



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:36 PM UTC

PDB ID : 1LBG / pdb_00001lbq
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

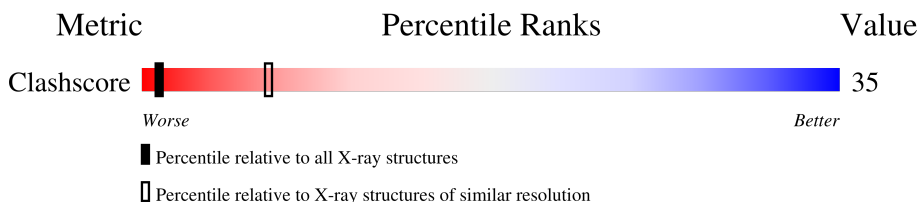
1 Overall quality at a glance

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	190562	1001 (5.60-3.98)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$.

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

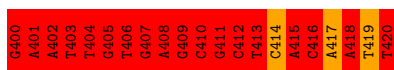
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

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:  14% 86%



- 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:  38% 62%



- 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:  24% 76%



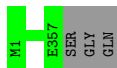
- Molecule 1: DNA (5'-D(*GP*AP*AP*TP*TP*GP*TP*GP*AP*GP*CP*GP*CP*TP*CP*AP*CP*AP*AP*TP*T)-3')

Chain H:  29% 71%

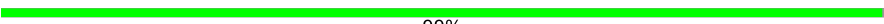


- Molecule 2: PROTEIN (LACTOSE OPERON REPRESSOR)

Chain A:  99%



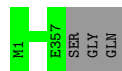
- Molecule 2: PROTEIN (LACTOSE OPERON REPRESSOR)

Chain B:  99% .

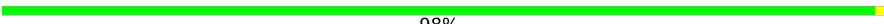


- Molecule 2: PROTEIN (LACTOSE OPERON REPRESSOR)

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 is therefore 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	1.84	14/481 (2.9%)	4.07	124/741 (16.7%)
1	F	1.65	9/481 (1.9%)	3.78	114/741 (15.4%)
1	G	2.01	19/481 (4.0%)	4.03	116/741 (15.7%)
1	H	1.71	12/481 (2.5%)	3.97	113/741 (15.2%)
All	All	1.81	54/1924 (2.8%)	3.97	467/2964 (15.8%)

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 (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	601	DA	O3'-P	13.59	1.81	1.61
1	G	620	DT	P-O5'	10.72	1.81	1.60
1	G	620	DT	C5'-C4'	10.56	1.73	1.52
1	E	401	DA	O3'-P	9.62	1.75	1.61
1	G	602	DA	O3'-P	9.37	1.75	1.61
1	G	602	DA	P-O5'	9.18	1.78	1.60
1	F	501	DA	O3'-P	8.85	1.74	1.61
1	H	701	DA	C1'-N9	8.48	1.63	1.46
1	G	600	DG	C1'-N9	8.22	1.62	1.46
1	G	602	DA	C5'-C4'	8.21	1.68	1.52
1	H	720	DT	P-O5'	8.17	1.76	1.60
1	H	701	DA	O3'-P	8.02	1.73	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	600	DG	O3'-P	7.65	1.72	1.61
1	G	620	DT	C4'-C3'	7.36	1.67	1.52
1	H	718	DA	O3'-P	7.28	1.72	1.61
1	F	500	DG	O3'-P	7.26	1.72	1.61
1	F	518	DA	P-O5'	7.19	1.74	1.60
1	F	500	DG	C1'-N9	7.15	1.60	1.46
1	G	601	DA	C3'-C2'	7.12	1.67	1.52
1	F	518	DA	O3'-P	7.04	1.71	1.61
1	E	406	DT	O3'-P	6.99	1.71	1.61
1	G	601	DA	C1'-N9	6.63	1.59	1.46
1	H	719	DT	O3'-P	6.60	1.71	1.61
1	H	718	DA	C4'-C3'	6.48	1.65	1.52
1	G	608	DA	O3'-P	6.47	1.70	1.61
1	H	719	DT	C5'-C4'	6.47	1.65	1.52
1	E	403	DT	O3'-P	6.40	1.70	1.61
1	E	401	DA	C5'-C4'	6.12	1.64	1.52
1	G	601	DA	C2'-C1'	6.09	1.65	1.52
1	E	404	DT	C4'-C3'	6.09	1.65	1.52
1	G	620	DT	O5'-C5'	5.89	1.60	1.42
1	E	418	DA	C5'-C4'	5.89	1.64	1.52
1	G	602	DA	C4'-C3'	5.83	1.64	1.52
1	E	416	DC	O3'-P	5.77	1.69	1.61
1	G	601	DA	C3'-O3'	5.70	1.59	1.42
1	F	518	DA	C5'-C4'	5.66	1.63	1.52
1	H	704	DT	O3'-P	5.65	1.69	1.61
1	F	518	DA	C4'-C3'	5.62	1.64	1.52
1	E	407	DG	O3'-P	5.58	1.69	1.61
1	E	404	DT	O3'-P	5.55	1.69	1.61
1	H	717	DA	O3'-P	5.54	1.69	1.61
1	H	719	DT	C4'-C3'	5.54	1.63	1.52
1	E	405	DG	O3'-P	5.53	1.69	1.61
1	G	617	DA	O3'-P	5.49	1.69	1.61
1	E	406	DT	P-O5'	5.46	1.71	1.60
1	E	406	DT	C5'-C4'	5.40	1.63	1.52
1	H	719	DT	P-O5'	5.39	1.71	1.60
1	F	504	DT	O3'-P	5.38	1.69	1.61
1	E	406	DT	C4'-C3'	5.37	1.63	1.52
1	H	718	DA	C5'-C4'	5.30	1.62	1.52
1	F	500	DG	C3'-C2'	5.29	1.63	1.52
1	G	605	DG	O3'-P	5.28	1.69	1.61
1	E	416	DC	C5'-C4'	5.20	1.62	1.52
1	G	619	DT	O3'-P	5.02	1.68	1.61

