



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:55 PM BST

PDB ID : 4C4Q
EMDB ID: : EMD-2450
Title : Cryo-EM map of the CSFV IRES in complex with the small ribosomal 40S subunit and DHX29
Authors : Hashem, Y.; desGeorges, A.; Dhote, V.; Langlois, R.; Liao, H.Y.; Grassucci, R.A.; Pestova, T.V.; Hellen, C.U.T.; Frank, J.
Deposited on : 2013-09-07
Resolution : 8.50 Å(reported)
Based on PDB ID : 2XZM

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

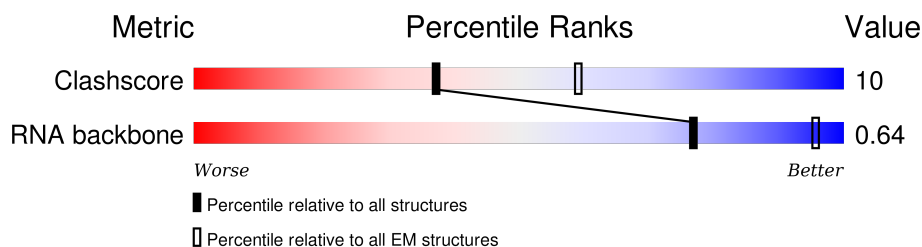
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

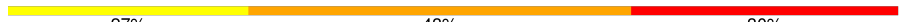
The reported resolution of this entry is 8.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
RNA backbone	3027	244

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	N	233	 27% 43% 30%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4986 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

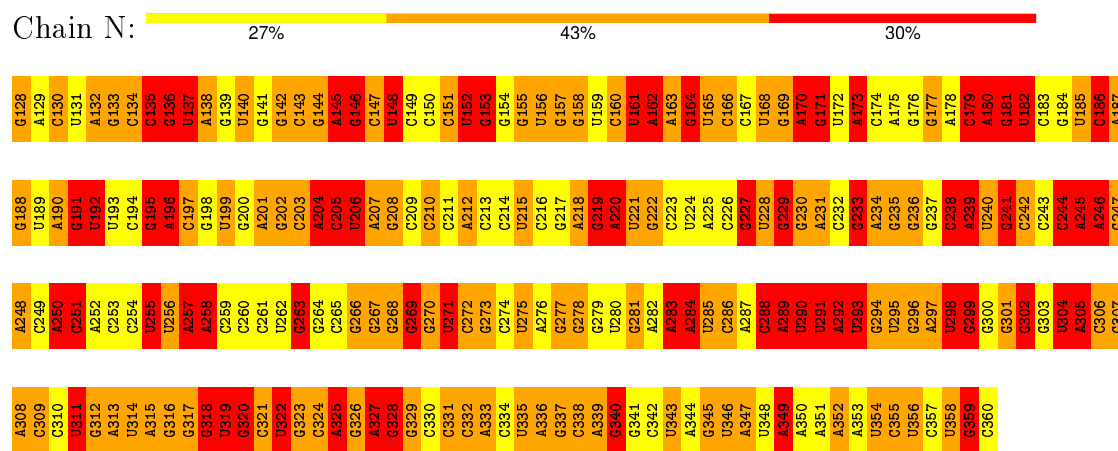
- Molecule 1 is a RNA chain called INTERNAL RIBOSOMAL ENTRY SITE.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	N	233	Total	C	N	O	P	0	0
			4986	2225	908	1621	232		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: INTERNAL RIBOSOMAL ENTRY SITE



4 Experimental information ⓘ

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	EACH PARTICLE	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	120	Depositor
Electron dose ($e^-/\text{\AA}^2$)	12	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN UTRASCAN 4000 CCD	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 2$	RMSZ	$\# Z > 2$
1	N	3.32	735/5579 (13.2%)	3.44	1129/8700 (13.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	N	0	122

