



Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 07:53 pm BST

PDB ID : 1K82
Title : Crystal structure of E.coli formamidopyrimidine-DNA glycosylase (Fpg) covalently trapped with DNA
Authors : Gilboa, R.; Zharkov, D.O.; Golan, G.; Fernandes, A.S.; Gerchman, S.E.; Matz, E.; Kycia, J.H.; Grollman, A.P.; Shoham, G.
Deposited on : 2001-10-22
Resolution : 2.10 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

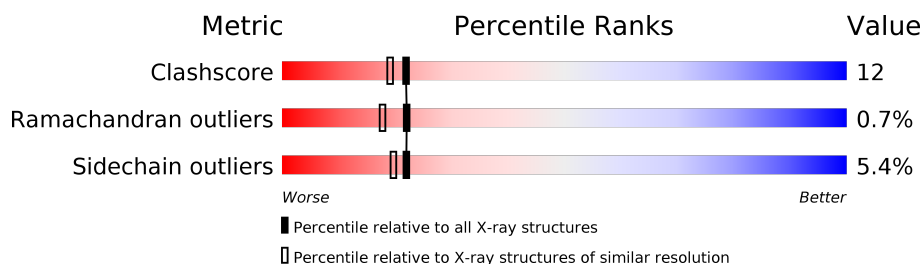
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)

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 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	13	62% 38%
1	F	13	69% 31%
1	G	13	69% 31%
1	H	13	69% 31%
2	I	13	8% 62% 31%
2	J	13	8% 54% 38%
2	K	13	8% 69% 23%
2	L	13	8% 54% 38%

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Mol	Chain	Length	Quality of chain
3	A	268	<div><div></div><div>72%22%</div><div></div><div></div></div>
3	B	268	<div><div></div><div>70%25%</div><div></div><div></div></div>
3	C	268	<div><div></div><div>72%21%</div><div></div><div></div></div>
3	D	268	<div><div></div><div>76%19%</div><div></div><div></div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10716 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 5'-D(*GP*GP*CP*TP*TP*CP*CP*TP*CP*CP*TP*GP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	13	Total	C	N	O	P	0	0	0
			260	125	43	80	12			
1	F	13	Total	C	N	O	P	0	0	0
			260	125	43	80	12			
1	G	13	Total	C	N	O	P	0	0	0
			260	125	43	80	12			
1	H	13	Total	C	N	O	P	0	0	0
			260	125	43	80	12			

- Molecule 2 is a DNA chain called 5'-D(*CP*CP*AP*GP*GP*AP*(PED)P*GP*AP*AP*GP*CP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	13	Total	C	N	O	P	0	0	0
			256	121	52	71	12			
2	J	13	Total	C	N	O	P	0	0	0
			256	121	52	71	12			
2	K	13	Total	C	N	O	P	0	0	0
			256	121	52	71	12			
2	L	13	Total	C	N	O	P	0	0	0
			256	121	52	71	12			

- Molecule 3 is a protein called formamidopyrimidine-DNA glycosylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	260	Total	C	N	O	S	0	0	0
			2038	1297	370	362	9			
3	B	260	Total	C	N	O	S	0	0	0
			2030	1293	367	361	9			
3	C	260	Total	C	N	O	S	0	0	0
			2042	1299	368	366	9			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	260	Total	C	N	O	S	0	0	0
			2039	1298	370	362	9			

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Zn	0	0
			1	1		
4	A	1	Total	Zn	0	0
			1	1		
4	D	1	Total	Zn	0	0
			1	1		
4	C	1	Total	Zn	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	15	Total	O	0	0
			15	15		
5	I	23	Total	O	0	0
			23	23		
5	F	16	Total	O	0	0
			16	16		
5	J	24	Total	O	0	0
			24	24		
5	G	18	Total	O	0	0
			18	18		
5	K	20	Total	O	0	0
			20	20		
5	H	18	Total	O	0	0
			18	18		
5	L	21	Total	O	0	0
			21	21		
5	A	93	Total	O	0	0
			93	93		
5	B	82	Total	O	0	0
			82	82		
5	C	77	Total	O	0	0
			77	77		
5	D	92	Total	O	0	0
			92	92		

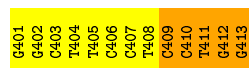
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

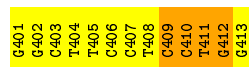
- Molecule 1: 5'-D(*GP*GP*CP*TP*TP*CP*CP*TP*CP*CP*TP*GP*G)-3'

Chain E: 



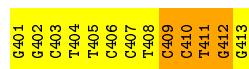
- Molecule 1: 5'-D(*GP*GP*CP*TP*TP*CP*CP*TP*CP*CP*TP*GP*G)-3'

Chain F: 



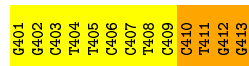
- Molecule 1: 5'-D(*GP*GP*CP*TP*TP*CP*CP*TP*CP*CP*TP*GP*G)-3'

Chain G: 




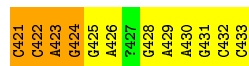
- Molecule 1: 5'-D(*GP*GP*CP*TP*TP*CP*CP*TP*CP*CP*TP*GP*G)-3'

Chain H: 



- Molecule 2: 5'-D(*CP*CP*AP*GP*GP*AP*(PED)P*GP*AP*AP*GP*CP*C)-3'

Chain I: 

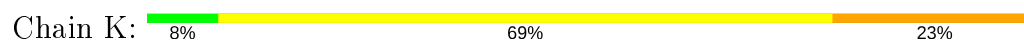


- Molecule 2: 5'-D(*CP*CP*AP*GP*GP*AP*(PED)P*GP*AP*AP*GP*CP*C)-3'

Chain J: 



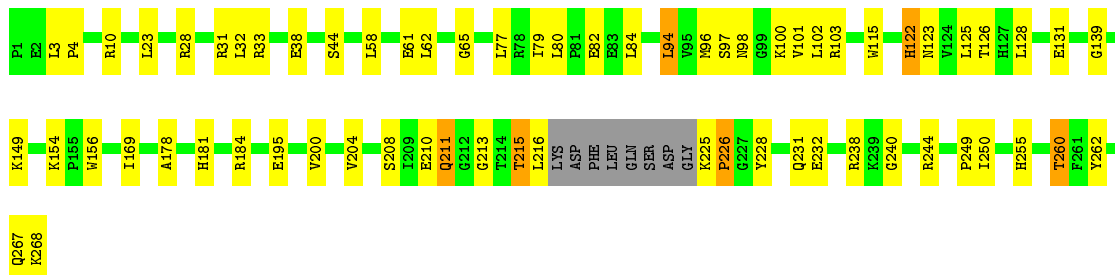
- Molecule 2: 5'-D(*CP*CP*AP*GP*GP*AP*(PED)P*GP*AP*AP*GP*CP*C)-3'



