC A   3       2.825  -3.646  -0.512  1.00  0.00           P
ATOM     41  OP1  DC A   3       3.654  -4.362  -1.541  1.00  0.00           O
ATOM     42  OP2  DC A   3       3.013  -3.823   0.970  1.00  0.00           O
ATOM     43  O5'  DC A   3       2.932  -2.003  -0.762  1.00  0.00           O
ATOM     44  C5'  DC A   3       3.332  -1.456  -2.022  1.00  0.00           C
ATOM     45  C4'  DC A   3       4.642  -0.698  -1.871  1.00  0.00           C
ATOM     46  O4'  DC A   3       4.449   0.499  -1.091  1.00  0.00           O
ATOM     47  C3'  DC A   3       5.738  -1.497  -1.152  1.00  0.00           C
ATOM     48  O3'  DC A   3       6.990  -1.067  -1.691  1.00  0.00           O
ATOM     49  C2'  DC A   3       5.571  -1.061   0.308  1.00  0.00           C
ATOM     50  C1'  DC A   3       5.109   0.398   0.169  1.00  0.00           C
ATOM     51  N1   DC A   3       4.188   0.856   1.218  1.00  0.00           N
ATOM     52  C2   DC A   3       4.412   2.123   1.857  1.00  0.00           C
ATOM     53  O2   DC A   3       5.445   2.746   1.609  1.00  0.00           O
ATOM     54  N3   DC A   3       3.450   2.586   2.709  1.00  0.00           N
ATOM     55  C4   DC A   3       2.357   1.869   2.943  1.00  0.00           C
ATOM     56  N4   DC A   3       1.421   2.385   3.771  1.00  0.00           N
ATOM     57  C5   DC A   3       2.126   0.584   2.350  1.00  0.00           C
ATOM     58  C6   DC A   3       3.062   0.136   1.471  1.00  0.00           C
END

COMPND    CCA / D-B3LYP / PO- MODEL / NEUTRAL
ATOM      1  O5'  DC A   1      -7.303  -0.945   0.089  1.00  0.00           O
ATOM      2  C5'  DC A   1      -6.980  -1.985  -0.834  1.00  0.00           C
ATOM      3  C4'  DC A   1      -5.470  -2.090  -0.995  1.00  0.00           C
ATOM      4  O4'  DC A   1      -4.961  -0.920  -1.662  1.00  0.00           O
ATOM      5  C3'  DC A   1      -4.693  -2.193   0.328  1.00  0.00           C
ATOM      6  O3'  DC A   1      -3.505  -2.955   0.065  1.00  0.00           O
ATOM      7  C2'  DC A   1      -4.353  -0.734   0.617  1.00  0.00           C
ATOM      8  C1'  DC A   1      -4.067  -0.210  -0.792  1.00  0.00           C
ATOM      9  N1   DC A   1      -4.272   1.224  -0.968  1.00  0.00           N
ATOM     10  C2   DC A   1      -3.291   1.994  -1.668  1.00  0.00           C
ATOM     11  O2   DC A   1      -2.343   1.420  -2.207  1.00  0.00           O
ATOM     12  N3   DC A   1      -3.455   3.349  -1.696  1.00  0.00           N
ATOM     13  C4   DC A   1      -4.553   3.902  -1.192  1.00  0.00           C
ATOM     14  N4   DC A   1      -4.628   5.252  -1.189  1.00  0.00           N
ATOM     15  C5   DC A   1      -5.637   3.135  -0.648  1.00  0.00           C
ATOM     16  C6   DC A   1      -5.443   1.794  -0.560  1.00  0.00           C
ATOM     17  P    DC A   2      -2.587  -3.461   1.353  1.00  0.00           P
ATOM     18  OP1  DC A   2      -3.310  -4.555   2.093  1.00  0.00           O
ATOM     19  OP2  DC A   2      -2.074  -2.271   2.136  1.00  0.00           O
ATOM     20  O5'  DC A   2      -1.362  -4.161   0.505  1.00  0.00           O
ATOM     21  C5'  DC A   2      -0.991  -3.912  -0.855  1.00  0.00           C
ATOM     22  C4'  DC A   2       0.145  -2.912  -1.024  1.00  0.00           C
ATOM     23  O4'  DC A   2      -0.358  -1.563  -1.003  1.00  0.00           O
