



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:39 PM GMT

PDB ID : 1LBG
Title : LACTOSE OPERON REPRESSOR BOUND TO 21-BASE PAIR SYMMETRIC OPERATOR DNA, ALPHA CARBONS ONLY
Authors : Lewis, M.; Chang, G.; Horton, N.C.; Kercher, M.A.; Pace, H.C.; Lu, P.
Deposited on : 1996-01-03
Resolution : 4.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
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) : trunk26865

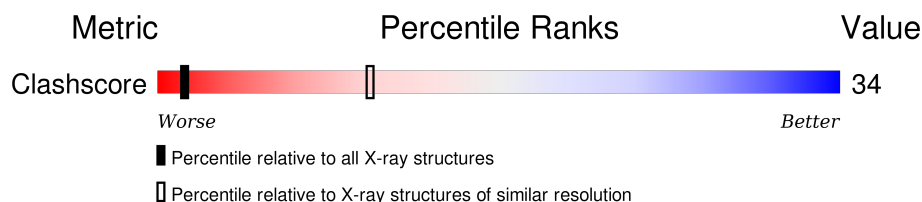
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.80 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1017 (5.96-3.64)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	E	21	 14% 86%
1	F	21	 38% 62%
1	G	21	 24% 76%
1	H	21	 29% 71%
2	A	360	 99% .
2	B	360	 99% .
2	C	360	 99% .
2	D	360	 98% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3144 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 DNA chain called DNA (5'-D(*GP*AP*AP*TP*TP*GP*TP*GP*AP*GP*CP*GP*CP*TP*CP*AP*CP*AP*AP*TP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	21	Total	C	N	O	P	0	0	0
			429	206	79	124	20			
1	F	21	Total	C	N	O	P	0	0	0
			429	206	79	124	20			
1	G	21	Total	C	N	O	P	0	0	0
			429	206	79	124	20			
1	H	21	Total	C	N	O	P	0	0	0
			429	206	79	124	20			

- Molecule 2 is a protein called PROTEIN (LACTOSE OPERON REPRESSOR).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
2	A	357	Total	C	0	0	357
			357	357			
2	B	357	Total	C	0	0	357
			357	357			
2	C	357	Total	C	0	0	357
			357	357			
2	D	357	Total	C	0	0	357
			357	357			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	109	THR	ALA	CONFLICT	UNP P03023
B	109	THR	ALA	CONFLICT	UNP P03023
C	109	THR	ALA	CONFLICT	UNP P03023
D	109	THR	ALA	CONFLICT	UNP P03023

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

Note EDS was not executed.

- Molecule 1: DNA (5'-D(*GP*AP*AP*TP*TP*GP*TP*GP*AP*GP*CP*GP*CP*TP*CP*AP*CP*AP*AP*TP*T)-3')

Chain E: 



- Molecule 1: DNA (5'-D(*GP*AP*AP*TP*TP*GP*TP*GP*AP*GP*CP*GP*CP*TP*CP*AP*CP*AP*AP*TP*T)-3')

Chain F: 



- Molecule 1: DNA (5'-D(*GP*AP*AP*TP*TP*GP*TP*GP*AP*GP*CP*GP*CP*TP*CP*AP*CP*AP*AP*TP*T)-3')

Chain G: 



- Molecule 1: DNA (5'-D(*GP*AP*AP*TP*TP*GP*TP*GP*AP*GP*CP*GP*CP*TP*CP*AP*CP*AP*AP*TP*T)-3')

Chain H: 



- Molecule 2: PROTEIN (LACTOSE OPERON REPRESSOR)

Chain A: 



- Molecule 2: PROTEIN (LACTOSE OPERON REPRESSOR)

Chain B:  99% .



- Molecule 2: PROTEIN (LACTOSE OPERON REPRESSOR)

Chain C:  99% .



- Molecule 2: PROTEIN (LACTOSE OPERON REPRESSOR)

Chain D:  98% ..



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	104.30Å 224.40Å 112.10Å 90.00° 95.70° 90.00°	Depositor
Resolution (Å)	15.00 – 4.80	Depositor
% Data completeness (in resolution range)	(Not available) (15.00-4.80)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.260 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3144	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

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	$\# Z > 5$	RMSZ	$\# Z > 5$
1	E	3.40	68/481 (14.1%)	5.71	203/741 (27.4%)
1	F	3.02	50/481 (10.4%)	5.29	200/741 (27.0%)
1	G	3.59	49/481 (10.2%)	5.52	204/741 (27.5%)
1	H	3.18	46/481 (9.6%)	5.51	203/741 (27.4%)
All	All	3.31	213/1924 (11.1%)	5.51	810/2964 (27.3%)

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	E	3	18
1	F	1	15
1	G	3	16
1	H	3	17
All	All	10	66

All (213) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	620	DT	P-O5'	22.13	1.81	1.59
1	G	620	DT	C5'-C4'	20.02	1.73	1.51
1	G	602	DA	P-O5'	19.05	1.78	1.59
1	H	720	DT	P-O5'	17.03	1.76	1.59
1	G	601	DA	O3'-P	16.98	1.81	1.61
1	G	602	DA	C5'-C4'	15.75	1.68	1.51
1	F	518	DA	P-O5'	15.07	1.74	1.59
1	G	620	DT	C4'-C3'	14.12	1.67	1.53
1	G	601	DA	C2'-C1'	12.78	1.65	1.52
1	H	719	DT	C5'-C4'	12.57	1.65	1.51
1	G	601	DA	C3'-C2'	12.46	1.67	1.52
1	H	718	DA	C4'-C3'	12.36	1.65	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	601	DA	C3'-O3'	12.16	1.59	1.44
1	E	401	DA	O3'-P	12.02	1.75	1.61
1	E	401	DA	C5'-C4'	11.95	1.64	1.51
1	G	602	DA	O3'-P	11.71	1.75	1.61
1	E	406	DT	P-O5'	11.62	1.71	1.59
1	E	404	DT	C4'-C3'	11.57	1.65	1.53
1	E	418	DA	C5'-C4'	11.52	1.64	1.51
1	H	719	DT	P-O5'	11.48	1.71	1.59
1	F	518	DA	C5'-C4'	11.10	1.63	1.51
1	F	501	DA	O3'-P	11.07	1.74	1.61
1	G	602	DA	C4'-C3'	11.07	1.64	1.53
1	H	701	DA	C1'-N9	10.90	1.63	1.49
1	H	701	DA	N9-C4	10.72	1.44	1.37
1	G	601	DA	N9-C4	10.72	1.44	1.37
1	F	518	DA	C4'-C3'	10.65	1.64	1.53
1	E	406	DT	C5'-C4'	10.64	1.63	1.51
1	G	600	DG	C1'-N9	10.49	1.62	1.49
1	H	719	DT	C4'-C3'	10.47	1.63	1.53
1	H	718	DA	C5'-C4'	10.46	1.62	1.51
1	E	416	DC	C5'-C4'	10.28	1.62	1.51
1	E	406	DT	C4'-C3'	10.13	1.63	1.53
1	E	418	DA	P-O5'	10.11	1.69	1.59
1	H	717	DA	P-O5'	10.08	1.69	1.59
1	E	401	DA	N9-C4	10.07	1.43	1.37
1	H	701	DA	O3'-P	10.02	1.73	1.61
1	E	401	DA	P-O5'	9.85	1.69	1.59
1	G	600	DG	O3'-P	9.57	1.72	1.61
1	E	404	DT	P-O5'	9.46	1.69	1.59
1	F	500	DG	C3'-C2'	9.40	1.63	1.52
1	H	718	DA	P-O5'	9.28	1.69	1.59
1	H	718	DA	O3'-P	9.10	1.72	1.61
1	F	504	DT	C4'-C3'	9.09	1.62	1.53
1	F	500	DG	O3'-P	9.08	1.72	1.61
1	H	716	DC	C5'-C4'	9.04	1.61	1.51
1	F	500	DG	C1'-N9	8.85	1.60	1.49
1	F	518	DA	O3'-P	8.80	1.71	1.61
1	E	401	DA	C4'-C3'	8.78	1.62	1.53
1	E	406	DT	O3'-P	8.74	1.71	1.61
1	E	420	DT	C1'-N1	8.73	1.60	1.49
1	H	701	DA	C2'-C1'	8.71	1.61	1.52
1	G	605	DG	C2'-C1'	8.63	1.60	1.52
1	H	717	DA	C2'-C1'	8.39	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	702	DA	C2'-C1'	8.30	1.60	1.52
1	H	719	DT	O3'-P	8.25	1.71	1.61
1	H	701	DA	C6-N1	-8.12	1.29	1.35
1	G	608	DA	O3'-P	8.08	1.70	1.61
1	G	601	DA	C1'-N9	8.05	1.59	1.49
1	E	403	DT	O3'-P	8.01	1.70	1.61
1	E	419	DT	C5'-C4'	7.93	1.60	1.51
1	F	515	DA	C5'-C4'	7.91	1.60	1.51
1	F	515	DA	P-O5'	7.90	1.67	1.59
1	F	504	DT	P-O5'	7.86	1.67	1.59
1	H	701	DA	C3'-C2'	7.85	1.61	1.52
1	F	502	DA	P-O5'	7.85	1.67	1.59
1	H	703	DT	C5-C7	7.83	1.54	1.50
1	H	719	DT	C2'-C1'	7.81	1.60	1.52
1	E	401	DA	C3'-O3'	7.81	1.54	1.44
1	G	619	DT	C5-C7	7.63	1.54	1.50
1	E	418	DA	C6-N1	-7.60	1.30	1.35
1	F	503	DT	C2'-C1'	7.59	1.59	1.52
1	F	509	DG	C2-N3	-7.57	1.26	1.32
1	E	419	DT	C5-C7	-7.51	1.45	1.50
1	E	420	DT	N1-C2	7.48	1.44	1.38
1	G	620	DT	O5'-C5'	7.27	1.60	1.42
1	F	500	DG	C3'-O3'	7.26	1.53	1.44
1	F	518	DA	N9-C4	7.25	1.42	1.37
1	E	402	DA	C2'-C1'	-7.24	1.45	1.52
1	E	416	DC	O3'-P	7.21	1.69	1.61
1	F	518	DA	C3'-O3'	7.14	1.53	1.44
1	H	720	DT	C5'-C4'	7.12	1.59	1.51
1	E	419	DT	N1-C2	7.12	1.43	1.38
1	E	407	DG	C2'-C1'	7.11	1.59	1.52
1	G	602	DA	N9-C8	-7.08	1.32	1.37
1	H	704	DT	O3'-P	7.07	1.69	1.61
1	H	718	DA	C3'-O3'	7.06	1.53	1.44
1	E	408	DA	P-O5'	7.06	1.66	1.59
1	E	419	DT	P-O5'	7.04	1.66	1.59
1	F	503	DT	P-O5'	7.02	1.66	1.59
1	G	606	DT	P-O5'	6.98	1.66	1.59
1	E	407	DG	O3'-P	6.97	1.69	1.61
1	E	402	DA	N9-C8	-6.95	1.32	1.37
1	E	402	DA	C4'-C3'	-6.95	1.45	1.52
1	E	404	DT	O3'-P	6.94	1.69	1.61
1	H	717	DA	O3'-P	6.92	1.69	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	405	DG	O3'-P	6.91	1.69	1.61
1	E	415	DA	C2'-C1'	6.90	1.59	1.52
1	G	602	DA	C3'-O3'	6.89	1.52	1.44
1	F	500	DG	C2'-C1'	6.88	1.59	1.52
1	G	617	DA	O3'-P	6.86	1.69	1.61
1	F	510	DC	P-O5'	6.85	1.66	1.59
1	F	510	DC	C2'-C1'	6.84	1.59	1.52
1	E	401	DA	C2'-C1'	6.83	1.59	1.52
1	E	407	DG	P-O5'	6.81	1.66	1.59
1	E	418	DA	C3'-O3'	6.79	1.52	1.44
1	G	615	DA	P-O5'	6.75	1.66	1.59
1	H	701	DA	O4'-C1'	6.73	1.50	1.42
1	H	700	DG	C5'-C4'	6.73	1.58	1.51
1	F	520	DT	C2'-C1'	6.73	1.59	1.52
1	F	504	DT	O3'-P	6.72	1.69	1.61
1	F	505	DG	P-O5'	6.68	1.66	1.59
1	G	613	DT	C5-C7	6.63	1.54	1.50
1	G	605	DG	O3'-P	6.60	1.69	1.61
1	G	620	DT	N3-C4	-6.58	1.33	1.38
1	E	403	DT	C4'-C3'	6.58	1.59	1.53
1	H	701	DA	C4'-O4'	6.57	1.51	1.45
1	H	710	DC	C2'-C1'	6.56	1.58	1.52
1	H	713	DT	C5-C7	6.56	1.53	1.50
1	E	406	DT	C3'-O3'	6.53	1.52	1.44
1	E	420	DT	O4'-C1'	6.53	1.50	1.42
1	F	505	DG	C5'-C4'	6.53	1.58	1.51
1	G	602	DA	C5-C6	-6.52	1.35	1.41
1	E	405	DG	P-O5'	6.50	1.66	1.59
1	F	509	DG	P-O5'	6.48	1.66	1.59
1	G	600	DG	C3'-O3'	6.45	1.52	1.44
1	G	617	DA	P-O5'	6.30	1.66	1.59
1	F	503	DT	C1'-N1	6.28	1.57	1.49
1	G	619	DT	O3'-P	6.27	1.68	1.61
1	E	403	DT	C5'-C4'	6.25	1.58	1.51
1	H	702	DA	C4'-C3'	-6.23	1.46	1.52
1	E	418	DA	C4'-C3'	6.18	1.59	1.53
1	H	702	DA	P-O5'	6.17	1.66	1.59
1	H	706	DT	P-O5'	6.14	1.65	1.59
1	E	419	DT	N3-C4	-6.13	1.33	1.38
1	H	716	DC	P-O5'	6.12	1.65	1.59
1	G	603	DT	P-O5'	6.12	1.65	1.59
1	G	602	DA	C3'-C2'	-6.12	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	407	DG	N9-C4	6.11	1.42	1.38
1	G	619	DT	C5'-C4'	-6.11	1.44	1.51
1	H	720	DT	N1-C6	-6.08	1.33	1.38
1	G	616	DC	P-O5'	6.06	1.65	1.59
1	E	417	DA	C6-N1	-6.04	1.31	1.35
1	F	509	DG	O3'-P	5.98	1.68	1.61
1	H	720	DT	N1-C2	5.98	1.42	1.38
1	E	420	DT	C5'-C4'	5.97	1.57	1.51
1	G	613	DT	O3'-P	5.95	1.68	1.61
1	H	717	DA	C6-N1	-5.95	1.31	1.35
1	E	401	DA	N9-C8	-5.94	1.32	1.37
1	E	410	DC	C2'-C1'	5.94	1.58	1.52
1	G	610	DC	P-O5'	5.91	1.65	1.59
1	E	404	DT	C3'-O3'	5.90	1.51	1.44
1	G	600	DG	C5'-C4'	5.86	1.57	1.51
1	H	701	DA	C5'-C4'	5.85	1.57	1.51
1	G	602	DA	C8-N7	-5.82	1.27	1.31
1	E	413	DT	C5'-C4'	5.80	1.57	1.51
1	G	618	DA	P-O5'	5.79	1.65	1.59
1	H	702	DA	C6-N1	-5.78	1.31	1.35
1	F	519	DT	C5-C7	5.73	1.53	1.50
1	E	404	DT	C5'-C4'	5.72	1.57	1.51
1	F	515	DA	C2'-C1'	5.71	1.58	1.52
1	F	502	DA	C5-C6	-5.70	1.35	1.41
1	G	606	DT	C2'-C1'	5.70	1.58	1.52
1	E	405	DG	C5-C4	-5.67	1.34	1.38
1	F	502	DA	O3'-P	5.65	1.68	1.61
1	H	718	DA	N9-C4	5.64	1.41	1.37
1	E	410	DC	P-O5'	5.62	1.65	1.59
1	E	420	DT	C4'-O4'	5.61	1.50	1.45
1	E	410	DC	O3'-P	5.61	1.67	1.61
1	G	615	DA	C5'-C4'	5.60	1.57	1.51
1	H	701	DA	C3'-O3'	5.57	1.51	1.44
1	F	505	DG	N9-C4	-5.57	1.33	1.38
1	F	520	DT	C5-C7	-5.57	1.46	1.50
1	F	518	DA	C2'-C1'	5.56	1.57	1.52
1	F	517	DA	C5'-C4'	5.55	1.57	1.51
1	F	519	DT	N1-C2	5.53	1.42	1.38
1	G	620	DT	C3'-C2'	5.53	1.58	1.52
1	E	402	DA	O3'-P	5.47	1.67	1.61
1	G	618	DA	O3'-P	5.46	1.67	1.61
1	G	600	DG	C4'-C3'	5.43	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	508	DA	C6-N1	-5.41	1.31	1.35
1	F	513	DT	C5-C7	5.40	1.53	1.50
1	E	407	DG	C1'-N9	5.40	1.56	1.49
1	F	508	DA	C5'-C4'	5.38	1.57	1.51
1	E	415	DA	C1'-N9	5.38	1.56	1.49
1	F	507	DG	P-O5'	5.37	1.65	1.59
1	H	720	DT	C4'-C3'	5.37	1.58	1.53
1	F	515	DA	O3'-P	5.35	1.67	1.61
1	E	413	DT	O3'-P	5.35	1.67	1.61
1	H	713	DT	C5'-C4'	5.34	1.57	1.51
1	G	620	DT	C5-C7	-5.34	1.46	1.50
1	F	509	DG	N3-C4	-5.34	1.31	1.35
1	G	614	DC	P-O5'	5.32	1.65	1.59
1	E	419	DT	O3'-P	5.31	1.67	1.61
1	F	509	DG	C5'-C4'	5.26	1.57	1.51
1	F	519	DT	P-O5'	5.26	1.65	1.59
1	F	509	DG	N9-C4	-5.24	1.33	1.38
1	E	405	DG	C6-O6	-5.19	1.19	1.24
1	H	705	DG	C4'-O4'	-5.18	1.39	1.45
1	E	416	DC	C2-N3	5.18	1.39	1.35
1	E	409	DG	O3'-P	5.14	1.67	1.61
1	F	506	DT	C5'-C4'	5.11	1.56	1.51
1	H	717	DA	C3'-C2'	5.11	1.58	1.52
1	E	417	DA	P-O5'	5.10	1.64	1.59
1	G	608	DA	C5'-C4'	5.10	1.56	1.51
1	E	415	DA	N9-C4	5.09	1.41	1.37
1	G	618	DA	C5'-C4'	5.09	1.56	1.51
1	H	719	DT	C3'-O3'	5.08	1.50	1.44
1	E	418	DA	O3'-P	5.07	1.67	1.61
1	E	414	DC	P-O5'	5.05	1.64	1.59
1	F	517	DA	C4'-C3'	5.04	1.58	1.53
1	E	403	DT	C3'-O3'	5.03	1.50	1.44
1	F	520	DT	N3-C4	-5.01	1.34	1.38