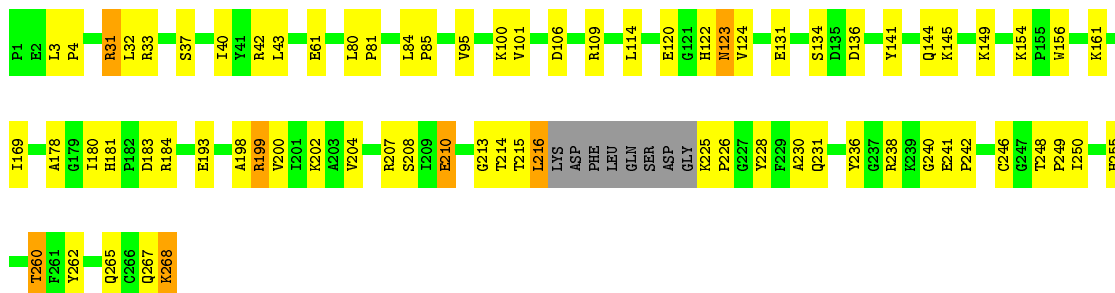
- Molecule 2: 5'-D(*CP*CP*AP*GP*GP*AP*(PED)P*GP*AP*AP*GP*CP*C)-3'



- Molecule 3: formamidopyrimidine-DNA glycosylase

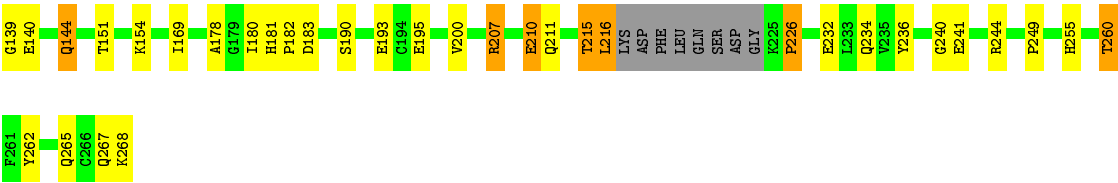


- Molecule 3: formamidopyrimidine-DNA glycosylase

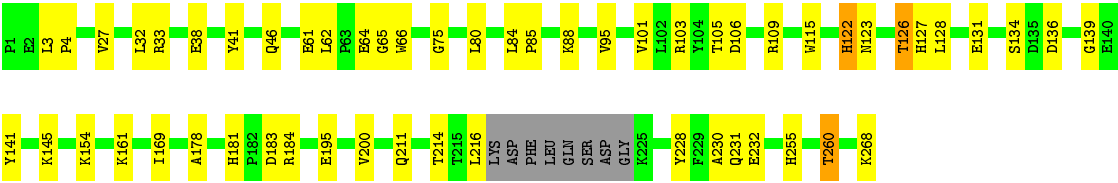


- Molecule 3: formamidopyrimidine-DNA glycosylase





• Molecule 3: formamidopyrimidine-DNA glycosylase



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.70 Å 96.03 Å 96.23 Å 90.00° 96.80° 90.00°	Depositor
Resolution (Å)	34.00 – 2.10	Depositor
% Data completeness (in resolution range)	(Not available) (34.00-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.214 , 0.265	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10716	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PED, ZN

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	3.03	18/289 (6.2%)	5.96	96/444 (21.6%)
1	F	2.97	19/289 (6.6%)	5.76	97/444 (21.8%)
1	G	2.99	17/289 (5.9%)	5.90	95/444 (21.4%)
1	H	2.98	18/289 (6.2%)	6.06	99/444 (22.3%)
2	I	1.76	10/275 (3.6%)	5.55	86/420 (20.5%)
2	J	1.74	9/275 (3.3%)	5.82	91/420 (21.7%)
2	K	1.73	9/275 (3.3%)	5.59	81/420 (19.3%)
2	L	1.74	10/275 (3.6%)	5.70	83/420 (19.8%)
3	A	0.33	0/2085	0.79	1/2826 (0.0%)
3	B	0.31	0/2076	0.80	3/2815 (0.1%)
3	C	0.33	0/2088	0.78	0/2830
3	D	0.32	0/2086	0.77	0/2828
All	All	1.17	110/10591 (1.0%)	2.89	732/14755 (5.0%)