All (735) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	283	A	N9-C4	17.10	1.48	1.37
1	N	307	G	O3'-P	-15.46	1.42	1.61
1	N	323	G	N9-C8	-15.46	1.27	1.37
1	N	151	C	N1-C6	14.29	1.45	1.37
1	N	183	C	N1-C6	13.73	1.45	1.37
1	N	326	G	N7-C5	13.58	1.47	1.39
1	N	297	A	N7-C5	-12.89	1.31	1.39
1	N	328	G	C6-N1	-12.78	1.30	1.39
1	N	157	G	C6-N1	12.71	1.48	1.39
1	N	160	C	N3-C4	12.45	1.42	1.33
1	N	273	G	N7-C5	12.25	1.46	1.39
1	N	208	G	C2-N3	11.77	1.42	1.32
1	N	208	G	N9-C4	11.76	1.47	1.38
1	N	294	G	N9-C8	11.63	1.46	1.37
1	N	155	G	C8-N7	11.59	1.38	1.30
1	N	152	U	N1-C6	-11.29	1.27	1.38
1	N	240	U	N1-C6	11.21	1.48	1.38
1	N	307	G	N7-C5	11.07	1.45	1.39
1	N	133	G	C4'-C3'	-11.06	1.41	1.53
1	N	284	A	O4'-C1'	-11.00	1.27	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	283	A	C5-C4	10.97	1.46	1.38
1	N	181	G	C8-N7	-10.81	1.24	1.30
1	N	186	C	C3'-O3'	10.67	1.57	1.42
1	N	252	A	N7-C5	-10.67	1.32	1.39
1	N	251	C	N1-C6	10.60	1.43	1.37
1	N	138	A	N3-C4	10.57	1.41	1.34
1	N	196	A	N3-C4	10.42	1.41	1.34
1	N	249	C	P-O5'	-10.28	1.49	1.59
1	N	303	G	C2-N3	10.16	1.40	1.32
1	N	342	C	N1-C6	-10.15	1.31	1.37
1	N	164	G	O3'-P	-10.15	1.49	1.61
1	N	315	A	N9-C4	-10.06	1.31	1.37
1	N	329	G	N9-C8	10.05	1.44	1.37
1	N	197	C	N1-C6	10.03	1.43	1.37
1	N	283	A	C3'-O3'	9.84	1.55	1.42
1	N	187	A	N3-C4	-9.79	1.28	1.34
1	N	175	A	N3-C4	9.73	1.40	1.34
1	N	208	G	P-O5'	-9.69	1.50	1.59
1	N	323	G	C6-N1	-9.68	1.32	1.39
1	N	327	A	C5'-C4'	9.64	1.62	1.51
1	N	344	A	O3'-P	-9.63	1.49	1.61
1	N	180	A	N3-C4	9.61	1.40	1.34
1	N	170	A	C6-N1	9.57	1.42	1.35
1	N	245	A	N3-C4	9.56	1.40	1.34
1	N	283	A	C8-N7	-9.52	1.24	1.31
1	N	264	G	N7-C5	9.49	1.45	1.39
1	N	277	G	N3-C4	9.41	1.42	1.35
1	N	233	G	C6-N1	9.39	1.46	1.39
1	N	336	A	O3'-P	-9.39	1.49	1.61
1	N	353	A	N7-C5	9.38	1.44	1.39
1	N	136	G	N7-C5	-9.37	1.33	1.39
1	N	282	A	N3-C4	-9.36	1.29	1.34
1	N	347	A	N9-C8	-9.35	1.30	1.37
1	N	257	A	N7-C5	-9.30	1.33	1.39
1	N	257	A	C6-N1	9.20	1.42	1.35
1	N	259	C	N3-C4	-9.18	1.27	1.33
1	N	352	A	C6-N6	-9.17	1.26	1.33
1	N	163	A	N3-C4	-9.14	1.29	1.34
1	N	198	G	N9-C8	9.14	1.44	1.37
1	N	264	G	C2'-C1'	-9.13	1.43	1.53
1	N	128	G	N9-C8	9.08	1.44	1.37
1	N	128	G	N7-C5	9.03	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	167	C	O3'-P	-9.03	1.50	1.61
1	N	354	U	N3-C4	9.03	1.46	1.38
1	N	248	A	C2'-C1'	-9.03	1.43	1.53
1	N	339	A	C3'-O3'	9.02	1.54	1.42
1	N	227	G	N9-C8	-9.00	1.31	1.37
1	N	267	G	N7-C5	8.97	1.44	1.39
1	N	250	A	N7-C5	-8.96	1.33	1.39
1	N	202	G	C2-N3	8.96	1.40	1.32
1	N	337	G	N7-C5	-8.95	1.33	1.39
1	N	273	G	O3'-P	-8.94	1.50	1.61
1	N	359	G	C4'-O4'	8.89	1.57	1.45
1	N	259	C	P-O5'	-8.89	1.50	1.59
1	N	281	G	N9-C8	-8.87	1.31	1.37
1	N	315	A	C8-N7	-8.83	1.25	1.31
1	N	219	G	N7-C5	8.80	1.44	1.39
1	N	231	A	N7-C5	-8.81	1.33	1.39
1	N	140	U	C4'-O4'	8.80	1.56	1.45
1	N	206	U	C4-C5	8.79	1.51	1.43
1	N	266	G	C4'-C3'	-8.73	1.43	1.53
1	N	169	G	N7-C5	8.72	1.44	1.39
1	N	250	A	O3'-P	-8.70	1.50	1.61
1	N	327	A	N9-C4	8.68	1.43	1.37
1	N	238	C	N1-C6	8.67	1.42	1.37
1	N	188	G	N3-C4	-8.66	1.29	1.35
1	N	309	C	C2-O2	8.66	1.32	1.24
1	N	279	G	C8-N7	-8.63	1.25	1.30
1	N	318	G	C3'-O3'	8.62	1.54	1.42
1	N	218	A	C5'-C4'	8.60	1.61	1.51
1	N	332	C	N3-C4	8.60	1.40	1.33
1	N	242	C	O3'-P	-8.57	1.50	1.61
1	N	200	G	O3'-P	-8.52	1.50	1.61
1	N	338	C	C4-N4	-8.52	1.26	1.33
1	N	274	C	P-O5'	-8.50	1.51	1.59
1	N	160	C	P-O5'	-8.49	1.51	1.59
1	N	284	A	P-O5'	8.48	1.68	1.59
1	N	233	G	C4'-C3'	8.48	1.62	1.53
1	N	240	U	C2'-C1'	-8.47	1.44	1.53
1	N	184	G	P-O5'	-8.46	1.51	1.59
1	N	142	G	N7-C5	-8.46	1.34	1.39
1	N	129	A	C8-N7	-8.41	1.25	1.31
1	N	188	G	N7-C5	8.41	1.44	1.39
1	N	239	A	N7-C5	8.40	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	154	G	N3-C4	-8.40	1.29	1.35
1	N	182	U	C4-C5	-8.39	1.35	1.43
1	N	217	G	O3'-P	-8.38	1.51	1.61
1	N	349	A	C6-N6	-8.36	1.27	1.33
1	N	200	G	N9-C4	8.36	1.44	1.38
1	N	278	G	C5-C4	8.35	1.44	1.38
1	N	231	A	N9-C4	-8.34	1.32	1.37
1	N	357	C	C5'-C4'	8.33	1.61	1.51
1	N	131	U	C5'-C4'	8.31	1.61	1.51
1	N	339	A	C4'-O4'	8.30	1.56	1.45
1	N	245	A	C3'-O3'	8.23	1.53	1.42
1	N	210	C	C4-N4	-8.22	1.26	1.33
1	N	194	C	P-O5'	-8.21	1.51	1.59
1	N	332	C	C2'-C1'	-8.13	1.44	1.53
1	N	258	A	P-O5'	-8.12	1.51	1.59
1	N	204	A	O3'-P	-8.11	1.51	1.61
1	N	164	G	N9-C4	-8.10	1.31	1.38
1	N	235	G	C8-N7	8.09	1.35	1.30
1	N	198	G	C8-N7	-8.07	1.26	1.30
1	N	171	G	C3'-O3'	8.06	1.53	1.42
1	N	141	G	N7-C5	8.04	1.44	1.39
1	N	351	A	N9-C4	-8.03	1.33	1.37
1	N	291	U	C2'-C1'	8.02	1.62	1.53
1	N	253	C	C5'-C4'	8.00	1.60	1.51
1	N	132	A	C5-C4	-8.00	1.33	1.38
1	N	315	A	N1-C2	8.00	1.41	1.34
1	N	248	A	P-O5'	-7.99	1.51	1.59
1	N	139	G	P-O5'	-7.95	1.51	1.59
1	N	333	A	N7-C5	-7.95	1.34	1.39
1	N	250	A	N9-C4	-7.95	1.33	1.37
1	N	358	U	C2'-C1'	-7.95	1.44	1.53
1	N	185	U	N1-C6	7.94	1.45	1.38
1	N	232	C	N3-C4	7.94	1.39	1.33
1	N	288	C	N1-C2	7.92	1.48	1.40
1	N	236	G	C2'-C1'	-7.91	1.44	1.53
1	N	256	U	C3'-C2'	7.91	1.61	1.52
1	N	207	A	P-O5'	-7.86	1.51	1.59
1	N	163	A	C6-N1	7.86	1.41	1.35
1	N	144	G	C2-N3	7.85	1.39	1.32
1	N	243	C	N1-C6	7.84	1.41	1.37
1	N	219	G	P-O5'	-7.83	1.51	1.59
1	N	277	G	O3'-P	-7.83	1.51	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	224	U	N1-C2	7.82	1.45	1.38
1	N	249	C	C4-C5	-7.82	1.36	1.43
1	N	246	A	C6-N6	7.82	1.40	1.33
1	N	242	C	C4-C5	-7.81	1.36	1.43
1	N	156	U	C1'-N1	7.79	1.60	1.48
1	N	148	U	C2-N3	7.78	1.43	1.37
1	N	153	G	C5-C4	7.77	1.43	1.38
1	N	129	A	C6-N1	-7.76	1.30	1.35
1	N	284	A	C5'-C4'	-7.73	1.42	1.51
1	N	135	C	C5'-C4'	7.71	1.60	1.51
1	N	342	C	N1-C2	7.71	1.47	1.40
1	N	158	G	P-O5'	-7.68	1.52	1.59
1	N	194	C	C4-C5	7.68	1.49	1.43
1	N	257	A	C2'-C1'	-7.68	1.44	1.53
1	N	269	G	N7-C5	7.67	1.43	1.39
1	N	279	G	C2-N3	7.66	1.38	1.32
1	N	336	A	N9-C4	7.66	1.42	1.37
1	N	162	A	N7-C5	-7.65	1.34	1.39
1	N	320	G	N3-C4	-7.63	1.30	1.35
1	N	302	G	C3'-C2'	-7.63	1.44	1.52
1	N	192	U	P-O5'	-7.61	1.52	1.59
1	N	165	U	C3'-C2'	7.61	1.61	1.52
1	N	245	A	N7-C5	-7.61	1.34	1.39
1	N	187	A	P-O5'	-7.61	1.52	1.59
1	N	155	G	C6-N1	-7.60	1.34	1.39
1	N	220	A	N9-C8	7.60	1.43	1.37
1	N	316	G	N3-C4	-7.58	1.30	1.35
1	N	299	G	N3-C4	-7.58	1.30	1.35
1	N	235	G	C5'-C4'	7.57	1.60	1.51
1	N	356	U	N1-C6	7.57	1.44	1.38
1	N	155	G	N9-C8	-7.53	1.32	1.37
1	N	242	C	C4-N4	-7.53	1.27	1.33
1	N	331	C	C3'-O3'	7.51	1.52	1.42
1	N	313	A	P-O5'	7.50	1.67	1.59
1	N	178	A	C6-N6	-7.50	1.27	1.33
1	N	177	G	C2-N3	7.49	1.38	1.32
1	N	279	G	C5-C4	-7.48	1.33	1.38
1	N	334	C	C2'-C1'	-7.48	1.45	1.53
1	N	328	G	N9-C8	-7.47	1.32	1.37
1	N	224	U	C4-O4	-7.47	1.17	1.23
1	N	318	G	C2'-C1'	-7.45	1.45	1.53
1	N	222	G	O3'-P	-7.45	1.52	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	345	G	C2-N3	7.45	1.38	1.32
1	N	165	U	P-O5'	-7.44	1.52	1.59
1	N	328	G	N7-C5	-7.44	1.34	1.39
1	N	301	G	N9-C4	7.44	1.43	1.38
1	N	289	A	N9-C8	7.43	1.43	1.37
1	N	325	A	C5-C4	7.43	1.44	1.38
1	N	144	G	N7-C5	-7.42	1.34	1.39
1	N	152	U	C4'-C3'	7.42	1.61	1.53
1	N	313	A	N3-C4	7.42	1.39	1.34
1	N	260	C	P-O5'	-7.41	1.52	1.59
1	N	302	G	C5'-C4'	7.40	1.60	1.51
1	N	305	A	C4'-O4'	7.39	1.55	1.45
1	N	291	U	C4-O4	-7.39	1.17	1.23
1	N	213	C	C5'-C4'	7.39	1.60	1.51
1	N	200	G	P-O5'	-7.38	1.52	1.59
1	N	354	U	C4-C5	-7.38	1.36	1.43
1	N	246	A	N9-C4	7.35	1.42	1.37
1	N	163	A	C5-C6	7.35	1.47	1.41
1	N	277	G	C2-N2	-7.34	1.27	1.34
1	N	132	A	C6-N1	7.33	1.40	1.35
1	N	269	G	C8-N7	-7.33	1.26	1.30
1	N	237	G	C2-N3	-7.32	1.26	1.32
1	N	253	C	C4-C5	-7.31	1.37	1.43
1	N	340	G	N9-C8	7.30	1.43	1.37
1	N	231	A	O3'-P	-7.28	1.52	1.61
1	N	142	G	C8-N7	-7.27	1.26	1.30
1	N	293	U	O3'-P	-7.27	1.52	1.61
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1	N	318	G	P-O5'	-7.24	1.52	1.59
1	N	138	A	N9-C8	7.23	1.43	1.37
1	N	159	U	C5'-C4'	7.23	1.60	1.51
1	N	181	G	N7-C5	7.20	1.43	1.39
1	N	230	G	C2'-C1'	7.18	1.61	1.53
1	N	275	U	C5'-C4'	7.17	1.59	1.51
1	N	238	C	C4-N4	-7.17	1.27	1.33
1	N	345	G	P-O5'	-7.16	1.52	1.59
1	N	282	A	O3'-P	-7.15	1.52	1.61
1	N	205	C	O3'-P	-7.15	1.52	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	288	C	N3-C4	-7.14	1.28	1.33
1	N	157	G	C5'-C4'	7.13	1.59	1.51
1	N	325	A	C2-N3	7.12	1.40	1.33
1	N	311	U	P-O5'	-7.12	1.52	1.59
1	N	178	A	N3-C4	7.12	1.39	1.34
1	N	154	G	P-O5'	-7.12	1.52	1.59
1	N	316	G	C3'-C2'	7.11	1.60	1.52
1	N	320	G	C5'-C4'	7.10	1.59	1.51
1	N	197	C	P-O5'	-7.09	1.52	1.59
1	N	329	G	C2'-C1'	-7.09	1.45	1.53
1	N	187	A	C5-C6	7.08	1.47	1.41
1	N	223	C	P-O5'	-7.08	1.52	1.59
1	N	243	C	C4-N4	-7.07	1.27	1.33
1	N	262	U	O3'-P	7.06	1.69	1.61
1	N	287	A	C8-N7	7.05	1.36	1.31
1	N	202	G	O4'-C1'	7.05	1.50	1.41
1	N	305	A	C2'-C1'	-7.04	1.45	1.53
1	N	133	G	C6-N1	7.04	1.44	1.39
1	N	324	C	C2'-C1'	-7.04	1.45	1.53
1	N	248	A	N9-C4	-7.04	1.33	1.37
1	N	261	C	C4-C5	7.04	1.48	1.43
1	N	294	G	O3'-P	-7.03	1.52	1.61
1	N	264	G	C1'-N9	7.02	1.59	1.48
1	N	189	U	C2-N3	-6.99	1.32	1.37
1	N	356	U	C4-C5	6.98	1.49	1.43
1	N	289	A	N7-C5	6.98	1.43	1.39
1	N	252	A	P-O5'	-6.97	1.52	1.59
1	N	208	G	N9-C8	6.96	1.42	1.37
1	N	197	C	C5-C6	-6.96	1.28	1.34
1	N	252	A	C5'-C4'	6.95	1.59	1.51
1	N	162	A	C8-N7	-6.94	1.26	1.31
1	N	180	A	N1-C2	6.94	1.40	1.34
1	N	276	A	C6-N1	-6.93	1.30	1.35
1	N	286	C	N1-C6	-6.93	1.32	1.37
1	N	298	U	O3'-P	-6.92	1.52	1.61
1	N	329	G	C6-N1	6.92	1.44	1.39
1	N	266	G	C8-N7	-6.91	1.26	1.30
1	N	319	U	C5'-C4'	6.91	1.59	1.51
1	N	293	U	P-O5'	-6.90	1.52	1.59
1	N	328	G	O3'-P	-6.90	1.52	1.61
1	N	146	G	N9-C8	-6.89	1.33	1.37
1	N	283	A	C5'-C4'	6.89	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	312	G	N7-C5	-6.89	1.35	1.39
1	N	336	A	C6-N1	6.87	1.40	1.35
1	N	154	G	C4'-C3'	6.86	1.60	1.53
1	N	154	G	C2'-C1'	-6.86	1.45	1.53
1	N	308	A	O3'-P	-6.85	1.52	1.61
1	N	188	G	P-O5'	-6.84	1.52	1.59
1	N	224	U	C2'-C1'	-6.84	1.45	1.53
1	N	315	A	N7-C5	-6.84	1.35	1.39
1	N	223	C	C3'-O3'	6.83	1.51	1.42
1	N	185	U	C4'-C3'	6.82	1.60	1.53
1	N	166	C	C4-N4	-6.79	1.27	1.33
1	N	254	C	C2-N3	6.77	1.41	1.35
1	N	144	G	C6-N1	6.77	1.44	1.39
1	N	353	A	C8-N7	6.76	1.36	1.31
1	N	307	G	C8-N7	-6.76	1.26	1.30
1	N	183	C	O3'-P	-6.75	1.53	1.61
1	N	312	G	C2'-C1'	6.75	1.60	1.53
1	N	272	C	C3'-O3'	6.74	1.51	1.42
1	N	325	A	C5'-C4'	6.72	1.59	1.51
1	N	217	G	N9-C4	6.70	1.43	1.38
1	N	204	A	C5'-C4'	6.69	1.59	1.51
1	N	238	C	C3'-C2'	6.69	1.60	1.52
1	N	288	C	C4'-C3'	6.68	1.60	1.53
1	N	235	G	C3'-C2'	-6.67	1.45	1.52
1	N	142	G	P-O5'	-6.67	1.53	1.59
1	N	229	G	C5-C4	6.67	1.43	1.38
1	N	171	G	C5'-C4'	6.66	1.59	1.51
1	N	141	G	C5-C4	-6.65	1.33	1.38
1	N	195	G	C2-N3	6.65	1.38	1.32
1	N	353	A	C4'-O4'	-6.63	1.36	1.45
1	N	261	C	C4-N4	-6.63	1.27	1.33
1	N	247	G	C5-C6	6.62	1.49	1.42
1	N	201	A	N7-C5	-6.62	1.35	1.39
1	N	167	C	O4'-C1'	6.62	1.50	1.41
1	N	271	U	N1-C6	6.60	1.43	1.38
1	N	332	C	N1-C6	-6.60	1.33	1.37
1	N	170	A	P-O5'	-6.60	1.53	1.59
1	N	204	A	N9-C8	6.60	1.43	1.37
1	N	200	G	N7-C5	6.59	1.43	1.39
1	N	214	C	C4-C5	-6.58	1.37	1.43
1	N	133	G	N3-C4	-6.57	1.30	1.35
1	N	155	G	N9-C4	6.57	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	339	A	P-O5'	-6.56	1.53	1.59
1	N	213	C	C4-C5	6.56	1.48	1.43
1	N	210	C	C2'-C1'	-6.56	1.46	1.53
1	N	315	A	C6-N6	6.56	1.39	1.33
1	N	277	G	C2-N3	6.55	1.38	1.32
1	N	225	A	C8-N7	-6.53	1.26	1.31
1	N	156	U	N3-C4	6.53	1.44	1.38
1	N	304	U	C5'-C4'	6.53	1.59	1.51
1	N	269	G	C5-C4	-6.53	1.33	1.38
1	N	203	C	N3-C4	6.53	1.38	1.33
1	N	318	G	C5-C4	6.52	1.43	1.38
1	N	187	A	C6-N1	-6.51	1.30	1.35
1	N	201	A	P-O5'	-6.51	1.53	1.59
1	N	204	A	N9-C4	6.51	1.41	1.37
1	N	133	G	P-O5'	-6.51	1.53	1.59
1	N	282	A	N1-C2	6.51	1.40	1.34
1	N	290	U	O4'-C1'	6.51	1.50	1.41
1	N	130	C	C5'-C4'	6.50	1.59	1.51
1	N	352	A	N3-C4	6.49	1.38	1.34
1	N	270	G	N3-C4	-6.48	1.30	1.35
1	N	197	C	C4'-C3'	-6.48	1.46	1.53
1	N	236	G	N1-C2	-6.48	1.32	1.37
1	N	351	A	C3'-C2'	6.48	1.60	1.52
1	N	163	A	O3'-P	-6.48	1.53	1.61
1	N	210	C	C2-N3	6.47	1.41	1.35
1	N	165	U	C2-N3	-6.47	1.33	1.37
1	N	229	G	N9-C8	-6.47	1.33	1.37
1	N	219	G	O3'-P	-6.47	1.53	1.61
1	N	206	U	C4'-C3'	6.46	1.60	1.53
1	N	219	G	O4'-C1'	6.45	1.50	1.41
1	N	346	U	C5'-C4'	6.45	1.59	1.51
1	N	258	A	N3-C4	6.44	1.38	1.34
1	N	317	G	C2-N2	-6.44	1.28	1.34
1	N	161	U	O3'-P	-6.42	1.53	1.61
1	N	169	G	C5'-C4'	6.42	1.59	1.51
1	N	135	C	C1'-N1	6.41	1.58	1.48
1	N	356	U	C5'-C4'	6.41	1.59	1.51
1	N	205	C	N1-C6	-6.39	1.33	1.37
1	N	273	G	C5-C4	6.39	1.42	1.38
1	N	142	G	N1-C2	6.38	1.42	1.37
1	N	302	G	N9-C4	6.38	1.43	1.38
1	N	135	C	C3'-C2'	-6.37	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	162	A	N3-C4	-6.36	1.31	1.34
1	N	272	C	C2'-C1'	-6.35	1.46	1.53
1	N	277	G	N7-C5	-6.34	1.35	1.39
1	N	250	A	N9-C8	-6.33	1.32	1.37
1	N	322	U	N3-C4	-6.31	1.32	1.38
1	N	220	A	O4'-C1'	6.30	1.49	1.41
1	N	151	C	C4-C5	-6.29	1.38	1.43
1	N	169	G	C5-C4	-6.27	1.33	1.38
1	N	236	G	N9-C4	6.27	1.43	1.38
1	N	327	A	C3'-C2'	-6.27	1.45	1.52
1	N	158	G	O3'-P	-6.26	1.53	1.61
1	N	208	G	N7-C5	6.26	1.43	1.39
1	N	307	G	N9-C4	6.25	1.43	1.38
1	N	344	A	N3-C4	-6.25	1.31	1.34
1	N	174	C	O3'-P	-6.25	1.53	1.61
1	N	305	A	C6-N1	-6.25	1.31	1.35
1	N	138	A	C5-C4	6.24	1.43	1.38
1	N	195	G	P-O5'	-6.24	1.53	1.59
1	N	151	C	C2-N3	6.23	1.40	1.35
1	N	190	A	C5-C4	6.23	1.43	1.38
1	N	266	G	N9-C4	6.23	1.43	1.38
1	N	252	A	N9-C4	-6.23	1.34	1.37
1	N	266	G	O3'-P	-6.22	1.53	1.61
1	N	173	A	N9-C4	6.22	1.41	1.37
1	N	184	G	N7-C5	6.21	1.43	1.39
1	N	306	C	N3-C4	6.21	1.38	1.33
1	N	240	U	P-O5'	-6.21	1.53	1.59
1	N	146	G	C5-C4	6.20	1.42	1.38
1	N	342	C	O4'-C1'	6.19	1.49	1.41
1	N	149	C	C2'-C1'	-6.19	1.46	1.53
1	N	273	G	C2-N3	-6.19	1.27	1.32
1	N	264	G	N1-C2	6.19	1.42	1.37
1	N	175	A	C5'-C4'	6.18	1.58	1.51
1	N	135	C	C4'-O4'	6.18	1.53	1.45
1	N	185	U	C2-N3	6.18	1.42	1.37
1	N	300	G	O5'-C5'	6.17	1.54	1.44
1	N	186	C	C3'-C2'	-6.17	1.46	1.52
1	N	170	A	C5-C4	-6.16	1.34	1.38
1	N	301	G	C5-C4	-6.16	1.34	1.38
1	N	306	C	C3'-O3'	6.16	1.50	1.42
1	N	147	C	N1-C6	-6.15	1.33	1.37
1	N	225	A	P-O5'	-6.15	1.53	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	192	U	C5'-C4'	6.15	1.58	1.51
1	N	357	C	N1-C6	6.15	1.40	1.37
1	N	353	A	N9-C4	6.14	1.41	1.37
1	N	142	G	C4'-C3'	6.14	1.59	1.53
1	N	342	C	C2-N3	6.13	1.40	1.35
1	N	344	A	P-O5'	6.13	1.65	1.59
1	N	235	G	N1-C2	6.13	1.42	1.37
1	N	153	G	C5'-C4'	6.12	1.58	1.51
1	N	146	G	C3'-C2'	6.12	1.59	1.52
1	N	244	C	C5'-C4'	6.12	1.58	1.51
1	N	135	C	N1-C2	6.12	1.46	1.40
1	N	153	G	C2-N2	-6.12	1.28	1.34
1	N	298	U	N3-C4	6.11	1.44	1.38
1	N	185	U	C5'-C4'	6.11	1.58	1.51
1	N	293	U	C5-C6	6.11	1.39	1.34
1	N	152	U	C4'-O4'	6.11	1.53	1.45
1	N	197	C	C4-N4	-6.09	1.28	1.33
1	N	240	U	N3-C4	6.09	1.44	1.38
1	N	280	U	C2-N3	-6.09	1.33	1.37
1	N	169	G	C3'-O3'	6.09	1.50	1.42
1	N	250	A	C4'-O4'	-6.08	1.37	1.45
1	N	359	G	O3'-P	-6.08	1.53	1.61
1	N	143	C	C2'-C1'	-6.07	1.46	1.53
1	N	302	G	N9-C8	6.07	1.42	1.37
1	N	192	U	C4-O4	-6.06	1.18	1.23
1	N	227	G	N7-C5	6.06	1.42	1.39
1	N	279	G	C6-N1	6.06	1.43	1.39
1	N	276	A	C5-C6	6.06	1.46	1.41
1	N	288	C	C1'-N1	6.06	1.57	1.48
1	N	224	U	O3'-P	-6.05	1.53	1.61
1	N	180	A	C5'-C4'	6.05	1.58	1.51
1	N	230	G	C2-N3	-6.03	1.27	1.32
1	N	137	U	O3'-P	-6.03	1.53	1.61
1	N	342	C	C3'-C2'	6.03	1.59	1.52
1	N	234	A	N3-C4	6.03	1.38	1.34
1	N	136	G	C2-N3	6.02	1.37	1.32
1	N	215	U	C5'-C4'	6.01	1.58	1.51
1	N	160	C	C3'-O3'	6.01	1.50	1.42
1	N	316	G	C4'-O4'	-6.00	1.37	1.45
1	N	202	G	P-O5'	-6.00	1.53	1.59
1	N	200	G	N9-C8	-5.99	1.33	1.37
1	N	304	U	O3'-P	-5.98	1.53	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	143	C	C5'-C4'	5.98	1.58	1.51
1	N	357	C	C2'-C1'	-5.98	1.46	1.53
1	N	323	G	P-O5'	-5.98	1.53	1.59
1	N	333	A	C4'-O4'	5.97	1.53	1.45
1	N	339	A	C3'-C2'	-5.97	1.46	1.52
1	N	299	G	C8-N7	-5.97	1.27	1.30
1	N	158	G	C2-N3	5.96	1.37	1.32
1	N	200	G	C2-N2	5.96	1.40	1.34
1	N	170	A	C6-N6	5.95	1.38	1.33
1	N	155	G	N3-C4	-5.95	1.31	1.35
1	N	344	A	C2'-C1'	-5.95	1.46	1.53
1	N	129	A	N3-C4	5.94	1.38	1.34
1	N	145	A	N9-C8	5.93	1.42	1.37
1	N	209	C	C4'-O4'	-5.93	1.37	1.45
1	N	318	G	C2-N3	5.91	1.37	1.32
1	N	196	A	N9-C8	-5.91	1.33	1.37
1	N	275	U	N1-C6	5.91	1.43	1.38
1	N	331	C	O3'-P	-5.90	1.54	1.61
1	N	274	C	C2'-C1'	-5.90	1.46	1.53
1	N	327	A	N7-C5	-5.90	1.35	1.39
1	N	338	C	N1-C6	5.89	1.40	1.37
1	N	356	U	C2'-C1'	-5.89	1.46	1.53
1	N	254	C	C4-N4	5.88	1.39	1.33
1	N	187	A	N7-C5	-5.87	1.35	1.39
1	N	235	G	C6-N1	5.86	1.43	1.39
1	N	233	G	N9-C8	5.86	1.42	1.37
1	N	318	G	N9-C8	5.86	1.42	1.37
1	N	338	C	C3'-O3'	5.86	1.50	1.42
1	N	132	A	C3'-C2'	5.85	1.59	1.52
1	N	151	C	C3'-O3'	5.84	1.50	1.42
1	N	262	U	O4'-C1'	5.84	1.49	1.41
1	N	176	G	C2-N3	5.84	1.37	1.32
1	N	295	U	P-O5'	-5.83	1.53	1.59
1	N	136	G	O3'-P	-5.83	1.54	1.61
1	N	336	A	C5-C4	5.82	1.42	1.38
1	N	329	G	C5-C6	-5.81	1.36	1.42
1	N	295	U	C5'-C4'	5.80	1.58	1.51
1	N	254	C	C5'-C4'	5.80	1.58	1.51
1	N	323	G	N9-C4	5.79	1.42	1.38
1	N	207	A	N9-C8	-5.79	1.33	1.37
1	N	258	A	C3'-C2'	5.79	1.59	1.52
1	N	141	G	N3-C4	-5.79	1.31	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	247	G	C8-N7	5.78	1.34	1.30
1	N	336	A	C2-N3	5.78	1.38	1.33
1	N	279	G	N3-C4	5.77	1.39	1.35
1	N	358	U	C2-N3	5.76	1.41	1.37
1	N	165	U	C4'-C3'	5.76	1.59	1.53
1	N	302	G	C6-O6	-5.76	1.19	1.24
1	N	264	G	C2-N2	-5.75	1.28	1.34
1	N	305	A	C5-C4	-5.75	1.34	1.38
1	N	138	A	C3'-O3'	5.74	1.50	1.42
1	N	283	A	N1-C2	5.74	1.39	1.34
1	N	206	U	C2'-C1'	-5.72	1.47	1.53
1	N	129	A	C4'-C3'	5.72	1.59	1.53
1	N	278	G	N9-C4	5.72	1.42	1.38
1	N	241	G	C5-C4	5.72	1.42	1.38
1	N	305	A	N9-C8	-5.72	1.33	1.37
1	N	134	C	N1-C6	-5.72	1.33	1.37
1	N	323	G	N7-C5	-5.71	1.35	1.39
1	N	243	C	P-O5'	-5.71	1.54	1.59
1	N	144	G	C4'-C3'	5.71	1.59	1.53
1	N	196	A	N7-C5	-5.70	1.35	1.39
1	N	317	G	C2'-C1'	-5.69	1.47	1.53
1	N	310	C	C2'-C1'	-5.69	1.47	1.53
1	N	299	G	N9-C8	5.69	1.41	1.37
1	N	331	C	N1-C6	5.68	1.40	1.37
1	N	196	A	O3'-P	-5.67	1.54	1.61
1	N	353	A	C5-C6	5.67	1.46	1.41
1	N	251	C	C5-C6	-5.67	1.29	1.34
1	N	223	C	O3'-P	-5.67	1.54	1.61
1	N	326	G	C6-N1	-5.67	1.35	1.39
1	N	196	A	C2-N3	5.66	1.38	1.33
1	N	229	G	N7-C5	5.66	1.42	1.39
1	N	166	C	O3'-P	-5.66	1.54	1.61
1	N	274	C	C4'-C3'	5.66	1.59	1.53
1	N	348	U	N1-C6	-5.66	1.32	1.38
1	N	184	G	C5'-C4'	5.66	1.58	1.51
1	N	166	C	C2-N3	5.65	1.40	1.35
1	N	179	C	C2'-C1'	-5.64	1.47	1.53
1	N	157	G	C2'-C1'	-5.64	1.47	1.53
1	N	304	U	O5'-C5'	5.64	1.53	1.44
1	N	355	C	C4-N4	5.64	1.39	1.33
1	N	250	A	N3-C4	5.63	1.38	1.34
1	N	357	C	C4'-C3'	-5.63	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	230	G	C5-C6	-5.63	1.36	1.42
1	N	175	A	P-O5'	-5.62	1.54	1.59
1	N	294	G	C2-N3	-5.62	1.28	1.32
1	N	177	G	N1-C2	5.61	1.42	1.37
1	N	190	A	O3'-P	-5.61	1.54	1.61
1	N	326	G	P-O5'	-5.61	1.54	1.59
1	N	310	C	C2-N3	-5.60	1.31	1.35
1	N	176	G	N7-C5	-5.60	1.35	1.39
1	N	142	G	C6-N1	5.59	1.43	1.39
1	N	318	G	C1'-N9	5.59	1.57	1.48
1	N	326	G	C2'-C1'	-5.59	1.47	1.53
1	N	355	C	C4'-C3'	5.59	1.59	1.53
1	N	219	G	C5'-C4'	5.59	1.58	1.51
1	N	137	U	N3-C4	-5.58	1.33	1.38
1	N	354	U	C2-O2	5.58	1.27	1.22
1	N	254	C	O3'-P	-5.58	1.54	1.61
1	N	128	G	C8-N7	5.57	1.34	1.30
1	N	311	U	C3'-C2'	5.57	1.59	1.52
1	N	145	A	N1-C2	-5.56	1.29	1.34
1	N	302	G	N7-C5	-5.56	1.35	1.39
1	N	166	C	P-O5'	-5.56	1.54	1.59
1	N	359	G	N9-C8	-5.55	1.33	1.37
1	N	154	G	C3'-O3'	5.55	1.50	1.42
1	N	285	U	C5-C6	-5.55	1.29	1.34
1	N	315	A	C4'-O4'	5.55	1.52	1.45
1	N	282	A	C5'-C4'	5.54	1.58	1.51
1	N	139	G	C4'-O4'	5.53	1.52	1.45
1	N	188	G	C4'-O4'	5.53	1.52	1.45
1	N	347	A	P-O5'	5.53	1.65	1.59
1	N	232	C	C1'-N1	5.53	1.57	1.48
1	N	197	C	C2'-C1'	-5.53	1.47	1.53
1	N	169	G	C5-C6	5.52	1.47	1.42
1	N	318	G	N3-C4	-5.52	1.31	1.35
1	N	357	C	O4'-C1'	-5.51	1.34	1.41
1	N	146	G	C3'-O3'	5.51	1.49	1.42
1	N	241	G	N1-C2	-5.50	1.33	1.37
1	N	315	A	N9-C8	-5.50	1.33	1.37
1	N	265	C	C5'-C4'	5.50	1.57	1.51
1	N	285	U	C5'-C4'	5.50	1.57	1.51
1	N	273	G	N9-C4	5.50	1.42	1.38
1	N	153	G	C4'-O4'	-5.50	1.38	1.45
1	N	200	G	N3-C4	5.50	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	236	G	C2-N3	5.50	1.37	1.32
1	N	144	G	N1-C2	5.49	1.42	1.37
1	N	356	U	C3'-O3'	5.49	1.49	1.42
1	N	288	C	P-O5'	-5.48	1.54	1.59
1	N	162	A	O3'-P	-5.47	1.54	1.61
1	N	274	C	C3'-O3'	5.47	1.49	1.42
1	N	314	U	C3'-O3'	5.47	1.49	1.42
1	N	180	A	O3'-P	-5.47	1.54	1.61
1	N	155	G	C2-N2	-5.46	1.29	1.34
1	N	358	U	C4'-C3'	5.46	1.59	1.53
1	N	143	C	N1-C2	5.46	1.45	1.40
1	N	181	G	C3'-O3'	5.45	1.49	1.42
1	N	317	G	N9-C4	5.45	1.42	1.38
1	N	160	C	N1-C6	5.45	1.40	1.37
1	N	348	U	N3-C4	-5.45	1.33	1.38
1	N	154	G	N7-C5	5.45	1.42	1.39
1	N	228	U	C4'-C3'	-5.45	1.47	1.52
1	N	228	U	C2-N3	-5.44	1.33	1.37
1	N	275	U	C4'-O4'	5.44	1.52	1.45
1	N	330	C	C2-O2	5.44	1.29	1.24
1	N	141	G	C5-C6	-5.43	1.36	1.42
1	N	142	G	C5-C4	5.43	1.42	1.38
1	N	223	C	C1'-N1	5.43	1.56	1.48
1	N	311	U	C4-O4	-5.42	1.19	1.23
1	N	150	C	C5-C6	5.42	1.38	1.34
1	N	236	G	N7-C5	-5.42	1.36	1.39
1	N	147	C	C4-C5	-5.41	1.38	1.43
1	N	184	G	C4'-C3'	-5.41	1.47	1.52
1	N	271	U	C3'-O3'	5.41	1.49	1.42
1	N	306	C	C3'-C2'	5.41	1.58	1.52
1	N	265	C	C5-C6	-5.41	1.30	1.34
1	N	150	C	C4'-C3'	-5.40	1.47	1.52
1	N	246	A	C3'-O3'	5.40	1.49	1.42
1	N	252	A	C8-N7	5.40	1.35	1.31
1	N	321	C	C3'-O3'	5.40	1.49	1.42
1	N	299	G	C2-N2	-5.39	1.29	1.34
1	N	323	G	N3-C4	5.38	1.39	1.35
1	N	192	U	C4'-O4'	5.38	1.52	1.45
1	N	285	U	C2-N3	-5.38	1.33	1.37
1	N	321	C	N3-C4	5.38	1.37	1.33
1	N	280	U	C2'-C1'	5.38	1.59	1.53
1	N	323	G	C8-N7	5.37	1.34	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	254	C	P-O5'	-5.37	1.54	1.59
1	N	330	C	C5'-C4'	5.37	1.57	1.51
1	N	296	G	C4'-O4'	-5.36	1.38	1.45
1	N	257	A	N9-C4	-5.35	1.34	1.37
1	N	331	C	C4'-O4'	5.35	1.52	1.45
1	N	138	A	C4'-O4'	-5.35	1.38	1.45
1	N	131	U	P-O5'	-5.35	1.54	1.59
1	N	266	G	C2'-C1'	-5.35	1.47	1.53
1	N	156	U	C4'-C3'	5.34	1.59	1.53
1	N	330	C	C2'-C1'	5.34	1.59	1.53
1	N	326	G	C2-N2	-5.33	1.29	1.34
1	N	199	U	C3'-C2'	-5.33	1.46	1.52
1	N	269	G	C2-N2	-5.33	1.29	1.34
1	N	318	G	C2-N2	-5.33	1.29	1.34
1	N	220	A	O3'-P	-5.33	1.54	1.61
1	N	193	U	N3-C4	-5.33	1.33	1.38
1	N	217	G	O4'-C1'	5.32	1.48	1.41
1	N	319	U	C3'-O3'	5.32	1.49	1.42
1	N	276	A	C6-N6	-5.32	1.29	1.33
1	N	314	U	O3'-P	-5.31	1.54	1.61
1	N	208	G	C2-N2	-5.31	1.29	1.34
1	N	289	A	C2'-C1'	-5.31	1.47	1.53
1	N	260	C	C4-N4	-5.30	1.29	1.33
1	N	166	C	C4'-C3'	5.29	1.58	1.53
1	N	305	A	C6-N6	5.29	1.38	1.33
1	N	156	U	C5-C6	-5.29	1.29	1.34
1	N	283	A	C6-N6	-5.29	1.29	1.33
1	N	300	G	C3'-C2'	5.29	1.58	1.52
1	N	320	G	C1'-N9	-5.29	1.39	1.46
1	N	185	U	C1'-N1	5.29	1.56	1.48
1	N	305	A	C3'-O3'	5.29	1.49	1.42
1	N	358	U	C4'-O4'	-5.28	1.38	1.45
1	N	161	U	N3-C4	5.28	1.43	1.38
1	N	250	A	C5-C6	-5.27	1.36	1.41
1	N	267	G	N3-C4	-5.26	1.31	1.35
1	N	132	A	N7-C5	5.25	1.42	1.39
1	N	292	A	N9-C4	5.25	1.41	1.37
1	N	232	C	P-O5'	-5.25	1.54	1.59
1	N	301	G	C8-N7	5.25	1.34	1.30
1	N	312	G	C3'-O3'	5.25	1.49	1.42
1	N	359	G	C4'-C3'	5.24	1.58	1.53
1	N	176	G	O3'-P	-5.23	1.54	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	207	A	C6-N6	5.23	1.38	1.33
1	N	260	C	O3'-P	-5.23	1.54	1.61
1	N	337	G	C6-O6	5.23	1.28	1.24
1	N	241	G	N9-C4	-5.22	1.33	1.38
1	N	222	G	C3'-C2'	-5.22	1.47	1.52
1	N	303	G	P-O5'	5.22	1.65	1.59
1	N	272	C	N1-C2	5.21	1.45	1.40
1	N	178	A	O3'-P	-5.21	1.54	1.61
1	N	237	G	N7-C5	-5.20	1.36	1.39
1	N	307	G	C6-O6	-5.20	1.19	1.24
1	N	218	A	C5-C6	5.20	1.45	1.41
1	N	257	A	C6-N6	-5.20	1.29	1.33
1	N	199	U	N1-C2	5.19	1.43	1.38
1	N	280	U	C4'-C3'	5.19	1.58	1.53
1	N	189	U	P-O5'	5.19	1.65	1.59
1	N	247	G	N1-C2	-5.19	1.33	1.37
1	N	341	G	C6-O6	-5.19	1.19	1.24
1	N	359	G	C3'-C2'	5.19	1.58	1.52
1	N	271	U	P-O5'	-5.18	1.54	1.59
1	N	201	A	N3-C4	5.18	1.38	1.34
1	N	347	A	C5-C4	-5.18	1.35	1.38
1	N	233	G	N7-C5	5.17	1.42	1.39
1	N	291	U	C4'-O4'	-5.17	1.38	1.45
1	N	183	C	C5'-C4'	5.17	1.57	1.51
1	N	195	G	O3'-P	-5.17	1.54	1.61
1	N	130	C	P-O5'	-5.16	1.54	1.59
1	N	202	G	N9-C4	5.16	1.42	1.38
1	N	190	A	C4'-O4'	5.16	1.52	1.45
1	N	301	G	C2'-C1'	5.16	1.59	1.53
1	N	225	A	N9-C8	5.16	1.41	1.37
1	N	237	G	C8-N7	-5.15	1.27	1.30
1	N	214	C	C3'-O3'	5.15	1.49	1.42
1	N	138	A	O3'-P	-5.15	1.54	1.61
1	N	295	U	C3'-O3'	5.14	1.49	1.42
1	N	135	C	C4-C5	-5.14	1.38	1.43
1	N	129	A	C6-N6	-5.14	1.29	1.33
1	N	137	U	C2-O2	5.14	1.26	1.22
1	N	138	A	C8-N7	5.13	1.35	1.31
1	N	343	U	O3'-P	-5.13	1.54	1.61
1	N	177	G	C3'-O3'	5.13	1.49	1.42
1	N	226	C	N1-C6	-5.12	1.34	1.37
1	N	233	G	C2-N3	5.12	1.36	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	181	G	C6-N1	-5.12	1.35	1.39
1	N	153	G	C6-N1	-5.11	1.35	1.39
1	N	221	U	C5'-C4'	5.11	1.57	1.51
1	N	215	U	C2'-C1'	-5.10	1.47	1.53
1	N	141	G	C3'-O3'	5.10	1.49	1.42
1	N	168	U	C1'-N1	5.10	1.56	1.48
1	N	344	A	C4'-O4'	5.09	1.52	1.45
1	N	185	U	C2'-C1'	-5.09	1.47	1.53
1	N	331	C	C5-C6	5.09	1.38	1.34
1	N	148	U	C4'-O4'	5.09	1.52	1.45
1	N	258	A	N1-C2	5.09	1.39	1.34
1	N	207	A	C5'-C4'	5.09	1.57	1.51
1	N	294	G	N1-C2	5.08	1.41	1.37
1	N	161	U	C2'-C1'	-5.07	1.47	1.53
1	N	320	G	O4'-C1'	-5.07	1.35	1.41
1	N	354	U	N1-C2	5.07	1.43	1.38
1	N	243	C	C4'-O4'	5.06	1.52	1.45
1	N	283	A	C2-N3	5.06	1.38	1.33
1	N	261	C	P-O5'	-5.06	1.54	1.59
1	N	222	G	C2-N3	5.06	1.36	1.32
1	N	148	U	P-O5'	-5.05	1.54	1.59
1	N	314	U	C3'-C2'	5.04	1.58	1.52
1	N	204	A	C4'-O4'	5.04	1.52	1.45
1	N	246	A	C2-N3	5.04	1.38	1.33
1	N	344	A	N7-C5	-5.04	1.36	1.39
1	N	163	A	C2'-C1'	-5.04	1.47	1.53
1	N	308	A	N7-C5	-5.04	1.36	1.39
1	N	158	G	N3-C4	-5.03	1.31	1.35
1	N	150	C	C4-C5	5.02	1.47	1.43
1	N	311	U	C1'-N1	5.02	1.56	1.48
1	N	343	U	C4'-O4'	5.02	1.52	1.45
1	N	129	A	C3'-C2'	5.01	1.58	1.52
1	N	282	A	C3'-C2'	-5.01	1.47	1.52
1	N	248	A	C8-N7	-5.01	1.28	1.31
1	N	224	U	C5-C6	5.01	1.38	1.34
1	N	301	G	C5'-C4'	5.01	1.57	1.51
1	N	344	A	O4'-C1'	5.01	1.48	1.41
1	N	239	A	C5-C4	-5.00	1.35	1.38
1	N	136	G	C3'-C2'	5.00	1.58	1.52
1	N	328	G	C2-N3	5.00	1.36	1.32
1	N	162	A	C3'-O3'	5.00	1.49	1.42
1	N	208	G	C6-N1	5.00	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	315	A	C5'-C4'	5.00	1.57	1.51