All (810) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	420	DT	O4'-C1'-N1	41.82	137.27	108.00
1	F	520	DT	O4'-C1'-N1	32.28	130.60	108.00
1	H	702	DA	O4'-C4'-C3'	-30.45	87.73	106.00
1	G	600	DG	O4'-C1'-N9	29.83	128.88	108.00
1	E	401	DA	P-O3'-C3'	28.34	153.71	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	620	DT	O4'-C4'-C3'	-27.34	89.60	106.00
1	E	405	DG	O4'-C1'-N9	25.42	125.80	108.00
1	F	515	DA	O4'-C1'-N9	24.80	125.36	108.00
1	E	402	DA	P-O3'-C3'	24.69	149.33	119.70
1	E	403	DT	O4'-C1'-N1	24.48	125.14	108.00
1	G	601	DA	C4'-C3'-C2'	-22.86	82.53	103.10
1	E	416	DC	O4'-C1'-C2'	-22.63	87.80	105.90
1	G	600	DG	P-O3'-C3'	22.50	146.69	119.70
1	E	420	DT	O4'-C1'-C2'	-22.41	87.97	105.90
1	G	601	DA	C8-N9-C4	-21.71	97.12	105.80
1	H	717	DA	C4'-C3'-C2'	-20.80	84.38	103.10
1	G	620	DT	C1'-O4'-C4'	-20.66	89.44	110.10
1	H	704	DT	O4'-C1'-N1	20.62	122.44	108.00
1	E	404	DT	O4'-C1'-N1	20.61	122.43	108.00
1	H	709	DG	O4'-C1'-N9	19.81	121.87	108.00
1	H	707	DG	O4'-C4'-C3'	-19.70	94.18	106.00
1	H	717	DA	C1'-O4'-C4'	-19.66	90.44	110.10
1	G	616	DC	O4'-C1'-N1	19.53	121.67	108.00
1	G	605	DG	C4'-C3'-C2'	-19.48	85.57	103.10
1	F	500	DG	C8-N9-C4	-19.22	98.71	106.40
1	E	416	DC	O4'-C1'-N1	19.16	121.41	108.00
1	G	604	DT	O4'-C1'-N1	19.11	121.38	108.00
1	G	620	DT	O4'-C1'-N1	19.02	121.31	108.00
1	H	701	DA	O4'-C1'-N9	18.77	121.14	108.00
1	F	506	DT	P-O3'-C3'	18.48	141.87	119.70
1	H	701	DA	C8-N9-C4	-18.28	98.49	105.80
1	E	415	DA	P-O3'-C3'	18.27	141.63	119.70
1	F	518	DA	P-O3'-C3'	18.19	141.53	119.70
1	E	409	DG	O4'-C1'-N9	18.00	120.60	108.00
1	H	719	DT	C1'-O4'-C4'	-17.89	92.21	110.10
1	F	509	DG	O4'-C1'-N9	17.71	120.40	108.00
1	H	715	DA	O4'-C1'-N9	17.68	120.38	108.00
1	G	601	DA	N9-C1'-C2'	17.67	146.17	112.60
1	G	602	DA	C5-N7-C8	-17.41	95.19	103.90
1	H	712	DC	O4'-C1'-N1	17.33	120.13	108.00
1	G	606	DT	O4'-C1'-N1	16.85	119.79	108.00
1	H	718	DA	C4'-C3'-O3'	16.80	151.69	109.70
1	G	606	DT	P-O3'-C3'	16.79	139.84	119.70
1	E	402	DA	N7-C8-N9	16.68	122.14	113.80
1	F	519	DT	O4'-C1'-N1	16.66	119.67	108.00
1	H	716	DC	P-O3'-C3'	16.53	139.54	119.70
1	F	502	DA	C4'-C3'-C2'	-16.48	88.27	103.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	703	DT	O4'-C1'-N1	16.47	119.53	108.00
1	H	710	DC	O4'-C1'-N1	16.34	119.44	108.00
1	F	500	DG	O4'-C1'-N9	16.22	119.36	108.00
1	F	515	DA	P-O3'-C3'	16.18	139.11	119.70
1	G	601	DA	O4'-C1'-C2'	-16.13	93.00	105.90
1	H	700	DG	P-O3'-C3'	16.06	138.98	119.70
1	G	601	DA	P-O3'-C3'	15.99	138.89	119.70
1	H	719	DT	C4'-C3'-C2'	-15.98	88.72	103.10
1	H	702	DA	N9-C1'-C2'	15.98	142.96	112.60
1	H	718	DA	C5'-C4'-C3'	15.90	142.72	114.10
1	H	705	DG	O4'-C4'-C3'	-15.84	96.50	106.00
1	E	403	DT	O4'-C1'-C2'	-15.83	93.23	105.90
1	H	701	DA	O4'-C4'-C3'	-15.79	96.53	106.00
1	F	512	DC	O4'-C4'-C3'	-15.53	96.68	106.00
1	G	617	DA	O4'-C1'-N9	15.48	118.83	108.00
1	F	512	DC	O4'-C1'-N1	15.46	118.82	108.00
1	G	608	DA	O4'-C4'-C3'	15.45	115.27	106.00
1	H	718	DA	C4'-C3'-C2'	-15.21	89.42	103.10
1	G	612	DC	O4'-C1'-N1	15.20	118.64	108.00
1	F	509	DG	N3-C2-N2	-15.19	109.27	119.90
1	H	719	DT	C5'-C4'-C3'	15.19	141.44	114.10
1	H	702	DA	O4'-C1'-C2'	-14.99	93.91	105.90
1	H	701	DA	O4'-C1'-C2'	-14.94	93.95	105.90
1	E	419	DT	P-O3'-C3'	14.85	137.51	119.70
1	G	611	DG	O4'-C1'-N9	14.81	118.36	108.00
1	F	500	DG	C2-N3-C4	-14.68	104.56	111.90
1	F	510	DC	O4'-C1'-N1	14.56	118.19	108.00
1	E	417	DA	C4'-C3'-C2'	-14.55	90.00	103.10
1	G	616	DC	O4'-C1'-C2'	-14.36	94.41	105.90
1	H	719	DT	O4'-C4'-C3'	-14.34	97.39	106.00
1	G	602	DA	P-O5'-C5'	14.29	143.77	120.90
1	E	411	DG	O4'-C1'-N9	14.23	117.96	108.00
1	E	402	DA	O4'-C1'-C2'	-14.19	94.55	105.90
1	F	508	DA	P-O3'-C3'	14.17	136.71	119.70
1	F	519	DT	O4'-C4'-C3'	-14.15	97.51	106.00
1	E	402	DA	C8-N9-C4	-14.14	100.14	105.80
1	H	702	DA	C8-N9-C4	-14.13	100.15	105.80
1	G	618	DA	O4'-C1'-N9	14.00	117.80	108.00
1	E	418	DA	O4'-C1'-N9	13.96	117.77	108.00
1	E	406	DT	C4'-C3'-C2'	-13.92	90.57	103.10
1	H	709	DG	N3-C2-N2	-13.90	110.17	119.90
1	F	514	DC	C4'-C3'-C2'	-13.81	90.67	103.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	420	DT	C6-N1-C2	-13.77	114.41	121.30
1	H	708	DA	P-O5'-C5'	13.64	142.72	120.90
1	F	517	DA	O4'-C1'-N9	13.63	117.54	108.00
1	H	702	DA	N1-C2-N3	13.60	136.10	129.30
1	F	514	DC	O4'-C1'-N1	13.50	117.45	108.00
1	F	501	DA	C4'-C3'-C2'	-13.43	91.01	103.10
1	H	717	DA	C2-N3-C4	-13.43	103.89	110.60
1	G	608	DA	O4'-C1'-N9	13.33	117.33	108.00
1	E	407	DG	O4'-C4'-C3'	-13.29	98.03	106.00
1	G	620	DT	C4-C5-C7	-13.24	111.06	119.00
1	E	402	DA	O4'-C1'-N9	13.20	117.24	108.00
1	G	610	DC	O4'-C1'-N1	13.20	117.24	108.00
1	G	601	DA	N7-C8-N9	13.19	120.39	113.80
1	F	506	DT	O4'-C1'-C2'	-13.17	95.36	105.90
1	F	507	DG	O4'-C1'-C2'	-13.15	95.38	105.90
1	F	507	DG	O4'-C1'-N9	13.05	117.14	108.00
1	H	701	DA	P-O3'-C3'	13.00	135.30	119.70
1	H	718	DA	O4'-C4'-C3'	-12.99	98.21	106.00
1	G	618	DA	P-O3'-C3'	12.88	135.15	119.70
1	H	700	DG	O4'-C1'-N9	12.81	116.97	108.00
1	E	407	DG	C8-N9-C4	-12.79	101.28	106.40
1	G	618	DA	C8-N9-C4	-12.77	100.69	105.80
1	E	401	DA	C8-N9-C4	-12.68	100.73	105.80
1	E	415	DA	O4'-C1'-N9	12.67	116.87	108.00
1	H	703	DT	O4'-C1'-C2'	-12.65	95.78	105.90
1	F	501	DA	O4'-C1'-C2'	-12.60	95.82	105.90
1	E	403	DT	C4'-C3'-C2'	-12.57	91.79	103.10
1	F	500	DG	P-O3'-C3'	12.44	134.62	119.70
1	G	608	DA	C4'-C3'-C2'	-12.42	91.92	103.10
1	F	501	DA	O4'-C1'-N9	12.39	116.67	108.00
1	F	520	DT	C4-C5-C6	12.38	125.43	118.00
1	H	715	DA	P-O5'-C5'	12.37	140.69	120.90
1	G	620	DT	C5'-C4'-C3'	12.32	136.28	114.10
1	H	700	DG	O4'-C4'-C3'	-12.25	98.65	106.00
1	E	401	DA	C5'-C4'-C3'	12.24	136.14	114.10
1	H	717	DA	O4'-C1'-N9	12.20	116.54	108.00
1	H	720	DT	O4'-C1'-N1	12.11	116.47	108.00
1	E	404	DT	C4'-C3'-C2'	-12.10	92.21	103.10
1	F	519	DT	P-O3'-C3'	-12.10	105.19	119.70
1	H	702	DA	C4'-C3'-C2'	-12.08	92.23	103.10
1	F	510	DC	P-O3'-C3'	12.08	134.19	119.70
1	E	417	DA	P-O5'-C5'	12.07	140.22	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	620	DT	C4-C5-C6	12.07	125.24	118.00
1	G	614	DC	O4'-C1'-N1	12.06	116.44	108.00
1	E	417	DA	O4'-C4'-C3'	12.05	113.23	106.00
1	E	416	DC	N3-C4-N4	12.01	126.41	118.00
1	E	409	DG	C4-N9-C1'	-11.94	110.98	126.50
1	E	401	DA	O4'-C1'-N9	11.93	116.35	108.00
1	F	504	DT	P-O3'-C3'	11.88	133.96	119.70
1	E	407	DG	P-O5'-C5'	11.84	139.84	120.90
1	E	415	DA	O4'-C1'-C2'	-11.83	96.44	105.90
1	G	602	DA	C4'-C3'-C2'	-11.80	92.48	103.10
1	E	408	DA	C8-N9-C4	-11.79	101.09	105.80
1	G	602	DA	C8-N9-C4	-11.77	101.09	105.80
1	F	500	DG	O4'-C1'-C2'	-11.74	96.50	105.90
1	G	609	DG	P-O5'-C5'	11.73	139.67	120.90
1	H	714	DC	O4'-C1'-N1	11.69	116.18	108.00
1	H	718	DA	P-O5'-C5'	11.64	139.52	120.90
1	F	500	DG	N9-C1'-C2'	11.60	134.64	112.60
1	F	500	DG	N7-C8-N9	11.54	118.87	113.10
1	H	710	DC	P-O3'-C3'	11.50	133.50	119.70
1	F	507	DG	P-O3'-C3'	11.40	133.38	119.70
1	G	607	DG	O4'-C1'-N9	11.40	115.98	108.00
1	E	417	DA	C2-N3-C4	-11.37	104.91	110.60
1	E	415	DA	C8-N9-C4	-11.31	101.28	105.80
1	E	412	DC	C4'-C3'-C2'	-11.30	92.93	103.10
1	H	701	DA	N1-C2-N3	11.24	134.92	129.30
1	H	709	DG	C8-N9-C4	-11.23	101.91	106.40