All (110) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	404	DT	C5-C7	18.17	1.60	1.50
1	F	411	DT	C5-C7	17.36	1.60	1.50
1	G	411	DT	C5-C7	17.27	1.60	1.50
1	G	404	DT	C5-C7	17.03	1.60	1.50
1	E	405	DT	C5-C7	16.97	1.60	1.50
1	G	408	DT	C5-C7	16.90	1.60	1.50
1	E	411	DT	C5-C7	16.89	1.60	1.50
1	H	411	DT	C5-C7	16.87	1.60	1.50
1	F	404	DT	C5-C7	16.79	1.60	1.50
1	E	408	DT	C5-C7	16.78	1.60	1.50
1	H	408	DT	C5-C7	16.49	1.59	1.50
1	F	405	DT	C5-C7	16.46	1.59	1.50
1	F	408	DT	C5-C7	16.37	1.59	1.50
1	H	405	DT	C5-C7	16.21	1.59	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	404	DT	C5-C7	16.15	1.59	1.50
1	G	405	DT	C5-C7	16.06	1.59	1.50
1	G	404	DT	C2-N3	11.19	1.46	1.37
1	E	404	DT	C2-N3	11.12	1.46	1.37
1	E	408	DT	C2-N3	11.12	1.46	1.37
1	H	411	DT	C2-N3	11.12	1.46	1.37
1	F	411	DT	C2-N3	11.08	1.46	1.37
1	H	405	DT	C2-N3	10.97	1.46	1.37
1	G	411	DT	C2-N3	10.96	1.46	1.37
1	F	404	DT	C2-N3	10.82	1.46	1.37
1	F	408	DT	C2-N3	10.62	1.46	1.37
1	F	405	DT	C2-N3	10.46	1.46	1.37
1	G	408	DT	C2-N3	10.45	1.46	1.37
1	E	411	DT	C2-N3	10.41	1.46	1.37
1	H	408	DT	C2-N3	10.39	1.46	1.37
1	E	405	DT	C2-N3	10.19	1.46	1.37
1	H	404	DT	C2-N3	10.08	1.45	1.37
1	G	405	DT	C2-N3	10.00	1.45	1.37
1	F	402	DG	C5-C4	6.34	1.42	1.38
1	H	413	DG	C5-C4	6.25	1.42	1.38
1	H	412	DG	C5-C4	6.15	1.42	1.38
1	E	402	DG	C5-C4	6.10	1.42	1.38
1	E	412	DG	C5-C4	6.05	1.42	1.38
1	E	413	DG	C5-C4	6.02	1.42	1.38
2	I	424	DG	C5-C4	5.94	1.42	1.38
2	L	428	DG	N3-C4	5.93	1.39	1.35
2	I	431	DG	C5-C4	5.87	1.42	1.38
2	K	431	DG	C5-C4	5.83	1.42	1.38
1	H	402	DG	C5-C4	5.80	1.42	1.38
2	L	428	DG	C5-C4	5.79	1.42	1.38
1	G	401	DG	C5-C4	5.77	1.42	1.38
1	G	401	DG	N3-C4	5.75	1.39	1.35
1	F	413	DG	C5-C4	5.72	1.42	1.38
1	H	401	DG	C5-C6	5.71	1.48	1.42
2	I	428	DG	C5-C4	5.68	1.42	1.38
2	J	431	DG	C5-C4	5.68	1.42	1.38
2	J	428	DG	C5-C4	5.68	1.42	1.38
1	G	401	DG	C5-C6	5.66	1.48	1.42
1	E	413	DG	C5-C6	5.64	1.48	1.42
2	L	424	DG	C5-C4	5.64	1.42	1.38
2	J	431	DG	C5-C6	5.63	1.48	1.42
2	K	424	DG	N3-C4	5.62	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	424	DG	C5-C4	5.61	1.42	1.38
1	F	412	DG	C5-C4	5.60	1.42	1.38
1	G	413	DG	C5-C4	5.57	1.42	1.38
2	L	424	DG	C5-C6	5.54	1.47	1.42
1	G	402	DG	C5-C6	5.50	1.47	1.42
1	E	401	DG	N3-C4	5.49	1.39	1.35
1	E	412	DG	C5-C6	5.49	1.47	1.42
1	H	413	DG	C5-C6	5.48	1.47	1.42
1	F	413	DG	C5-C6	5.48	1.47	1.42
1	E	401	DG	C5-C4	5.47	1.42	1.38
2	J	425	DG	C5-C4	5.47	1.42	1.38
2	K	425	DG	C5-C4	5.46	1.42	1.38
2	K	431	DG	N3-C4	5.45	1.39	1.35
2	K	424	DG	C5-C6	5.42	1.47	1.42
2	K	425	DG	C5-C6	5.41	1.47	1.42
1	F	401	DG	N3-C4	5.41	1.39	1.35
2	J	428	DG	N3-C4	5.39	1.39	1.35
2	I	424	DG	C5-C6	5.38	1.47	1.42
2	K	428	DG	C5-C6	5.37	1.47	1.42
2	I	425	DG	C5-C6	5.36	1.47	1.42
2	K	424	DG	C5-C4	5.36	1.42	1.38
1	E	401	DG	C5-C6	5.33	1.47	1.42
2	I	431	DG	C5-C6	5.33	1.47	1.42
1	H	401	DG	N3-C4	5.33	1.39	1.35
1	G	413	DG	C5-C6	5.29	1.47	1.42
2	L	424	DG	N3-C4	5.27	1.39	1.35
2	I	428	DG	N3-C4	5.26	1.39	1.35
1	H	412	DG	C5-C6	5.26	1.47	1.42
1	F	412	DG	C5-C6	5.25	1.47	1.42
2	L	425	DG	C5-C6	5.25	1.47	1.42
1	F	401	DG	C5-C6	5.24	1.47	1.42
2	L	431	DG	C5-C6	5.24	1.47	1.42
2	I	431	DG	N3-C4	5.24	1.39	1.35
1	F	412	DG	N3-C4	5.24	1.39	1.35
1	F	401	DG	C5-C4	5.22	1.42	1.38
1	G	402	DG	C5-C4	5.21	1.42	1.38
1	F	402	DG	C5-C6	5.20	1.47	1.42
2	L	425	DG	C5-C4	5.20	1.42	1.38
1	H	413	DG	N3-C4	5.19	1.39	1.35
2	J	424	DG	C5-C6	5.18	1.47	1.42
1	E	402	DG	C5-C6	5.18	1.47	1.42
2	J	424	DG	N3-C4	5.14	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	413	DG	N3-C4	5.14	1.39	1.35
2	L	428	DG	C5-C6	5.14	1.47	1.42
2	I	428	DG	C5-C6	5.13	1.47	1.42
1	H	402	DG	C5-C6	5.12	1.47	1.42
1	F	413	DG	N3-C4	5.12	1.39	1.35
2	J	425	DG	C5-C6	5.12	1.47	1.42
2	I	425	DG	C5-C4	5.08	1.42	1.38
2	L	425	DG	N3-C4	5.07	1.39	1.35
2	K	428	DG	C5-C4	5.05	1.41	1.38
1	H	401	DG	C5-C4	5.03	1.41	1.38
1	G	412	DG	C5-C4	5.02	1.41	1.38
1	E	412	DG	N3-C4	5.00	1.39	1.35