All (467) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	718	DA	C4'-C3'-O3'	27.79	151.69	110.00
1	E	401	DA	P-O3'-C3'	22.34	153.71	120.20
1	G	601	DA	N9-C1'-C2'	21.78	146.17	113.50
1	H	702	DA	N9-C1'-C2'	19.64	142.96	113.50
1	E	402	DA	P-O3'-C3'	19.42	149.33	120.20
1	E	420	DT	O4'-C1'-N1	19.25	137.27	108.40
1	H	718	DA	C5'-C4'-C3'	18.55	142.72	114.90
1	H	719	DT	C4'-C3'-O3'	17.95	136.93	110.00
1	H	719	DT	C5'-C4'-C3'	17.69	141.44	114.90
1	G	600	DG	P-O3'-C3'	17.66	146.69	120.20
1	G	601	DA	C2'-C3'-O3'	15.87	135.30	111.50
1	G	602	DA	P-O5'-C5'	15.84	143.77	120.00
1	E	420	DT	O5'-C5'-C4'	15.38	133.87	110.80
1	E	401	DA	C4'-C3'-O3'	15.28	132.92	110.00
1	H	708	DA	P-O5'-C5'	15.15	142.72	120.00
1	F	520	DT	O4'-C1'-N1	14.80	130.60	108.40
1	F	506	DT	P-O3'-C3'	14.45	141.87	120.20
1	E	415	DA	P-O3'-C3'	14.28	141.63	120.20
1	G	620	DT	C5'-C4'-C3'	14.26	136.28	114.90
1	F	518	DA	P-O3'-C3'	14.22	141.53	120.20
1	E	401	DA	C5'-C4'-C3'	14.16	136.14	114.90
1	F	500	DG	N9-C1'-C2'	14.09	134.64	113.50
1	H	718	DA	O3'-P-O5'	13.80	124.70	104.00
1	H	715	DA	P-O5'-C5'	13.79	140.69	120.00
1	G	608	DA	O5'-C5'-C4'	13.75	131.43	110.80
1	G	600	DG	O4'-C1'-N9	13.65	128.88	108.40
1	E	402	DA	C4'-C3'-O3'	13.62	130.44	110.00
1	G	620	DT	C1'-O4'-C4'	-13.51	89.44	109.70
1	E	417	DA	P-O5'-C5'	13.48	140.22	120.00
1	G	602	DA	C4'-C3'-O3'	13.41	130.11	110.00
1	G	601	DA	C4'-C3'-C2'	-13.25	82.53	102.40
1	E	407	DG	P-O5'-C5'	13.23	139.84	120.00
1	E	415	DA	C4'-C3'-O3'	13.17	129.76	110.00
1	E	418	DA	O3'-P-O5'	13.13	123.69	104.00
1	G	609	DG	P-O5'-C5'	13.11	139.67	120.00
1	G	606	DT	P-O3'-C3'	13.10	139.84	120.20
1	E	417	DA	O5'-C5'-C4'	13.05	130.38	110.80
1	H	718	DA	P-O5'-C5'	13.01	139.52	120.00
1	H	716	DC	P-O3'-C3'	12.89	139.54	120.20
1	H	717	DA	C1'-O4'-C4'	-12.84	90.44	109.70
1	E	407	DG	N9-C1'-C2'	12.80	132.69	113.50
1	F	517	DA	O5'-C5'-C4'	12.71	129.86	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	515	DA	P-O3'-C3'	12.61	139.11	120.20
1	H	701	DA	N9-C1'-C2'	12.55	132.33	113.50
1	H	700	DG	P-O3'-C3'	12.52	138.98	120.20
1	F	516	DC	O5'-C5'-C4'	12.50	129.54	110.80
1	G	619	DT	O3'-P-O5'	12.46	122.69	104.00
1	G	601	DA	P-O3'-C3'	12.46	138.89	120.20
1	E	416	DC	O4'-C1'-C2'	-12.40	87.80	106.40
1	F	508	DA	O5'-C5'-C4'	12.38	129.37	110.80
1	F	502	DA	C4'-C3'-O3'	12.33	128.49	110.00
1	G	601	DA	O3'-P-O5'	12.31	122.47	104.00
1	F	514	DC	P-O5'-C5'	12.31	138.46	120.00
1	E	420	DT	O4'-C1'-C2'	-12.28	87.97	106.40
1	F	520	DT	C5'-C4'-C3'	12.11	133.06	114.90
1	E	406	DT	C4'-C3'-O3'	12.07	128.11	110.00
1	G	608	DA	P-O5'-C5'	12.05	138.07	120.00
1	F	501	DA	C4'-C3'-O3'	12.04	128.06	110.00
1	H	717	DA	C4'-C3'-C2'	-12.01	84.38	102.40
1	E	420	DT	C5'-C4'-O4'	11.95	127.33	109.40
1	E	409	DG	N9-C1'-C2'	11.88	131.32	113.50
1	G	602	DA	N9-C1'-C2'	-11.83	95.75	113.50
1	H	702	DA	O4'-C4'-C3'	-11.78	87.73	105.40
1	G	620	DT	N1-C1'-C2'	11.73	131.09	113.50
1	H	719	DT	C1'-O4'-C4'	-11.66	92.21	109.70
1	H	710	DC	P-O5'-C5'	11.64	137.46	120.00
1	E	405	DG	O4'-C1'-N9	11.60	125.80	108.40
1	E	419	DT	P-O3'-C3'	11.54	137.51	120.20
1	G	604	DT	C2'-C3'-O3'	-11.49	94.27	111.50
1	F	506	DT	C4'-C3'-O3'	11.45	127.18	110.00
1	G	620	DT	P-O5'-C5'	11.39	137.08	120.00
1	G	601	DA	C4'-C3'-O3'	11.38	127.07	110.00
1	F	515	DA	O4'-C1'-N9	11.30	125.36	108.40
1	G	620	DT	C4'-C3'-O3'	11.26	126.89	110.00
1	F	503	DT	N1-C1'-C2'	11.25	130.38	113.50
1	E	420	DT	P-O5'-C5'	11.25	136.87	120.00