1	E	419	DT	C4-C5-C6	11.14	124.69	118.00
1	E	403	DT	N3-C2-O2	-11.10	115.64	122.30
1	G	600	DG	N3-C4-C5	-10.99	123.11	128.60
1	F	509	DG	N9-C4-C5	10.99	109.80	105.40
1	F	514	DC	P-O5'-C5'	10.98	138.46	120.90
1	F	502	DA	O4'-C4'-C3'	-10.96	99.42	106.00
1	H	718	DA	O3'-P-O5'	10.89	124.70	104.00
1	H	719	DT	C4'-C3'-O3'	10.89	136.93	109.70
1	H	720	DT	C4-C5-C6	10.88	124.53	118.00
1	E	419	DT	N3-C2-O2	-10.78	115.83	122.30
1	E	406	DT	O4'-C1'-N1	10.76	115.53	108.00
1	E	417	DA	N1-C2-N3	10.75	134.68	129.30
1	G	608	DA	P-O5'-C5'	10.73	138.07	120.90
1	H	717	DA	N1-C2-N3	10.65	134.63	129.30
1	H	715	DA	O4'-C4'-C3'	10.63	112.38	106.00
1	F	509	DG	N1-C2-N2	10.63	125.76	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	413	DT	O4'-C1'-C2'	-10.59	97.43	105.90
1	E	407	DG	N9-C1'-C2'	10.57	132.69	112.60
1	G	615	DA	O4'-C1'-N9	10.54	115.38	108.00
1	E	409	DG	N3-C2-N2	-10.54	112.52	119.90
1	F	520	DT	C5'-C4'-C3'	10.53	133.06	114.10
1	F	520	DT	C4-C5-C7	-10.48	112.71	119.00
1	F	509	DG	C8-N9-C4	-10.43	102.23	106.40
1	H	719	DT	P-O3'-C3'	10.41	132.19	119.70
1	F	503	DT	O4'-C1'-C2'	-10.40	97.58	105.90
1	H	701	DA	N9-C1'-C2'	10.38	132.33	112.60
1	E	417	DA	O4'-C1'-C2'	-10.38	97.60	105.90
1	F	518	DA	C4'-C3'-C2'	-10.37	93.77	103.10
1	E	418	DA	O3'-P-O5'	10.36	123.69	104.00
1	H	710	DC	P-O5'-C5'	10.35	137.46	120.90
1	G	600	DG	C8-N9-C4	-10.30	102.28	106.40
1	F	500	DG	C5-C6-N1	-10.26	106.37	111.50
1	H	718	DA	C1'-O4'-C4'	-10.26	99.84	110.10
1	G	617	DA	C4'-C3'-C2'	-10.25	93.88	103.10
1	E	417	DA	O4'-C1'-N9	10.24	115.17	108.00
1	G	601	DA	N1-C2-N3	10.21	134.41	129.30
1	H	705	DG	O4'-C1'-N9	-10.20	100.86	108.00
1	E	402	DA	C5-N7-C8	-10.19	98.80	103.90
1	G	620	DT	P-O5'-C5'	10.11	137.08	120.90
1	E	416	DC	C5-C4-N4	-10.10	113.13	120.20
1	E	401	DA	C3'-C2'-C1'	10.08	114.60	102.50
1	F	509	DG	N3-C4-N9	-10.08	119.95	126.00
1	H	701	DA	N7-C8-N9	10.02	118.81	113.80
1	E	420	DT	P-O5'-C5'	9.98	136.87	120.90
1	G	609	DG	P-O3'-C3'	9.95	131.64	119.70
1	H	709	DG	N9-C4-C5	9.94	109.38	105.40
1	F	512	DC	N1-C2-O2	9.88	124.83	118.90
1	E	408	DA	N1-C2-N3	9.86	134.23	129.30
1	E	409	DG	N1-C2-N2	9.86	125.07	116.20
1	E	409	DG	N9-C1'-C2'	9.85	131.32	112.60
1	G	605	DG	C1'-O4'-C4'	-9.85	100.25	110.10
1	E	405	DG	P-O5'-C5'	9.84	136.64	120.90
1	G	619	DT	O3'-P-O5'	9.84	122.69	104.00
1	H	702	DA	C5-N7-C8	-9.82	98.99	103.90
1	F	518	DA	O4'-C1'-N9	9.81	114.86	108.00
1	E	411	DG	P-O5'-C5'	9.78	136.55	120.90
1	F	506	DT	C4-C5-C6	9.77	123.86	118.00
1	F	514	DC	P-O3'-C3'	9.74	131.39	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	603	DT	N3-C2-O2	-9.74	116.45	122.30
1	G	620	DT	N1-C1'-C2'	9.73	131.09	112.60
1	G	618	DA	N7-C8-N9	9.72	118.66	113.80
1	G	601	DA	O3'-P-O5'	9.72	122.47	104.00
1	G	607	DG	C4'-C3'-C2'	-9.70	94.37	103.10
1	G	620	DT	C5-C6-N1	-9.64	117.92	123.70
1	G	602	DA	O4'-C1'-N9	9.59	114.72	108.00
1	G	602	DA	C5-C6-N6	-9.57	116.04	123.70
1	G	606	DT	C4-C5-C6	9.57	123.74	118.00
1	H	712	DC	N1-C2-O2	9.57	124.64	118.90
1	E	420	DT	C4-C5-C6	9.54	123.72	118.00
1	G	619	DT	C3'-C2'-C1'	-9.53	91.07	102.50
1	E	406	DT	P-O3'-C3'	9.53	131.13	119.70
1	H	712	DC	O4'-C4'-C3'	-9.51	100.30	106.00
1	E	420	DT	C5'-C4'-O4'	9.49	127.33	109.30
1	E	404	DT	C4-C5-C7	-9.48	113.31	119.00
1	E	403	DT	C6-N1-C2	-9.48	116.56	121.30
1	F	518	DA	C8-N9-C4	-9.48	102.01	105.80
1	F	507	DG	C8-N9-C4	-9.47	102.61	106.40
1	G	602	DA	N1-C6-N6	9.43	124.26	118.60
1	E	420	DT	C3'-C2'-C1'	9.43	113.81	102.50
1	G	607	DG	C8-N9-C4	-9.40	102.64	106.40
1	H	717	DA	C5-C6-N1	-9.39	113.00	117.70
1	E	416	DC	C4'-C3'-C2'	-9.38	94.66	103.10
1	F	502	DA	P-O5'-C5'	9.37	135.90	120.90
1	F	501	DA	N1-C2-N3	9.37	133.99	129.30
1	H	717	DA	C8-N9-C4	-9.37	102.05	105.80
1	F	501	DA	N7-C8-N9	9.36	118.48	113.80
1	F	503	DT	N1-C1'-C2'	9.36	130.38	112.60
1	F	513	DT	O4'-C1'-C2'	-9.36	98.41	105.90
1	F	504	DT	O4'-C1'-N1	9.33	114.53	108.00
1	F	519	DT	N3-C2-O2	-9.32	116.71	122.30
1	E	408	DA	N7-C8-N9	9.30	118.45	113.80
1	F	503	DT	O4'-C4'-C3'	-9.30	100.42	106.00
1	E	401	DA	C4'-C3'-O3'	9.29	132.92	109.70
1	G	603	DT	O4'-C1'-C2'	-9.24	98.51	105.90
1	H	707	DG	C8-N9-C4	-9.20	102.72	106.40
1	F	516	DC	O4'-C4'-C3'	-9.19	100.48	106.00
1	H	713	DT	O4'-C1'-C2'	-9.15	98.58	105.90
1	E	420	DT	O5'-C5'-C4'	9.15	133.87	111.00
1	H	720	DT	N3-C2-O2	-9.11	116.83	122.30
1	G	617	DA	N1-C2-N3	9.10	133.85	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	516	DC	P-O5'-C5'	9.09	135.45	120.90
1	E	410	DC	N1-C2-O2	9.09	124.36	118.90
1	G	606	DT	C4-C5-C7	-9.07	113.56	119.00
1	E	417	DA	C8-N9-C4	-9.06	102.18	105.80
1	H	709	DG	N1-C2-N2	9.04	124.34	116.20
1	E	401	DA	N7-C8-N9	9.03	118.31	113.80
1	H	717	DA	N9-C1'-C2'	9.01	129.73	112.60
1	H	719	DT	O4'-C1'-N1	8.99	114.30	108.00
1	F	517	DA	N1-C2-N3	8.99	133.79	129.30
1	E	420	DT	N3-C2-O2	-8.97	116.92	122.30
1	H	707	DG	N9-C1'-C2'	8.97	129.64	112.60
1	H	717	DA	C5-C6-N6	8.96	130.87	123.70
1	F	501	DA	C8-N9-C4	-8.96	102.22	105.80
1	F	510	DC	P-O5'-C5'	8.95	135.21	120.90
1	E	401	DA	O4'-C1'-C2'	-8.94	98.75	105.90
1	G	600	DG	C6-N1-C2	-8.92	119.75	125.10
1	G	611	DG	C4'-C3'-C2'	-8.92	95.07	103.10
1	G	609	DG	O4'-C1'-N9	8.90	114.23	108.00
1	G	600	DG	N9-C4-C5	8.90	108.96	105.40
1	E	417	DA	N9-C4-C5	8.88	109.35	105.80
1	G	602	DA	N9-C1'-C2'	-8.87	95.75	112.60
1	F	500	DG	C3'-C2'-C1'	8.87	113.14	102.50
1	F	517	DA	C2-N3-C4	-8.85	106.17	110.60
1	H	712	DC	C4'-C3'-C2'	-8.84	95.15	103.10
1	F	502	DA	C2-N3-C4	-8.81	106.20	110.60
1	E	405	DG	N1-C2-N2	8.78	124.10	116.20
1	G	607	DG	O4'-C1'-C2'	-8.76	98.89	105.90
1	E	416	DC	P-O3'-C3'	8.74	130.19	119.70
1	H	717	DA	O4'-C1'-C2'	-8.73	98.92	105.90
1	F	519	DT	O5'-P-OP1	-8.68	97.89	105.70
1	H	715	DA	C4'-C3'-C2'	-8.66	95.31	103.10
1	E	404	DT	C4-C5-C6	8.65	123.19	118.00
1	H	702	DA	C2-N3-C4	-8.65	106.28	110.60
1	F	516	DC	N3-C4-N4	8.64	124.05	118.00
1	H	704	DT	P-O3'-C3'	8.64	130.07	119.70
1	E	407	DG	N7-C8-N9	8.64	117.42	113.10
1	G	605	DG	C5'-C4'-C3'	8.64	129.65	114.10
1	E	406	DT	O4'-C1'-C2'	-8.62	99.00	105.90
1	G	613	DT	P-O3'-C3'	8.62	130.05	119.70
1	E	404	DT	O4'-C4'-C3'	8.61	111.16	106.00
1	G	618	DA	N1-C6-N6	-8.60	113.44	118.60
1	G	612	DC	C4'-C3'-C2'	-8.59	95.37	103.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	515	DA	O4'-C4'-C3'	8.58	111.15	106.00
1	G	600	DG	N3-C2-N2	-8.54	113.92	119.90
1	F	504	DT	C4-C5-C6	8.54	123.12	118.00
1	H	717	DA	N9-C4-C5	8.53	109.21	105.80
1	F	508	DA	O4'-C1'-C2'	-8.51	99.09	105.90
1	G	601	DA	O5'-P-OP2	-8.51	98.04	105.70
1	F	504	DT	C4'-C3'-C2'	-8.51	95.44	103.10
1	F	520	DT	C5-C6-N1	-8.50	118.60	123.70
1	H	707	DG	N7-C8-N9	8.44	117.32	113.10
1	H	701	DA	N9-C4-C5	8.42	109.17	105.80
1	G	606	DT	O4'-C1'-C2'	-8.41	99.17	105.90
1	F	514	DC	C6-N1-C2	-8.40	116.94	120.30
1	H	720	DT	O4'-C1'-C2'	-8.39	99.18	105.90
1	F	515	DA	C4'-C3'-C2'	-8.38	95.56	103.10
1	E	417	DA	C5-C6-N6	8.37	130.40	123.70
1	F	519	DT	N1-C1'-C2'	8.35	128.46	112.60
1	H	703	DT	P-O3'-C3'	8.35	129.71	119.70
1	G	618	DA	N9-C4-C5	8.34	109.14	105.80
1	E	420	DT	C4-C5-C7	-8.34	114.00	119.00
1	E	404	DT	P-O3'-C3'	8.32	129.69	119.70
1	F	515	DA	P-O5'-C5'	8.31	134.19	120.90