All (732) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	413	DG	N7-C8-N9	22.34	124.27	113.10
1	H	413	DG	N7-C8-N9	21.92	124.06	113.10
1	F	412	DG	N7-C8-N9	21.85	124.02	113.10
2	L	424	DG	N7-C8-N9	21.82	124.01	113.10
2	J	431	DG	N7-C8-N9	21.74	123.97	113.10
2	L	431	DG	N7-C8-N9	21.72	123.96	113.10
1	E	412	DG	N7-C8-N9	21.66	123.93	113.10
1	H	412	DG	N3-C4-C5	-21.61	117.79	128.60
2	J	422	DC	C2-N3-C4	21.54	130.67	119.90
2	I	424	DG	N7-C8-N9	21.50	123.85	113.10
1	G	413	DG	N7-C8-N9	21.39	123.80	113.10
1	H	402	DG	N7-C8-N9	21.37	123.78	113.10
2	L	425	DG	N7-C8-N9	21.33	123.77	113.10
2	J	424	DG	N7-C8-N9	21.26	123.73	113.10
1	H	412	DG	N7-C8-N9	21.19	123.69	113.10
1	F	402	DG	N7-C8-N9	21.18	123.69	113.10
1	G	402	DG	N7-C8-N9	21.14	123.67	113.10
1	G	412	DG	N7-C8-N9	21.11	123.66	113.10
2	K	424	DG	N7-C8-N9	20.94	123.57	113.10
1	E	402	DG	N7-C8-N9	20.75	123.48	113.10
2	K	431	DG	N7-C8-N9	20.75	123.47	113.10
1	F	413	DG	N7-C8-N9	20.70	123.45	113.10
1	E	413	DG	C8-N9-C4	-20.66	98.13	106.40
2	J	428	DG	N7-C8-N9	20.64	123.42	113.10
2	J	431	DG	C8-N9-C4	-20.60	98.16	106.40
2	K	425	DG	N3-C4-C5	-20.59	118.31	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	428	DG	N7-C8-N9	20.55	123.38	113.10
2	I	425	DG	N7-C8-N9	20.21	123.21	113.10
2	L	428	DG	N7-C8-N9	20.17	123.19	113.10
1	H	413	DG	N3-C4-C5	-20.12	118.54	128.60
2	I	424	DG	C8-N9-C4	-20.08	98.37	106.40
1	E	412	DG	C8-N9-C4	-20.06	98.38	106.40
1	H	413	DG	C8-N9-C4	-20.06	98.38	106.40
2	L	433	DC	C2-N3-C4	19.98	129.89	119.90
2	K	425	DG	N7-C8-N9	19.96	123.08	113.10
1	G	401	DG	N7-C8-N9	19.88	123.04	113.10
1	E	412	DG	N3-C4-C5	-19.86	118.67	128.60
2	K	428	DG	N7-C8-N9	19.77	122.98	113.10
1	H	401	DG	N7-C8-N9	19.72	122.96	113.10
1	F	413	DG	C8-N9-C4	-19.71	98.52	106.40
1	G	412	DG	N3-C4-C5	-19.70	118.75	128.60
1	G	413	DG	N3-C4-C5	-19.67	118.76	128.60
2	L	424	DG	C8-N9-C4	-19.66	98.53	106.40
1	F	412	DG	C8-N9-C4	-19.60	98.56	106.40
2	J	421	DC	C2-N3-C4	19.54	129.67	119.90
1	E	402	DG	N3-C4-C5	-19.37	118.91	128.60
2	J	431	DG	N3-C4-C5	-19.28	118.96	128.60
1	G	402	DG	C8-N9-C4	-19.26	98.69	106.40
1	H	401	DG	N3-C4-C5	-19.26	118.97	128.60
2	K	424	DG	C8-N9-C4	-19.25	98.70	106.40
2	J	428	DG	N3-C4-C5	-19.25	118.98	128.60
1	H	410	DC	C2-N3-C4	19.24	129.52	119.90
1	H	402	DG	C8-N9-C4	-19.22	98.71	106.40
2	I	425	DG	N3-C4-C5	-19.21	118.99	128.60
1	G	413	DG	C8-N9-C4	-19.19	98.72	106.40
1	G	402	DG	N3-C4-C5	-19.17	119.01	128.60
2	K	431	DG	N3-C4-C5	-19.16	119.02	128.60
2	J	425	DG	N7-C8-N9	19.07	122.63	113.10
2	J	424	DG	N3-C4-C5	-18.99	119.10	128.60
1	G	412	DG	C8-N9-C4	-18.98	98.81	106.40
1	F	401	DG	N7-C8-N9	18.93	122.57	113.10
1	H	402	DG	N3-C4-C5	-18.86	119.17	128.60
1	E	401	DG	N7-C8-N9	18.86	122.53	113.10
1	H	412	DG	C8-N9-C4	-18.85	98.86	106.40
1	F	402	DG	C8-N9-C4	-18.85	98.86	106.40
1	E	401	DG	N3-C4-C5	-18.72	119.24	128.60
2	J	424	DG	C8-N9-C4	-18.67	98.93	106.40
2	I	424	DG	N3-C4-C5	-18.60	119.30	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	428	DG	C8-N9-C4	-18.60	98.96	106.40
2	I	425	DG	C8-N9-C4	-18.57	98.97	106.40
2	L	431	DG	C8-N9-C4	-18.55	98.98	106.40
2	L	431	DG	N3-C4-C5	-18.52	119.34	128.60
1	F	406	DC	C2-N3-C4	18.48	129.14	119.90
2	L	425	DG	C8-N9-C4	-18.43	99.03	106.40
2	K	431	DG	C8-N9-C4	-18.36	99.06	106.40
1	E	413	DG	N3-C4-C5	-18.36	119.42	128.60
1	G	413	DG	C2-N3-C4	18.36	121.08	111.90
1	F	402	DG	N3-C4-C5	-18.30	119.45	128.60
2	I	422	DC	C2-N3-C4	18.27	129.04	119.90
2	K	425	DG	C8-N9-C4	-18.23	99.11	106.40
2	J	422	DC	N3-C4-C5	-18.21	114.62	121.90
2	J	428	DG	C8-N9-C4	-18.16	99.14	106.40
1	H	403	DC	N3-C4-C5	-18.05	114.68	121.90
1	G	401	DG	N3-C4-C5	-18.05	119.58	128.60
1	E	402	DG	C8-N9-C4	-17.95	99.22	106.40
2	I	428	DG	N3-C4-C5	-17.95	119.63	128.60
1	G	401	DG	C8-N9-C4	-17.89	99.24	106.40
1	H	401	DG	C2-N3-C4	17.88	120.84	111.90
2	K	425	DG	C2-N3-C4	17.87	120.84	111.90
1	H	401	DG	C8-N9-C4	-17.84	99.26	106.40
2	L	432	DC	C2-N3-C4	17.81	128.81	119.90
2	I	425	DG	C2-N3-C4	17.80	120.80	111.90
2	K	428	DG	N3-C4-C5	-17.78	119.71	128.60
2	L	433	DC	N3-C4-C5	-17.74	114.81	121.90
1	F	413	DG	N3-C4-C5	-17.73	119.74	128.60
2	K	424	DG	N3-C4-C5	-17.71	119.75	128.60
2	I	428	DG	C8-N9-C4	-17.67	99.33	106.40
2	L	428	DG	N3-C4-C5	-17.67	119.77	128.60
1	F	401	DG	N3-C4-C5	-17.65	119.78	128.60
2	L	424	DG	N3-C4-C5	-17.52	119.84	128.60
1	H	412	DG	C2-N3-C4	17.44	120.62	111.90
1	H	409	DC	N3-C4-C5	-17.42	114.93	121.90
2	I	431	DG	N7-C8-N9	17.36	121.78	113.10