ATOM     24  C3'  DC A   2       1.247  -2.991   0.062  1.00  0.00           C
ATOM     25  O3'  DC A   2       2.510  -2.957  -0.623  1.00  0.00           O
ATOM     26  C2'  DC A   2       0.990  -1.726   0.879  1.00  0.00           C
ATOM     27  C1'  DC A   2       0.562  -0.772  -0.230  1.00  0.00           C
ATOM     28  N1   DC A   2      -0.097   0.462   0.160  1.00  0.00           N
ATOM     29  C2   DC A   2       0.272   1.687  -0.478  1.00  0.00           C
ATOM     30  O2   DC A   2       1.169   1.689  -1.323  1.00  0.00           O
ATOM     31  N3   DC A   2      -0.383   2.824  -0.098  1.00  0.00           N
ATOM     32  C4   DC A   2      -1.360   2.769   0.791  1.00  0.00           C
ATOM     33  N4   DC A   2      -1.946   3.948   1.161  1.00  0.00           N
ATOM     34  C5   DC A   2      -1.778   1.554   1.417  1.00  0.00           C
ATOM     35  C6   DC A   2      -1.118   0.420   1.059  1.00  0.00           C
ATOM     36  P    DA A   3       3.933  -3.190   0.203  1.00  0.00           P
ATOM     37  OP1  DA A   3       4.589  -4.430  -0.340  1.00  0.00           O
ATOM     38  OP2  DA A   3       3.737  -2.960   1.677  1.00  0.00           O
ATOM     39  O5'  DA A   3       4.756  -1.853  -0.340  1.00  0.00           O
ATOM     40  C5'  DA A   3       4.953  -1.689  -1.742  1.00  0.00           C
ATOM     41  C4'  DA A   3       5.586  -0.332  -2.004  1.00  0.00           C
ATOM     42  O4'  DA A   3       4.678   0.719  -1.621  1.00  0.00           O
ATOM     43  C3'  DA A   3       6.885  -0.067  -1.231  1.00  0.00           C
ATOM     44  O3'  DA A   3       7.676   0.805  -2.039  1.00  0.00           O
ATOM     45  C2'  DA A   3       6.381   0.632   0.031  1.00  0.00           C
ATOM     46  C1'  DA A   3       5.182   1.432  -0.494  1.00  0.00           C
ATOM     47  N9   DA A   3       4.129   1.608   0.490  1.00  0.00           N
ATOM     48  C8   DA A   3       3.507   0.632   1.246  1.00  0.00           C
ATOM     49  N7   DA A   3       2.529   1.091   1.994  1.00  0.00           N
ATOM     50  C5   DA A   3       2.495   2.445   1.711  1.00  0.00           C
ATOM     51  C6   DA A   3       1.648   3.486   2.136  1.00  0.00           C
ATOM     52  N6   DA A   3       0.646   3.286   3.040  1.00  0.00           N
ATOM     53  N1   DA A   3       1.855   4.728   1.654  1.00  0.00           N
ATOM     54  C2   DA A   3       2.847   4.908   0.766  1.00  0.00           C
ATOM     55  N3   DA A   3       3.698   4.005   0.263  1.00  0.00           N
ATOM     56  C4   DA A   3       3.470   2.785   0.769  1.00  0.00           C
END

COMPND    CCA / D-B3LYP / PO- MODEL / SINGLY IONIZED
ATOM      1  O5'  DC A   1      -7.234  -0.406   0.138  1.00  0.00           O
ATOM      2  C5'  DC A   1      -7.023  -1.552  -0.686  1.00  0.00           C
ATOM      3  C4'  DC A   1      -5.535  -1.838  -0.817  1.00  0.00           C
ATOM      4  O4'  DC A   1      -4.891  -0.794  -1.573  1.00  0.00           O
ATOM      5  C3'  DC A   1      -4.772  -1.916   0.517  1.00  0.00           C
ATOM      6  O3'  DC A   1      -3.672  -2.811   0.308  1.00  0.00           O
ATOM      7  C2'  DC A   1      -4.287  -0.481   0.687  1.00  0.00           C
ATOM      8  C1'  DC A   1      -3.920  -0.126  -0.756  1.00  0.00           C