1	E	402	DA	C4'-C3'-O3'	8.29	130.44	109.70
1	E	400	DG	O4'-C1'-N9	8.29	113.80	108.00
1	H	704	DT	O4'-C1'-C2'	-8.28	99.28	105.90
1	H	702	DA	P-O3'-C3'	-8.27	109.77	119.70
1	G	607	DG	O4'-C4'-C3'	8.27	110.96	106.00
1	H	715	DA	N1-C6-N6	8.27	123.56	118.60
1	F	503	DT	C6-N1-C2	-8.26	117.17	121.30
1	E	407	DG	O4'-C1'-C2'	-8.26	99.29	105.90
1	F	502	DA	N1-C6-N6	8.25	123.55	118.60
1	G	603	DT	O4'-C1'-N1	8.23	113.76	108.00
1	H	712	DC	C1'-O4'-C4'	-8.21	101.89	110.10
1	G	604	DT	N3-C4-O4	8.20	124.82	119.90
1	G	601	DA	N9-C4-C5	8.18	109.07	105.80
1	G	608	DA	O5'-C5'-C4'	8.17	131.43	111.00
1	G	602	DA	C4'-C3'-O3'	8.16	130.11	109.70
1	E	400	DG	C2-N3-C4	-8.16	107.82	111.90
1	F	500	DG	C1'-O4'-C4'	8.16	118.26	110.10
1	H	713	DT	C5-C4-O4	-8.15	119.20	124.90
1	F	514	DC	N3-C2-O2	-8.14	116.20	121.90
1	G	616	DC	C4'-C3'-C2'	-8.14	95.78	103.10
1	F	520	DT	O4'-C4'-C3'	-8.10	101.14	106.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	601	DA	C3'-C2'-C1'	8.08	112.19	102.50
1	G	602	DA	O4'-C1'-C2'	-8.07	99.44	105.90
1	H	713	DT	N3-C4-O4	8.07	124.74	119.90
1	E	416	DC	C6-N1-C2	-8.06	117.08	120.30
1	G	615	DA	N9-C4-C5	8.05	109.02	105.80
1	G	618	DA	C5-C6-N6	8.05	130.14	123.70
1	G	608	DA	C8-N9-C4	-8.04	102.59	105.80
1	H	711	DG	O4'-C1'-C2'	-8.03	99.47	105.90
1	F	500	DG	N9-C4-C5	8.03	108.61	105.40
1	E	415	DA	C4'-C3'-O3'	8.02	129.76	109.70
1	G	601	DA	C5-C6-N6	8.02	130.12	123.70
1	H	700	DG	O4'-C1'-C2'	-8.01	99.49	105.90
1	H	718	DA	P-O3'-C3'	8.01	129.31	119.70
1	G	618	DA	O4'-C1'-C2'	-8.00	99.50	105.90
1	G	604	DT	O4'-C4'-C3'	7.98	110.79	106.00
1	H	707	DG	O4'-C1'-C2'	-7.97	99.52	105.90
1	E	410	DC	N3-C2-O2	-7.97	116.32	121.90
1	H	700	DG	C8-N9-C4	-7.96	103.21	106.40
1	E	407	DG	N3-C4-C5	-7.95	124.62	128.60
1	H	719	DT	N1-C1'-C2'	7.93	127.66	112.60
1	E	406	DT	C4-C5-C6	7.92	122.75	118.00
1	F	504	DT	N3-C4-O4	7.90	124.64	119.90
1	H	702	DA	C1'-O4'-C4'	-7.87	102.23	110.10
1	G	619	DT	O4'-C4'-C3'	-7.85	101.29	106.00
1	F	511	DG	P-O3'-C3'	7.84	129.11	119.70
1	F	503	DT	C4'-C3'-C2'	-7.84	96.05	103.10
1	H	710	DC	N3-C2-O2	-7.80	116.44	121.90
1	H	714	DC	O4'-C1'-C2'	-7.79	99.67	105.90
1	F	515	DA	N1-C2-N3	7.79	133.19	129.30
1	G	613	DT	C4'-C3'-C2'	-7.78	96.10	103.10
1	E	405	DG	C2-N3-C4	7.77	115.79	111.90
1	E	409	DG	O4'-C4'-C3'	7.77	110.66	106.00
1	G	610	DC	N1-C2-O2	7.77	123.56	118.90
1	E	417	DA	O5'-C5'-C4'	7.75	130.38	111.00
1	H	716	DC	O4'-C1'-C2'	-7.75	99.70	105.90
1	G	611	DG	C5'-C4'-C3'	-7.73	100.18	114.10
1	E	405	DG	C5-C6-O6	-7.73	123.97	128.60
1	E	420	DT	N1-C2-N3	7.71	119.23	114.60
1	H	714	DC	O4'-C4'-C3'	-7.70	101.38	106.00
1	E	405	DG	C5-C6-N1	7.67	115.34	111.50
1	E	417	DA	C5-C6-N1	-7.67	113.86	117.70
1	F	508	DA	C2-N3-C4	-7.67	106.77	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	515	DA	C2-N3-C4	-7.65	106.77	110.60
1	H	710	DC	N1-C2-O2	7.65	123.49	118.90
1	E	415	DA	N1-C2-N3	7.64	133.12	129.30
1	F	503	DT	O3'-P-O5'	7.63	118.50	104.00
1	G	608	DA	O3'-P-O5'	7.63	118.49	104.00
1	H	708	DA	O4'-C1'-N9	7.62	113.33	108.00
1	F	508	DA	C4'-C3'-C2'	-7.61	96.25	103.10
1	F	514	DC	O4'-C4'-C3'	7.61	110.56	106.00
1	E	408	DA	N9-C1'-C2'	7.59	127.02	112.60
1	E	401	DA	P-O5'-C5'	7.59	133.04	120.90
1	G	602	DA	C5'-C4'-C3'	7.59	127.75	114.10
1	E	410	DC	O4'-C1'-N1	7.56	113.30	108.00
1	G	617	DA	C2-N3-C4	-7.56	106.82	110.60
1	E	414	DC	P-O5'-C5'	7.55	132.97	120.90
1	F	517	DA	O5'-C5'-C4'	7.54	129.86	111.00
1	F	502	DA	C4'-C3'-O3'	7.52	128.49	109.70
1	F	503	DT	N1-C2-N3	7.49	119.10	114.60
1	H	717	DA	N3-C4-N9	-7.48	121.41	127.40
1	G	601	DA	C2-N3-C4	-7.48	106.86	110.60
1	H	713	DT	O4'-C1'-N1	7.47	113.23	108.00
1	E	414	DC	P-O3'-C3'	7.46	128.65	119.70
1	H	701	DA	C5-C6-N6	7.44	129.65	123.70
1	H	704	DT	C4-C5-C6	7.43	122.46	118.00
1	F	516	DC	O5'-C5'-C4'	7.42	129.54	111.00
1	G	615	DA	C8-N9-C4	-7.42	102.83	105.80
1	G	619	DT	P-O3'-C3'	7.42	128.60	119.70
1	G	602	DA	C3'-C2'-C1'	7.38	111.36	102.50
1	H	716	DC	N1-C2-O2	7.38	123.33	118.90
1	E	406	DT	C4'-C3'-O3'	7.36	128.11	109.70
1	E	408	DA	O4'-C1'-C2'	-7.35	100.02	105.90
1	F	508	DA	O5'-C5'-C4'	7.35	129.37	111.00
1	F	500	DG	C5-N7-C8	-7.34	100.63	104.30
1	F	501	DA	C4'-C3'-O3'	7.34	128.06	109.70
1	E	405	DG	C1'-O4'-C4'	-7.34	102.76	110.10
1	E	415	DA	N7-C8-N9	7.33	117.47	113.80
1	H	702	DA	C6-N1-C2	-7.33	114.20	118.60
1	E	415	DA	N1-C6-N6	7.33	123.00	118.60
1	E	418	DA	C5'-C4'-C3'	7.33	127.28	114.10
1	H	709	DG	N7-C8-N9	7.32	116.76	113.10
1	E	405	DG	C4-N9-C1'	-7.32	116.99	126.50
1	F	502	DA	C5'-C4'-O4'	-7.32	95.40	109.30
1	G	612	DC	O4'-C4'-C3'	-7.31	101.58	104.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	506	DT	C6-C5-C7	-7.31	118.51	122.90
1	G	614	DC	N3-C4-C5	-7.31	118.98	121.90
1	G	614	DC	P-O5'-C5'	7.29	132.57	120.90
1	F	506	DT	O4'-C1'-N1	7.28	113.09	108.00
1	E	418	DA	C2-N3-C4	-7.25	106.97	110.60
1	H	704	DT	O4'-C4'-C3'	7.25	110.35	106.00
1	H	701	DA	C1'-O4'-C4'	7.25	117.35	110.10
1	H	715	DA	O4'-C1'-C2'	-7.25	100.10	105.90
1	G	608	DA	C1'-O4'-C4'	-7.25	102.85	110.10
1	G	607	DG	P-O3'-C3'	7.24	128.39	119.70
1	H	719	DT	P-O5'-C5'	7.23	132.47	120.90
1	E	416	DC	O5'-P-OP2	-7.21	99.21	105.70
1	E	405	DG	C8-N9-C1'	7.21	136.37	127.00
1	G	606	DT	C6-N1-C2	-7.21	117.70	121.30
1	H	704	DT	C4'-C3'-C2'	-7.19	96.63	103.10
1	F	520	DT	C4'-C3'-C2'	-7.17	96.65	103.10
1	G	606	DT	O5'-P-OP2	-7.14	99.28	105.70
1	E	418	DA	C4'-C3'-C2'	-7.14	96.68	103.10
1	E	414	DC	C6-N1-C2	-7.13	117.45	120.30
1	H	711	DG	N3-C4-N9	7.13	130.28	126.00
1	F	519	DT	C4-C5-C6	7.13	122.28	118.00
1	E	413	DT	P-O5'-C5'	7.12	132.29	120.90
1	G	616	DC	N3-C2-O2	-7.12	116.92	121.90
1	F	520	DT	P-O5'-C5'	7.11	132.28	120.90
1	F	505	DG	C4-N9-C1'	-7.08	117.29	126.50
1	F	501	DA	C2-N3-C4	-7.08	107.06	110.60
1	H	718	DA	C8-N9-C4	-7.08	102.97	105.80
1	G	609	DG	C5'-C4'-O4'	-7.06	95.89	109.30
1	H	714	DC	N3-C4-C5	-7.06	119.08	121.90
1	H	706	DT	O4'-C4'-C3'	7.05	110.23	106.00
1	G	601	DA	C5-C6-N1	-7.04	114.18	117.70
1	G	611	DG	O4'-C1'-C2'	-7.03	100.28	105.90
1	E	420	DT	C4'-C3'-C2'	-7.03	96.78	103.10
1	E	418	DA	C8-N9-C4	-7.02	102.99	105.80
1	G	610	DC	N3-C2-O2	-7.01	116.99	121.90
1	E	404	DT	C5'-C4'-O4'	-7.00	96.00	109.30
1	F	506	DT	C4'-C3'-O3'	6.99	127.18	109.70
1	H	719	DT	C4-C5-C6	6.98	122.19	118.00
1	H	705	DG	O4'-C1'-C2'	-6.97	100.33	105.90
1	G	600	DG	C2-N3-C4	6.96	115.38	111.90
1	G	601	DA	C4'-C3'-O3'	6.95	127.07	109.70
1	E	409	DG	C5-C6-O6	-6.93	124.44	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	607	DG	N7-C8-N9	6.92	116.56	113.10
1	H	702	DA	N7-C8-N9	6.91	117.26	113.80
1	F	516	DC	O4'-C1'-C2'	-6.90	100.38	105.90
1	G	601	DA	C2'-C3'-O3'	6.88	135.30	112.60
1	G	620	DT	C4'-C3'-O3'	6.88	126.89	109.70
1	H	709	DG	N3-C4-N9	-6.87	121.88	126.00
1	H	705	DG	N9-C1'-C2'	6.85	125.61	112.60
1	H	715	DA	C5-C6-N6	-6.85	118.22	123.70
1	F	512	DC	C1'-O4'-C4'	-6.83	103.27	110.10
1	G	606	DT	P-O5'-C5'	6.82	131.82	120.90
1	H	718	DA	O4'-C1'-N9	6.82	112.78	108.00
1	G	606	DT	C4'-C3'-O3'	6.80	126.71	109.70
1	F	515	DA	C4'-C3'-O3'	6.80	126.70	109.70
1	H	719	DT	N1-C2-N3	6.80	118.68	114.60
1	E	415	DA	C3'-C2'-C1'	6.79	110.65	102.50
1	F	508	DA	P-O5'-C5'	6.79	131.76	120.90