1	G	605	DG	C4'-C3'-C2'	-11.22	85.57	102.40
1	E	403	DT	O4'-C1'-N1	11.16	125.14	108.40
1	G	606	DT	C4'-C3'-O3'	11.14	126.71	110.00
1	F	515	DA	C4'-C3'-O3'	11.13	126.70	110.00
1	E	405	DG	P-O5'-C5'	11.09	136.64	120.00
1	E	411	DG	P-O5'-C5'	11.03	136.55	120.00
1	F	508	DA	P-O3'-C3'	11.00	136.71	120.20
1	G	602	DA	C2'-C3'-O3'	-10.97	95.04	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	618	DA	C4'-C3'-O3'	10.95	126.42	110.00
1	H	717	DA	N9-C1'-C2'	10.82	129.73	113.50
1	H	707	DG	N9-C1'-C2'	10.76	129.64	113.50
1	E	419	DT	C2'-C3'-O3'	10.75	127.62	111.50
1	H	714	DC	C4'-C3'-O3'	10.69	126.04	110.00
1	E	409	DG	C4-N9-C1'	-10.68	110.98	127.00
1	F	502	DA	P-O5'-C5'	10.60	135.90	120.00
1	G	620	DT	O4'-C4'-C3'	-10.53	89.60	105.40
1	F	500	DG	C2'-C3'-O3'	10.52	127.28	111.50
1	E	402	DA	C2'-C3'-O3'	10.49	127.23	111.50
1	G	602	DA	O5'-C5'-C4'	10.38	126.37	110.80
1	F	516	DC	P-O5'-C5'	10.30	135.45	120.00
1	F	517	DA	C4'-C3'-O3'	10.24	125.36	110.00
1	F	510	DC	P-O5'-C5'	10.14	135.21	120.00
1	H	701	DA	P-O3'-C3'	10.07	135.30	120.20
1	F	519	DT	P-O3'-C3'	-10.01	105.19	120.20
1	F	519	DT	N1-C1'-C2'	9.98	128.46	113.50
1	G	618	DA	P-O3'-C3'	9.97	135.15	120.20
1	H	715	DA	O5'-C5'-C4'	9.91	125.67	110.80
1	H	702	DA	C2'-C3'-O3'	9.84	126.27	111.50
1	G	604	DT	O5'-C5'-C4'	9.84	125.55	110.80
1	G	605	DG	C5'-C4'-C3'	9.83	129.65	114.90
1	E	403	DT	C4'-C3'-O3'	9.82	124.73	110.00
1	G	611	DG	C5'-C4'-C3'	-9.81	100.18	114.90
1	H	701	DA	C4'-C3'-O3'	9.78	124.68	110.00
1	F	503	DT	O3'-P-O5'	9.67	118.50	104.00
1	G	608	DA	O3'-P-O5'	9.66	118.49	104.00
1	F	500	DG	P-O3'-C3'	9.62	134.62	120.20
1	E	407	DG	C4'-C3'-O3'	9.57	124.36	110.00
1	F	518	DA	O5'-C5'-C4'	9.57	125.15	110.80
1	F	509	DG	C4'-C3'-O3'	9.53	124.29	110.00
1	G	600	DG	C2'-C3'-O3'	9.49	125.74	111.50
1	F	515	DA	P-O5'-C5'	9.46	134.19	120.00
1	H	719	DT	N1-C1'-C2'	9.44	127.66	113.50
1	F	502	DA	C4'-C3'-C2'	-9.42	88.27	102.40
1	H	700	DG	C4'-C3'-O3'	9.39	124.09	110.00
1	H	704	DT	O4'-C1'-N1	9.36	122.44	108.40
1	E	404	DT	O4'-C1'-N1	9.35	122.43	108.40
1	F	502	DA	C5'-C4'-O4'	-9.33	95.40	109.40
1	F	510	DC	P-O3'-C3'	9.33	134.19	120.20
1	F	508	DA	C4'-C3'-O3'	9.22	123.83	110.00
1	G	620	DT	O5'-C5'-C4'	9.21	124.61	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	619	DT	C2'-C3'-O3'	9.19	125.29	111.50
1	F	504	DT	P-O3'-C3'	9.17	133.96	120.20
1	H	719	DT	C4'-C3'-C2'	-9.12	88.72	102.40
1	E	408	DA	N9-C1'-C2'	9.01	127.02	113.50
1	G	609	DG	C5'-C4'-O4'	-9.01	95.89	109.40
1	H	709	DG	O4'-C1'-N9	8.98	121.87	108.40
1	G	605	DG	C2'-C3'-O3'	8.98	124.97	111.50
1	F	514	DC	O5'-C5'-C4'	8.97	124.25	110.80
1	F	507	DG	C4'-C3'-O3'	8.96	123.45	110.00
1	G	601	DA	O4'-C1'-C2'	-8.94	93.00	106.40
1	G	605	DG	C4'-C3'-O3'	8.93	123.40	110.00
1	E	404	DT	C5'-C4'-O4'	-8.93	96.00	109.40
1	F	519	DT	C4'-C3'-O3'	8.88	123.32	110.00
1	H	710	DC	P-O3'-C3'	8.86	133.50	120.20
1	G	616	DC	O4'-C1'-N1	8.85	121.67	108.40
1	F	507	DG	P-O3'-C3'	8.79	133.38	120.20
1	E	403	DT	O4'-C1'-C2'	-8.78	93.23	106.40
1	E	404	DT	C4'-C3'-O3'	8.72	123.08	110.00
1	E	401	DA	P-O5'-C5'	8.69	133.04	120.00
1	E	416	DC	O4'-C1'-N1	8.67	121.41	108.40
1	H	701	DA	O5'-C5'-C4'	8.67	123.81	110.80
1	E	401	DA	C3'-C2'-C1'	8.67	114.60	101.60
1	H	718	DA	C4'-C3'-C2'	-8.66	89.42	102.40
1	G	604	DT	O4'-C1'-N1	8.65	121.38	108.40
1	E	414	DC	P-O5'-C5'	8.65	132.97	120.00
1	G	620	DT	O4'-C1'-N1	8.61	121.31	108.40
1	G	602	DA	C5'-C4'-C3'	8.57	127.75	114.90
1	H	701	DA	O4'-C1'-N9	8.49	121.14	108.40