All (1129) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	307	G	P-O3'-C3'	30.70	156.54	119.70
1	N	135	C	P-O3'-C3'	30.11	155.83	119.70
1	N	195	G	P-O3'-C3'	26.18	151.12	119.70
1	N	191	G	P-O3'-C3'	24.78	149.43	119.70
1	N	142	G	P-O3'-C3'	23.54	147.95	119.70
1	N	256	U	P-O3'-C3'	19.46	143.06	119.70
1	N	257	A	N1-C6-N6	18.42	129.65	118.60
1	N	135	C	C6-N1-C2	-18.05	113.08	120.30
1	N	136	G	P-O3'-C3'	17.98	141.27	119.70
1	N	181	G	P-O3'-C3'	17.60	140.82	119.70
1	N	328	G	P-O3'-C3'	17.07	140.19	119.70
1	N	144	G	C8-N9-C4	-16.77	99.69	106.40
1	N	179	C	P-O3'-C3'	15.51	138.31	119.70
1	N	188	G	C5-C6-O6	-15.43	119.34	128.60
1	N	222	G	P-O3'-C3'	14.96	137.65	119.70
1	N	310	C	C6-N1-C2	-14.83	114.37	120.30
1	N	163	A	P-O3'-C3'	14.79	137.44	119.70
1	N	284	A	C5'-C4'-C3'	14.68	139.50	116.00
1	N	188	G	N1-C6-O6	14.51	128.61	119.90
1	N	340	G	C5-C6-O6	-14.48	119.91	128.60
1	N	323	G	C5-C6-O6	-14.34	120.00	128.60
1	N	245	A	P-O3'-C3'	-14.27	102.58	119.70
1	N	233	G	C5-C6-O6	-13.93	120.24	128.60
1	N	244	C	P-O3'-C3'	13.88	136.35	119.70
1	N	325	A	N1-C6-N6	13.87	126.92	118.60
1	N	290	U	P-O3'-C3'	13.74	136.19	119.70
1	N	155	G	C5-C6-O6	-13.59	120.45	128.60
1	N	233	G	P-O3'-C3'	13.40	135.78	119.70
1	N	331	C	P-O5'-C5'	13.35	142.26	120.90
1	N	308	A	P-O3'-C3'	13.35	135.72	119.70
1	N	161	U	P-O3'-C3'	13.33	135.70	119.70
1	N	283	A	C8-N9-C1'	-13.30	103.76	127.70
1	N	155	G	N1-C6-O6	13.29	127.88	119.90
1	N	210	C	C2-N3-C4	-13.28	113.26	119.90
1	N	283	A	N9-C4-C5	-13.12	100.55	105.80
1	N	158	G	N1-C6-O6	13.01	127.71	119.90
1	N	272	C	C6-N1-C2	-12.98	115.11	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	274	C	C6-N1-C2	-12.84	115.16	120.30
1	N	283	A	O4'-C1'-N9	12.81	118.45	108.20
1	N	305	A	O4'-C1'-N9	12.79	118.43	108.20
1	N	158	G	C5-C6-O6	-12.75	120.95	128.60
1	N	207	A	N1-C6-N6	-12.70	110.98	118.60
1	N	239	A	N9-C4-C5	12.67	110.87	105.80
1	N	196	A	O4'-C1'-N9	12.57	118.26	108.20
1	N	250	A	P-O3'-C3'	12.56	134.78	119.70
1	N	297	A	P-O3'-C3'	12.55	134.76	119.70
1	N	334	C	O4'-C1'-N1	12.54	118.23	108.20
1	N	142	G	C5-C6-O6	-12.53	121.08	128.60
1	N	282	A	P-O3'-C3'	12.53	134.74	119.70
1	N	144	G	N1-C6-O6	12.46	127.38	119.90
1	N	202	G	C8-N9-C4	-12.45	101.42	106.40
1	N	181	G	N7-C8-N9	12.29	119.24	113.10
1	N	153	G	C5-C6-O6	-12.27	121.24	128.60
1	N	260	C	O4'-C1'-N1	12.27	118.02	108.20
1	N	320	G	P-O5'-C5'	12.26	140.52	120.90
1	N	265	C	O4'-C1'-N1	12.15	117.92	108.20
1	N	135	C	C2-N1-C1'	-12.10	105.49	118.80
1	N	305	A	C2-N3-C4	-12.06	104.57	110.60
1	N	162	A	C8-N9-C4	-12.05	100.98	105.80
1	N	351	A	C5-N7-C8	-12.00	97.90	103.90
1	N	180	A	C8-N9-C4	-11.97	101.01	105.80
1	N	306	C	N3-C4-C5	-11.96	117.12	121.90
1	N	135	C	C5'-C4'-C3'	11.88	135.00	116.00
1	N	266	G	O4'-C1'-N9	11.86	117.69	108.20
1	N	283	A	N1-C2-N3	11.81	135.21	129.30
1	N	181	G	C5'-C4'-C3'	11.75	134.80	116.00
1	N	325	A	C5-C6-N6	-11.73	114.31	123.70
1	N	259	C	N3-C4-C5	-11.71	117.22	121.90
1	N	320	G	C5'-C4'-C3'	11.69	134.70	116.00
1	N	157	G	P-O3'-C3'	11.66	133.69	119.70
1	N	219	G	N1-C6-O6	11.61	126.86	119.90
1	N	152	U	C4'-C3'-C2'	-11.51	91.09	102.60
1	N	331	C	N3-C4-C5	11.47	126.49	121.90
1	N	257	A	C5-C6-N6	-11.45	114.54	123.70
1	N	345	G	C5-C6-O6	-11.26	121.84	128.60
1	N	222	G	C5-C6-O6	-11.15	121.91	128.60
1	N	270	G	C5-C6-O6	-11.14	121.91	128.60
1	N	148	U	O4'-C1'-N1	11.10	117.08	108.20
1	N	142	G	N1-C6-O6	11.09	126.56	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	169	G	C4-C5-N7	11.06	115.22	110.80
1	N	241	G	C5-C6-O6	10.98	135.19	128.60
1	N	231	A	C2-N3-C4	-10.95	105.13	110.60
1	N	237	G	C4-C5-N7	10.95	115.18	110.80
1	N	157	G	C4'-C3'-C2'	-10.92	91.68	102.60
1	N	306	C	C5-C4-N4	10.91	127.83	120.20
1	N	308	A	N1-C6-N6	10.81	125.09	118.60
1	N	168	U	O4'-C1'-N1	10.72	116.78	108.20
1	N	151	C	C6-N1-C2	-10.69	116.02	120.30
1	N	204	A	C8-N9-C4	-10.68	101.53	105.80
1	N	329	G	C8-N9-C4	-10.67	102.13	106.40
1	N	319	U	C5-C6-N1	-10.65	117.38	122.70
1	N	337	G	N1-C6-O6	10.64	126.29	119.90
1	N	336	A	N1-C6-N6	10.63	124.98	118.60
1	N	180	A	P-O3'-C3'	10.62	132.45	119.70
1	N	137	U	O4'-C1'-N1	10.60	116.68	108.20
1	N	333	A	C8-N9-C4	-10.58	101.57	105.80
1	N	245	A	P-O5'-C5'	10.57	137.81	120.90
1	N	337	G	O4'-C1'-N9	10.57	116.65	108.20
1	N	298	U	C2'-C3'-O3'	10.55	132.72	109.50
1	N	336	A	P-O3'-C3'	10.55	132.37	119.70
1	N	298	U	C5-C6-N1	10.49	127.94	122.70
1	N	244	C	N3-C4-C5	10.45	126.08	121.90
1	N	294	G	C5-C6-O6	10.45	134.87	128.60
1	N	258	A	N1-C6-N6	-10.42	112.35	118.60
1	N	234	A	P-O3'-C3'	10.42	132.20	119.70
1	N	241	G	C4-C5-N7	-10.42	106.63	110.80
1	N	169	G	O4'-C1'-N9	10.41	116.53	108.20
1	N	156	U	O4'-C1'-N1	10.39	116.51	108.20
1	N	136	G	C1'-O4'-C4'	10.36	118.19	109.90
1	N	335	U	O4'-C1'-N1	10.34	116.47	108.20
1	N	153	G	C5-C6-N1	10.32	116.66	111.50
1	N	339	A	N1-C6-N6	-10.29	112.42	118.60
1	N	251	C	N3-C4-N4	10.25	125.18	118.00
1	N	186	C	C6-N1-C2	-10.21	116.22	120.30
1	N	207	A	C8-N9-C4	10.21	109.88	105.80
1	N	217	G	P-O3'-C3'	10.20	131.94	119.70
1	N	291	U	O4'-C1'-N1	10.18	116.35	108.20
1	N	268	G	C5-C6-O6	-10.17	122.50	128.60
1	N	175	A	C5-C6-N1	10.15	122.77	117.70
1	N	326	G	C5-C6-O6	-10.11	122.53	128.60
1	N	239	A	C4-C5-N7	-10.06	105.67	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	173	A	N1-C6-N6	-10.06	112.56	118.60
1	N	336	A	C5-C6-N6	-10.05	115.66	123.70
1	N	302	G	C2-N3-C4	10.00	116.90	111.90
1	N	199	U	O4'-C1'-N1	9.97	116.18	108.20
1	N	194	C	C6-N1-C2	9.94	124.28	120.30
1	N	208	G	N3-C2-N2	9.93	126.85	119.90
1	N	147	C	C4-C5-C6	9.88	122.34	117.40
1	N	334	C	C6-N1-C2	-9.87	116.35	120.30
1	N	181	G	C5-C6-O6	-9.84	122.69	128.60
1	N	353	A	C5-N7-C8	-9.79	99.00	103.90
1	N	277	G	N7-C8-N9	-9.78	108.21	113.10
1	N	345	G	N1-C6-O6	9.71	125.72	119.90
1	N	214	C	C6-N1-C2	-9.70	116.42	120.30
1	N	279	G	C5-C6-O6	-9.69	122.79	128.60
1	N	351	A	N7-C8-N9	9.67	118.63	113.80
1	N	211	C	C6-N1-C2	-9.65	116.44	120.30
1	N	284	A	C5'-C4'-O4'	-9.64	97.53	109.10
1	N	208	G	P-O5'-C5'	9.63	136.30	120.90
1	N	232	C	O4'-C1'-N1	9.63	115.90	108.20
1	N	243	C	O4'-C1'-N1	9.60	115.88	108.20
1	N	236	G	C4-C5-N7	9.60	114.64	110.80
1	N	304	U	C5'-C4'-C3'	9.60	131.35	116.00
1	N	270	G	N1-C6-O6	9.57	125.64	119.90
1	N	136	G	C8-N9-C4	-9.56	102.58	106.40
1	N	144	G	N7-C8-N9	9.53	117.86	113.10
1	N	304	U	P-O3'-C3'	9.50	131.10	119.70
1	N	210	C	O4'-C1'-N1	9.49	115.80	108.20
1	N	268	G	N1-C6-O6	9.49	125.60	119.90
1	N	135	C	O4'-C4'-C3'	-9.49	94.51	104.00
1	N	324	C	C5-C6-N1	9.47	125.74	121.00
1	N	195	G	C5-C6-O6	-9.46	122.92	128.60
1	N	319	U	C2-N1-C1'	-9.46	106.35	117.70
1	N	350	A	C4-C5-C6	-9.45	112.28	117.00
1	N	219	G	C4-C5-N7	-9.43	107.03	110.80
1	N	242	C	P-O3'-C3'	9.42	131.00	119.70
1	N	341	G	C5-C6-O6	-9.41	122.95	128.60
1	N	358	U	N1-C2-O2	-9.38	116.24	122.80
1	N	196	A	C5-C6-N6	-9.30	116.26	123.70
1	N	332	C	O4'-C1'-N1	9.30	115.64	108.20
1	N	220	A	P-O3'-C3'	9.29	130.85	119.70
1	N	200	G	O4'-C1'-N9	9.29	115.63	108.20
1	N	202	G	P-O3'-C3'	9.27	130.83	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	152	U	C3'-C2'-C1'	9.26	108.91	101.50
1	N	233	G	C4'-C3'-C2'	-9.26	93.34	102.60
1	N	328	G	C4-C5-N7	-9.24	107.10	110.80
1	N	283	A	C2-N3-C4	-9.24	105.98	110.60
1	N	202	G	N7-C8-N9	9.23	117.72	113.10
1	N	167	C	N3-C4-N4	-9.23	111.54	118.00
1	N	217	G	N7-C8-N9	9.22	117.71	113.10
1	N	330	C	N3-C4-C5	-9.22	118.21	121.90
1	N	340	G	N1-C6-O6	9.22	125.43	119.90
1	N	219	G	C5-C6-N1	-9.22	106.89	111.50
1	N	353	A	N7-C8-N9	9.20	118.40	113.80
1	N	190	A	N1-C6-N6	-9.20	113.08	118.60
1	N	271	U	N3-C4-C5	-9.17	109.10	114.60
1	N	237	G	C6-C5-N7	-9.16	124.90	130.40
1	N	201	A	N1-C2-N3	9.15	133.88	129.30
1	N	273	G	C5-C6-O6	-9.15	123.11	128.60
1	N	350	A	N1-C2-N3	-9.14	124.73	129.30
1	N	137	U	C5-C4-O4	-9.13	120.42	125.90
1	N	275	U	O4'-C1'-N1	9.11	115.49	108.20
1	N	328	G	N3-C4-C5	-9.10	124.05	128.60
1	N	269	G	C5-C6-O6	-9.09	123.15	128.60
1	N	301	G	N1-C6-O6	9.08	125.35	119.90
1	N	180	A	N9-C4-C5	9.08	109.43	105.80
1	N	301	G	O4'-C1'-N9	9.07	115.46	108.20
1	N	233	G	C5-C6-N1	9.07	116.03	111.50
1	N	218	A	N1-C6-N6	9.07	124.04	118.60
1	N	316	G	C2-N3-C4	9.05	116.43	111.90
1	N	352	A	C2-N3-C4	-9.05	106.07	110.60
1	N	349	A	N9-C4-C5	-9.05	102.18	105.80
1	N	143	C	N3-C4-C5	9.04	125.52	121.90
1	N	163	A	C6-N1-C2	-9.04	113.18	118.60
1	N	178	A	O4'-C1'-N9	9.02	115.42	108.20
1	N	323	G	C5-C6-N1	9.02	116.01	111.50
1	N	328	G	O3'-P-O5'	-9.00	86.91	104.00
1	N	214	C	O4'-C1'-N1	8.99	115.39	108.20
1	N	173	A	C5-C6-N6	8.98	130.88	123.70
1	N	211	C	C5-C6-N1	8.97	125.49	121.00
1	N	245	A	C4-C5-N7	8.97	115.18	110.70
1	N	320	G	O4'-C1'-N9	8.95	115.36	108.20
1	N	243	C	N3-C4-C5	8.95	125.48	121.90
1	N	255	U	O4'-C1'-N1	8.94	115.36	108.20
1	N	232	C	P-O5'-C5'	8.93	135.18	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	136	G	O4'-C1'-C2'	-8.92	96.88	105.80
1	N	339	A	O4'-C1'-N9	8.92	115.34	108.20
1	N	226	C	C5-C6-N1	8.92	125.46	121.00
1	N	229	G	C4-C5-N7	-8.90	107.24	110.80
1	N	181	G	C8-N9-C4	-8.89	102.84	106.40
1	N	144	G	N9-C4-C5	8.89	108.95	105.40
1	N	302	G	N1-C2-N3	-8.88	118.57	123.90
1	N	307	G	O4'-C1'-N9	8.88	115.30	108.20
1	N	275	U	N3-C2-O2	-8.87	115.99	122.20
1	N	349	A	C4-C5-N7	8.83	115.11	110.70
1	N	232	C	C6-N1-C2	8.81	123.82	120.30
1	N	284	A	C8-N9-C4	-8.79	102.28	105.80
1	N	323	G	C8-N9-C4	8.78	109.91	106.40
1	N	342	C	C6-N1-C2	-8.78	116.79	120.30
1	N	137	U	P-O5'-C5'	8.74	134.88	120.90
1	N	250	A	O4'-C1'-N9	8.73	115.19	108.20
1	N	133	G	C2-N3-C4	8.72	116.26	111.90
1	N	201	A	C2-N3-C4	-8.72	106.24	110.60
1	N	149	C	C5-C4-N4	8.69	126.28	120.20
1	N	349	A	N3-C4-C5	8.69	132.88	126.80
1	N	169	G	C4-C5-C6	-8.69	113.59	118.80
1	N	277	G	C6-N1-C2	8.69	130.31	125.10
1	N	171	G	C4-C5-N7	8.68	114.27	110.80
1	N	324	C	O4'-C1'-N1	8.68	115.14	108.20
1	N	144	G	C5-C6-O6	-8.67	123.40	128.60
1	N	128	G	N1-C6-O6	8.66	125.10	119.90
1	N	313	A	C5'-C4'-O4'	8.66	119.50	109.10
1	N	210	C	N3-C2-O2	-8.66	115.84	121.90
1	N	167	C	C6-N1-C2	-8.66	116.84	120.30
1	N	244	C	C2-N3-C4	-8.65	115.58	119.90
1	N	223	C	N3-C4-C5	-8.62	118.45	121.90
1	N	283	A	C5'-C4'-O4'	-8.60	98.78	109.10
1	N	148	U	N3-C4-O4	-8.57	113.40	119.40
1	N	351	A	C4-C5-C6	-8.57	112.72	117.00
1	N	202	G	N3-C4-C5	-8.55	124.32	128.60
1	N	147	C	O4'-C1'-N1	8.55	115.04	108.20
1	N	284	A	O5'-C5'-C4'	8.55	127.94	111.70
1	N	175	A	C6-N1-C2	-8.53	113.48	118.60
1	N	232	C	N1-C2-O2	8.53	124.02	118.90
1	N	331	C	C4-C5-C6	-8.53	113.14	117.40
1	N	294	G	C8-N9-C4	-8.53	102.99	106.40
1	N	329	G	C6-C5-N7	-8.53	125.28	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	160	C	C5-C6-N1	8.52	125.26	121.00
1	N	349	A	C4-C5-C6	-8.52	112.74	117.00
1	N	139	G	C2-N3-C4	8.49	116.15	111.90
1	N	304	U	O4'-C1'-N1	8.49	115.00	108.20
1	N	233	G	C2-N3-C4	8.49	116.14	111.90
1	N	315	A	C8-N9-C4	8.48	109.19	105.80
1	N	355	C	C2-N3-C4	8.48	124.14	119.90
1	N	155	G	O4'-C1'-N9	8.48	114.98	108.20
1	N	264	G	C8-N9-C4	8.46	109.78	106.40
1	N	215	U	P-O3'-C3'	8.45	129.84	119.70
1	N	234	A	O4'-C1'-N9	8.44	114.95	108.20
1	N	333	A	N9-C4-C5	8.42	109.17	105.80
1	N	213	C	N3-C4-C5	-8.41	118.54	121.90
1	N	143	C	C6-N1-C2	-8.35	116.96	120.30
1	N	217	G	O4'-C1'-N9	8.34	114.87	108.20
1	N	285	U	P-O5'-C5'	-8.34	107.56	120.90
1	N	357	C	N3-C2-O2	-8.33	116.07	121.90
1	N	203	C	C2-N3-C4	-8.33	115.74	119.90
1	N	284	A	C4-N9-C1'	-8.33	111.31	126.30
1	N	295	U	P-O3'-C3'	-8.31	109.72	119.70
1	N	218	A	C4-C5-C6	-8.31	112.85	117.00
1	N	164	G	N7-C8-N9	8.30	117.25	113.10
1	N	355	C	N3-C4-C5	-8.29	118.58	121.90
1	N	326	G	N1-C6-O6	8.27	124.86	119.90
1	N	169	G	N9-C4-C5	-8.26	102.10	105.40
1	N	223	C	N1-C2-O2	8.25	123.85	118.90
1	N	255	U	N1-C2-N3	8.25	119.85	114.90
1	N	179	C	C5-C4-N4	-8.24	114.43	120.20
1	N	193	U	P-O3'-C3'	-8.24	109.81	119.70
1	N	161	U	C4'-C3'-C2'	-8.23	94.37	102.60
1	N	195	G	O4'-C1'-N9	8.23	114.78	108.20
1	N	360	C	N3-C2-O2	-8.22	116.14	121.90
1	N	328	G	O4'-C1'-N9	8.22	114.77	108.20
1	N	147	C	N3-C4-C5	-8.20	118.62	121.90
1	N	315	A	N9-C4-C5	-8.20	102.52	105.80
1	N	218	A	C5-C6-N6	-8.18	117.16	123.70
1	N	144	G	N3-C2-N2	8.15	125.60	119.90
1	N	145	A	C5-C6-N1	-8.14	113.63	117.70
1	N	320	G	C2-N3-C4	8.14	115.97	111.90
1	N	207	A	P-O5'-C5'	8.13	133.91	120.90
1	N	272	C	C5-C4-N4	-8.13	114.51	120.20
1	N	144	G	P-O3'-C3'	8.12	129.44	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	261	C	O4'-C1'-N1	8.12	114.69	108.20
1	N	331	C	C5'-C4'-C3'	8.12	128.99	116.00
1	N	177	G	N1-C6-O6	-8.10	115.04	119.90
1	N	141	G	C6-N1-C2	-8.10	120.24	125.10
1	N	310	C	O4'-C1'-N1	8.10	114.68	108.20
1	N	342	C	C4-C5-C6	8.10	121.45	117.40
1	N	277	G	C8-N9-C4	8.08	109.63	106.40
1	N	325	A	N7-C8-N9	8.08	117.84	113.80
1	N	347	A	N1-C2-N3	8.08	133.34	129.30
1	N	164	G	C8-N9-C4	-8.07	103.17	106.40
1	N	174	C	P-O3'-C3'	8.05	129.36	119.70
1	N	227	G	O4'-C1'-N9	8.04	114.63	108.20
1	N	174	C	O3'-P-O5'	-8.04	88.73	104.00
1	N	180	A	C1'-O4'-C4'	8.02	116.32	109.90
1	N	143	C	C5-C6-N1	8.01	125.01	121.00
1	N	215	U	C6-N1-C2	-8.00	116.20	121.00
1	N	256	U	N1-C2-N3	8.00	119.70	114.90
1	N	326	G	C8-N9-C4	8.00	109.60	106.40
1	N	186	C	O4'-C1'-N1	8.00	114.60	108.20
1	N	273	G	O4'-C1'-N9	8.00	114.60	108.20
1	N	263	G	C5-C6-O6	-7.97	123.82	128.60
1	N	152	U	P-O3'-C3'	7.97	129.26	119.70
1	N	163	A	N1-C2-N3	7.95	133.28	129.30
1	N	208	G	C6-C5-N7	-7.91	125.66	130.40
1	N	262	U	C2-N3-C4	7.91	131.74	127.00
1	N	359	G	N1-C6-O6	7.90	124.64	119.90
1	N	308	A	C5-C6-N6	-7.88	117.39	123.70
1	N	244	C	C4'-C3'-C2'	7.88	110.48	102.60
1	N	202	G	C2-N3-C4	7.87	115.83	111.90
1	N	317	G	O4'-C1'-N9	7.87	114.50	108.20
1	N	171	G	N9-C4-C5	-7.86	102.26	105.40
1	N	135	C	O4'-C1'-N1	7.84	114.48	108.20
1	N	219	G	C4-C5-C6	7.83	123.50	118.80
1	N	179	C	O4'-C1'-N1	7.83	114.46	108.20
1	N	203	C	C5-C4-N4	-7.82	114.73	120.20
1	N	347	A	C6-N1-C2	-7.80	113.92	118.60
1	N	301	G	C5-C6-O6	-7.80	123.92	128.60
1	N	144	G	O4'-C1'-N9	7.80	114.44	108.20
1	N	219	G	N3-C4-C5	-7.79	124.70	128.60
1	N	298	U	C2-N3-C4	-7.79	122.33	127.00
1	N	284	A	N9-C1'-C2'	7.78	124.12	114.00
1	N	273	G	C5-N7-C8	-7.78	100.41	104.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	136	G	C6-C5-N7	-7.75	125.75	130.40
1	N	313	A	N1-C2-N3	7.74	133.17	129.30
1	N	195	G	N3-C2-N2	7.74	125.32	119.90
1	N	271	U	C4-C5-C6	7.74	124.34	119.70
1	N	360	C	O4'-C1'-N1	7.73	114.39	108.20
1	N	251	C	C5'-C4'-C3'	7.73	128.37	116.00
1	N	359	G	O4'-C1'-N9	7.73	114.38	108.20
1	N	323	G	N9-C4-C5	-7.71	102.32	105.40
1	N	272	C	C2-N1-C1'	7.70	127.27	118.80
1	N	327	A	C5'-C4'-C3'	7.68	128.29	116.00
1	N	207	A	N7-C8-N9	-7.68	109.96	113.80
1	N	195	G	N1-C6-O6	7.68	124.51	119.90
1	N	151	C	P-O3'-C3'	-7.67	110.50	119.70
1	N	349	A	C2-N3-C4	-7.66	106.77	110.60
1	N	237	G	O4'-C1'-N9	7.66	114.32	108.20
1	N	258	A	N9-C4-C5	7.63	108.85	105.80
1	N	270	G	O4'-C1'-C2'	-7.62	98.18	105.80
1	N	294	G	C6-C5-N7	-7.61	125.83	130.40
1	N	342	C	N3-C4-C5	-7.61	118.86	121.90
1	N	271	U	O3'-P-O5'	7.59	118.43	104.00
1	N	324	C	C6-N1-C2	-7.59	117.26	120.30
1	N	181	G	O3'-P-O5'	7.58	118.40	104.00
1	N	162	A	C4-N9-C1'	7.57	139.92	126.30
1	N	290	U	O4'-C1'-N1	7.56	114.25	108.20
1	N	299	G	O5'-C5'-C4'	7.56	126.07	111.70
1	N	235	G	P-O5'-C5'	7.56	132.99	120.90
1	N	350	A	C5-C6-N1	7.55	121.48	117.70
1	N	277	G	N9-C4-C5	-7.55	102.38	105.40
1	N	152	U	C5-C6-N1	7.54	126.47	122.70
1	N	340	G	N3-C4-C5	-7.54	124.83	128.60
1	N	319	U	C5'-C4'-O4'	-7.53	100.06	109.10
1	N	330	C	C4-C5-C6	7.53	121.16	117.40
1	N	142	G	N7-C8-N9	7.51	116.86	113.10
1	N	256	U	C4-C5-C6	7.51	124.20	119.70
1	N	246	A	N1-C2-N3	-7.50	125.55	129.30
1	N	174	C	C5-C6-N1	-7.50	117.25	121.00
1	N	136	G	N3-C4-C5	-7.49	124.86	128.60
1	N	264	G	C6-N1-C2	-7.47	120.62	125.10
1	N	303	G	C6-C5-N7	-7.46	125.92	130.40
1	N	305	A	C3'-C2'-C1'	7.46	107.47	101.50
1	N	180	A	P-O5'-C5'	7.45	132.83	120.90
1	N	323	G	C6-C5-N7	7.45	134.87	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	168	U	C2-N3-C4	-7.44	122.54	127.00
1	N	283	A	N1-C6-N6	7.43	123.06	118.60
1	N	358	U	N3-C2-O2	7.43	127.40	122.20
1	N	258	A	C8-N9-C4	-7.43	102.83	105.80
1	N	230	G	P-O3'-C3'	7.43	128.61	119.70
1	N	133	G	N3-C2-N2	7.42	125.10	119.90
1	N	234	A	N1-C6-N6	-7.42	114.15	118.60
1	N	316	G	C4'-C3'-C2'	-7.42	95.18	102.60
1	N	140	U	C5-C4-O4	-7.39	121.46	125.90
1	N	304	U	C6-N1-C2	-7.39	116.56	121.00
1	N	149	C	N3-C4-N4	-7.38	112.83	118.00
1	N	197	C	C6-N1-C2	-7.38	117.35	120.30
1	N	181	G	C6-N1-C2	-7.37	120.68	125.10
1	N	187	A	C6-N1-C2	-7.37	114.18	118.60
1	N	303	G	C3'-C2'-C1'	-7.37	95.60	101.50
1	N	139	G	C5-C6-N1	7.37	115.18	111.50
1	N	169	G	N3-C4-C5	7.37	132.28	128.60
1	N	179	C	N3-C4-N4	7.36	123.15	118.00
1	N	169	G	C3'-C2'-C1'	7.35	107.38	101.50
1	N	223	C	P-O5'-C5'	7.33	132.63	120.90
1	N	241	G	N1-C6-O6	-7.32	115.51	119.90
1	N	305	A	N3-C4-C5	7.32	131.92	126.80
1	N	171	G	N1-C6-O6	-7.31	115.51	119.90
1	N	261	C	C6-N1-C2	7.31	123.22	120.30
1	N	356	U	OP1-P-OP2	-7.28	108.68	119.60
1	N	350	A	N9-C4-C5	-7.27	102.89	105.80
1	N	325	A	O4'-C1'-N9	7.27	114.02	108.20
1	N	211	C	C4'-C3'-C2'	-7.26	95.34	102.60
1	N	283	A	N3-C4-N9	7.26	133.21	127.40
1	N	318	G	P-O3'-C3'	-7.25	111.00	119.70
1	N	159	U	O4'-C1'-N1	7.23	113.98	108.20
1	N	138	A	N9-C4-C5	7.21	108.69	105.80
1	N	145	A	N1-C6-N6	7.21	122.93	118.60
1	N	148	U	N3-C4-C5	7.20	118.92	114.60
1	N	292	A	O4'-C1'-N9	7.20	113.96	108.20
1	N	256	U	N1-C2-O2	-7.20	117.76	122.80
1	N	339	A	P-O3'-C3'	-7.20	111.06	119.70
1	N	158	G	N1-C2-N3	-7.19	119.58	123.90
1	N	143	C	C4-C5-C6	-7.18	113.81	117.40
1	N	190	A	P-O3'-C3'	-7.18	111.08	119.70
1	N	137	U	C1'-O4'-C4'	-7.17	104.16	109.90
1	N	320	G	O5'-C5'-C4'	7.17	125.33	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	271	U	C5-C6-N1	-7.17	119.11	122.70
1	N	332	C	C2-N3-C4	-7.17	116.32	119.90
1	N	177	G	N3-C4-N9	-7.16	121.71	126.00
1	N	186	C	C5-C6-N1	7.14	124.57	121.00
1	N	273	G	N9-C4-C5	-7.14	102.54	105.40
1	N	226	C	C6-N1-C2	-7.14	117.44	120.30
1	N	258	A	C5-C6-N1	7.14	121.27	117.70
1	N	137	U	C2-N1-C1'	7.14	126.26	117.70
1	N	339	A	C5-C6-N6	7.13	129.41	123.70
1	N	206	U	N3-C4-C5	-7.12	110.33	114.60
1	N	342	C	P-O5'-C5'	-7.12	109.50	120.90
1	N	316	G	C5'-C4'-C3'	-7.12	104.61	116.00
1	N	157	G	C5-C6-O6	7.10	132.86	128.60
1	N	162	A	C8-N9-C1'	-7.10	114.92	127.70
1	N	164	G	N1-C6-O6	-7.10	115.64	119.90
1	N	283	A	N7-C8-N9	7.10	117.35	113.80
1	N	307	G	C2-N3-C4	7.09	115.45	111.90
1	N	351	A	C4-C5-N7	7.09	114.25	110.70
1	N	233	G	C4-C5-N7	7.09	113.64	110.80
1	N	278	G	N9-C4-C5	-7.09	102.56	105.40
1	N	278	G	O4'-C1'-N9	7.09	113.87	108.20
1	N	215	U	O3'-P-O5'	7.08	117.45	104.00
1	N	297	A	O4'-C1'-N9	7.08	113.86	108.20
1	N	165	U	P-O3'-C3'	-7.08	111.21	119.70
1	N	191	G	C5-C6-O6	-7.07	124.36	128.60
1	N	143	C	O4'-C1'-N1	7.07	113.86	108.20
1	N	281	G	C5-C6-O6	-7.06	124.36	128.60
1	N	209	C	O4'-C1'-N1	7.05	113.84	108.20
1	N	306	C	C4-C5-C6	7.05	120.93	117.40
1	N	134	C	O4'-C1'-N1	7.05	113.84	108.20
1	N	204	A	N9-C1'-C2'	-7.05	104.24	112.00
1	N	256	U	C6-N1-C2	-7.05	116.77	121.00
1	N	196	A	C5-C6-N1	7.04	121.22	117.70
1	N	295	U	N3-C2-O2	7.04	127.12	122.20
1	N	351	A	N1-C6-N6	-7.04	114.38	118.60
1	N	236	G	C2-N3-C4	7.03	115.42	111.90
1	N	172	U	N3-C4-O4	-7.03	114.48	119.40
1	N	160	C	O4'-C1'-N1	7.03	113.82	108.20
1	N	346	U	C4-C5-C6	-7.03	115.48	119.70
1	N	205	C	P-O3'-C3'	7.02	128.13	119.70
1	N	324	C	P-O5'-C5'	7.02	132.13	120.90
1	N	157	G	N3-C4-C5	7.02	132.11	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	170	A	P-O3'-C3'	7.02	128.12	119.70
1	N	341	G	N9-C4-C5	7.01	108.20	105.40
1	N	302	G	C8-N9-C4	-7.01	103.60	106.40
1	N	270	G	N9-C4-C5	7.00	108.20	105.40
1	N	263	G	OP1-P-OP2	-6.98	109.12	119.60
1	N	167	C	C5-C4-N4	6.98	125.09	120.20
1	N	137	U	N3-C4-O4	6.97	124.28	119.40
1	N	162	A	O4'-C1'-N9	6.97	113.78	108.20
1	N	251	C	N3-C4-C5	-6.97	119.11	121.90
1	N	342	C	O4'-C1'-N1	6.97	113.77	108.20
1	N	188	G	P-O3'-C3'	-6.96	111.35	119.70
1	N	304	U	C4'-C3'-C2'	6.96	109.56	102.60
1	N	321	C	C6-N1-C2	-6.96	117.52	120.30
1	N	157	G	C2-N3-C4	-6.95	108.42	111.90
1	N	153	G	C4-C5-C6	-6.95	114.63	118.80
1	N	301	G	C6-C5-N7	-6.95	126.23	130.40
1	N	247	G	P-O3'-C3'	-6.94	111.37	119.70
1	N	304	U	C5-C4-O4	-6.94	121.73	125.90
1	N	319	U	O5'-P-OP2	-6.92	99.47	105.70
1	N	191	G	N1-C6-O6	6.92	124.05	119.90
1	N	321	C	N3-C4-C5	-6.92	119.13	121.90
1	N	329	G	C4-C5-C6	6.92	122.95	118.80
1	N	162	A	C1'-O4'-C4'	6.91	115.43	109.90
1	N	210	C	N1-C2-N3	6.91	124.04	119.20
1	N	297	A	C8-N9-C4	-6.91	103.04	105.80
1	N	265	C	C5-C6-N1	6.90	124.45	121.00
1	N	354	U	N1-C2-O2	-6.90	117.97	122.80
1	N	242	C	C6-N1-C1'	-6.89	112.53	120.80
1	N	172	U	C5-C4-O4	6.89	130.03	125.90
1	N	271	U	O4'-C1'-N1	6.89	113.71	108.20
1	N	314	U	O4'-C1'-N1	6.89	113.71	108.20
1	N	317	G	C8-N9-C4	-6.89	103.64	106.40
1	N	141	G	C5-C6-N1	6.88	114.94	111.50
1	N	305	A	C5'-C4'-C3'	6.88	127.01	116.00
1	N	210	C	C5-C4-N4	-6.88	115.39	120.20
1	N	324	C	C5'-C4'-O4'	6.87	117.35	109.10
1	N	180	A	C5-C6-N6	-6.87	118.21	123.70
1	N	283	A	C6-N1-C2	-6.86	114.48	118.60
1	N	346	U	C5'-C4'-O4'	6.85	117.32	109.10
1	N	182	U	C5'-C4'-C3'	6.85	126.96	116.00
1	N	320	G	C4'-C3'-C2'	-6.84	95.76	102.60
1	N	185	U	C4'-C3'-C2'	-6.83	95.77	102.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	328	G	C5-N7-C8	6.83	107.71	104.30
1	N	141	G	C8-N9-C4	6.82	109.13	106.40
1	N	337	G	P-O3'-C3'	6.82	127.88	119.70
1	N	236	G	C8-N9-C4	-6.80	103.68	106.40
1	N	180	A	C6-N1-C2	-6.80	114.52	118.60
1	N	275	U	C6-N1-C2	-6.79	116.92	121.00
1	N	176	G	C8-N9-C4	-6.79	103.68	106.40
1	N	228	U	C1'-O4'-C4'	-6.79	104.47	109.90
1	N	297	A	C4-C5-N7	6.79	114.09	110.70
1	N	177	G	N3-C4-C5	6.78	131.99	128.60
1	N	173	A	P-O3'-C3'	6.78	127.84	119.70
1	N	340	G	C2-N3-C4	6.78	115.29	111.90
1	N	200	G	C1'-O4'-C4'	-6.78	104.48	109.90
1	N	230	G	C5-C6-O6	-6.77	124.54	128.60
1	N	304	U	O3'-P-O5'	-6.76	91.15	104.00
1	N	169	G	C5-N7-C8	-6.76	100.92	104.30
1	N	306	C	N1-C1'-C2'	-6.75	104.58	112.00
1	N	153	G	N9-C4-C5	-6.75	102.70	105.40
1	N	281	G	C5'-C4'-C3'	6.74	126.78	116.00
1	N	192	U	N3-C2-O2	-6.74	117.48	122.20
1	N	246	A	C8-N9-C4	-6.74	103.11	105.80
1	N	241	G	O4'-C1'-N9	6.73	113.58	108.20
1	N	209	C	C4'-C3'-C2'	-6.73	95.87	102.60
1	N	298	U	C6-N1-C2	-6.73	116.96	121.00
1	N	216	C	O4'-C1'-N1	6.72	113.58	108.20
1	N	255	U	C6-N1-C2	-6.72	116.97	121.00
1	N	276	A	N1-C6-N6	6.71	122.62	118.60
1	N	341	G	C8-N9-C4	-6.71	103.72	106.40
1	N	284	A	P-O5'-C5'	-6.71	110.17	120.90
1	N	153	G	N7-C8-N9	6.70	116.45	113.10
1	N	199	U	C5-C6-N1	6.70	126.05	122.70
1	N	164	G	C5'-C4'-C3'	-6.70	105.28	116.00
1	N	192	U	N1-C2-N3	6.69	118.92	114.90
1	N	350	A	C4'-C3'-C2'	-6.68	95.92	102.60
1	N	330	C	O4'-C1'-N1	6.68	113.55	108.20
1	N	188	G	C4-C5-N7	-6.68	108.13	110.80
1	N	252	A	C8-N9-C4	-6.67	103.13	105.80
1	N	323	G	N1-C6-O6	6.67	123.90	119.90
1	N	231	A	N1-C2-N3	6.67	132.63	129.30
1	N	320	G	C3'-C2'-C1'	6.67	106.83	101.50
1	N	160	C	C6-N1-C2	-6.67	117.63	120.30
1	N	177	G	C5-C6-N1	6.67	114.83	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	204	A	P-O3'-C3'	6.66	127.70	119.70
1	N	258	A	O4'-C1'-N9	6.66	113.53	108.20
1	N	306	C	O4'-C1'-N1	6.66	113.53	108.20
1	N	227	G	N1-C6-O6	-6.65	115.91	119.90
1	N	309	C	N3-C4-C5	-6.63	119.25	121.90
1	N	154	G	P-O5'-C5'	6.63	131.51	120.90
1	N	294	G	N1-C6-O6	-6.63	115.92	119.90
1	N	218	A	P-O5'-C5'	-6.63	110.30	120.90
1	N	291	U	P-O3'-C3'	6.62	127.65	119.70
1	N	270	G	C4-C5-N7	-6.62	108.15	110.80
1	N	157	G	O4'-C1'-N9	6.62	113.49	108.20
1	N	284	A	C2'-C3'-O3'	6.62	124.28	113.70
1	N	153	G	C2-N3-C4	-6.61	108.59	111.90
1	N	201	A	C4-C5-C6	6.61	120.31	117.00
1	N	187	A	P-O5'-C5'	6.61	131.47	120.90
1	N	212	A	O4'-C1'-N9	6.61	113.48	108.20
1	N	164	G	N3-C4-C5	-6.60	125.30	128.60
1	N	339	A	O4'-C4'-C3'	-6.60	97.40	104.00
1	N	171	G	N1-C2-N3	-6.60	119.94	123.90
1	N	232	C	N1-C2-N3	-6.60	114.58	119.20
1	N	273	G	C2-N3-C4	6.60	115.20	111.90
1	N	295	U	N3-C4-C5	6.60	118.56	114.60