1	E	412	DC	C2-N3-C4	6.78	123.29	119.90
1	G	619	DT	P-O5'-C5'	-6.78	110.05	120.90
1	H	705	DG	N7-C8-N9	6.78	116.49	113.10
1	F	506	DT	O5'-P-OP2	-6.77	99.60	105.70
1	E	415	DA	C2-N3-C4	-6.77	107.21	110.60
1	E	405	DG	O4'-C4'-C3'	6.77	110.06	106.00
1	G	604	DT	C4'-C3'-C2'	-6.77	97.01	103.10
1	F	508	DA	O4'-C4'-C3'	6.75	110.05	106.00
1	E	407	DG	C4'-C3'-C2'	-6.74	97.03	103.10
1	F	500	DG	C4'-C3'-C2'	-6.74	97.03	103.10
1	G	605	DG	C8-N9-C4	-6.72	103.71	106.40
1	F	505	DG	C5-N7-C8	-6.72	100.94	104.30
1	H	707	DG	C8-N9-C1'	-6.71	118.27	127.00
1	F	507	DG	N3-C2-N2	-6.71	115.20	119.90
1	G	618	DA	C4'-C3'-O3'	6.69	126.42	109.70
1	G	602	DA	O5'-P-OP2	-6.68	99.69	105.70
1	F	516	DC	C4'-C3'-C2'	-6.67	97.10	103.10
1	H	708	DA	C8-N9-C4	-6.66	103.14	105.80
1	H	707	DG	O3'-P-O5'	6.66	116.65	104.00
1	E	405	DG	N3-C2-N2	-6.66	115.24	119.90
1	F	509	DG	C4-N9-C1'	-6.61	117.90	126.50
1	G	604	DT	O4'-C1'-C2'	-6.61	100.61	105.90
1	E	404	DT	N3-C2-O2	-6.61	118.34	122.30
1	H	704	DT	C6-C5-C7	-6.60	118.94	122.90
1	H	702	DA	O4'-C1'-N9	-6.60	103.38	108.00
1	H	706	DT	P-O5'-C5'	-6.60	110.34	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	612	DC	N1-C2-O2	6.59	122.86	118.90
1	F	508	DA	N1-C2-N3	6.58	132.59	129.30
1	G	606	DT	N3-C2-O2	-6.58	118.35	122.30
1	E	407	DG	C4-N9-C1'	6.58	135.06	126.50
1	E	419	DT	C6-N1-C2	-6.57	118.01	121.30
1	E	419	DT	N1-C1'-C2'	6.55	125.06	112.60
1	E	401	DA	C4-C5-C6	6.55	120.27	117.00
1	E	418	DA	N1-C2-N3	6.55	132.57	129.30
1	F	518	DA	C3'-C2'-C1'	6.54	110.35	102.50
1	F	507	DG	C4'-C3'-C2'	-6.54	97.22	103.10
1	H	714	DC	C4'-C3'-O3'	6.54	126.04	109.70
1	H	709	DG	P-O3'-C3'	6.53	127.54	119.70
1	G	616	DC	N3-C4-C5	-6.53	119.29	121.90
1	E	408	DA	C2-N3-C4	-6.52	107.34	110.60
1	F	512	DC	N1-C1'-C2'	6.52	124.98	112.60
1	E	404	DT	N1-C2-N3	6.51	118.51	114.60
1	G	605	DG	O3'-P-O5'	6.50	116.35	104.00
1	F	509	DG	N7-C8-N9	6.49	116.35	113.10
1	F	510	DC	N3-C2-O2	-6.49	117.36	121.90
1	G	610	DC	P-O3'-C3'	6.49	127.48	119.70
1	E	418	DA	O4'-C1'-C2'	-6.49	100.71	105.90
1	H	702	DA	C5'-C4'-C3'	6.49	125.77	114.10
1	G	618	DA	P-O5'-C5'	6.48	131.27	120.90
1	H	703	DT	O5'-P-OP2	-6.47	99.88	105.70
1	G	603	DT	O3'-P-O5'	6.46	116.27	104.00
1	H	720	DT	P-O5'-C5'	6.46	131.24	120.90
1	H	706	DT	C6-C5-C7	-6.44	119.04	122.90
1	F	520	DT	O4'-C1'-C2'	-6.44	100.75	105.90
1	H	705	DG	C8-N9-C4	-6.43	103.83	106.40
1	E	419	DT	P-O5'-C5'	6.40	131.14	120.90
1	F	518	DA	C5'-C4'-C3'	6.40	125.61	114.10
1	G	615	DA	P-O3'-C3'	-6.39	112.03	119.70
1	H	716	DC	N3-C2-O2	-6.39	117.43	121.90
1	H	717	DA	N7-C8-N9	6.38	116.99	113.80
1	E	411	DG	C8-N9-C4	-6.37	103.85	106.40
1	H	719	DT	O3'-P-O5'	6.37	116.11	104.00
1	H	701	DA	C3'-C2'-C1'	6.37	110.14	102.50
1	F	504	DT	C5'-C4'-O4'	-6.34	97.24	109.30
1	H	709	DG	C3'-C2'-C1'	6.34	110.11	102.50
1	F	506	DT	C3'-C2'-C1'	6.33	110.09	102.50
1	F	509	DG	C4'-C3'-C2'	-6.32	97.41	103.10
1	F	519	DT	P-O5'-C5'	6.32	131.00	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	616	DC	P-O5'-C5'	6.31	131.00	120.90
1	H	701	DA	C4-C5-C6	6.31	120.16	117.00
1	G	620	DT	C3'-C2'-C1'	-6.31	94.93	102.50
1	E	405	DG	O5'-P-OP1	-6.30	100.03	105.70
1	G	614	DC	O4'-C4'-C3'	-6.30	101.98	104.50
1	H	706	DT	C4-C5-C6	6.30	121.78	118.00
1	H	715	DA	C1'-O4'-C4'	-6.29	103.81	110.10
1	F	520	DT	C5'-C4'-O4'	6.29	121.25	109.30
1	H	701	DA	C2-N3-C4	-6.28	107.46	110.60
1	G	607	DG	N3-C2-N2	-6.28	115.51	119.90
1	E	413	DT	N1-C1'-C2'	6.28	124.52	112.60
1	E	419	DT	C4-C5-C7	-6.27	115.24	119.00
1	E	406	DT	O3'-P-O5'	6.27	115.91	104.00
1	F	517	DA	C4'-C3'-O3'	6.26	125.36	109.70
1	F	510	DC	O4'-C1'-C2'	-6.26	100.89	105.90
1	E	410	DC	O3'-P-O5'	6.25	115.88	104.00
1	G	605	DG	O4'-C1'-C2'	-6.23	100.91	105.90
1	H	708	DA	N1-C2-N3	6.23	132.42	129.30
1	G	607	DG	N9-C4-C5	6.22	107.89	105.40
1	H	713	DT	P-O5'-C5'	6.22	130.85	120.90
1	F	506	DT	O3'-P-O5'	6.22	115.82	104.00
1	E	403	DT	O3'-P-O5'	6.21	115.80	104.00
1	H	712	DC	N3-C2-O2	-6.21	117.55	121.90
1	H	704	DT	C6-N1-C2	-6.20	118.20	121.30
1	H	713	DT	C4'-C3'-C2'	-6.20	97.52	103.10
1	F	509	DG	C5-N7-C8	-6.18	101.21	104.30
1	H	700	DG	O3'-P-O5'	6.17	115.72	104.00
1	F	506	DT	P-O5'-C5'	6.16	130.76	120.90
1	F	504	DT	N3-C4-C5	-6.15	111.51	115.20
1	G	602	DA	O5'-C5'-C4'	6.15	126.37	111.00
1	H	717	DA	C5'-C4'-O4'	6.14	120.96	109.30
1	E	401	DA	C8-N9-C1'	-6.13	116.66	127.70
1	F	517	DA	O4'-C1'-C2'	-6.12	101.00	105.90
1	F	514	DC	N1-C2-N3	6.11	123.48	119.20
1	G	604	DT	O5'-P-OP1	-6.11	100.20	105.70
1	E	400	DG	P-O3'-C3'	6.10	127.02	119.70
1	E	412	DC	C1'-O4'-C4'	-6.09	104.01	110.10
1	E	404	DT	C1'-O4'-C4'	-6.09	104.01	110.10
1	H	709	DG	C5-N7-C8	-6.08	101.26	104.30
1	H	705	DG	P-O5'-C5'	6.08	130.62	120.90
1	F	512	DC	C2-N3-C4	6.06	122.93	119.90
1	G	614	DC	C6-N1-C2	-6.06	117.88	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	609	DG	C8-N9-C4	-6.05	103.98	106.40
1	H	707	DG	C4-N9-C1'	6.05	134.37	126.50
1	F	518	DA	O4'-C4'-C3'	6.05	109.63	106.00
1	F	507	DG	N7-C8-N9	6.03	116.11	113.10
1	H	709	DG	C4-N9-C1'	-6.03	118.67	126.50
1	F	505	DG	N3-C4-N9	-6.02	122.39	126.00
1	F	502	DA	C1'-O4'-C4'	-6.02	104.08	110.10
1	E	403	DT	C4-C5-C6	6.02	121.61	118.00
1	F	518	DA	N7-C8-N9	6.02	116.81	113.80
1	F	510	DC	N1-C2-O2	6.01	122.51	118.90
1	H	716	DC	O4'-C1'-N1	6.01	112.21	108.00
1	E	403	DT	C4'-C3'-O3'	6.01	124.73	109.70
1	F	515	DA	C8-N9-C4	-6.01	103.39	105.80
1	G	605	DG	P-O5'-C5'	6.00	130.50	120.90
1	F	516	DC	N1-C2-O2	6.00	122.50	118.90
1	F	516	DC	C5-C4-N4	-6.00	116.00	120.20
1	G	620	DT	N3-C4-C5	-5.99	111.60	115.20
1	H	701	DA	C4'-C3'-O3'	5.99	124.68	109.70
1	F	517	DA	O4'-C4'-C3'	5.99	109.59	106.00
1	H	711	DG	N3-C4-C5	-5.99	125.61	128.60
1	E	415	DA	P-O5'-C5'	5.99	130.48	120.90
1	G	601	DA	C4-N9-C1'	5.98	137.06	126.30
1	E	419	DT	O5'-P-OP1	-5.96	100.33	105.70
1	H	714	DC	C6-N1-C2	-5.96	117.92	120.30
1	F	509	DG	P-O3'-C3'	5.94	126.83	119.70
1	F	514	DC	N3-C4-C5	-5.94	119.53	121.90
1	H	710	DC	O4'-C1'-C2'	-5.92	101.17	105.90
1	E	403	DT	C3'-C2'-C1'	5.91	109.59	102.50
1	F	517	DA	N7-C8-N9	5.91	116.75	113.80
1	G	619	DT	C5'-C4'-C3'	-5.90	103.48	114.10
1	F	505	DG	C4'-C3'-C2'	-5.89	97.80	103.10
1	G	606	DT	C3'-C2'-C1'	5.89	109.56	102.50
1	E	412	DC	O4'-C4'-C3'	-5.88	102.15	104.50
1	E	407	DG	C4'-C3'-O3'	5.87	124.36	109.70
1	E	417	DA	N3-C4-N9	-5.87	122.71	127.40
1	H	715	DA	O5'-C5'-C4'	5.87	125.67	111.00
1	E	416	DC	C5'-C4'-O4'	5.86	120.42	109.30
1	H	706	DT	C4'-C3'-C2'	-5.86	97.83	103.10
1	E	403	DT	C6-C5-C7	-5.85	119.39	122.90
1	E	401	DA	C1'-O4'-C4'	5.85	115.95	110.10
1	F	509	DG	C4'-C3'-O3'	5.84	124.29	109.70
1	F	516	DC	P-O3'-C3'	-5.83	112.71	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	604	DT	O5'-C5'-C4'	5.82	125.55	111.00
1	G	613	DT	N1-C1'-C2'	5.82	123.66	112.60
1	F	519	DT	C6-N1-C2	-5.81	118.39	121.30
1	F	513	DT	N1-C1'-C2'	5.81	123.63	112.60
1	E	407	DG	C5'-C4'-C3'	5.80	124.54	114.10
1	E	413	DT	C4-C5-C6	5.80	121.48	118.00
1	F	505	DG	C1'-O4'-C4'	-5.79	104.31	110.10
1	G	617	DA	O4'-C4'-C3'	5.79	109.47	106.00
1	G	608	DA	C2-N3-C4	-5.78	107.71	110.60
1	F	520	DT	N3-C4-C5	-5.77	111.74	115.20
1	H	700	DG	C4'-C3'-O3'	5.75	124.09	109.70