ATOM      9  N1   DC A   1      -3.951   1.301  -1.061  1.00  0.00           N
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ATOM     10  C2   DC A   1      -2.861   1.902  -1.765  1.00  0.00           C
ATOM     11  O2   DC A   1      -1.929   1.191  -2.153  1.00  0.00           O
ATOM     12  N3   DC A   1      -2.897   3.250  -1.958  1.00  0.00           N
ATOM     13  C4   DC A   1      -3.961   3.954  -1.584  1.00  0.00           C
ATOM     14  N4   DC A   1      -3.916   5.292  -1.751  1.00  0.00           N
ATOM     15  C5   DC A   1      -5.137   3.354  -1.017  1.00  0.00           C
ATOM     16  C6   DC A   1      -5.080   2.018  -0.781  1.00  0.00           C
ATOM     17  P    DC A   2      -2.698  -3.257   1.572  1.00  0.00           P
ATOM     18  OP2  DC A   2      -2.054  -2.037   2.203  1.00  0.00           O
ATOM     19  OP1  DC A   2      -3.419  -4.230   2.463  1.00  0.00           O
ATOM     20  O5'  DC A   2      -1.579  -4.100   0.707  1.00  0.00           O
ATOM     21  C5'  DC A   2      -1.309  -3.984  -0.693  1.00  0.00           C
ATOM     22  C4'  DC A   2      -0.143  -3.068  -1.028  1.00  0.00           C
ATOM     23  O4'  DC A   2      -0.561  -1.683  -1.012  1.00  0.00           O
ATOM     24  C3'  DC A   2       1.072  -3.180  -0.067  1.00  0.00           C
ATOM     25  O3'  DC A   2       2.247  -3.319  -0.889  1.00  0.00           O
ATOM     26  C2'  DC A   2       0.978  -1.866   0.707  1.00  0.00           C
ATOM     27  C1'  DC A   2       0.499  -0.941  -0.405  1.00  0.00           C
ATOM     28  N1   DC A   2      -0.008   0.363   0.016  1.00  0.00           N
ATOM     29  C2   DC A   2       0.494   1.564  -0.616  1.00  0.00           C
ATOM     30  O2   DC A   2       1.374   1.463  -1.466  1.00  0.00           O
ATOM     31  N3   DC A   2      -0.011   2.763  -0.215  1.00  0.00           N
ATOM     32  C4   DC A   2      -1.021   2.814   0.644  1.00  0.00           C
ATOM     33  N4   DC A   2      -1.512   4.020   0.986  1.00  0.00           N
ATOM     34  C5   DC A   2      -1.541   1.639   1.281  1.00  0.00           C
ATOM     35  C6   DC A   2      -0.997   0.425   0.920  1.00  0.00           C
ATOM     36  P    DA A   3       3.759  -2.803  -0.458  1.00  0.00           P
ATOM     37  OP1  DA A   3       4.702  -3.437  -1.442  1.00  0.00           O
ATOM     38  OP2  DA A   3       3.964  -2.884   1.036  1.00  0.00           O
ATOM     39  O5'  DA A   3       3.630  -1.179  -0.764  1.00  0.00           O
ATOM     40  C5'  DA A   3       3.924  -0.642  -2.057  1.00  0.00           C
ATOM     41  C4'  DA A   3       5.168   0.229  -1.986  1.00  0.00           C
ATOM     42  O4'  DA A   3       4.942   1.414  -1.194  1.00  0.00           O
ATOM     43  C3'  DA A   3       6.374  -0.452  -1.333  1.00  0.00           C
ATOM     44  O3'  DA A   3       7.545   0.134  -1.901  1.00  0.00           O
ATOM     45  C2'  DA A   3       6.214  -0.090   0.157  1.00  0.00           C
ATOM     46  C1'  DA A   3       5.394   1.215   0.128  1.00  0.00           C
ATOM     47  N9   DA A   3       4.238   1.218   1.053  1.00  0.00           N
ATOM     48  C8   DA A   3       3.630   0.195   1.732  1.00  0.00           C
ATOM     49  N7   DA A   3       2.535   0.562   2.395  1.00  0.00           N