1	G	616	DC	C4'-C3'-O3'	8.49	122.74	110.00
1	E	405	DG	C4'-C3'-O3'	8.47	122.71	110.00
1	H	707	DG	O3'-P-O5'	8.44	116.65	104.00
1	G	608	DA	C4'-C3'-O3'	8.40	122.60	110.00
1	G	614	DC	P-O5'-C5'	8.38	132.57	120.00
1	H	702	DA	O4'-C1'-C2'	-8.33	93.91	106.40
1	H	719	DT	P-O5'-C5'	8.31	132.47	120.00
1	H	701	DA	O4'-C1'-C2'	-8.30	93.95	106.40
1	F	503	DT	C4'-C3'-O3'	8.30	122.44	110.00
1	E	403	DT	C2'-C3'-O3'	-8.28	99.08	111.50
1	E	417	DA	C4'-C3'-C2'	-8.26	90.00	102.40
1	E	418	DA	C5'-C4'-C3'	8.26	127.28	114.90
1	H	710	DC	O5'-C5'-C4'	8.24	123.16	110.80
1	G	605	DG	O3'-P-O5'	8.23	116.35	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	410	DC	C4'-C3'-O3'	8.22	122.33	110.00
1	H	709	DG	C4'-C3'-O3'	8.22	122.33	110.00
1	E	413	DT	P-O5'-C5'	8.20	132.29	120.00
1	F	520	DT	P-O5'-C5'	8.19	132.28	120.00
1	G	603	DT	O3'-P-O5'	8.18	116.27	104.00
1	E	420	DT	C3'-C2'-C1'	8.14	113.81	101.60
1	E	409	DG	O4'-C1'-N9	8.13	120.60	108.40
1	H	719	DT	O5'-C5'-C4'	8.13	123.00	110.80
1	F	504	DT	C5'-C4'-O4'	-8.10	97.24	109.40
1	H	705	DG	N9-C1'-C2'	8.07	125.61	113.50
1	H	719	DT	O3'-P-O5'	8.07	116.11	104.00
1	G	616	DC	C2'-C3'-O3'	-8.06	99.41	111.50
1	E	400	DG	C2'-C3'-O3'	-8.04	99.44	111.50
1	F	509	DG	O4'-C1'-N9	8.00	120.40	108.40
1	H	719	DT	P-O3'-C3'	7.99	132.19	120.20
1	G	616	DC	O4'-C1'-C2'	-7.99	94.41	106.40
1	H	715	DA	O4'-C1'-N9	7.99	120.38	108.40
1	E	406	DT	O3'-P-O5'	7.94	115.91	104.00
1	F	508	DA	C2'-C3'-O3'	-7.92	99.61	111.50
1	E	410	DC	O3'-P-O5'	7.92	115.88	104.00
1	E	402	DA	O4'-C1'-C2'	-7.90	94.55	106.40
1	F	520	DT	C5'-C4'-O4'	7.90	121.25	109.40
1	E	406	DT	C4'-C3'-C2'	-7.88	90.57	102.40
1	F	506	DT	O3'-P-O5'	7.88	115.82	104.00
1	G	606	DT	P-O5'-C5'	7.88	131.82	120.00
1	E	403	DT	O3'-P-O5'	7.87	115.80	104.00
1	F	501	DA	O5'-C5'-C4'	7.85	122.57	110.80
1	F	508	DA	P-O5'-C5'	7.84	131.76	120.00
1	H	712	DC	O4'-C1'-N1	7.82	120.13	108.40
1	F	514	DC	C4'-C3'-C2'	-7.82	90.67	102.40
1	H	700	DG	O3'-P-O5'	7.81	115.72	104.00
1	G	618	DA	O5'-C5'-C4'	7.81	122.51	110.80
1	H	717	DA	C5'-C4'-O4'	7.71	120.96	109.40
1	E	419	DT	N1-C1'-C2'	7.70	125.06	113.50
1	F	500	DG	C3'-C2'-C1'	7.69	113.14	101.60
1	F	512	DC	N1-C1'-C2'	7.66	124.98	113.50
1	E	401	DA	C2'-C3'-O3'	7.63	122.95	111.50
1	G	609	DG	P-O3'-C3'	7.62	131.64	120.20
1	G	619	DT	C5'-C4'-C3'	-7.61	103.48	114.90
1	G	606	DT	O4'-C1'-N1	7.59	119.79	108.40
1	F	501	DA	C4'-C3'-C2'	-7.59	91.01	102.40
1	G	607	DG	C4'-C3'-O3'	7.59	121.39	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	620	DT	C4-C5-C7	-7.56	111.06	122.40
1	G	618	DA	P-O5'-C5'	7.51	131.27	120.00
1	F	519	DT	O4'-C1'-N1	7.51	119.67	108.40
1	H	720	DT	P-O5'-C5'	7.49	131.24	120.00
1	H	707	DG	O4'-C4'-C3'	-7.48	94.18	105.40
1	F	514	DC	P-O3'-C3'	7.46	131.39	120.20
1	E	416	DC	O5'-C5'-C4'	7.45	121.98	110.80
1	G	609	DG	C4'-C3'-O3'	7.45	121.18	110.00
1	E	419	DT	P-O5'-C5'	7.43	131.14	120.00
1	H	703	DT	O4'-C1'-N1	7.42	119.53	108.40
1	E	403	DT	O5'-C5'-C4'	7.38	121.86	110.80
1	H	710	DC	O4'-C1'-N1	7.36	119.44	108.40
1	F	506	DT	O4'-C1'-C2'	-7.36	95.36	106.40
1	H	704	DT	O5'-C5'-C4'	7.36	121.83	110.80
1	E	413	DT	N1-C1'-C2'	7.35	124.52	113.50
1	E	416	DC	C5'-C4'-O4'	7.35	120.42	109.40
1	F	507	DG	O4'-C1'-C2'	-7.35	95.38	106.40
1	F	519	DT	P-O5'-C5'	7.34	131.00	120.00
1	G	616	DC	P-O5'-C5'	7.33	131.00	120.00
1	F	500	DG	O4'-C1'-N9	7.30	119.36	108.40
1	H	707	DG	C4'-C3'-O3'	7.30	120.95	110.00
1	E	406	DT	P-O3'-C3'	7.29	131.13	120.20
1	H	702	DA	C5'-C4'-C3'	7.25	125.77	114.90