1	F	508	DA	O4'-C1'-N9	5.75	112.03	108.00
1	H	719	DT	O5'-P-OP1	-5.75	100.52	105.70
1	E	406	DT	O4'-C4'-C3'	5.75	109.45	106.00
1	H	710	DC	C4'-C3'-C2'	-5.75	97.92	103.10
1	G	617	DA	N7-C8-N9	5.75	116.67	113.80
1	F	517	DA	C5'-C4'-C3'	5.75	124.44	114.10
1	E	413	DT	C6-C5-C7	-5.74	119.45	122.90
1	H	701	DA	N1-C6-N6	-5.74	115.16	118.60
1	H	704	DT	N3-C2-O2	-5.74	118.86	122.30
1	H	719	DT	C6-C5-C7	-5.74	119.46	122.90
1	E	406	DT	C4-C5-C7	-5.73	115.56	119.00
1	F	513	DT	N3-C4-O4	5.73	123.34	119.90
1	H	707	DG	P-O3'-C3'	5.73	126.57	119.70
1	H	720	DT	C3'-C2'-C1'	5.72	109.36	102.50
1	H	708	DA	P-O3'-C3'	5.72	126.56	119.70
1	E	415	DA	C4-C5-C6	5.71	119.86	117.00
1	F	502	DA	C5'-C4'-C3'	5.69	124.33	114.10
1	G	611	DG	N3-C4-C5	-5.68	125.76	128.60
1	E	412	DC	N1-C2-O2	5.68	122.31	118.90
1	H	720	DT	C5-C6-N1	-5.67	120.30	123.70
1	G	619	DT	N3-C4-C5	-5.67	111.80	115.20
1	F	509	DG	C5'-C4'-O4'	-5.66	98.54	109.30
1	F	503	DT	C4-C5-C6	5.66	121.40	118.00
1	F	518	DA	O5'-C5'-C4'	5.66	125.15	111.00
1	E	411	DG	C4'-C3'-C2'	-5.66	98.01	103.10
1	F	507	DG	C3'-C2'-C1'	5.66	109.29	102.50
1	F	508	DA	C4'-C3'-O3'	5.65	123.83	109.70
1	E	407	DG	O5'-P-OP2	-5.65	100.62	105.70
1	G	606	DT	N1-C2-N3	5.65	117.99	114.60
1	H	705	DG	P-O3'-C3'	-5.65	112.92	119.70
1	H	705	DG	C4'-C3'-C2'	-5.65	98.02	103.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	520	DT	N1-C2-N3	5.64	117.99	114.60
1	H	709	DG	P-O5'-C5'	5.64	129.93	120.90
1	E	414	DC	O4'-C1'-N1	5.64	111.95	108.00
1	E	419	DT	C2-N3-C4	-5.64	123.82	127.20
1	H	708	DA	N7-C8-N9	5.63	116.62	113.80
1	F	505	DG	C8-N9-C1'	5.63	134.32	127.00
1	H	718	DA	N9-C1'-C2'	5.63	123.29	112.60
1	E	419	DT	O4'-C1'-C2'	-5.62	101.40	105.90
1	E	403	DT	N1-C2-N3	5.62	117.97	114.60
1	F	508	DA	N1-C6-N6	5.62	121.97	118.60
1	G	618	DA	C3'-C2'-C1'	5.62	109.24	102.50
1	H	711	DG	C6-C5-N7	-5.61	127.04	130.40
1	E	404	DT	C5-C6-N1	-5.60	120.34	123.70
1	F	517	DA	C5-N7-C8	-5.60	101.10	103.90
1	F	503	DT	C3'-C2'-C1'	5.60	109.22	102.50
1	F	503	DT	O4'-C1'-N1	5.60	111.92	108.00
1	H	720	DT	C4-C5-C7	-5.60	115.64	119.00
1	F	502	DA	C5-C6-N1	-5.59	114.90	117.70
1	E	419	DT	N1-C2-N3	5.57	117.94	114.60
1	H	703	DT	C4-C5-C6	5.57	121.34	118.00
1	G	603	DT	C6-N1-C2	-5.57	118.52	121.30
1	E	407	DG	C4-C5-C6	5.56	122.14	118.80
1	G	604	DT	C4-C5-C6	5.56	121.33	118.00
1	G	619	DT	O4'-C1'-N1	5.56	111.89	108.00
1	G	604	DT	C2'-C3'-O3'	-5.55	94.27	112.60
1	E	416	DC	C3'-C2'-C1'	5.55	109.16	102.50
1	G	604	DT	OP1-P-OP2	5.54	127.92	119.60
1	G	611	DG	N3-C4-N9	5.54	129.33	126.00
1	F	510	DC	C3'-C2'-C1'	5.54	109.15	102.50
1	E	405	DG	N1-C2-N3	-5.54	120.58	123.90
1	F	516	DC	O3'-P-O5'	5.53	114.51	104.00
1	G	615	DA	C2-N3-C4	-5.53	107.83	110.60
1	H	720	DT	N1-C2-N3	5.53	117.92	114.60
1	H	720	DT	C1'-O4'-C4'	5.52	115.62	110.10
1	G	610	DC	C4'-C3'-C2'	-5.52	98.13	103.10
1	G	612	DC	N3-C2-O2	-5.52	118.04	121.90
1	G	615	DA	P-O5'-C5'	5.52	129.73	120.90
1	F	511	DG	N3-C4-N9	5.50	129.30	126.00
1	G	602	DA	P-O3'-C3'	5.50	126.30	119.70
1	F	507	DG	C4'-C3'-O3'	5.50	123.45	109.70
1	G	615	DA	N3-C4-N9	-5.50	123.00	127.40
1	G	617	DA	C5-N7-C8	-5.49	101.16	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	605	DG	N9-C1'-C2'	5.49	123.03	112.60
1	H	708	DA	C2-N3-C4	-5.49	107.86	110.60
1	G	605	DG	C4'-C3'-O3'	5.48	123.40	109.70
1	H	701	DA	C4-N9-C1'	5.47	136.14	126.30
1	G	612	DC	C2-N3-C4	5.45	122.63	119.90
1	F	519	DT	C4'-C3'-O3'	5.45	123.32	109.70
1	G	601	DA	C4-C5-C6	5.45	119.72	117.00
1	G	604	DT	C4-C5-C7	-5.45	115.73	119.00
1	G	620	DT	O5'-C5'-C4'	5.44	124.61	111.00
1	H	719	DT	N3-C4-C5	-5.44	111.94	115.20
1	F	512	DC	C6-N1-C1'	-5.44	114.27	120.80
1	G	602	DA	N9-C4-C5	-5.43	103.63	105.80
1	G	613	DT	C3'-C2'-C1'	5.43	109.01	102.50
1	G	612	DC	C1'-O4'-C4'	-5.42	104.68	110.10
1	F	520	DT	N3-C2-O2	-5.41	119.05	122.30
1	F	501	DA	C5'-C4'-C3'	5.41	123.84	114.10
1	F	511	DG	N3-C4-C5	-5.41	125.90	128.60
1	E	418	DA	P-O3'-C3'	5.40	126.18	119.70
1	H	710	DC	N3-C4-C5	-5.40	119.74	121.90
1	E	410	DC	O4'-C1'-C2'	-5.40	101.58	105.90
1	G	616	DC	O5'-P-OP2	-5.38	100.85	105.70
1	E	406	DT	N3-C2-O2	-5.38	119.07	122.30
1	F	508	DA	C8-N9-C4	-5.38	103.65	105.80
1	E	401	DA	N3-C4-C5	-5.37	123.04	126.80
1	G	620	DT	N3-C2-O2	-5.37	119.08	122.30
1	E	404	DT	C4'-C3'-O3'	5.35	123.08	109.70
1	G	602	DA	C2'-C3'-O3'	-5.32	95.04	112.60
1	H	710	DC	C3'-C2'-C1'	5.32	108.88	102.50
1	H	700	DG	C5-C6-N1	5.32	114.16	111.50
1	G	608	DA	N9-C4-C5	5.30	107.92	105.80
1	E	419	DT	C5-C6-N1	-5.30	120.52	123.70
1	E	407	DG	C8-N9-C1'	-5.30	120.11	127.00
1	F	514	DC	O5'-C5'-C4'	5.30	124.25	111.00
1	E	414	DC	N3-C2-O2	-5.29	118.19	121.90
1	G	617	DA	C8-N9-C4	-5.27	103.69	105.80
1	F	517	DA	C4'-C3'-C2'	-5.26	98.37	103.10
1	F	518	DA	N3-C4-C5	-5.23	123.14	126.80
1	G	616	DC	C2-N1-C1'	-5.23	113.05	118.80
1	G	614	DC	P-O3'-C3'	-5.23	113.42	119.70
1	H	707	DG	C6-C5-N7	-5.23	127.26	130.40
1	G	616	DC	C4'-C3'-O3'	5.21	122.74	109.70
1	E	401	DA	N3-C4-N9	5.21	131.57	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	405	DG	C4'-C3'-O3'	5.20	122.71	112.30
1	F	516	DC	C5-C6-N1	5.20	123.60	121.00
1	F	517	DA	O3'-P-O5'	5.20	113.88	104.00
1	E	400	DG	C3'-C2'-C1'	5.20	108.74	102.50
1	G	615	DA	C5-C6-N1	-5.20	115.10	117.70
1	E	406	DT	C3'-C2'-C1'	5.19	108.73	102.50
1	H	700	DG	N3-C4-C5	-5.19	126.00	128.60
1	H	712	DC	N1-C1'-C2'	5.19	122.46	112.60
1	F	500	DG	C5-C6-O6	5.19	131.71	128.60
1	G	602	DA	N7-C8-N9	5.18	116.39	113.80
1	G	608	DA	C5-C6-N1	-5.18	115.11	117.70
1	G	603	DT	N1-C2-N3	5.18	117.71	114.60
1	E	409	DG	P-O5'-C5'	5.17	129.18	120.90
1	H	710	DC	C6-N1-C2	-5.17	118.23	120.30
1	H	711	DG	O4'-C1'-N9	5.17	111.62	108.00
1	G	600	DG	N9-C1'-C2'	5.17	122.42	112.60
1	G	605	DG	N9-C4-C5	5.16	107.47	105.40
1	F	520	DT	C2-N1-C1'	-5.16	109.95	118.20
1	G	608	DA	C4'-C3'-O3'	5.15	122.60	112.30
1	H	717	DA	C5'-C4'-C3'	5.15	123.37	114.10
1	E	402	DA	C4'-C3'-C2'	-5.15	98.47	103.10
1	G	609	DG	N7-C8-N9	5.14	115.67	113.10
1	H	701	DA	C5-C6-N1	-5.14	115.13	117.70
1	E	411	DG	N7-C8-N9	5.13	115.67	113.10
1	H	701	DA	O5'-C5'-C4'	5.12	123.81	111.00
1	H	720	DT	C6-C5-C7	-5.12	119.83	122.90
1	F	505	DG	C5-C6-N1	-5.09	108.95	111.50
1	E	402	DA	C4-N9-C1'	5.09	135.46	126.30
1	H	719	DT	N3-C2-O2	-5.08	119.25	122.30
1	G	608	DA	O4'-C1'-C2'	-5.08	101.84	105.90
1	F	503	DT	C4'-C3'-O3'	5.07	122.44	112.30
1	F	505	DG	C6-N1-C2	5.07	128.14	125.10
1	G	613	DT	O4'-C1'-N1	5.05	111.54	108.00
1	E	416	DC	N3-C2-O2	-5.05	118.37	121.90
1	G	603	DT	C4-C5-C6	5.04	121.02	118.00
1	G	620	DT	N1-C2-N3	5.04	117.62	114.60
1	H	714	DC	C4'-C3'-C2'	-5.04	98.56	103.10
1	G	612	DC	N3-C4-C5	-5.04	119.89	121.90
1	E	402	DA	C1'-O4'-C4'	5.02	115.12	110.10
1	F	513	DT	P-O3'-C3'	5.02	125.72	119.70
1	E	414	DC	N3-C4-C5	-5.02	119.89	121.90
1	E	404	DT	N3-C4-C5	-5.01	112.19	115.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	613	DT	O4'-C1'-C2'	-5.01	101.89	105.90
1	H	707	DG	N3-C4-C5	-5.01	126.09	128.60
1	H	709	DG	C4'-C3'-O3'	5.01	122.33	112.30
1	E	410	DC	C4'-C3'-O3'	5.01	122.33	112.30
1	E	404	DT	C6-N1-C2	-5.01	118.80	121.30
1	G	617	DA	N9-C4-C5	5.00	107.80	105.80
1	E	418	DA	P-O5'-C5'	5.00	128.90	120.90