2	I	422	DC	N3-C4-C5	-17.30	114.98	121.90
2	J	425	DG	C8-N9-C4	-17.26	99.50	106.40
1	H	410	DC	N3-C4-C5	-17.14	115.05	121.90
1	H	409	DC	C2-N3-C4	17.07	128.43	119.90
2	I	421	DC	C2-N3-C4	16.99	128.40	119.90
1	E	402	DG	C2-N3-C4	16.96	120.38	111.90
1	G	412	DG	C2-N3-C4	16.95	120.38	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	401	DG	C2-N3-C4	16.92	120.36	111.90
2	J	425	DG	N3-C4-C5	-16.86	120.17	128.60
2	J	421	DC	N3-C4-C5	-16.82	115.17	121.90
1	F	401	DG	C8-N9-C4	-16.81	99.68	106.40
1	E	406	DC	C2-N3-C4	16.76	128.28	119.90
2	K	428	DG	C8-N9-C4	-16.72	99.71	106.40
2	L	431	DG	C2-N3-C4	16.71	120.26	111.90
2	I	431	DG	N3-C4-C5	-16.71	120.25	128.60
2	J	431	DG	C2-N3-C4	16.66	120.23	111.90
2	K	428	DG	C2-N3-C4	16.63	120.21	111.90
1	E	412	DG	C2-N3-C4	16.58	120.19	111.90
2	I	432	DC	C2-N3-C4	16.40	128.10	119.90
2	J	428	DG	C2-N3-C4	16.39	120.10	111.90
1	G	402	DG	C2-N3-C4	16.38	120.09	111.90
1	F	406	DC	N3-C4-C5	-16.33	115.37	121.90
2	I	431	DG	C8-N9-C4	-16.29	99.88	106.40
1	E	403	DC	N3-C4-C5	-16.28	115.39	121.90
2	L	421	DC	C2-N3-C4	16.18	127.99	119.90
2	L	425	DG	N3-C4-C5	-16.11	120.54	128.60
1	H	413	DG	C2-N3-C4	16.09	119.95	111.90
1	F	409	DC	C2-N3-C4	16.03	127.91	119.90
1	E	407	DC	C2-N3-C4	16.00	127.90	119.90
2	J	432	DC	C2-N3-C4	15.99	127.90	119.90
2	L	424	DG	C2-N3-C4	15.98	119.89	111.90
1	G	407	DC	C2-N3-C4	15.91	127.85	119.90
2	J	425	DG	C2-N3-C4	15.89	119.85	111.90
2	J	424	DG	C2-N3-C4	15.85	119.82	111.90
1	G	410	DC	C2-N3-C4	15.84	127.82	119.90
1	H	402	DG	C2-N3-C4	15.81	119.80	111.90
2	I	421	DC	N3-C4-C5	-15.75	115.60	121.90
1	H	403	DC	C2-N3-C4	15.66	127.73	119.90
2	K	422	DC	C2-N3-C4	15.64	127.72	119.90
1	F	410	DC	N3-C4-C5	-15.61	115.66	121.90
2	I	433	DC	C2-N3-C4	15.56	127.68	119.90
2	L	421	DC	N3-C4-C5	-15.56	115.68	121.90
1	F	413	DG	C2-N3-C4	15.55	119.67	111.90
1	E	410	DC	C2-N3-C4	15.52	127.66	119.90
1	E	406	DC	N3-C4-C5	-15.51	115.70	121.90
2	I	428	DG	C2-N3-C4	15.50	119.65	111.90
2	I	424	DG	C2-N3-C4	15.49	119.64	111.90
2	J	432	DC	N3-C4-C5	-15.38	115.75	121.90
1	E	403	DC	C2-N3-C4	15.37	127.59	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	422	DC	N3-C4-C5	-15.37	115.75	121.90
1	F	407	DC	C2-N3-C4	15.31	127.55	119.90
2	L	432	DC	N3-C4-C5	-15.30	115.78	121.90
1	F	402	DG	C2-N3-C4	15.23	119.52	111.90
1	E	413	DG	C2-N3-C4	15.22	119.51	111.90
1	G	403	DC	C2-N3-C4	15.10	127.45	119.90
1	F	407	DC	N3-C4-C5	-15.09	115.86	121.90
1	F	410	DC	C2-N3-C4	15.08	127.44	119.90
1	E	401	DG	C8-N9-C4	-15.04	100.38	106.40
1	G	409	DC	C2-N3-C4	15.00	127.40	119.90
1	E	410	DC	N3-C4-C5	-14.98	115.91	121.90
2	I	432	DC	N3-C4-C5	-14.93	115.93	121.90
2	L	431	DG	C5-N7-C8	-14.93	96.84	104.30
1	H	406	DC	C2-N3-C4	14.90	127.35	119.90
2	K	431	DG	C2-N3-C4	14.88	119.34	111.90
1	H	407	DC	C2-N3-C4	14.88	127.34	119.90
1	F	412	DG	N3-C4-C5	-14.84	121.18	128.60
1	G	410	DC	N3-C4-C5	-14.82	115.97	121.90
2	L	425	DG	C2-N3-C4	14.78	119.29	111.90
2	K	421	DC	C2-N3-C4	14.75	127.27	119.90
2	I	431	DG	C2-N3-C4	14.70	119.25	111.90
2	K	432	DC	C2-N3-C4	14.68	127.24	119.90
1	G	409	DC	N3-C4-C5	-14.64	116.04	121.90
1	H	406	DC	N3-C4-C5	-14.64	116.04	121.90
1	E	409	DC	C2-N3-C4	14.64	127.22	119.90
2	K	426	DA	O4'-C1'-N9	14.63	118.24	108.00
1	G	403	DC	N3-C4-C5	-14.63	116.05	121.90
1	F	401	DG	C2-N3-C4	14.61	119.21	111.90
1	E	404	DT	N3-C2-O2	-14.57	113.56	122.30
2	K	424	DG	C2-N3-C4	14.56	119.18	111.90
2	L	425	DG	C5-N7-C8	-14.56	97.02	104.30
2	L	428	DG	C2-N3-C4	14.56	119.18	111.90
1	F	403	DC	C2-N3-C4	14.51	127.15	119.90
2	K	422	DC	N3-C4-C5	-14.47	116.11	121.90
2	L	422	DC	C2-N3-C4	14.43	127.11	119.90
2	K	433	DC	C2-N3-C4	14.42	127.11	119.90
2	K	421	DC	N3-C4-C5	-14.37	116.15	121.90
1	H	402	DG	C5-N7-C8	-14.34	97.13	104.30
1	E	407	DC	N3-C4-C5	-14.14	116.24	121.90
2	J	424	DG	C5-N7-C8	-14.09	97.26	104.30
2	L	424	DG	C5-N7-C8	-14.07	97.27	104.30
1	H	412	DG	C5-N7-C8	-13.99	97.30	104.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	403	DC	N3-C4-C5	-13.99	116.30	121.90
1	F	409	DC	N3-C4-C5	-13.99	116.31	121.90
2	K	431	DG	C5-N7-C8	-13.98	97.31	104.30
2	J	433	DC	C2-N3-C4	13.98	126.89	119.90
2	K	432	DC	N3-C4-C5	-13.95	116.32	121.90
1	H	412	DG	N3-C4-N9	13.94	134.36	126.00
1	G	401	DG	C2-N3-C4	13.92	118.86	111.90
2	I	428	DG	C5-N7-C8	-13.88	97.36	104.30
1	H	413	DG	C5-N7-C8	-13.86	97.37	104.30
2	L	431	DG	C5-C6-O6	-13.85	120.29	128.60
1	E	411	DT	O4'-C1'-N1	13.85	117.69	108.00
1	F	411	DT	C2-N3-C4	-13.82	118.91	127.20
1	G	412	DG	C5-N7-C8	-13.81	97.39	104.30