ATOM     50  C5   DA A   3       2.410   1.885   2.115  1.00  0.00           C
ATOM     51  C6   DA A   3       1.463   2.867   2.496  1.00  0.00           C
ATOM     52  N6   DA A   3       0.396   2.558   3.244  1.00  0.00           N
ATOM     53  N1   DA A   3       1.621   4.144   2.070  1.00  0.00           N
ATOM     54  C2   DA A   3       2.663   4.414   1.291  1.00  0.00           C
ATOM     55  N3   DA A   3       3.630   3.572   0.842  1.00  0.00           N
ATOM     56  C4   DA A   3       3.461   2.335   1.280  1.00  0.00           C
END

COMPND    CAA / D-B3LYP / PO- MODEL / NEUTRAL
ATOM      1  O5'  DC A   1      -7.203  -0.623   0.231  1.00  0.00           O
ATOM      2  C5'  DC A   1      -7.004  -1.710  -0.672  1.00  0.00           C
ATOM      3  C4'  DC A   1      -5.515  -1.952  -0.879  1.00  0.00           C
ATOM      4  O4'  DC A   1      -4.928  -0.842  -1.582  1.00  0.00           O
ATOM      5  C3'  DC A   1      -4.707  -2.101   0.420  1.00  0.00           C
ATOM      6  O3'  DC A   1      -3.588  -2.954   0.131  1.00  0.00           O
ATOM      7  C2'  DC A   1      -4.243  -0.671   0.676  1.00  0.00           C
ATOM      8  C1'  DC A   1      -3.949  -0.201  -0.751  1.00  0.00           C
ATOM      9  N1   DC A   1      -4.019   1.240  -0.962  1.00  0.00           N
ATOM     10  C2   DC A   1      -3.034   1.875  -1.782  1.00  0.00           C
ATOM     11  O2   DC A   1      -2.194   1.189  -2.365  1.00  0.00           O
ATOM     12  N3   DC A   1      -3.070   3.237  -1.871  1.00  0.00           N
ATOM     13  C4   DC A   1      -4.041   3.924  -1.286  1.00  0.00           C
ATOM     14  N4   DC A   1      -3.959   5.278  -1.326  1.00  0.00           N
ATOM     15  C5   DC A   1      -5.140   3.301  -0.608  1.00  0.00           C
ATOM     16  C6   DC A   1      -5.083   1.949  -0.483  1.00  0.00           C
ATOM     17  P    DA A   2      -2.730  -3.583   1.405  1.00  0.00           P
ATOM     18  OP1  DA A   2      -3.542  -4.659   2.075  1.00  0.00           O
ATOM     19  OP2  DA A   2      -2.149  -2.473   2.255  1.00  0.00           O
ATOM     20  O5'  DA A   2      -1.518  -4.302   0.553  1.00  0.00           O
ATOM     21  C5'  DA A   2      -1.206  -4.162  -0.835  1.00  0.00           C
ATOM     22  C4'  DA A   2       0.021  -3.295  -1.095  1.00  0.00           C
ATOM     23  O4'  DA A   2      -0.334  -1.895  -1.108  1.00  0.00           O
ATOM     24  C3'  DA A   2       1.146  -3.452  -0.048  1.00  0.00           C
ATOM     25  O3'  DA A   2       2.383  -3.482  -0.775  1.00  0.00           O
ATOM     26  C2'  DA A   2       0.965  -2.195   0.800  1.00  0.00           C
ATOM     27  C1'  DA A   2       0.584  -1.181  -0.269  1.00  0.00           C
ATOM     28  N9   DA A   2      -0.053   0.019   0.209  1.00  0.00           N
ATOM     29  C8   DA A   2      -0.983   0.119   1.220  1.00  0.00           C
ATOM     30  N7   DA A   2      -1.420   1.346   1.412  1.00  0.00           N
ATOM     31  C5   DA A   2      -0.728   2.097   0.477  1.00  0.00           C
ATOM     32  C6   DA A   2      -0.742   3.466   0.166  1.00  0.00           C
ATOM     33  N6   DA A   2      -1.545   4.347   0.837  1.00  0.00           N
ATOM     34  N1   DA A   2       0.099   3.923  -0.780  1.00  0.00           N