All (10) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	E	402	DA	C3'
1	E	405	DG	C1'
1	E	409	DG	C1'
1	F	520	DT	C4'
1	G	600	DG	C1'
1	G	601	DA	C1'
1	G	620	DT	C1'
1	H	702	DA	C1'
1	H	718	DA	C3'
1	H	719	DT	C4'

All (66) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	400	DG	Sidechain
1	E	401	DA	Sidechain
1	E	402	DA	Sidechain
1	E	403	DT	Sidechain
1	E	404	DT	Sidechain
1	E	405	DG	Sidechain
1	E	406	DT	Sidechain
1	E	407	DG	Sidechain
1	E	408	DA	Sidechain
1	E	409	DG	Sidechain
1	E	410	DC	Sidechain
1	E	411	DG	Sidechain
1	E	412	DC	Sidechain
1	E	413	DT	Sidechain
1	E	415	DA	Sidechain
1	E	416	DC	Sidechain
1	E	418	DA	Sidechain

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Mol	Chain	Res	Type	Group
1	E	420	DT	Sidechain
1	F	500	DG	Sidechain
1	F	501	DA	Sidechain
1	F	503	DT	Sidechain
1	F	504	DT	Sidechain
1	F	505	DG	Sidechain
1	F	508	DA	Sidechain
1	F	509	DG	Sidechain
1	F	510	DC	Sidechain
1	F	512	DC	Sidechain
1	F	513	DT	Sidechain
1	F	515	DA	Sidechain
1	F	516	DC	Sidechain
1	F	517	DA	Sidechain
1	F	519	DT	Sidechain
1	F	520	DT	Sidechain
1	G	600	DG	Sidechain
1	G	601	DA	Sidechain
1	G	602	DA	Sidechain
1	G	604	DT	Sidechain
1	G	606	DT	Sidechain
1	G	608	DA	Sidechain
1	G	609	DG	Sidechain
1	G	610	DC	Sidechain
1	G	611	DG	Sidechain
1	G	612	DC	Sidechain
1	G	613	DT	Sidechain
1	G	614	DC	Sidechain
1	G	615	DA	Sidechain
1	G	616	DC	Sidechain
1	G	619	DT	Sidechain
1	G	620	DT	Sidechain
1	H	700	DG	Sidechain
1	H	701	DA	Sidechain
1	H	702	DA	Sidechain
1	H	704	DT	Sidechain
1	H	706	DT	Sidechain
1	H	707	DG	Sidechain
1	H	708	DA	Sidechain
1	H	709	DG	Sidechain
1	H	710	DC	Sidechain
1	H	712	DC	Sidechain