2	I	433	DC	N3-C4-C5	-13.80	116.38	121.90
1	F	412	DG	C5-N7-C8	-13.79	97.41	104.30
1	G	411	DT	C2-N3-C4	-13.72	118.97	127.20
1	G	402	DG	C5-N7-C8	-13.70	97.45	104.30
1	G	413	DG	C5-N7-C8	-13.68	97.46	104.30
1	E	401	DG	N3-C4-N9	13.57	134.14	126.00
1	E	413	DG	C5-N7-C8	-13.57	97.51	104.30
1	E	401	DG	C5-N7-C8	-13.56	97.52	104.30
1	F	402	DG	C5-N7-C8	-13.51	97.55	104.30
1	E	409	DC	N3-C4-C5	-13.49	116.50	121.90
1	E	402	DG	C5-N7-C8	-13.49	97.56	104.30
1	E	408	DT	N3-C2-O2	-13.46	114.22	122.30
1	E	412	DG	C5-N7-C8	-13.45	97.58	104.30
2	K	428	DG	C5-N7-C8	-13.41	97.59	104.30
2	J	429	DA	O4'-C1'-N9	13.39	117.38	108.00
1	F	412	DG	C2-N3-C4	13.37	118.58	111.90
2	J	428	DG	C5-N7-C8	-13.34	97.63	104.30
2	K	424	DG	C5-N7-C8	-13.33	97.63	104.30
1	G	413	DG	C5-C6-N1	13.30	118.15	111.50
2	L	428	DG	C5-N7-C8	-13.26	97.67	104.30
2	J	431	DG	C5-N7-C8	-13.24	97.68	104.30
2	K	425	DG	N3-C4-N9	13.23	133.94	126.00
1	G	406	DC	C2-N3-C4	13.20	126.50	119.90
1	G	407	DC	N3-C4-C5	-13.15	116.64	121.90
2	I	424	DG	C5-N7-C8	-13.07	97.77	104.30
1	H	412	DG	C6-N1-C2	-13.04	117.28	125.10
1	F	401	DG	C5-N7-C8	-13.03	97.78	104.30
2	J	433	DC	N3-C4-C5	-13.03	116.69	121.90
2	I	425	DG	C5-N7-C8	-12.99	97.80	104.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	401	DG	C5-N7-C8	-12.96	97.82	104.30
1	F	413	DG	C5-N7-C8	-12.95	97.83	104.30
2	J	424	DG	C6-N1-C2	-12.88	117.37	125.10
2	J	425	DG	C5-N7-C8	-12.87	97.86	104.30
1	H	408	DT	C2-N3-C4	-12.86	119.48	127.20
2	K	425	DG	C5-N7-C8	-12.84	97.88	104.30
1	H	401	DG	C5-N7-C8	-12.78	97.91	104.30
1	E	413	DG	C6-N1-C2	-12.74	117.45	125.10
1	G	413	DG	C6-N1-C2	-12.72	117.47	125.10
2	L	425	DG	O4'-C1'-N9	12.72	116.90	108.00
2	K	431	DG	N3-C4-N9	12.72	133.63	126.00
1	H	405	DT	C2-N3-C4	-12.69	119.59	127.20
1	G	412	DG	C6-N1-C2	-12.66	117.50	125.10
1	G	405	DT	O4'-C1'-N1	12.66	116.86	108.00
2	K	431	DG	C6-N1-C2	-12.63	117.52	125.10
2	J	424	DG	C5-C6-O6	-12.62	121.03	128.60
1	H	401	DG	N3-C4-N9	12.52	133.51	126.00
1	E	402	DG	N3-C4-N9	12.52	133.51	126.00
1	E	401	DG	C5-C6-O6	-12.51	121.09	128.60
2	J	428	DG	N3-C4-N9	12.47	133.48	126.00
1	E	404	DT	C2-N3-C4	-12.46	119.72	127.20
2	K	433	DC	N3-C4-C5	-12.44	116.92	121.90
1	G	413	DG	N3-C4-N9	12.41	133.44	126.00
1	F	401	DG	C5-C6-O6	-12.39	121.17	128.60
1	H	401	DG	C5-C6-N1	12.38	117.69	111.50
1	H	413	DG	C6-N1-C2	-12.37	117.68	125.10
1	G	412	DG	N3-C4-N9	12.36	133.42	126.00
1	H	413	DG	N3-C4-N9	12.36	133.42	126.00
1	G	406	DC	N3-C4-C5	-12.36	116.96	121.90
1	F	405	DT	C2-N3-C4	-12.34	119.80	127.20
2	J	424	DG	C5-C6-N1	12.27	117.64	111.50
2	L	431	DG	N3-C4-N9	12.24	133.34	126.00
1	G	404	DT	C2-N3-C4	-12.16	119.90	127.20
2	J	424	DG	N3-C4-N9	12.03	133.22	126.00
1	H	407	DC	N3-C4-C5	-11.98	117.11	121.90
2	K	431	DG	C5-C6-O6	-11.97	121.42	128.60
1	E	412	DG	O4'-C1'-N9	11.96	116.37	108.00
1	E	412	DG	N3-C4-N9	11.94	133.16	126.00
2	J	428	DG	C6-N1-C2	-11.94	117.94	125.10
2	L	431	DG	C5-C6-N1	11.94	117.47	111.50
2	J	428	DG	C5-C6-N1	11.94	117.47	111.50
1	E	402	DG	C6-N1-C2	-11.93	117.94	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	425	DG	C6-N1-C2	-11.89	117.97	125.10
2	L	431	DG	C6-N1-C2	-11.88	117.97	125.10
1	G	412	DG	C5-C6-N1	11.86	117.43	111.50
2	K	425	DG	C6-N1-C2	-11.85	117.99	125.10
2	K	425	DG	C5-C6-O6	-11.83	121.50	128.60
1	E	402	DG	C5-C6-N1	11.79	117.40	111.50
1	G	413	DG	C5-C6-O6	-11.78	121.53	128.60
2	I	425	DG	N3-C4-N9	11.74	133.04	126.00
2	I	428	DG	N3-C4-N9	11.73	133.04	126.00
1	G	402	DG	N3-C4-N9	11.72	133.03	126.00
2	I	425	DG	C5-C6-N1	11.70	117.35	111.50
1	F	411	DT	O4'-C1'-N1	11.69	116.19	108.00
2	I	424	DG	C6-N1-C2	-11.69	118.09	125.10
1	E	404	DT	C6-C5-C7	-11.68	115.89	122.90
2	I	428	DG	C5-C6-N1	11.68	117.34	111.50
1	H	402	DG	C6-N1-C2	-11.64	118.12	125.10
2	I	428	DG	C6-N1-C2	-11.61	118.13	125.10
1	E	413	DG	C5-C6-N1	11.61	117.30	111.50
2	K	431	DG	O4'-C1'-N9	11.52	116.06	108.00
1	G	402	DG	C5-C6-O6	-11.51	121.70	128.60
2	J	425	DG	C5-C6-N1	11.50	117.25	111.50
2	K	431	DG	C5-C6-N1	11.48	117.24	111.50
1	E	405	DT	C2-N3-C4	-11.47	120.32	127.20
1	F	401	DG	C5-C6-N1	11.46	117.23	111.50
1	E	411	DT	N3-C2-O2	-11.45	115.43	122.30
2	J	431	DG	C6-N1-C2	-11.45	118.23	125.10
1	G	401	DG	C6-N1-C2	-11.41	118.25	125.10
2	L	425	DG	C5-C6-O6	-11.37	121.78	128.60
1	G	401	DG	C5-C6-O6	-11.35	121.79	128.60
1	F	402	DG	N3-C4-N9	11.34	132.80	126.00
1	G	401	DG	N3-C4-N9	11.33	132.80	126.00
1	H	402	DG	N3-C4-N9	11.30	132.78	126.00
1	H	412	DG	C5-C6-N1	11.27	117.14	111.50