1	N	340	G	C6-N1-C2	-6.59	121.14	125.10
1	N	312	G	C2-N3-C4	6.59	115.19	111.90
1	N	350	A	C8-N9-C4	6.58	108.43	105.80
1	N	243	C	C4-C5-C6	-6.58	114.11	117.40
1	N	201	A	C8-N9-C4	-6.56	103.18	105.80
1	N	237	G	OP1-P-OP2	-6.56	109.77	119.60
1	N	257	A	N3-C4-N9	-6.56	122.15	127.40
1	N	221	U	C6-N1-C2	6.55	124.93	121.00
1	N	263	G	O4'-C1'-N9	6.55	113.44	108.20
1	N	211	C	N1-C1'-C2'	-6.55	104.80	112.00
1	N	323	G	C4-C5-C6	-6.54	114.88	118.80
1	N	248	A	OP1-P-OP2	-6.53	109.80	119.60
1	N	320	G	P-O3'-C3'	-6.53	111.86	119.70
1	N	298	U	O4'-C1'-C2'	-6.52	99.28	105.80
1	N	217	G	N1-C2-N3	-6.52	119.99	123.90
1	N	283	A	C1'-O4'-C4'	6.51	115.11	109.90
1	N	310	C	N1-C2-O2	-6.51	114.99	118.90
1	N	155	G	O4'-C4'-C3'	-6.50	97.50	104.00
1	N	174	C	P-O5'-C5'	6.50	131.30	120.90
1	N	315	A	C3'-C2'-C1'	6.50	106.70	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	262	U	P-O5'-C5'	-6.49	110.51	120.90
1	N	277	G	N3-C4-N9	6.48	129.89	126.00
1	N	306	C	C2-N3-C4	6.48	123.14	119.90
1	N	274	C	C4'-C3'-C2'	-6.47	96.12	102.60
1	N	354	U	N3-C2-O2	6.47	126.73	122.20
1	N	211	C	O4'-C1'-N1	6.47	113.38	108.20
1	N	152	U	P-O5'-C5'	6.46	131.24	120.90
1	N	277	G	C5-N7-C8	6.46	107.53	104.30
1	N	153	G	O5'-P-OP1	-6.45	99.89	105.70
1	N	288	C	O4'-C1'-N1	6.45	113.36	108.20
1	N	222	G	N1-C6-O6	6.45	123.77	119.90
1	N	360	C	C3'-C2'-C1'	-6.45	96.34	101.50
1	N	218	A	C5'-C4'-C3'	-6.44	105.69	116.00
1	N	147	C	C4'-C3'-C2'	-6.43	96.17	102.60
1	N	353	A	OP1-P-OP2	-6.43	109.95	119.60
1	N	351	A	C5'-C4'-C3'	6.43	126.29	116.00
1	N	149	C	N3-C4-C5	-6.43	119.33	121.90
1	N	189	U	O4'-C1'-N1	6.42	113.34	108.20
1	N	251	C	C5-C4-N4	-6.42	115.70	120.20
1	N	171	G	C5-C6-O6	6.42	132.45	128.60
1	N	302	G	N3-C2-N2	6.42	124.39	119.90
1	N	257	A	O4'-C1'-N9	6.41	113.33	108.20
1	N	181	G	N1-C6-O6	6.41	123.74	119.90
1	N	210	C	C6-N1-C2	-6.40	117.74	120.30
1	N	210	C	C5-C6-N1	6.40	124.20	121.00
1	N	266	G	N9-C4-C5	-6.40	102.84	105.40
1	N	138	A	C4'-C3'-C2'	-6.39	96.20	102.60
1	N	337	G	C5-C6-O6	-6.39	124.76	128.60
1	N	130	C	O4'-C1'-N1	6.39	113.31	108.20
1	N	280	U	P-O3'-C3'	6.39	127.37	119.70
1	N	133	G	N1-C2-N3	-6.38	120.07	123.90
1	N	136	G	N3-C4-N9	6.38	129.83	126.00
1	N	288	C	C4-C5-C6	6.38	120.59	117.40
1	N	138	A	P-O3'-C3'	-6.37	112.05	119.70
1	N	180	A	C5-C6-N1	6.37	120.89	117.70
1	N	238	C	C4'-C3'-C2'	-6.37	96.23	102.60
1	N	279	G	C6-N1-C2	-6.37	121.28	125.10
1	N	319	U	C5'-C4'-C3'	6.36	126.18	116.00
1	N	233	G	N1-C6-O6	6.36	123.72	119.90
1	N	272	C	C1'-O4'-C4'	-6.35	104.82	109.90
1	N	242	C	C5-C4-N4	-6.35	115.75	120.20
1	N	190	A	C2-N3-C4	-6.35	107.43	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	319	U	C6-N1-C2	6.35	124.81	121.00
1	N	271	U	C5-C4-O4	6.34	129.71	125.90
1	N	153	G	C6-N1-C2	-6.34	121.29	125.10
1	N	357	C	N1-C2-O2	6.34	122.70	118.90
1	N	129	A	C4-C5-C6	6.34	120.17	117.00
1	N	245	A	N9-C4-C5	-6.34	103.27	105.80
1	N	302	G	N3-C4-C5	-6.34	125.43	128.60
1	N	326	G	N1-C2-N3	6.34	127.70	123.90
1	N	206	U	O4'-C1'-N1	6.33	113.27	108.20
1	N	261	C	C2-N3-C4	-6.33	116.73	119.90
1	N	152	U	C5'-C4'-C3'	-6.33	105.87	116.00
1	N	154	G	C2-N3-C4	6.33	115.07	111.90
1	N	189	U	C5'-C4'-C3'	6.33	126.13	116.00
1	N	313	A	C5-N7-C8	-6.33	100.74	103.90
1	N	344	A	N1-C2-N3	-6.33	126.14	129.30
1	N	289	A	C8-N9-C4	-6.32	103.27	105.80
1	N	264	G	N9-C4-C5	-6.32	102.87	105.40
1	N	186	C	C4-C5-C6	-6.31	114.24	117.40
1	N	202	G	N9-C4-C5	6.31	107.92	105.40
1	N	242	C	O4'-C1'-N1	6.31	113.25	108.20
1	N	192	U	C5-C6-N1	-6.30	119.55	122.70
1	N	144	G	N3-C4-N9	-6.30	122.22	126.00
1	N	193	U	C5-C6-N1	-6.30	119.55	122.70
1	N	203	C	C6-N1-C2	-6.29	117.78	120.30
1	N	285	U	N3-C4-O4	6.28	123.80	119.40
1	N	311	U	C3'-C2'-C1'	6.27	106.52	101.50
1	N	321	C	N3-C4-N4	6.27	122.39	118.00
1	N	331	C	C6-N1-C2	-6.27	117.79	120.30
1	N	340	G	C5-C6-N1	6.27	114.63	111.50
1	N	226	C	O4'-C1'-N1	6.26	113.21	108.20
1	N	209	C	C6-N1-C2	-6.26	117.80	120.30
1	N	202	G	C5-C6-N1	6.26	114.63	111.50
1	N	334	C	N3-C2-O2	-6.25	117.53	121.90
1	N	146	G	N9-C4-C5	-6.25	102.90	105.40
1	N	250	A	N1-C6-N6	-6.24	114.85	118.60
1	N	141	G	C5-C6-O6	-6.24	124.86	128.60
1	N	274	C	C2-N3-C4	-6.24	116.78	119.90
1	N	346	U	N1-C2-N3	-6.23	111.16	114.90
1	N	247	G	C5-C6-N1	-6.23	108.39	111.50
1	N	201	A	C5-C6-N1	-6.23	114.59	117.70
1	N	303	G	C5-C6-O6	6.23	132.34	128.60
1	N	283	A	P-O3'-C3'	-6.22	112.23	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	177	G	O4'-C1'-N9	6.22	113.18	108.20
1	N	308	A	P-O5'-C5'	6.21	130.84	120.90
1	N	283	A	N9-C1'-C2'	6.21	122.08	114.00
1	N	249	C	N3-C4-N4	-6.21	113.65	118.00
1	N	243	C	N1-C1'-C2'	-6.21	105.17	112.00
1	N	170	A	O4'-C1'-N9	6.20	113.16	108.20
1	N	158	G	O4'-C1'-N9	6.20	113.16	108.20
1	N	275	U	C5-C6-N1	6.20	125.80	122.70
1	N	219	G	C8-N9-C4	6.19	108.88	106.40
1	N	331	C	O5'-P-OP1	-6.19	100.13	105.70
1	N	281	G	N7-C8-N9	6.19	116.19	113.10
1	N	336	A	N3-C4-N9	6.19	132.35	127.40
1	N	294	G	C5-C6-N1	-6.19	108.41	111.50
1	N	154	G	C5'-C4'-C3'	6.18	125.89	116.00
1	N	312	G	N1-C2-N3	-6.18	120.19	123.90
1	N	289	A	N9-C4-C5	6.18	108.27	105.80
1	N	132	A	N1-C2-N3	-6.17	126.21	129.30
1	N	230	G	N9-C4-C5	6.17	107.87	105.40
1	N	259	C	C4-C5-C6	6.17	120.48	117.40
1	N	273	G	N3-C4-N9	6.16	129.70	126.00
1	N	169	G	C8-N9-C4	6.15	108.86	106.40
1	N	187	A	C5-N7-C8	-6.15	100.83	103.90
1	N	237	G	N3-C2-N2	6.15	124.20	119.90
1	N	338	C	P-O3'-C3'	-6.15	112.32	119.70
1	N	200	G	C4'-C3'-C2'	-6.14	96.46	102.60
1	N	275	U	N1-C2-O2	6.14	127.10	122.80
1	N	135	C	N1-C2-O2	6.14	122.58	118.90
1	N	219	G	C1'-O4'-C4'	-6.13	104.99	109.90
1	N	283	A	C5-C6-N1	-6.12	114.64	117.70
1	N	148	U	C2-N3-C4	-6.11	123.34	127.00
1	N	206	U	N3-C2-O2	-6.11	117.92	122.20
1	N	156	U	N1-C1'-C2'	-6.10	105.29	112.00
1	N	315	A	C4'-C3'-C2'	-6.10	96.50	102.60
1	N	183	C	O4'-C1'-N1	6.10	113.08	108.20
1	N	343	U	O4'-C1'-N1	6.09	113.08	108.20
1	N	291	U	C4-C5-C6	6.08	123.35	119.70
1	N	304	U	P-O5'-C5'	-6.08	111.17	120.90
1	N	309	C	O4'-C1'-N1	6.08	113.06	108.20
1	N	234	A	C5-N7-C8	6.07	106.94	103.90
1	N	291	U	N3-C4-C5	-6.07	110.96	114.60
1	N	230	G	N3-C2-N2	-6.07	115.65	119.90
1	N	286	C	P-O3'-C3'	-6.07	112.42	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	358	U	C4'-C3'-C2'	-6.07	96.53	102.60
1	N	339	A	OP2-P-O3'	6.06	118.54	105.20
1	N	172	U	C4'-C3'-C2'	-6.06	96.54	102.60
1	N	268	G	P-O5'-C5'	6.06	130.59	120.90
1	N	279	G	P-O5'-C5'	6.06	130.59	120.90
1	N	331	C	N3-C4-N4	-6.06	113.76	118.00
1	N	254	C	O4'-C1'-N1	6.06	113.05	108.20
1	N	262	U	P-O3'-C3'	-6.05	112.44	119.70
1	N	284	A	C3'-C2'-C1'	6.04	106.33	101.50
1	N	303	G	C5-C6-N1	-6.03	108.48	111.50
1	N	203	C	N3-C4-C5	6.03	124.31	121.90
1	N	221	U	C4'-C3'-C2'	6.03	108.63	102.60
1	N	135	C	C4'-C3'-C2'	6.02	108.62	102.60
1	N	302	G	C5-C6-N1	6.02	114.51	111.50
1	N	245	A	C6-C5-N7	-6.02	128.09	132.30
1	N	310	C	N1-C2-N3	6.02	123.41	119.20
1	N	163	A	N1-C6-N6	-6.01	114.99	118.60
1	N	216	C	N3-C2-O2	-6.01	117.69	121.90
1	N	136	G	C6-N1-C2	-6.01	121.49	125.10
1	N	327	A	C8-N9-C4	-6.01	103.39	105.80
1	N	171	G	N3-C4-N9	6.01	129.60	126.00
1	N	231	A	C3'-C2'-C1'	-6.01	96.69	101.50
1	N	281	G	C5-N7-C8	-6.01	101.30	104.30
1	N	181	G	C5'-C4'-O4'	-6.00	101.90	109.10
1	N	329	G	C5'-C4'-C3'	6.00	125.60	116.00
1	N	340	G	P-O3'-C3'	-6.00	112.50	119.70
1	N	328	G	C4-C5-C6	6.00	122.40	118.80
1	N	195	G	N1-C2-N2	-6.00	110.80	116.20
1	N	219	G	C5-N7-C8	6.00	107.30	104.30
1	N	277	G	C5-C6-O6	6.00	132.20	128.60
1	N	176	G	N1-C2-N2	5.99	121.59	116.20
1	N	234	A	N7-C8-N9	-5.98	110.81	113.80
1	N	258	A	P-O5'-C5'	5.97	130.46	120.90
1	N	252	A	C4-C5-N7	5.97	113.68	110.70
1	N	187	A	C1'-O4'-C4'	5.96	114.67	109.90
1	N	188	G	C2-N3-C4	5.96	114.88	111.90
1	N	128	G	C6-N1-C2	5.96	128.67	125.10
1	N	186	C	OP1-P-OP2	-5.95	110.67	119.60
1	N	187	A	C4-C5-N7	5.95	113.68	110.70
1	N	301	G	C8-N9-C4	-5.95	104.02	106.40
1	N	136	G	C5-C6-O6	-5.95	125.03	128.60
1	N	227	G	C6-C5-N7	5.95	133.97	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	136	G	C5-C6-N1	5.94	114.47	111.50
1	N	267	G	N1-C6-O6	5.94	123.46	119.90
1	N	257	A	C5'-C4'-O4'	-5.93	101.99	109.10
1	N	273	G	N7-C8-N9	5.93	116.06	113.10
1	N	259	C	C6-N1-C2	-5.92	117.93	120.30
1	N	279	G	C5-C6-N1	5.92	114.46	111.50
1	N	176	G	N1-C2-N3	-5.91	120.35	123.90
1	N	273	G	C4-C5-N7	5.91	113.17	110.80
1	N	274	C	C1'-O4'-C4'	-5.91	105.17	109.90
1	N	286	C	C4-C5-C6	5.91	120.35	117.40
1	N	244	C	N3-C4-N4	-5.90	113.87	118.00
1	N	340	G	N3-C4-N9	5.90	129.54	126.00
1	N	298	U	C1'-O4'-C4'	-5.89	105.19	109.90
1	N	268	G	C2-N3-C4	-5.88	108.96	111.90
1	N	198	G	C5-N7-C8	5.88	107.24	104.30
1	N	231	A	C5-N7-C8	-5.88	100.96	103.90
1	N	355	C	N3-C2-O2	5.88	126.02	121.90
1	N	267	G	O4'-C1'-N9	5.87	112.90	108.20
1	N	268	G	C5'-C4'-C3'	5.87	125.40	116.00
1	N	175	A	N1-C2-N3	5.87	132.24	129.30
1	N	314	U	C5-C6-N1	-5.87	119.76	122.70
1	N	268	G	N3-C4-C5	5.86	131.53	128.60
1	N	282	A	O4'-C1'-N9	5.86	112.89	108.20
1	N	207	A	C5-C6-N1	5.86	120.63	117.70
1	N	325	A	N9-C4-C5	-5.86	103.46	105.80
1	N	156	U	C2-N3-C4	-5.85	123.49	127.00
1	N	197	C	O4'-C1'-N1	5.85	112.88	108.20
1	N	249	C	N1-C2-O2	5.85	122.41	118.90
1	N	354	U	C5'-C4'-O4'	5.84	116.11	109.10
1	N	239	A	C8-N9-C4	-5.84	103.46	105.80
1	N	144	G	C5-C6-N1	-5.84	108.58	111.50
1	N	213	C	O4'-C1'-N1	5.84	112.87	108.20
1	N	163	A	O4'-C4'-C3'	-5.83	98.17	104.00
1	N	360	C	C2-N3-C4	-5.83	116.98	119.90
1	N	318	G	N1-C2-N3	-5.83	120.40	123.90
1	N	303	G	C6-N1-C2	5.82	128.59	125.10
1	N	324	C	C4-C5-C6	-5.82	114.49	117.40
1	N	216	C	N1-C2-O2	5.82	122.39	118.90
1	N	353	A	N1-C2-N3	-5.82	126.39	129.30
1	N	135	C	C5'-C4'-O4'	-5.82	102.12	109.10
1	N	299	G	C4-C5-N7	-5.82	108.47	110.80
1	N	218	A	C5'-C4'-O4'	5.81	116.07	109.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	136	G	C5'-C4'-C3'	5.80	125.28	116.00
1	N	259	C	O4'-C1'-N1	5.80	112.84	108.20
1	N	151	C	O4'-C4'-C3'	-5.79	98.20	104.00
1	N	226	C	N3-C4-N4	5.79	122.05	118.00
1	N	355	C	N1-C2-N3	-5.79	115.15	119.20
1	N	191	G	O4'-C1'-N9	5.79	112.83	108.20
1	N	207	A	C5-C6-N6	5.79	128.33	123.70
1	N	235	G	O5'-P-OP2	-5.79	100.49	105.70
1	N	146	G	C5-C6-O6	5.78	132.07	128.60
1	N	235	G	O4'-C4'-C3'	-5.78	98.22	104.00
1	N	283	A	C4-C5-C6	5.78	119.89	117.00
1	N	145	A	P-O3'-C3'	5.77	126.62	119.70
1	N	247	G	O4'-C1'-N9	5.77	112.82	108.20
1	N	142	G	C8-N9-C4	-5.77	104.09	106.40
1	N	208	G	C4-C5-C6	5.77	122.26	118.80
1	N	360	C	C6-N1-C2	-5.77	117.99	120.30
1	N	158	G	N9-C1'-C2'	-5.77	105.66	112.00
1	N	226	C	C2-N3-C4	5.76	122.78	119.90
1	N	273	G	N1-C6-O6	5.76	123.35	119.90
1	N	343	U	N3-C4-O4	5.76	123.43	119.40
1	N	221	U	OP1-P-OP2	-5.75	110.97	119.60
1	N	158	G	C1'-O4'-C4'	-5.75	105.30	109.90
1	N	226	C	C4-C5-C6	-5.75	114.53	117.40
1	N	285	U	C2-N1-C1'	5.74	124.59	117.70
1	N	269	G	O4'-C1'-N9	5.74	112.79	108.20
1	N	294	G	N9-C4-C5	5.74	107.69	105.40
1	N	188	G	C6-N1-C2	-5.74	121.66	125.10
1	N	174	C	C1'-O4'-C4'	-5.73	105.31	109.90
1	N	198	G	N1-C2-N3	-5.73	120.46	123.90
1	N	193	U	C4'-C3'-C2'	-5.73	96.87	102.60
1	N	322	U	C4'-C3'-C2'	-5.73	96.87	102.60
1	N	180	A	N3-C4-N9	-5.72	122.82	127.40
1	N	231	A	C5-C6-N6	5.72	128.28	123.70
1	N	245	A	C5'-C4'-C3'	5.72	125.16	116.00
1	N	190	A	C5-C6-N6	5.72	128.28	123.70
1	N	150	C	O4'-C1'-N1	5.71	112.77	108.20
1	N	205	C	N1-C2-O2	5.71	122.33	118.90
1	N	195	G	O3'-P-O5'	5.71	114.85	104.00
1	N	263	G	C5-C6-N1	5.71	114.35	111.50
1	N	274	C	N1-C2-N3	5.70	123.19	119.20
1	N	326	G	C8-N9-C1'	-5.70	119.59	127.00
1	N	164	G	C5-N7-C8	-5.69	101.45	104.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	187	A	N7-C8-N9	5.69	116.65	113.80
1	N	267	G	P-O5'-C5'	-5.69	111.79	120.90
1	N	185	U	P-O5'-C5'	5.69	130.00	120.90
1	N	206	U	C4'-C3'-C2'	-5.69	96.91	102.60
1	N	244	C	O4'-C1'-N1	5.68	112.75	108.20
1	N	295	U	N1-C2-N3	-5.68	111.49	114.90
1	N	245	A	C5-N7-C8	-5.68	101.06	103.90
1	N	220	A	C5'-C4'-C3'	5.68	125.09	116.00
1	N	238	C	C5'-C4'-O4'	5.68	115.91	109.10
1	N	291	U	C5-C6-N1	-5.67	119.86	122.70
1	N	176	G	N1-C6-O6	-5.67	116.50	119.90
1	N	238	C	C5-C4-N4	-5.67	116.23	120.20
1	N	341	G	N3-C2-N2	-5.67	115.93	119.90
1	N	145	A	C8-N9-C4	-5.66	103.53	105.80
1	N	222	G	O4'-C1'-N9	5.66	112.73	108.20
1	N	223	C	C4'-C3'-C2'	-5.66	96.94	102.60
1	N	221	U	C2-N3-C4	-5.66	123.60	127.00
1	N	241	G	C5-N7-C8	5.66	107.13	104.30
1	N	264	G	O4'-C1'-N9	5.65	112.72	108.20
1	N	304	U	OP2-P-O3'	5.64	117.61	105.20
1	N	148	U	N1-C2-O2	5.63	126.74	122.80
1	N	164	G	C5-C6-O6	5.63	131.98	128.60
1	N	323	G	C4-N9-C1'	-5.63	119.18	126.50
1	N	235	G	C3'-C2'-C1'	-5.63	97.00	101.50
1	N	319	U	O3'-P-O5'	5.63	114.69	104.00
1	N	209	C	N3-C4-N4	5.63	121.94	118.00
1	N	193	U	P-O5'-C5'	5.62	129.90	120.90
1	N	210	C	N3-C4-C5	5.62	124.15	121.90
1	N	341	G	N1-C6-O6	5.62	123.27	119.90
1	N	221	U	P-O5'-C5'	5.62	129.89	120.90
1	N	303	G	C5-N7-C8	-5.61	101.49	104.30
1	N	356	U	C5-C6-N1	-5.61	119.89	122.70
1	N	307	G	N1-C2-N3	-5.61	120.54	123.90
1	N	155	G	C2-N3-C4	-5.60	109.10	111.90
1	N	143	C	C5-C4-N4	-5.60	116.28	120.20
1	N	132	A	C2-N3-C4	5.59	113.39	110.60
1	N	265	C	O4'-C4'-C3'	-5.59	98.41	104.00
1	N	279	G	C2-N3-C4	-5.58	109.11	111.90
1	N	171	G	C6-C5-N7	-5.58	127.05	130.40
1	N	233	G	C6-N1-C2	-5.57	121.76	125.10
1	N	128	G	C5-C6-N1	-5.57	108.72	111.50
1	N	279	G	N3-C4-C5	5.57	131.38	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	186	C	P-O3'-C3'	-5.57	113.02	119.70
1	N	256	U	O4'-C1'-N1	5.57	112.66	108.20
1	N	300	G	O4'-C1'-N9	5.57	112.65	108.20
1	N	227	G	C8-N9-C4	5.57	108.63	106.40
1	N	130	C	P-O5'-C5'	5.56	129.80	120.90
1	N	281	G	N9-C4-C5	-5.56	103.18	105.40
1	N	327	A	O3'-P-O5'	5.56	114.57	104.00
1	N	346	U	C5'-C4'-C3'	-5.56	107.10	116.00
1	N	325	A	C5-N7-C8	-5.56	101.12	103.90
1	N	158	G	C6-N1-C2	5.55	128.43	125.10
1	N	247	G	C4'-C3'-C2'	-5.55	97.05	102.60
1	N	278	G	C5-C6-O6	-5.54	125.27	128.60
1	N	280	U	N3-C4-O4	-5.54	115.52	119.40
1	N	187	A	N9-C4-C5	-5.54	103.58	105.80
1	N	250	A	C2-N3-C4	-5.54	107.83	110.60
1	N	192	U	C6-N1-C2	-5.53	117.68	121.00
1	N	347	A	N7-C8-N9	-5.53	111.03	113.80
1	N	360	C	N1-C2-N3	5.53	123.07	119.20
1	N	152	U	C4-C5-C6	-5.53	116.39	119.70
1	N	304	U	N3-C2-O2	-5.53	118.33	122.20
1	N	313	A	O4'-C1'-N9	5.53	112.62	108.20
1	N	326	G	O4'-C1'-N9	5.53	112.62	108.20
1	N	237	G	C5-N7-C8	-5.52	101.54	104.30
1	N	246	A	C5'-C4'-O4'	-5.52	102.48	109.10
1	N	189	U	C2-N3-C4	5.51	130.31	127.00
1	N	257	A	C4'-C3'-C2'	-5.51	97.09	102.60
1	N	348	U	OP1-P-OP2	-5.51	111.34	119.60
1	N	237	G	N9-C4-C5	-5.50	103.20	105.40
1	N	175	A	C3'-C2'-C1'	-5.49	97.11	101.50
1	N	293	U	C3'-C2'-C1'	-5.49	97.11	101.50
1	N	344	A	C8-N9-C4	-5.49	103.61	105.80
1	N	247	G	N3-C2-N2	5.48	123.74	119.90
1	N	131	U	C4'-C3'-C2'	-5.48	97.12	102.60
1	N	169	G	N3-C2-N2	5.48	123.73	119.90
1	N	222	G	C5-C6-N1	5.47	114.24	111.50
1	N	223	C	N3-C2-O2	-5.47	118.07	121.90
1	N	329	G	N7-C8-N9	5.47	115.83	113.10
1	N	192	U	O4'-C4'-C3'	-5.46	98.54	104.00
1	N	250	A	C2'-C3'-O3'	5.46	122.44	113.70
1	N	255	U	C5'-C4'-C3'	-5.46	107.26	116.00
1	N	293	U	P-O3'-C3'	5.46	126.25	119.70
1	N	305	A	N3-C4-N9	-5.46	123.03	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	210	C	OP1-P-OP2	-5.46	111.42	119.60
1	N	212	A	C2-N3-C4	-5.46	107.87	110.60
1	N	313	A	C6-C5-N7	-5.45	128.48	132.30
1	N	214	C	C1'-O4'-C4'	5.45	114.26	109.90
1	N	291	U	P-O5'-C5'	-5.45	112.19	120.90
1	N	328	G	N9-C4-C5	5.45	107.58	105.40
1	N	338	C	C6-N1-C2	-5.44	118.12	120.30
1	N	238	C	N3-C2-O2	-5.44	118.09	121.90
1	N	153	G	C5-N7-C8	-5.44	101.58	104.30
1	N	219	G	N3-C4-N9	5.43	129.26	126.00
1	N	191	G	C6-C5-N7	-5.43	127.14	130.40
1	N	201	A	C5'-C4'-O4'	-5.43	102.58	109.10
1	N	181	G	C1'-O4'-C4'	5.43	114.24	109.90
1	N	316	G	O4'-C1'-N9	5.43	112.54	108.20
1	N	135	C	C6-N1-C1'	-5.42	114.29	120.80
1	N	288	C	C6-N1-C2	-5.42	118.13	120.30
1	N	229	G	N1-C6-O6	5.42	123.15	119.90
1	N	170	A	C4-C5-C6	5.42	119.71	117.00
1	N	352	A	N1-C2-N3	5.42	132.01	129.30
1	N	178	A	C5-C6-N6	5.42	128.03	123.70
1	N	236	G	C6-C5-N7	-5.42	127.15	130.40
1	N	239	A	C4'-C3'-C2'	-5.42	97.18	102.60
1	N	208	G	N1-C2-N2	-5.42	111.33	116.20
1	N	202	G	O4'-C1'-N9	5.41	112.53	108.20
1	N	316	G	C6-C5-N7	-5.41	127.15	130.40
1	N	139	G	N1-C2-N3	-5.41	120.65	123.90
1	N	169	G	C5-C6-O6	-5.41	125.36	128.60
1	N	171	G	C1'-O4'-C4'	-5.41	105.57	109.90
1	N	350	A	C5-C6-N6	-5.41	119.38	123.70
1	N	311	U	C4'-C3'-C2'	-5.40	97.20	102.60
1	N	220	A	N7-C8-N9	-5.40	111.10	113.80
1	N	136	G	O5'-C5'-C4'	5.40	121.96	111.70
1	N	185	U	O3'-P-O5'	5.40	114.26	104.00
1	N	229	G	N3-C4-C5	-5.39	125.91	128.60
1	N	329	G	N9-C4-C5	5.38	107.55	105.40
1	N	350	A	C2-N3-C4	5.38	113.29	110.60
1	N	164	G	N9-C4-C5	5.38	107.55	105.40
1	N	311	U	P-O5'-C5'	5.37	129.50	120.90
1	N	307	G	C4-C5-N7	-5.37	108.65	110.80
1	N	247	G	N7-C8-N9	-5.37	110.42	113.10
1	N	147	C	N3-C2-O2	-5.36	118.15	121.90
1	N	321	C	O4'-C1'-N1	5.36	112.49	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	329	G	C4-N9-C1'	5.36	133.47	126.50
1	N	360	C	N1-C1'-C2'	-5.36	106.11	112.00
1	N	236	G	N1-C2-N3	-5.36	120.69	123.90
1	N	307	G	O3'-P-O5'	5.36	114.17	104.00
1	N	146	G	N7-C8-N9	5.35	115.78	113.10
1	N	242	C	C2-N1-C1'	5.35	124.69	118.80
1	N	339	A	C8-N9-C4	-5.35	103.66	105.80
1	N	356	U	O4'-C1'-N1	5.35	112.48	108.20
1	N	236	G	O4'-C1'-N9	5.35	112.48	108.20
1	N	332	C	C6-N1-C1'	-5.34	114.39	120.80
1	N	136	G	C4-C5-N7	5.34	112.94	110.80
1	N	165	U	C4-C5-C6	-5.34	116.50	119.70
1	N	308	A	N3-C4-C5	-5.34	123.06	126.80
1	N	224	U	C6-N1-C2	-5.34	117.80	121.00
1	N	341	G	P-O3'-C3'	-5.34	113.29	119.70
1	N	228	U	N3-C4-C5	-5.34	111.40	114.60
1	N	278	G	C5-N7-C8	5.34	106.97	104.30
1	N	313	A	C4-C5-N7	5.34	113.37	110.70
1	N	201	A	OP1-P-OP2	-5.33	111.60	119.60
1	N	303	G	C4-C5-C6	5.33	122.00	118.80
1	N	337	G	C5-C6-N1	-5.33	108.83	111.50
1	N	341	G	C4-C5-N7	-5.33	108.67	110.80
1	N	308	A	O3'-P-O5'	5.32	114.11	104.00
1	N	139	G	C5-C6-O6	-5.32	125.41	128.60
1	N	253	C	P-O5'-C5'	-5.32	112.40	120.90
1	N	297	A	C1'-O4'-C4'	5.32	114.15	109.90
1	N	217	G	C8-N9-C4	-5.31	104.28	106.40
1	N	359	G	C6-N1-C2	5.31	128.29	125.10
1	N	141	G	C2-N3-C4	5.31	114.55	111.90
1	N	194	C	C2-N1-C1'	-5.31	112.96	118.80
1	N	332	C	C3'-C2'-C1'	5.31	105.75	101.50
1	N	317	G	N1-C6-O6	5.31	123.08	119.90
1	N	190	A	N1-C2-N3	5.30	131.95	129.30
1	N	284	A	C4'-C3'-C2'	-5.30	97.30	102.60
1	N	311	U	C5-C4-O4	-5.30	122.72	125.90
1	N	272	C	C4'-C3'-C2'	-5.30	97.30	102.60
1	N	227	G	C4-C5-C6	-5.30	115.62	118.80
1	N	262	U	O4'-C1'-N1	5.30	112.44	108.20
1	N	322	U	N1-C2-O2	-5.30	119.09	122.80
1	N	191	G	C4-N9-C1'	-5.29	119.62	126.50
1	N	167	C	C5-C6-N1	5.29	123.64	121.00
1	N	277	G	O4'-C1'-N9	5.29	112.43	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	247	G	C8-N9-C4	5.28	108.51	106.40
1	N	345	G	C2-N3-C4	-5.27	109.27	111.90
1	N	157	G	C3'-C2'-C1'	5.27	105.71	101.50
1	N	311	U	N1-C2-O2	-5.27	119.11	122.80
1	N	137	U	C6-N1-C2	-5.26	117.84	121.00
1	N	217	G	C2-N3-C4	5.26	114.53	111.90
1	N	227	G	C5-N7-C8	-5.26	101.67	104.30
1	N	251	C	C2-N3-C4	5.26	122.53	119.90
1	N	204	A	N7-C8-N9	5.26	116.43	113.80
1	N	283	A	C6-C5-N7	-5.26	128.62	132.30
1	N	180	A	C5'-C4'-C3'	5.26	124.41	116.00
1	N	217	G	N3-C2-N2	5.26	123.58	119.90
1	N	136	G	O3'-P-O5'	-5.25	94.02	104.00
1	N	323	G	C2-N3-C4	-5.25	109.27	111.90
1	N	142	G	C8-N9-C1'	5.25	133.83	127.00
1	N	228	U	O4'-C1'-N1	5.25	112.40	108.20
1	N	320	G	N3-C2-N2	5.25	123.57	119.90
1	N	199	U	O5'-P-OP1	5.25	117.00	110.70
1	N	240	U	OP1-P-OP2	-5.25	111.73	119.60
1	N	165	U	C4'-C3'-C2'	-5.24	97.36	102.60
1	N	158	G	N3-C4-C5	5.24	131.22	128.60
1	N	198	G	C3'-C2'-C1'	-5.24	97.31	101.50
1	N	285	U	C5-C4-O4	-5.24	122.76	125.90
1	N	298	U	P-O5'-C5'	5.24	129.28	120.90
1	N	333	A	N3-C4-N9	-5.24	123.21	127.40
1	N	341	G	N3-C4-C5	-5.24	125.98	128.60
1	N	220	A	C5-C6-N1	5.23	120.31	117.70
1	N	266	G	C5-C6-O6	-5.23	125.46	128.60
1	N	215	U	C2-N1-C1'	5.22	123.97	117.70
1	N	227	G	C1'-O4'-C4'	-5.22	105.72	109.90
1	N	205	C	N3-C2-O2	-5.21	118.25	121.90
1	N	282	A	C4-C5-N7	-5.21	108.09	110.70
1	N	204	A	P-O5'-C5'	5.21	129.24	120.90
1	N	266	G	C5-C6-N1	5.21	114.11	111.50
1	N	177	G	C6-N1-C2	-5.21	121.97	125.10
1	N	233	G	N1-C2-N3	-5.21	120.78	123.90
1	N	337	G	N3-C2-N2	5.21	123.55	119.90
1	N	217	G	N9-C4-C5	-5.20	103.32	105.40
1	N	236	G	N7-C8-N9	5.20	115.70	113.10
1	N	334	C	OP1-P-OP2	-5.20	111.80	119.60
1	N	285	U	N1-C2-O2	-5.20	119.16	122.80
1	N	282	A	N9-C4-C5	5.20	107.88	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	311	U	C5'-C4'-O4'	-5.19	102.87	109.10
1	N	204	A	C1'-O4'-C4'	-5.19	105.75	109.90
1	N	270	G	C6-N1-C2	-5.18	121.99	125.10
1	N	276	A	C5-C6-N1	-5.18	115.11	117.70
1	N	360	C	N3-C4-N4	-5.18	114.38	118.00
1	N	179	C	C4'-C3'-C2'	-5.18	97.42	102.60
1	N	190	A	C4'-C3'-C2'	-5.17	97.43	102.60
1	N	175	A	N1-C6-N6	-5.16	115.50	118.60
1	N	349	A	C5-N7-C8	-5.16	101.32	103.90
1	N	196	A	C4-C5-C6	-5.16	114.42	117.00
1	N	170	A	C6-C5-N7	-5.16	128.69	132.30
1	N	308	A	C8-N9-C4	-5.16	103.74	105.80
1	N	334	C	C5'-C4'-O4'	5.15	115.28	109.10
1	N	308	A	C2-N3-C4	5.15	113.18	110.60
1	N	346	U	O3'-P-O5'	5.15	113.79	104.00
1	N	329	G	C5-C6-N1	-5.15	108.93	111.50
1	N	331	C	O4'-C1'-N1	5.14	112.32	108.20
1	N	274	C	N1-C2-O2	-5.14	115.82	118.90
1	N	164	G	P-O3'-C3'	5.14	125.86	119.70
1	N	320	G	N3-C4-C5	-5.13	126.03	128.60
1	N	200	G	C4-C5-N7	-5.13	108.75	110.80
1	N	196	A	N1-C6-N6	5.13	121.68	118.60
1	N	322	U	N3-C2-O2	5.12	125.79	122.20
1	N	339	A	C2-N3-C4	5.12	113.16	110.60
1	N	354	U	C3'-C2'-C1'	5.12	105.60	101.50
1	N	159	U	OP2-P-O3'	5.12	116.46	105.20
1	N	157	G	N1-C6-O6	-5.12	116.83	119.90
1	N	161	U	C5-C6-N1	-5.11	120.14	122.70
1	N	175	A	C4-C5-C6	-5.11	114.44	117.00
1	N	229	G	C6-N1-C2	5.11	128.17	125.10
1	N	233	G	C4-C5-C6	-5.11	115.73	118.80
1	N	216	C	N3-C4-C5	-5.11	119.86	121.90
1	N	226	C	C2-N1-C1'	5.11	124.42	118.80
1	N	167	C	N1-C2-N3	5.11	122.78	119.20
1	N	259	C	P-O3'-C3'	-5.10	113.58	119.70
1	N	313	A	OP1-P-OP2	-5.10	111.95	119.60
1	N	162	A	C5'-C4'-C3'	5.10	124.16	116.00
1	N	315	A	C5-C6-N1	-5.09	115.15	117.70
1	N	231	A	C6-C5-N7	-5.09	128.74	132.30
1	N	281	G	C5'-C4'-O4'	-5.09	102.99	109.10
1	N	318	G	C4-N9-C1'	5.09	133.11	126.50
1	N	269	G	N1-C6-O6	5.08	122.95	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	272	C	N3-C4-C5	5.08	123.93	121.90
1	N	252	A	N9-C4-C5	5.08	107.83	105.80
1	N	274	C	C5-C6-N1	5.08	123.54	121.00
1	N	228	U	N3-C4-O4	5.08	122.95	119.40
1	N	239	A	C5-N7-C8	5.07	106.44	103.90
1	N	273	G	C4-C5-C6	-5.07	115.76	118.80
1	N	318	G	C2-N3-C4	5.07	114.44	111.90
1	N	161	U	C1'-O4'-C4'	5.07	113.96	109.90
1	N	178	A	O4'-C4'-C3'	-5.07	98.93	104.00
1	N	236	G	N3-C4-N9	5.06	129.04	126.00
1	N	153	G	P-O5'-C5'	-5.06	112.80	120.90
1	N	170	A	C5-C6-N1	-5.06	115.17	117.70
1	N	227	G	C4'-C3'-C2'	-5.06	97.54	102.60
1	N	180	A	C4-C5-N7	-5.06	108.17	110.70
1	N	241	G	C5-C6-N1	-5.06	108.97	111.50
1	N	291	U	C5'-C4'-O4'	5.06	115.17	109.10
1	N	233	G	N1-C2-N2	5.05	120.75	116.20
1	N	155	G	N1-C2-N2	-5.05	111.66	116.20
1	N	286	C	N3-C4-C5	-5.05	119.88	121.90
1	N	326	G	N3-C2-N2	-5.05	116.37	119.90
1	N	191	G	O5'-P-OP2	-5.04	101.16	105.70
1	N	281	G	N1-C2-N3	-5.04	120.87	123.90
1	N	282	A	N3-C4-N9	-5.04	123.36	127.40
1	N	328	G	C8-N9-C1'	5.04	133.55	127.00
1	N	198	G	C2-N3-C4	5.04	114.42	111.90
1	N	219	G	O4'-C1'-N9	5.04	112.23	108.20
1	N	252	A	C4'-C3'-C2'	5.04	107.64	102.60
1	N	142	G	C4-C5-C6	-5.03	115.78	118.80
1	N	204	A	C4'-C3'-C2'	-5.03	97.57	102.60
1	N	194	C	N3-C4-N4	5.03	121.52	118.00
1	N	307	G	C6-C5-N7	5.03	133.41	130.40
1	N	183	C	C5'-C4'-C3'	5.02	124.04	116.00
1	N	151	C	C2-N1-C1'	5.02	124.32	118.80
1	N	295	U	C4-C5-C6	-5.02	116.69	119.70
1	N	302	G	OP1-P-OP2	-5.02	112.07	119.60
1	N	275	U	C5-C4-O4	5.01	128.91	125.90
1	N	262	U	N3-C4-C5	-5.01	111.59	114.60
1	N	128	G	C6-C5-N7	-5.01	127.39	130.40
1	N	183	C	P-O3'-C3'	5.01	125.71	119.70
1	N	335	U	P-O3'-C3'	-5.00	113.69	119.70
1	N	156	U	C6-N1-C2	-5.00	118.00	121.00
1	N	224	U	C5-C4-O4	-5.00	122.90	125.90