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Mol	Chain	Res	Type	Group
1	H	713	DT	Sidechain
1	H	714	DC	Sidechain
1	H	715	DA	Sidechain
1	H	716	DC	Sidechain
1	H	717	DA	Sidechain
1	H	718	DA	Sidechain
1	H	719	DT	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	E	429	0	239	40	0
1	F	429	0	239	37	0
1	G	429	0	239	42	6
1	H	429	0	239	38	0
2	A	357	0	0	0	0
2	B	357	0	0	0	0
2	C	357	0	0	0	0
2	D	357	0	0	1	6
All	All	3144	0	956	139	6

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 34.

All (139) 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:F:501:DA:H2'	1:F:502:DA:H1'	1.40	1.01
1:G:601:DA:H3'	1:G:602:DA:N7	1.94	0.82
1:H:701:DA:H3'	1:H:702:DA:C8	2.16	0.80
1:F:511:DG:N3	1:F:512:DC:H1'	1.98	0.78
1:E:405:DG:H2''	1:E:406:DT:H71	1.66	0.77
1:E:416:DC:H42	1:F:505:DG:H1	1.33	0.76
1:G:611:DG:H2''	1:G:612:DC:C6	2.22	0.74
1:G:611:DG:N3	1:G:612:DC:H1'	2.01	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:712:DC:H2'	1:H:713:DT:C6	2.24	0.73
1:H:711:DG:N3	1:H:712:DC:H1'	2.04	0.72
1:G:617:DA:H2''	1:G:618:DA:N7	2.04	0.72
1:F:512:DC:H2'	1:F:513:DT:C6	2.24	0.72
1:H:709:DG:H2''	1:H:710:DC:C6	2.25	0.71
1:G:619:DT:H3	1:H:702:DA:H2	1.40	0.70
1:E:410:DC:H3'	1:E:411:DG:C8	2.27	0.69
1:E:408:DA:H5''	1:E:408:DA:H8	1.57	0.69
1:H:708:DA:H8	1:H:708:DA:H5''	1.57	0.69
1:G:602:DA:H2''	1:G:603:DT:OP2	1.94	0.68
1:G:603:DT:H2''	1:G:604:DT:C6	2.28	0.68
1:F:518:DA:H2''	1:F:519:DT:H4'	1.75	0.68
1:E:401:DA:H2''	1:E:402:DA:C8	2.27	0.67
1:E:403:DT:OP2	1:E:403:DT:H6	1.77	0.67
1:E:419:DT:H3'	1:E:420:DT:H3'	1.77	0.67
1:E:402:DA:C8	1:E:402:DA:OP2	2.49	0.66
1:G:604:DT:H2'	1:G:604:DT:OP1	1.96	0.66
1:E:414:DC:H2'	1:E:415:DA:C8	2.31	0.66
1:F:506:DT:H2''	1:F:507:DG:H5'	1.78	0.66
1:H:701:DA:H2'	1:H:702:DA:H2''	1.76	0.65
1:H:704:DT:H2'	1:H:704:DT:OP2	1.97	0.65
1:F:519:DT:H2'	1:F:520:DT:H4'	1.79	0.65
1:G:611:DG:H2''	1:G:612:DC:H6	1.62	0.64
1:E:414:DC:O5'	1:E:414:DC:H6	1.82	0.63
1:H:715:DA:H2''	1:H:716:DC:C5	2.34	0.63
1:H:709:DG:H2''	1:H:710:DC:C5	2.34	0.63
1:E:401:DA:H2''	1:E:402:DA:N9	2.13	0.62
1:E:415:DA:H2''	1:E:416:DC:H6	1.64	0.62
1:G:618:DA:C2	1:G:619:DT:H1'	2.35	0.62
1:H:704:DT:H1'	1:H:705:DG:OP2	2.00	0.62
1:E:402:DA:H8	1:E:402:DA:OP2	1.83	0.62
1:H:718:DA:H2'	1:H:719:DT:OP2	1.99	0.62
1:H:708:DA:C8	1:H:708:DA:H5''	2.33	0.61
1:E:403:DT:H2''	1:E:404:DT:C6	2.36	0.61
1:F:513:DT:H2'	1:F:514:DC:O4'	2.01	0.61
1:G:600:DG:H4'	1:G:601:DA:H2''	1.82	0.61
1:E:419:DT:O4	1:F:502:DA:N1	2.33	0.60
1:G:617:DA:H2''	1:G:618:DA:C8	2.36	0.60
1:H:701:DA:H3'	1:H:702:DA:N7	2.15	0.60
1:G:605:DG:H3'	1:G:606:DT:C6	2.37	0.60
1:G:605:DG:H2'	1:G:605:DG:N3	2.16	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:609:DG:H2'	1:G:610:DC:C6	2.37	0.59
1:H:704:DT:H6	1:H:704:DT:OP2	1.85	0.59
1:F:514:DC:H2'	1:F:515:DA:C8	2.38	0.59
1:G:607:DG:H2''	1:G:608:DA:C8	2.37	0.58
1:E:400:DG:H2'	1:E:401:DA:H8	1.66	0.58
1:E:402:DA:H2'	1:E:403:DT:C5	2.39	0.57
1:E:403:DT:H2''	1:E:404:DT:C5	2.39	0.57
1:E:408:DA:H2	1:F:513:DT:H3	1.52	0.57
1:H:711:DG:C2	1:H:712:DC:H1'	2.39	0.57
1:E:406:DT:H2''	1:E:407:DG:C8	2.39	0.57
1:F:518:DA:N3	1:F:519:DT:H1'	2.19	0.57
1:F:502:DA:C6	1:F:503:DT:H1'	2.39	0.56
1:E:405:DG:O6	1:F:516:DC:N4	2.35	0.56
1:F:515:DA:H2''	1:F:516:DC:C5	2.41	0.56
1:G:603:DT:H2''	1:G:604:DT:H6	1.71	0.56
1:F:502:DA:C5	1:F:503:DT:H1'	2.41	0.55
1:G:619:DT:H2'	1:H:701:DA:N1	2.21	0.55
1:E:407:DG:H2'	1:E:408:DA:O4'	2.06	0.55
1:F:513:DT:H3'	1:F:514:DC:C6	2.42	0.55
1:E:418:DA:N1	1:F:503:DT:O2	2.39	0.55
1:H:716:DC:H2''	1:H:717:DA:C8	2.42	0.55
1:G:617:DA:H2'	1:G:617:DA:O5'	2.06	0.55
1:G:602:DA:C8	1:G:602:DA:O5'	2.60	0.54
1:F:513:DT:H3'	1:F:514:DC:H6	1.72	0.54
1:G:604:DT:OP1	1:G:604:DT:H6	1.91	0.53
1:H:715:DA:OP2	1:H:715:DA:H2'	2.08	0.53
1:H:700:DG:H2''	1:H:701:DA:H5''	1.89	0.53
1:F:511:DG:C2	1:F:512:DC:H1'	2.43	0.52
1:G:608:DA:N1	1:H:713:DT:O4	2.42	0.52
1:E:417:DA:H2'	1:E:417:DA:OP2	2.09	0.52
1:E:416:DC:N4	1:F:505:DG:H1	2.04	0.52
1:H:703:DT:H3'	2:D:30:VAL:CA	2.40	0.52
1:G:619:DT:N3	1:H:702:DA:H2	2.08	0.52
1:E:419:DT:P	1:E:419:DT:H73	2.51	0.51
1:F:506:DT:C2'	1:F:507:DG:H5'	2.39	0.51
1:E:406:DT:H6	1:E:406:DT:OP2	1.94	0.50
1:F:501:DA:H3'	1:F:501:DA:H8	1.76	0.50
1:F:501:DA:C8	1:F:501:DA:H3'	2.46	0.50
1:H:700:DG:N2	1:H:702:DA:N1	2.60	0.50
1:G:600:DG:H4'	1:G:601:DA:C2'	2.41	0.50
1:G:604:DT:O4	1:H:717:DA:N1	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:504:DT:OP2	1:F:504:DT:H6	1.95	0.50
1:F:519:DT:H2'	1:F:520:DT:C4'	2.41	0.50
1:E:419:DT:H3'	1:E:420:DT:C3'	2.41	0.49
1:F:500:DG:H2''	1:F:501:DA:C8	2.47	0.49
1:H:719:DT:H6	1:H:719:DT:OP1	1.96	0.49
1:F:518:DA:C2	1:F:519:DT:H1'	2.47	0.49
1:E:413:DT:H3'	1:E:414:DC:C5	2.48	0.49
1:F:508:DA:H1'	1:F:509:DG:H5'	1.95	0.48
1:G:616:DC:H2''	1:G:617:DA:C8	2.49	0.48
1:H:703:DT:H2''	1:H:704:DT:OP2	2.13	0.47
1:G:604:DT:O4'	1:G:604:DT:OP2	2.32	0.47
1:F:515:DA:H2''	1:F:516:DC:H5	1.80	0.47
1:H:704:DT:OP2	1:H:704:DT:C6	2.66	0.47
1:G:602:DA:C2	1:H:720:DT:O4'	2.68	0.47
1:G:613:DT:H3	1:H:708:DA:H2	1.61	0.47
1:G:601:DA:H3'	1:G:602:DA:C5	2.50	0.46
1:F:518:DA:H2''	1:F:519:DT:C4'	2.44	0.46
1:E:402:DA:H3'	1:E:403:DT:O4'	2.14	0.46
1:F:501:DA:C3'	1:F:501:DA:C8	2.99	0.46
1:H:708:DA:H2'	1:H:709:DG:C8	2.51	0.46
1:H:712:DC:H2'	1:H:713:DT:C5	2.51	0.46
1:E:419:DT:OP2	1:E:419:DT:H73	2.17	0.45
1:E:404:DT:OP2	1:E:404:DT:H6	1.99	0.45
1:E:403:DT:OP2	1:E:403:DT:C6	2.65	0.45
1:G:618:DA:N1	1:H:703:DT:O4	2.50	0.45
1:E:415:DA:H2''	1:E:416:DC:C6	2.49	0.45
1:F:516:DC:H3'	1:F:516:DC:OP2	2.17	0.44
1:G:615:DA:OP2	1:G:615:DA:H8	2.00	0.44
1:H:713:DT:C6	1:H:713:DT:H5''	2.53	0.44
1:F:502:DA:H2'	1:F:502:DA:N3	2.33	0.44
1:G:606:DT:C2'	1:G:607:DG:H5'	2.48	0.44
1:G:613:DT:H2'	1:G:614:DC:C6	2.53	0.44
1:E:417:DA:N1	1:F:504:DT:O4	2.51	0.44
1:G:601:DA:H3'	1:G:602:DA:C8	2.52	0.43
1:E:412:DC:H5''	1:E:413:DT:OP2	2.18	0.43
1:H:712:DC:H5''	1:H:713:DT:OP2	2.19	0.43
1:G:620:DT:O4	1:H:700:DG:C2	2.72	0.43
1:H:714:DC:H6	1:H:714:DC:O5'	2.02	0.42
1:G:603:DT:H6	1:G:603:DT:OP2	2.02	0.41
1:E:408:DA:H5''	1:E:408:DA:C8	2.47	0.41
1:E:402:DA:N3	1:F:519:DT:O4	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:401:DA:H2''	1:E:402:DA:C1'	2.50	0.41
1:G:604:DT:O4'	1:G:604:DT:P	2.78	0.41
1:G:602:DA:C8	1:G:602:DA:P	3.13	0.41
1:G:618:DA:H2	1:H:703:DT:H3	1.68	0.41
1:G:612:DC:H2'	1:G:613:DT:C6	2.55	0.41
1:F:511:DG:H4'	1:F:512:DC:OP1	2.20	0.41
1:E:408:DA:H2'	1:E:409:DG:N9	2.36	0.40
1:G:608:DA:H2''	1:G:609:DG:C8	2.57	0.40

All (6) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:600:DG:N7	2:D:351:ARG:CA[1_455]	0.37	1.83
1:G:600:DG:C5	2:D:351:ARG:CA[1_455]	1.25	0.95
1:G:600:DG:O6	2:D:350:ALA:CA[1_455]	1.38	0.82
1:G:600:DG:C8	2:D:351:ARG:CA[1_455]	1.46	0.74
1:G:600:DG:C6	2:D:350:ALA:CA[1_455]	2.06	0.14
1:G:600:DG:C4	2:D:351:ARG:CA[1_455]	2.18	0.02

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

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.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.