2	K	428	DG	N3-C4-N9	11.27	132.76	126.00
1	E	401	DG	C5-C6-N1	11.26	117.13	111.50
1	E	412	DG	C6-N1-C2	-11.25	118.35	125.10
2	L	428	DG	C6-N1-C2	-11.22	118.37	125.10
1	H	412	DG	C5-C6-O6	-11.17	121.90	128.60
2	K	428	DG	C6-N1-C2	-11.15	118.41	125.10
1	H	401	DG	O4'-C1'-N9	11.14	115.80	108.00
1	F	405	DT	C6-C5-C7	-11.13	116.22	122.90
1	G	402	DG	C6-N1-C2	-11.09	118.44	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	408	DT	C6-C5-C7	-11.08	116.25	122.90
1	G	408	DT	O4'-C1'-N1	11.03	115.72	108.00
2	I	425	DG	C5-C6-O6	-11.02	121.99	128.60
1	H	401	DG	C6-N1-C2	-11.02	118.49	125.10
2	K	428	DG	C5-C6-N1	11.01	117.00	111.50
1	F	405	DT	N3-C2-O2	-10.95	115.73	122.30
2	K	425	DG	C5-C6-N1	10.95	116.97	111.50
1	F	401	DG	N3-C4-N9	10.94	132.56	126.00
1	F	413	DG	C5-C6-N1	10.93	116.97	111.50
1	H	413	DG	C5-C6-N1	10.90	116.95	111.50
1	F	413	DG	C6-N1-C2	-10.89	118.57	125.10
2	I	424	DG	C5-C6-N1	10.82	116.91	111.50
1	G	411	DT	O4'-C1'-N1	10.82	115.57	108.00
1	H	404	DT	C2-N3-C4	-10.80	120.72	127.20
2	I	431	DG	C5-C6-N1	10.79	116.90	111.50
1	G	412	DG	C5-C6-O6	-10.78	122.13	128.60
2	J	425	DG	N3-C4-N9	10.76	132.46	126.00
2	L	428	DG	N3-C4-N9	10.73	132.44	126.00
2	L	428	DG	C5-C6-N1	10.73	116.87	111.50
1	G	404	DT	C6-C5-C7	-10.72	116.47	122.90
1	F	404	DT	C6-C5-C7	-10.68	116.49	122.90
1	H	402	DG	C5-C6-N1	10.68	116.84	111.50
1	E	405	DT	C6-C5-C7	-10.67	116.50	122.90
2	I	431	DG	C5-N7-C8	-10.66	98.97	104.30
2	J	431	DG	N3-C4-N9	10.65	132.39	126.00
1	F	404	DT	C2-N3-C4	-10.62	120.83	127.20
1	F	402	DG	C6-N1-C2	-10.62	118.73	125.10
1	F	401	DG	C6-N1-C2	-10.61	118.73	125.10
2	J	431	DG	C5-C6-N1	10.61	116.81	111.50
1	E	413	DG	C5-C6-O6	-10.56	122.26	128.60
2	I	431	DG	C6-N1-C2	-10.56	118.76	125.10
1	F	411	DT	C6-C5-C7	-10.54	116.58	122.90
2	J	425	DG	C6-N1-C2	-10.50	118.80	125.10
1	E	401	DG	C6-N1-C2	-10.50	118.80	125.10
2	L	424	DG	N3-C4-N9	10.50	132.30	126.00
2	K	428	DG	C5-C6-O6	-10.46	122.32	128.60
2	I	428	DG	C5-C6-O6	-10.45	122.33	128.60
2	K	424	DG	C6-N1-C2	-10.45	118.83	125.10
1	G	402	DG	C5-C6-N1	10.43	116.71	111.50
1	F	404	DT	N3-C2-O2	-10.41	116.06	122.30
1	G	408	DT	C2-N3-C4	-10.40	120.96	127.20
2	I	424	DG	N3-C4-N9	10.38	132.23	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	413	DG	N3-C4-N9	10.34	132.20	126.00
1	G	401	DG	C5-C6-N1	10.30	116.65	111.50
1	H	401	DG	C5-C6-O6	-10.30	122.42	128.60
2	L	424	DG	C5-C6-N1	10.29	116.64	111.50
1	G	408	DT	N3-C2-O2	-10.27	116.14	122.30
1	E	411	DT	C6-C5-C7	-10.22	116.77	122.90
2	K	424	DG	N3-C4-N9	10.20	132.12	126.00
1	F	411	DT	N3-C2-O2	-10.20	116.18	122.30
1	F	402	DG	C5-C6-N1	10.17	116.58	111.50
1	G	411	DT	C6-C5-C7	-10.17	116.80	122.90
1	F	413	DG	N3-C4-N9	10.16	132.10	126.00
2	J	425	DG	C5-C6-O6	-10.15	122.51	128.60
1	H	411	DT	C2-N3-C4	-10.14	121.11	127.20
2	L	425	DG	N3-C4-N9	10.10	132.06	126.00
1	F	402	DG	C5-C6-O6	-10.06	122.56	128.60
1	G	405	DT	C2-N3-C4	-10.04	121.17	127.20
1	H	411	DT	C6-C5-C7	-10.03	116.88	122.90
1	E	412	DG	C5-C6-N1	10.02	116.51	111.50
2	L	424	DG	C6-N1-C2	-10.02	119.09	125.10
1	F	411	DT	N1-C2-N3	10.01	120.61	114.60
1	H	404	DT	C6-C5-C7	-9.99	116.91	122.90
1	F	408	DT	C2-N3-C4	-9.97	121.22	127.20
1	F	408	DT	N3-C2-O2	-9.97	116.32	122.30
1	E	411	DT	C2-N3-C4	-9.86	121.28	127.20
1	G	405	DT	C6-C5-C7	-9.78	117.03	122.90
1	G	411	DT	N3-C2-O2	-9.78	116.43	122.30
2	K	424	DG	C5-C6-N1	9.74	116.37	111.50
1	H	405	DT	C6-C5-C7	-9.72	117.07	122.90
1	H	405	DT	O4'-C1'-N1	9.69	114.78	108.00
2	I	431	DG	N3-C4-N9	9.68	131.81	126.00
2	K	432	DC	O4'-C1'-N1	9.66	114.77	108.00
1	F	411	DT	C4-C5-C6	9.65	123.79	118.00
1	E	405	DT	C4-C5-C6	9.62	123.77	118.00
1	H	413	DG	C5-C6-O6	-9.59	122.85	128.60
2	J	428	DG	C5-C6-O6	-9.58	122.85	128.60
1	H	405	DT	N1-C2-N3	9.54	120.33	114.60
1	G	411	DT	N1-C2-N3	9.53	120.32	114.60
2	L	425	DG	C5-C6-N1	9.48	116.24	111.50
1	E	408	DT	C6-C5-C7	-9.48	117.21	122.90
2	L	424	DG	C5-C6-O6	-9.47	122.92	128.60
1	G	404	DT	N3-C2-O2	-9.45	116.63	122.30
1	F	410	DC	N3-C4-N4	9.34	124.53	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	404	DT	N1-C2-N3	9.32	120.19	114.60
1	G	408	DT	C6-C5-C7	-9.31	117.31	122.90
1	E	412	DG	C5-C6-O6	-9.29	123.03	128.60
1	H	403	DC	N3-C4-N4	9.21	124.45	118.00
1	E	408	DT	C2-N3-C4	-9.17	121.70	127.20
2	J	431	DG	C5-C6-O6	-9.16	123.11	128.60
2	I	431	DG	O4'-C1'-N9	9.14	114.40	108.00
1	H	411	DT	N3-C2-O2	-9.11	116.83	122.30
2	J	432	DC	N3-C4-N4	9.04	124.33	118.00
1	H	402	DG	C5-C6-O6	-8.99	123.21	128.60