There are no chirality outliers.

All (122) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	N	128	G	Sidechain
1	N	130	C	Sidechain
1	N	132	A	Sidechain
1	N	135	C	Sidechain
1	N	136	G	Sidechain
1	N	137	U	Sidechain
1	N	138	A	Sidechain
1	N	140	U	Sidechain
1	N	142	G	Sidechain
1	N	144	G	Sidechain
1	N	145	A	Sidechain
1	N	146	G	Sidechain
1	N	147	C	Sidechain
1	N	148	U	Sidechain
1	N	151	C	Sidechain
1	N	152	U	Sidechain
1	N	153	G	Sidechain
1	N	155	G	Sidechain
1	N	156	U	Sidechain
1	N	160	C	Sidechain
1	N	162	A	Sidechain
1	N	164	G	Sidechain
1	N	165	U	Sidechain
1	N	166	C	Sidechain
1	N	168	U	Sidechain
1	N	169	G	Sidechain
1	N	170	A	Sidechain
1	N	171	G	Sidechain
1	N	173	A	Sidechain
1	N	177	G	Sidechain
1	N	179	C	Sidechain
1	N	180	A	Sidechain
1	N	181	G	Sidechain
1	N	182	U	Sidechain
1	N	186	C	Sidechain
1	N	188	G	Sidechain
1	N	191	G	Sidechain
1	N	192	U	Sidechain
1	N	195	G	Sidechain
1	N	197	C	Sidechain