ATOM     35  C2   DA A   2       0.895   3.036  -1.400  1.00  0.00           C
ATOM     36  N3   DA A   2       0.974   1.713  -1.227  1.00  0.00           N
ATOM     37  C4   DA A   2       0.132   1.295  -0.275  1.00  0.00           C
ATOM     38  P    DA A   3       3.853  -3.502  -0.001  1.00  0.00           P
ATOM     39  OP1  DA A   3       4.713  -4.500  -0.727  1.00  0.00           O
ATOM     40  OP2  DA A   3       3.677  -3.510   1.491  1.00  0.00           O
ATOM     41  O5'  DA A   3       4.369  -1.964  -0.383  1.00  0.00           O
ATOM     42  C5'  DA A   3       4.568  -1.666  -1.765  1.00  0.00           C
ATOM     43  C4'  DA A   3       5.296  -0.342  -1.915  1.00  0.00           C
ATOM     44  O4'  DA A   3       4.465   0.747  -1.470  1.00  0.00           O
ATOM     45  C3'  DA A   3       6.596  -0.236  -1.106  1.00  0.00           C
ATOM     46  O3'  DA A   3       7.469   0.629  -1.835  1.00  0.00           O
ATOM     47  C2'  DA A   3       6.120   0.407   0.197  1.00  0.00           C
ATOM     48  C1'  DA A   3       4.998   1.335  -0.287  1.00  0.00           C
ATOM     49  N9   DA A   3       3.934   1.516   0.683  1.00  0.00           N
ATOM     50  C8   DA A   3       3.212   0.532   1.330  1.00  0.00           C
ATOM     51  N7   DA A   3       2.235   0.999   2.075  1.00  0.00           N
ATOM     52  C5   DA A   3       2.304   2.371   1.899  1.00  0.00           C
ATOM     53  C6   DA A   3       1.515   3.440   2.368  1.00  0.00           C
ATOM     54  N6   DA A   3       0.434   3.256   3.180  1.00  0.00           N
ATOM     55  N1   DA A   3       1.849   4.697   2.010  1.00  0.00           N
ATOM     56  C2   DA A   3       2.893   4.870   1.184  1.00  0.00           C
ATOM     57  N3   DA A   3       3.690   3.946   0.636  1.00  0.00           N
ATOM     58  C4   DA A   3       3.348   2.712   1.031  1.00  0.00           C
END

COMPND    CAA / D-B3LYP / PO- MODEL / SINGLY IONIZED
ATOM      1  O5'  DC A   1      -7.105  -0.754  -0.217  1.00  0.00           O
ATOM      2  C5'  DC A   1      -6.688  -1.783  -1.115  1.00  0.00           C
ATOM      3  C4'  DC A   1      -5.173  -1.909  -1.089  1.00  0.00           C
ATOM      4  O4'  DC A   1      -4.565  -0.750  -1.694  1.00  0.00           O
ATOM      5  C3'  DC A   1      -4.567  -2.015   0.319  1.00  0.00           C
ATOM      6  O3'  DC A   1      -3.373  -2.801   0.218  1.00  0.00           O
ATOM      7  C2'  DC A   1      -4.226  -0.561   0.640  1.00  0.00           C
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ATOM      8  C1'  DC A   1      -3.788  -0.037  -0.733  1.00  0.00           C
ATOM      9  N1   DC A   1      -4.016   1.400  -0.928  1.00  0.00           N
ATOM     10  C2   DC A   1      -2.982   2.235  -1.424  1.00  0.00           C
ATOM     11  O2   DC A   1      -1.894   1.727  -1.751  1.00  0.00           O
ATOM     12  N3   DC A   1      -3.209   3.569  -1.515  1.00  0.00           N
ATOM     13  C4   DC A   1      -4.420   4.063  -1.242  1.00  0.00           C
ATOM     14  N4   DC A   1      -4.578   5.395  -1.319  1.00  0.00           N
ATOM     15  C5   DC A   1      -5.530   3.226  -0.894  1.00  0.00           C
ATOM     16  C6   DC A   1      -5.275   1.899  -0.749  1.00  0.00           C
ATOM     17  P    DA A   2      -2.753  -3.433   1.619  1.00  0.00           P