1	G	615	DA	C4'-C3'-O3'	7.25	120.87	110.00
1	F	509	DG	C5'-C4'-O4'	-7.24	98.54	109.40
1	H	713	DT	P-O5'-C5'	7.24	130.85	120.00
1	F	518	DA	C4'-C3'-O3'	7.19	120.78	110.00
1	E	413	DT	O5'-C5'-C4'	7.18	121.56	110.80
1	F	506	DT	P-O5'-C5'	7.17	130.76	120.00
1	F	518	DA	C5'-C4'-C3'	7.14	125.61	114.90
1	H	703	DT	O4'-C1'-C2'	-7.08	95.78	106.40
1	H	705	DG	P-O5'-C5'	7.08	130.62	120.00
1	E	403	DT	C4'-C3'-C2'	-7.07	91.79	102.40
1	G	601	DA	C3'-C2'-C1'	7.06	112.19	101.60
1	F	501	DA	O4'-C1'-C2'	-7.05	95.82	106.40
1	G	619	DT	C3'-C2'-C1'	-7.02	91.07	101.60
1	F	516	DC	O3'-P-O5'	7.01	114.51	104.00
1	G	605	DG	P-O5'-C5'	7.00	130.50	120.00
1	E	415	DA	P-O5'-C5'	6.99	130.48	120.00
1	G	608	DA	C4'-C3'-C2'	-6.98	91.92	102.40
1	G	617	DA	O4'-C1'-N9	6.96	118.83	108.40
1	F	509	DG	N3-C2-N2	-6.95	109.27	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	702	DA	P-O3'-C3'	-6.95	109.77	120.20
1	F	512	DC	O4'-C1'-N1	6.95	118.82	108.40
1	E	401	DA	C8-N9-C1'	-6.93	116.66	127.05
1	E	413	DT	C4'-C3'-O3'	6.86	120.28	110.00
1	H	708	DA	O5'-C5'-C4'	6.83	121.05	110.80
1	F	520	DT	O5'-C5'-C4'	6.83	121.04	110.80
1	G	612	DC	O4'-C1'-N1	6.83	118.64	108.40
1	H	716	DC	C4'-C3'-O3'	6.82	120.23	110.00
1	G	614	DC	C4'-C3'-O3'	6.80	120.20	110.00
1	E	404	DT	C4'-C3'-C2'	-6.79	92.21	102.40
1	H	702	DA	C4'-C3'-C2'	-6.78	92.23	102.40
1	G	613	DT	N1-C1'-C2'	6.77	123.66	113.50
1	F	504	DT	C4'-C3'-O3'	6.76	120.15	110.00
1	F	513	DT	N1-C1'-C2'	6.75	123.63	113.50
1	H	713	DT	C4'-C3'-O3'	6.74	120.11	110.00
1	E	414	DC	C2'-C3'-O3'	6.70	121.55	111.50
1	E	405	DG	C4-N9-C1'	-6.68	116.99	127.00
1	G	601	DA	C4-N9-C1'	6.68	137.06	127.05
1	E	419	DT	C4'-C3'-O3'	6.67	120.00	110.00
1	E	416	DC	P-O3'-C3'	6.66	130.19	120.20
1	E	415	DA	O4'-C1'-C2'	-6.64	96.44	106.40
1	G	611	DG	O4'-C1'-N9	6.64	118.36	108.40
1	G	619	DT	P-O5'-C5'	-6.64	110.05	120.00
1	F	505	DG	C2'-C3'-O3'	-6.62	101.57	111.50
1	H	709	DG	P-O5'-C5'	6.62	129.93	120.00
1	G	602	DA	C4'-C3'-C2'	-6.61	92.48	102.40
1	F	500	DG	O4'-C1'-C2'	-6.60	96.50	106.40
1	F	517	DA	O3'-P-O5'	6.59	113.88	104.00
1	G	608	DA	O4'-C4'-C3'	6.58	115.27	105.40
1	H	704	DT	P-O3'-C3'	6.58	130.07	120.20
1	H	718	DA	C1'-O4'-C4'	-6.57	99.84	109.70
1	G	613	DT	P-O3'-C3'	6.56	130.05	120.20
1	E	415	DA	C2'-C3'-O3'	6.55	121.33	111.50
1	F	520	DT	C4'-C3'-O3'	6.55	119.83	110.00
1	F	510	DC	O4'-C1'-N1	6.53	118.19	108.40
1	H	718	DA	N9-C1'-C2'	6.53	123.29	113.50
1	G	602	DA	C3'-C2'-C1'	6.51	111.36	101.60
1	F	510	DC	C4'-C3'-O3'	6.49	119.74	110.00
1	G	615	DA	P-O5'-C5'	6.48	129.73	120.00
1	E	403	DT	N1-C1'-C2'	-6.47	103.79	113.50
1	F	505	DG	C4-N9-C1'	-6.47	117.29	127.00
1	H	703	DT	C2'-C3'-O3'	6.46	121.19	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	520	DT	C4-C5-C7	-6.46	112.71	122.40
1	H	716	DC	O5'-C5'-C4'	6.46	120.49	110.80
1	F	503	DT	C2'-C3'-O3'	6.44	121.16	111.50
1	H	706	DT	P-O5'-C5'	-6.44	110.34	120.00
1	E	407	DG	C5'-C4'-C3'	6.43	124.54	114.90
1	E	401	DA	O5'-C5'-C4'	6.38	120.37	110.80
1	E	411	DG	O4'-C1'-N9	6.37	117.96	108.40
1	F	515	DA	C4-N9-C1'	-6.37	117.50	127.05
1	F	517	DA	C5'-C4'-C3'	6.36	124.44	114.90
1	H	709	DG	N3-C2-N2	-6.35	110.17	119.70
1	G	605	DG	N9-C1'-C2'	6.35	123.03	113.50
1	H	703	DT	P-O3'-C3'	6.34	129.71	120.20
1	G	602	DA	O3'-P-O5'	6.33	113.50	104.00
1	F	518	DA	C5'-C4'-O4'	-6.33	99.91	109.40
1	E	404	DT	P-O3'-C3'	6.32	129.69	120.20
1	E	412	DC	C4'-C3'-C2'	-6.31	92.93	102.40
1	F	509	DG	N1-C2-N2	6.31	125.76	116.30