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Mol	Chain	Res	Type	Group
1	N	199	U	Sidechain
1	N	202	G	Sidechain
1	N	203	C	Sidechain
1	N	204	A	Sidechain
1	N	206	U	Sidechain
1	N	212	A	Sidechain
1	N	215	U	Sidechain
1	N	219	G	Sidechain
1	N	220	A	Sidechain
1	N	227	G	Sidechain
1	N	229	G	Sidechain
1	N	233	G	Sidechain
1	N	239	A	Sidechain
1	N	241	G	Sidechain
1	N	242	C	Sidechain
1	N	244	C	Sidechain
1	N	245	A	Sidechain
1	N	246	A	Sidechain
1	N	247	G	Sidechain
1	N	248	A	Sidechain
1	N	250	A	Sidechain
1	N	251	C	Sidechain
1	N	255	U	Sidechain
1	N	257	A	Sidechain
1	N	258	A	Sidechain
1	N	263	G	Sidechain
1	N	266	G	Sidechain
1	N	268	G	Sidechain
1	N	269	G	Sidechain
1	N	271	U	Sidechain
1	N	272	C	Sidechain
1	N	273	G	Sidechain
1	N	277	G	Sidechain
1	N	278	G	Sidechain
1	N	281	G	Sidechain
1	N	283	A	Sidechain
1	N	284	A	Sidechain
1	N	285	U	Sidechain
1	N	286	C	Sidechain
1	N	288	C	Sidechain
1	N	289	A	Sidechain
1	N	290	U	Sidechain