ATOM     18  OP1  DA A   2      -3.774  -4.339   2.253  1.00  0.00           O
ATOM     19  OP2  DA A   2      -2.129  -2.335   2.458  1.00  0.00           O
ATOM     20  O5'  DA A   2      -1.531  -4.330   0.976  1.00  0.00           O
ATOM     21  C5'  DA A   2      -1.229  -4.503  -0.409  1.00  0.00           C
ATOM     22  C4'  DA A   2      -0.043  -3.656  -0.843  1.00  0.00           C
ATOM     23  O4'  DA A   2      -0.435  -2.264  -0.933  1.00  0.00           O
ATOM     24  C3'  DA A   2       1.168  -3.708   0.127  1.00  0.00           C
ATOM     25  O3'  DA A   2       2.357  -3.768  -0.685  1.00  0.00           O
ATOM     26  C2'  DA A   2       0.989  -2.406   0.903  1.00  0.00           C
ATOM     27  C1'  DA A   2       0.543  -1.500  -0.233  1.00  0.00           C
ATOM     28  N9   DA A   2      -0.021  -0.232   0.177  1.00  0.00           N
ATOM     29  C8   DA A   2      -0.906   0.012   1.185  1.00  0.00           C
ATOM     30  N7   DA A   2      -1.183   1.316   1.350  1.00  0.00           N
ATOM     31  C5   DA A   2      -0.419   1.928   0.422  1.00  0.00           C
ATOM     32  C6   DA A   2      -0.267   3.292   0.030  1.00  0.00           C
ATOM     33  N6   DA A   2      -1.020   4.245   0.562  1.00  0.00           N
ATOM     34  N1   DA A   2       0.663   3.607  -0.904  1.00  0.00           N
ATOM     35  C2   DA A   2       1.348   2.616  -1.461  1.00  0.00           C
ATOM     36  N3   DA A   2       1.229   1.274  -1.259  1.00  0.00           N
ATOM     37  C4   DA A   2       0.351   0.992  -0.327  1.00  0.00           C
ATOM     38  P    DA A   3       3.817  -3.061  -0.333  1.00  0.00           P
ATOM     39  OP1  DA A   3       4.810  -3.691  -1.269  1.00  0.00           O
ATOM     40  OP2  DA A   3       4.036  -2.971   1.156  1.00  0.00           O
ATOM     41  O5'  DA A   3       3.530  -1.495  -0.799  1.00  0.00           O
ATOM     42  C5'  DA A   3       3.790  -1.033  -2.124  1.00  0.00           C
ATOM     43  C4'  DA A   3       4.903   0.005  -2.099  1.00  0.00           C
ATOM     44  O4'  DA A   3       4.484   1.209  -1.428  1.00  0.00           O
ATOM     45  C3'  DA A   3       6.159  -0.458  -1.352  1.00  0.00           C
ATOM     46  O3'  DA A   3       7.268   0.226  -1.937  1.00  0.00           O
ATOM     47  C2'  DA A   3       5.893   0.011   0.087  1.00  0.00           C
ATOM     48  C1'  DA A   3       5.005   1.252  -0.106  1.00  0.00           C
ATOM     49  N9   DA A   3       3.913   1.362   0.863  1.00  0.00           N
ATOM     50  C8   DA A   3       3.185   0.377   1.504  1.00  0.00           C
ATOM     51  N7   DA A   3       2.182   0.841   2.220  1.00  0.00           N
ATOM     52  C5   DA A   3       2.240   2.211   2.034  1.00  0.00           C
ATOM     53  C6   DA A   3       1.485   3.289   2.545  1.00  0.00           C
ATOM     54  N6   DA A   3       0.437   3.112   3.383  1.00  0.00           N
ATOM     55  N1   DA A   3       1.826   4.547   2.190  1.00  0.00           N
ATOM     56  C2   DA A   3       2.869   4.716   1.363  1.00  0.00           C
ATOM     57  N3   DA A   3       3.663   3.788   0.814  1.00  0.00           N
ATOM     58  C4   DA A   3       3.309   2.554   1.192  1.00  0.00           C
END
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