1	G	605	DG	C1'-O4'-C4'	-6.30	100.25	109.70
1	F	505	DG	O5'-C5'-C4'	6.30	120.24	110.80
1	F	502	DA	C5'-C4'-C3'	6.29	124.33	114.90
1	F	520	DT	C2-N1-C1'	-6.26	109.95	119.35
1	G	618	DA	O4'-C1'-N9	6.26	117.80	108.40
1	E	418	DA	O4'-C1'-N9	6.25	117.77	108.40
1	E	405	DG	C8-N9-C1'	6.25	136.37	127.00
1	E	401	DA	O3'-P-O5'	6.21	113.32	104.00
1	F	512	DC	C4'-C3'-O3'	6.15	119.22	110.00
1	H	708	DA	C2'-C3'-O3'	-6.13	102.31	111.50
1	F	507	DG	O5'-C5'-C4'	6.13	119.99	110.80
1	H	703	DT	O5'-C5'-C4'	6.12	119.98	110.80
1	E	409	DG	P-O5'-C5'	6.12	129.18	120.00
1	G	619	DT	C4'-C3'-O3'	6.10	119.15	110.00
1	F	517	DA	O4'-C1'-N9	6.09	117.54	108.40
1	G	605	DG	O5'-C5'-C4'	-6.09	101.67	110.80
1	G	606	DT	C5'-C4'-O4'	-6.08	100.27	109.40
1	H	718	DA	P-O3'-C3'	6.07	129.31	120.20
1	F	520	DT	N1-C1'-C2'	-6.07	104.40	113.50
1	F	509	DG	C4-N9-C1'	-6.07	117.90	127.00
1	H	701	DA	C4-N9-C1'	6.06	136.14	127.05
1	E	404	DT	C4-C5-C7	-6.06	113.31	122.40
1	H	705	DG	C5'-C4'-O4'	-6.05	100.32	109.40
1	G	603	DT	O5'-C5'-C4'	6.04	119.86	110.80
1	E	415	DA	C3'-C2'-C1'	6.03	110.65	101.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	514	DC	O4'-C1'-N1	6.03	117.45	108.40
1	F	506	DT	O5'-C5'-C4'	6.01	119.82	110.80
1	E	413	DT	O4'-C1'-C2'	-5.98	97.43	106.40
1	H	712	DC	N1-C1'-C2'	5.97	122.46	113.50
1	F	501	DA	C5'-C4'-C3'	5.96	123.84	114.90
1	G	608	DA	O4'-C1'-N9	5.95	117.33	108.40
1	E	406	DT	O5'-C5'-C4'	5.95	119.72	110.80
1	G	600	DG	N9-C1'-C2'	5.95	122.42	113.50
1	F	511	DG	P-O3'-C3'	5.94	129.11	120.20
1	E	418	DA	P-O5'-C5'	5.93	128.90	120.00
1	H	705	DG	O4'-C4'-C3'	-5.93	96.50	105.40
1	F	510	DC	O5'-C5'-C4'	5.92	119.68	110.80
1	H	701	DA	O4'-C4'-C3'	-5.92	96.53	105.40
1	H	709	DG	C5'-C4'-C3'	-5.91	106.04	114.90
1	G	615	DA	O3'-P-O5'	5.90	112.85	104.00
1	E	402	DA	O4'-C1'-N9	5.89	117.24	108.40
1	G	606	DT	C4-C5-C7	-5.89	113.56	122.40
1	G	610	DC	O4'-C1'-N1	5.89	117.24	108.40
1	F	503	DT	O4'-C1'-C2'	-5.88	97.58	106.40
1	H	711	DG	C5'-C4'-O4'	5.88	118.21	109.40
1	E	417	DA	O4'-C1'-C2'	-5.87	97.60	106.40
1	G	601	DA	C8-N9-C4	-5.86	97.12	105.90
1	E	409	DG	N1-C2-N2	5.85	125.07	116.30
1	H	718	DA	O5'-C5'-C4'	5.84	119.57	110.80
1	F	504	DT	C2'-C3'-O3'	-5.84	102.74	111.50
1	F	517	DA	P-O5'-C5'	5.84	128.75	120.00
1	F	518	DA	C3'-C2'-C1'	5.83	110.35	101.60
1	H	716	DC	C2'-C3'-O3'	-5.83	102.75	111.50
1	F	507	DG	O4'-C1'-N9	5.83	117.14	108.40
1	H	707	DG	C8-N9-C1'	-5.82	118.27	127.00
1	F	512	DC	O4'-C4'-C3'	-5.81	96.68	105.40
1	G	602	DA	C5-N7-C8	-5.80	95.19	103.90
1	G	601	DA	O5'-C5'-C4'	-5.80	102.11	110.80
1	G	600	DG	O3'-P-O5'	5.79	112.68	104.00
1	E	418	DA	C4'-C3'-O3'	5.78	118.67	110.00
1	E	400	DG	O3'-P-O5'	5.78	112.67	104.00
1	H	717	DA	P-O5'-C5'	5.77	128.65	120.00
1	F	518	DA	C4'-C3'-C2'	-5.75	93.77	102.40
1	H	712	DC	C4'-C3'-O3'	5.75	118.63	110.00
1	E	405	DG	C5'-C4'-C3'	-5.72	106.32	114.90
1	H	700	DG	O4'-C1'-N9	5.71	116.97	108.40
1	F	500	DG	C1'-O4'-C4'	5.71	118.26	109.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	717	DA	C2'-C3'-O3'	5.70	120.05	111.50
1	H	701	DA	C3'-C2'-C1'	5.69	110.14	101.60
1	G	617	DA	C4'-C3'-C2'	-5.68	93.88	102.40
1	H	709	DG	C3'-C2'-C1'	5.68	110.11	101.60
1	E	416	DC	N3-C4-N4	5.67	126.41	117.90
1	F	506	DT	C3'-C2'-C1'	5.66	110.09	101.60
1	G	619	DT	O5'-C5'-C4'	-5.66	102.32	110.80
1	E	415	DA	O4'-C1'-N9	5.65	116.87	108.40
1	H	717	DA	C5'-C4'-C3'	5.64	123.37	114.90
1	E	414	DC	P-O3'-C3'	5.64	128.65	120.20
1	E	402	DA	C4-N9-C1'	5.61	135.46	127.05