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Mol	Chain	Res	Type	Group
1	N	291	U	Sidechain
1	N	292	A	Sidechain
1	N	293	U	Sidechain
1	N	295	U	Sidechain
1	N	296	G	Sidechain
1	N	297	A	Sidechain
1	N	298	U	Sidechain
1	N	299	G	Sidechain
1	N	301	G	Sidechain
1	N	302	G	Sidechain
1	N	304	U	Sidechain
1	N	311	U	Sidechain
1	N	312	G	Sidechain
1	N	314	U	Sidechain
1	N	315	A	Sidechain
1	N	317	G	Sidechain
1	N	318	G	Sidechain
1	N	319	U	Sidechain
1	N	320	G	Sidechain
1	N	321	C	Sidechain
1	N	322	U	Sidechain
1	N	323	G	Sidechain
1	N	325	A	Sidechain
1	N	326	G	Sidechain
1	N	327	A	Sidechain
1	N	328	G	Sidechain
1	N	332	C	Sidechain
1	N	333	A	Sidechain
1	N	335	U	Sidechain
1	N	336	A	Sidechain
1	N	339	A	Sidechain
1	N	340	G	Sidechain
1	N	343	U	Sidechain
1	N	345	G	Sidechain
1	N	346	U	Sidechain
1	N	349	A	Sidechain
1	N	352	A	Sidechain
1	N	355	C	Sidechain
1	N	356	U	Sidechain
1	N	359	G	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	N	4986	0	2463	72	0
All	All	4986	0	2463	72	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (72) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:283:A:H3'	1:N:284:A:H5'	1.38	1.05
1:N:283:A:C3'	1:N:284:A:H5'	1.94	0.96
1:N:283:A:H3'	1:N:284:A:C5'	2.10	0.79
1:N:263:G:H1	1:N:275:U:H3	1.35	0.72
1:N:319:U:H2'	1:N:320:G:C5'	2.20	0.72
1:N:153:G:H1	1:N:255:U:H3	1.37	0.71
1:N:204:A:C2	1:N:208:G:C6	2.81	0.69
1:N:244:C:H3'	1:N:245:A:C4'	2.24	0.67
1:N:283:A:N9	1:N:284:A:N9	2.43	0.67
1:N:164:G:C2	1:N:180:A:C2	2.84	0.65
1:N:283:A:C8	1:N:284:A:C8	2.84	0.65
1:N:135:C:N1	1:N:136:G:N9	2.46	0.63
1:N:135:C:C6	1:N:136:G:C8	2.87	0.62
1:N:318:G:C2	1:N:319:U:C2	2.88	0.61
1:N:135:C:C2	1:N:136:G:H1'	2.35	0.61
1:N:164:G:N1	1:N:180:A:C2	2.69	0.61
1:N:180:A:C2	1:N:181:G:C5	2.89	0.61
1:N:283:A:C4	1:N:284:A:C4	2.88	0.60
1:N:201:A:H61	1:N:210:C:N4	2.03	0.57
1:N:283:A:N1	1:N:284:A:N1	2.54	0.55
1:N:319:U:H2'	1:N:320:G:H5'	1.90	0.53
1:N:358:U:H2'	1:N:359:G:C8	2.43	0.53
1:N:135:C:C5	1:N:136:G:C5	2.97	0.52
1:N:190:A:C6	1:N:191:G:C5	2.97	0.52
1:N:148:U:H3	1:N:302:G:H1	1.57	0.52
1:N:170:A:H2'	1:N:173:A:H61	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:185:U:C4	1:N:186:C:C4	2.98	0.52
1:N:283:A:C2	1:N:284:A:C2	2.99	0.51
1:N:162:A:C4	1:N:246:A:C2	2.98	0.51
1:N:181:G:H2'	1:N:182:U:C6	2.45	0.50
1:N:255:U:O2	1:N:257:A:C6	2.64	0.50
1:N:170:A:H2'	1:N:173:A:N6	2.26	0.50
1:N:283:A:C2'	1:N:284:A:H5'	2.42	0.50
1:N:283:A:N9	1:N:284:A:C8	2.80	0.49
1:N:135:C:N1	1:N:136:G:C8	2.80	0.49
1:N:244:C:H3'	1:N:245:A:H4'	1.95	0.49
1:N:179:C:H2'	1:N:180:A:C8	2.48	0.48
1:N:135:C:H3'	1:N:136:G:O4'	2.12	0.48
1:N:135:C:C4	1:N:136:G:C4	3.02	0.48
1:N:173:A:H5''	1:N:236:G:H21	1.78	0.48
1:N:161:U:C2	1:N:162:A:C8	3.01	0.48
1:N:250:A:C2	1:N:251:C:C4	3.01	0.48
1:N:250:A:H2'	1:N:251:C:C6	2.48	0.47
1:N:180:A:C2	1:N:181:G:C8	3.03	0.47
1:N:283:A:N1	1:N:284:A:C2	2.82	0.47
1:N:267:G:H1	1:N:271:U:H3	1.61	0.47
1:N:289:A:N1	1:N:294:G:C6	2.82	0.47
1:N:133:G:H2'	1:N:134:C:H6	1.80	0.47
1:N:319:U:H2'	1:N:320:G:H5''	1.94	0.47
1:N:283:A:C6	1:N:284:A:N1	2.84	0.46
1:N:134:C:C4	1:N:135:C:C5	3.04	0.46
1:N:195:G:H2'	1:N:196:A:C8	2.50	0.46
1:N:238:C:H3'	1:N:239:A:C5'	2.45	0.46
1:N:244:C:C4	1:N:245:A:C4	3.04	0.45
1:N:283:A:C6	1:N:284:A:C6	3.05	0.45
1:N:186:C:C2	1:N:231:A:N1	2.85	0.44
1:N:283:A:C4	1:N:284:A:N9	2.85	0.44
1:N:311:U:H3	1:N:316:G:H1	1.64	0.44
1:N:244:C:H3'	1:N:245:A:O4'	2.18	0.44
1:N:230:G:H2'	1:N:231:A:C8	2.53	0.44
1:N:204:A:C2	1:N:208:G:C5	3.06	0.43
1:N:305:A:C2	1:N:306:C:C4	3.05	0.43
1:N:204:A:H3'	1:N:205:C:C5'	2.49	0.43
1:N:283:A:C5	1:N:284:A:C5	3.08	0.42
1:N:327:A:H3'	1:N:328:G:H5''	2.02	0.42
1:N:187:A:H2	1:N:229:G:O6	2.03	0.41
1:N:133:G:C6	1:N:134:C:C4	3.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:133:G:H2'	1:N:134:C:C6	2.55	0.41
1:N:135:C:C6	1:N:136:G:N9	2.89	0.41
1:N:288:C:H2'	1:N:289:A:O4'	2.21	0.41
1:N:146:G:H4'	1:N:146:G:OP1	2.21	0.41
1:N:289:A:C2	1:N:294:G:C2	3.09	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein molecules in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein molecules in this entry.