1	E	420	DT	C4-C5-C7	-5.60	114.00	122.40
1	G	619	DT	P-O3'-C3'	5.60	128.60	120.20
1	G	616	DC	N1-C1'-C2'	-5.59	105.12	113.50
1	H	704	DT	C4'-C3'-O3'	5.57	118.36	110.00
1	E	402	DA	N7-C8-N9	5.56	122.14	113.80
1	H	709	DG	C4-N9-C1'	-5.55	118.67	127.00
1	E	410	DC	P-O5'-C5'	5.54	128.31	120.00
1	G	603	DT	C2'-C3'-O3'	5.53	119.79	111.50
1	F	501	DA	O4'-C1'-N9	5.51	116.67	108.40
1	E	415	DA	O5'-C5'-C4'	5.50	119.05	110.80
1	G	603	DT	C4'-C3'-O3'	5.49	118.23	110.00
1	H	703	DT	C5'-C4'-O4'	5.48	117.62	109.40
1	H	716	DC	P-O5'-C5'	5.48	128.22	120.00
1	G	607	DG	P-O3'-C3'	5.46	128.39	120.20
1	G	615	DA	P-O3'-C3'	-5.45	112.03	120.20
1	H	717	DA	O4'-C1'-N9	5.43	116.54	108.40
1	G	607	DG	C5'-C4'-C3'	-5.42	106.76	114.90
1	E	404	DT	C2-N1-C1'	-5.42	111.22	119.35
1	H	709	DG	N9-C1'-C2'	-5.42	105.37	113.50
1	H	720	DT	O5'-C5'-C4'	5.41	118.91	110.80
1	H	702	DA	C4-N9-C1'	5.39	135.14	127.05
1	H	713	DT	C5'-C4'-O4'	-5.39	101.32	109.40
1	H	720	DT	O4'-C1'-N1	5.38	116.47	108.40
1	E	411	DG	O5'-C5'-C4'	5.38	118.87	110.80
1	E	407	DG	C4-N9-C1'	5.37	135.06	127.00
1	G	614	DC	O4'-C1'-N1	5.36	116.44	108.40
1	H	709	DG	N1-C2-N2	5.36	124.34	116.30
1	G	607	DG	C4'-C3'-C2'	-5.36	94.37	102.40
1	E	418	DA	O5'-C5'-C4'	5.35	118.83	110.80
1	H	719	DT	O4'-C4'-C3'	-5.34	97.39	105.40
1	E	403	DT	C3'-C2'-C1'	5.33	109.59	101.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	513	DT	O4'-C1'-C2'	-5.32	98.41	106.40
1	F	504	DT	P-O5'-C5'	5.32	127.98	120.00
1	F	516	DC	C4'-C3'-O3'	5.32	117.97	110.00
1	G	606	DT	C3'-C2'-C1'	5.31	109.56	101.60
1	E	401	DA	O4'-C1'-N9	5.30	116.35	108.40
1	F	500	DG	C5'-C4'-O4'	-5.30	101.45	109.40
1	H	707	DG	P-O5'-C5'	5.28	127.92	120.00
1	G	620	DT	C6-N1-C1'	5.27	127.26	119.35
1	G	603	DT	O4'-C1'-C2'	-5.26	98.51	106.40
1	F	519	DT	O4'-C4'-C3'	-5.26	97.51	105.40
1	F	507	DG	C2'-C3'-O3'	-5.26	103.61	111.50
1	H	710	DC	C5'-C4'-O4'	5.23	117.25	109.40
1	E	417	DA	O4'-C4'-C3'	5.22	113.23	105.40
1	E	417	DA	N9-C1'-C2'	5.22	121.33	113.50
1	H	713	DT	O4'-C1'-C2'	-5.21	98.58	106.40
1	G	603	DT	P-O5'-C5'	5.21	127.82	120.00
1	H	712	DC	C1'-O4'-C4'	-5.21	101.89	109.70
1	E	408	DA	O3'-P-O5'	5.20	111.81	104.00
1	G	601	DA	C8-N9-C1'	-5.20	119.24	127.05
1	E	405	DG	N1-C2-N2	5.20	124.10	116.30
1	H	714	DC	O4'-C1'-N1	5.19	116.18	108.40
1	G	616	DC	O3'-P-O5'	5.18	111.77	104.00
1	H	720	DT	C3'-C2'-C1'	5.17	109.36	101.60
1	E	405	DG	C2'-C3'-O3'	5.17	119.26	111.50
1	E	405	DG	N9-C1'-C2'	5.17	121.25	113.50
1	E	416	DC	C4'-C3'-C2'	-5.16	94.66	102.40
1	E	407	DG	C2'-C3'-O3'	5.14	119.21	111.50
1	F	507	DG	C3'-C2'-C1'	5.12	109.29	101.60
1	H	720	DT	C5'-C4'-C3'	5.12	122.58	114.90
1	E	404	DT	P-O5'-C5'	5.12	127.67	120.00
1	F	508	DA	C5'-C4'-O4'	5.11	117.07	109.40
1	G	610	DC	C4'-C3'-O3'	5.11	117.67	110.00
1	E	414	DC	O3'-P-O5'	-5.11	96.34	104.00
1	E	401	DA	O4'-C1'-C2'	-5.10	98.75	106.40
1	H	701	DA	C1'-O4'-C4'	5.10	117.35	109.70
1	E	401	DA	C4-N9-C1'	5.10	134.69	127.05
1	G	618	DA	C3'-C2'-C1'	5.09	109.24	101.60
1	F	503	DT	C3'-C2'-C1'	5.08	109.22	101.60
1	E	408	DA	P-O5'-C5'	5.07	127.60	120.00
1	E	416	DC	P-O5'-C5'	5.06	127.58	120.00
1	G	607	DG	O4'-C1'-N9	5.05	115.98	108.40
1	E	416	DC	N1-C1'-C2'	-5.04	105.94	113.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	416	DC	C3'-C2'-C1'	5.04	109.16	101.60
1	F	510	DC	C3'-C2'-C1'	5.03	109.15	101.60
1	H	705	DG	O4'-C1'-N9	-5.03	100.86	108.40
1	H	714	DC	O3'-P-O5'	-5.01	96.48	104.00
1	G	607	DG	O4'-C1'-C2'	-5.00	98.89	106.40