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	N	232/233 (99%)	63 (27%)	21 (9%)

All (63) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	N	136	G
1	N	137	U
1	N	143	C
1	N	145	A
1	N	146	G
1	N	152	U
1	N	153	G
1	N	158	G
1	N	162	A
1	N	163	A
1	N	164	G
1	N	171	G
1	N	173	A

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Mol	Chain	Res	Type
1	N	180	A
1	N	182	U
1	N	192	U
1	N	196	A
1	N	205	C
1	N	206	U
1	N	207	A
1	N	218	A
1	N	219	G
1	N	220	A
1	N	221	U
1	N	222	G
1	N	227	G
1	N	228	U
1	N	229	G
1	N	234	A
1	N	235	G
1	N	238	C
1	N	239	A
1	N	240	U
1	N	241	G
1	N	245	A
1	N	250	A
1	N	256	U
1	N	257	A
1	N	258	A
1	N	269	G
1	N	270	G
1	N	284	A
1	N	291	U
1	N	292	A
1	N	293	U
1	N	299	G
1	N	305	A
1	N	308	A
1	N	309	C
1	N	313	A
1	N	322	U
1	N	324	C
1	N	325	A
1	N	327	A
1	N	328	G

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Mol	Chain	Res	Type
1	N	329	G
1	N	331	C
1	N	337	G
1	N	338	C
1	N	340	G
1	N	347	A
1	N	349	A
1	N	354	U

All (21) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	N	135	C
1	N	136	G
1	N	152	U
1	N	157	G
1	N	161	U
1	N	163	A
1	N	179	C
1	N	181	G
1	N	191	G
1	N	195	G
1	N	233	G
1	N	234	A
1	N	256	U
1	N	257	A
1	N	284	A
1	N	290	U
1	N	298	U
1	N	304	U
1	N	307	G
1	N	308	A
1	N	313	A

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.