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
1	E	420	DT	Sidechain
1	F	500	DG	Sidechain

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Mol	Chain	Res	Type	Group
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
1	H	713	DT	Sidechain
1	H	714	DC	Sidechain

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Mol	Chain	Res	Type	Group
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	41	0
1	F	429	0	239	37	0
1	G	429	0	239	43	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	141	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 35.

All (141) 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:416:DC:H42	1:F:505:DG:H1	1.33	0.76
1:E:405:DG:H2''	1:E:406:DT:H72	1.69	0.74
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H8	1:E:408:DA:H5''	1.57	0.69
1:H:708:DA:H5''	1:H:708:DA:H8	1.57	0.69
1:G:602:DA:H2'	1:G:603:DT:H71	1.73	0.69
1:G:602:DA:H2''	1:G:603:DT:OP2	1.94	0.68
1:F:518:DA:H2''	1:F:519:DT:H4'	1.75	0.68
1:G:603:DT:H2''	1:G:604:DT:C6	2.28	0.68
1:E:401:DA:H2''	1:E:402:DA:C8	2.27	0.67
1:E:403:DT:H6	1:E:403:DT:OP2	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:E:414:DC:H2'	1:E:415:DA:C8	2.31	0.66
1:G:604:DT:H2'	1:G:604:DT:OP1	1.96	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:H6	1:E:414:DC:O5'	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:E:402:DA:OP2	1:E:402:DA:H8	1.83	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:H:718:DA:H2'	1:H:719:DT:OP2	1.99	0.62
1:H:708:DA:H5''	1:H:708:DA:C8	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
1:G:609:DG:H2'	1:G:610:DC:C6	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:704:DT:OP2	1:H:704:DT:H6	1.85	0.59
1:F:514:DC:H2'	1:F:515:DA:C8	2.38	0.59
1:E:400:DG:H2'	1:E:401:DA:H8	1.66	0.58
1:G:607:DG:H2''	1:G:608:DA:C8	2.37	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:G:617:DA:O5'	1:G:617:DA:H2'	2.06	0.55
1:H:716:DC:H2''	1:H:717:DA:C8	2.42	0.55
1:G:602:DA:O5'	1:G:602:DA:C8	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:H2'	1:H:715:DA:OP2	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:H73	1:E:419:DT:P	2.51	0.51
1:F:506:DT:C2'	1:F:507:DG:H5'	2.39	0.51
1:E:406:DT:OP2	1:E:406:DT:H6	1.94	0.50
1:F:501:DA:H3'	1:F:501:DA:H8	1.76	0.50
1:F:501:DA:H3'	1:F:501:DA:C8	2.46	0.50
1:H:700:DG:N2	1:H:702:DA:N1	2.60	0.50
1:F:504:DT:OP2	1:F:504:DT:H6	1.95	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: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:F:518:DA:C2	1:F:519:DT:H1'	2.47	0.49
1:H:719:DT:H6	1:H:719:DT:OP1	1.96	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:F:515:DA:H2''	1:F:516:DC:H5	1.80	0.47
1:G:604:DT:O4'	1:G:604:DT:OP2	2.32	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:F:518:DA:H2''	1:F:519:DT:C4'	2.44	0.46
1:G:601:DA:H3'	1:G:602:DA:C5	2.50	0.46
1:E:402:DA:H3'	1:E:403:DT:O4'	2.14	0.46
1:F:501:DA:C8	1:F:501:DA:C3'	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:H73	1:E:419:DT:OP2	2.17	0.45
1:E:404:DT:H6	1:E:404:DT:OP2	1.99	0.45
1:E:403:DT:OP2	1:E:403:DT:C6	2.65	0.45
1:E:415:DA:H2''	1:E:416:DC:C6	2.49	0.45
1:G:618:DA:N1	1:H:703:DT:O4	2.50	0.45
1:F:516:DC:H3'	1:F:516:DC:OP2	2.17	0.44
1:G:615:DA:H8	1:G:615:DA:OP2	2.00	0.44
1:H:713:DT:C6	1:H:713:DT:H5''	2.53	0.44
1:F:502:DA:N3	1:F:502:DA:H2'	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:OP2	1:G:603:DT:H6	2.02	0.41
1:E:402:DA:N3	1:F:519:DT:O4	2.52	0.41
1:E:408:DA:H5''	1:E:408:DA:C8	2.47	0.41
1:E:401:DA:H2''	1:E:402:DA:C1'	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:612:DC:H2'	1:G:613:DT:C6	2.55	0.41
1:G:618:DA:H2	1:H:703:DT:H3	1.68	0.41
1:F:511:DG:H4'	1:F:512:DC:OP1	2.20	0.41
1:E:405:DG:H2''	1:E:406:DT:C7	2.46	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 oligosaccharides 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	G	1
1	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	601:DA	O3'	602:DA	P	1.81
1	E	401:DA	O3'	402:DA	P	1.75

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.