2	K	425	DG	O4'-C1'-N9	8.97	114.28	108.00
3	B	31	ARG	CD-NE-CZ	8.93	136.11	123.60
1	H	408	DT	C4-C5-C6	8.91	123.35	118.00
1	E	402	DG	C5-C6-O6	-8.90	123.26	128.60
1	H	405	DT	N3-C2-O2	-8.90	116.96	122.30
1	H	408	DT	N3-C2-O2	-8.83	117.00	122.30
2	L	432	DC	N3-C4-N4	8.83	124.18	118.00
1	H	408	DT	N1-C2-N3	8.82	119.89	114.60
1	E	405	DT	N1-C2-N3	8.80	119.88	114.60
1	H	405	DT	C4-C5-C6	8.78	123.27	118.00
2	L	425	DG	C6-N1-C2	-8.77	119.84	125.10
1	G	402	DG	O4'-C1'-N9	8.77	114.14	108.00
1	G	411	DT	C4-C5-C6	8.71	123.22	118.00
1	F	412	DG	C8-N9-C1'	8.66	138.26	127.00
1	F	408	DT	C6-C5-C7	-8.62	117.73	122.90
1	H	409	DC	N3-C4-N4	8.56	124.00	118.00
1	E	411	DT	C4-C5-C6	8.51	123.11	118.00
1	H	404	DT	C4-C5-C6	8.41	123.04	118.00
1	G	412	DG	O4'-C1'-N9	8.40	113.88	108.00
2	J	422	DC	C5-C6-N1	8.39	125.20	121.00
1	G	408	DT	C4-C5-C6	8.35	123.01	118.00
1	H	410	DC	C5-C6-N1	8.34	125.17	121.00
2	L	433	DC	N3-C4-N4	8.31	123.81	118.00
1	F	412	DG	C5-C6-N1	8.28	115.64	111.50
1	F	412	DG	N3-C4-N9	8.23	130.94	126.00
2	L	433	DC	C5-C6-N1	8.22	125.11	121.00
2	L	432	DC	C5-C6-N1	8.20	125.10	121.00
1	F	413	DG	C5-C6-O6	-8.18	123.69	128.60
2	J	433	DC	O4'-C1'-N1	8.18	113.73	108.00
2	J	426	DA	O4'-C1'-N9	8.18	113.72	108.00
2	L	423	DA	O4'-C1'-N9	8.16	113.71	108.00
1	G	410	DC	N3-C4-N4	8.13	123.69	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	407	DC	O4'-C1'-N1	8.08	113.66	108.00
2	J	431	DG	N9-C4-C5	8.06	108.62	105.40
1	E	405	DT	N3-C2-O2	-8.02	117.49	122.30
2	J	421	DC	C5-C6-N1	8.01	125.01	121.00
2	I	422	DC	C5-C6-N1	8.00	125.00	121.00
1	F	413	DG	O4'-C1'-N9	7.97	113.58	108.00
1	H	403	DC	C6-N1-C2	-7.93	117.13	120.30
1	E	404	DT	C4-C5-C6	7.90	122.74	118.00
2	L	428	DG	C5-C6-O6	-7.89	123.87	128.60
1	E	411	DT	N1-C2-N3	7.86	119.32	114.60
1	G	404	DT	C4-C5-C6	7.83	122.70	118.00
1	H	410	DC	O4'-C1'-N1	7.83	113.48	108.00
2	L	430	DA	C2-N3-C4	7.81	114.51	110.60
2	J	422	DC	O4'-C4'-C3'	-7.79	101.33	106.00
1	F	406	DC	C5-C6-N1	7.79	124.89	121.00
2	I	424	DG	C5-C6-O6	-7.78	123.93	128.60
1	E	408	DT	C4-C5-C6	7.78	122.67	118.00
2	J	433	DC	O4'-C4'-C3'	-7.76	101.35	106.00
1	G	408	DT	N1-C2-N3	7.74	119.24	114.60
2	J	423	DA	O4'-C1'-N9	7.73	113.41	108.00
2	I	432	DC	C5-C6-N1	7.72	124.86	121.00
2	I	424	DG	N9-C4-C5	7.68	108.47	105.40
1	F	412	DG	C5-C6-O6	-7.67	124.00	128.60
2	K	422	DC	N3-C4-N4	7.64	123.35	118.00
2	J	421	DC	N3-C4-N4	7.64	123.35	118.00
1	F	408	DT	C4-C5-C6	7.61	122.57	118.00
1	E	403	DC	N3-C4-N4	7.58	123.31	118.00
2	J	422	DC	N1-C2-N3	-7.58	113.89	119.20
1	F	412	DG	C6-N1-C2	-7.58	120.55	125.10
2	J	425	DG	O4'-C1'-N9	7.58	113.30	108.00
1	G	405	DT	N3-C2-O2	-7.54	117.78	122.30
2	K	432	DC	N3-C4-N4	7.49	123.24	118.00
1	H	404	DT	N3-C2-O2	-7.46	117.82	122.30
1	E	413	DG	N9-C4-C5	7.45	108.38	105.40
1	E	408	DT	N1-C2-N3	7.43	119.06	114.60
2	L	422	DC	N3-C4-N4	7.41	123.19	118.00
1	G	413	DG	O4'-C1'-N9	7.39	113.17	108.00
2	J	433	DC	N3-C4-N4	7.37	123.16	118.00
1	G	405	DT	C4-C5-C6	7.33	122.40	118.00
1	G	404	DT	N1-C2-N3	7.33	119.00	114.60
2	I	421	DC	C5-C6-N1	7.28	124.64	121.00
2	J	432	DC	C5-C6-N1	7.28	124.64	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	421	DC	O4'-C1'-N1	7.26	113.08	108.00
1	F	403	DC	C5-C6-N1	7.21	124.61	121.00
2	L	433	DC	N1-C2-N3	-7.18	114.17	119.20
2	J	421	DC	N1-C2-N3	-7.18	114.17	119.20
1	F	406	DC	N3-C4-N4	7.18	123.02	118.00
1	E	409	DC	N3-C4-N4	7.16	123.02	118.00
2	K	429	DA	C5-C6-N1	-7.16	114.12	117.70
1	H	403	DC	C5-C6-N1	7.16	124.58	121.00
2	J	432	DC	O4'-C1'-N1	7.12	112.98	108.00
2	K	429	DA	C6-N1-C2	7.10	122.86	118.60
2	K	424	DG	C5-C6-O6	-7.08	124.35	128.60
1	H	411	DT	C4-C5-C6	7.08	122.25	118.00
2	K	422	DC	C5-C6-N1	7.04	124.52	121.00
1	E	410	DC	N3-C4-N4	7.04	122.93	118.00
1	H	404	DT	N1-C2-N3	7.03	118.82	114.60
1	E	413	DG	O4'-C1'-N9	7.00	112.90	108.00
2	I	422	DC	O4'-C1'-N1	7.00	112.90	108.00
2	I	433	DC	O4'-C4'-C3'	-6.98	101.71	104.50
2	L	431	DG	O4'-C1'-N9	6.97	112.88	108.00
2	L	433	DC	O4'-C4'-C3'	-6.95	101.72	104.50
1	F	405	DT	C4-C5-C6	6.94	122.16	118.00
1	E	412	DG	N9-C4-C5	6.90	108.16	105.40
1	F	413	DG	N9-C4-C5	6.89	108.16	105.40
2	L	432	DC	N1-C2-N3	-6.88	114.38	119.20
1	F	405	DT	N1-C2-N3	6.84	118.71	114.60
2	K	423	DA	C4-C5-C6	6.82	120.41	117.00
1	F	404	DT	C4-C5-C6	6.82	122.09	118.00
2	K	424	DG	N9-C4-C5	6.80	108.12	105.40
1	F	406	DC	N1-C2-N3	-6.79	114.45	119.20
2	K	433	DC	C5-C6-N1	6.76	124.38	121.00
1	G	409	DC	C5-C6-N1	6.73	124.36	121.00
1	F	404	DT	N1-C2-N3	6.73	118.64	114.60
1	H	410	DC	N1-C2-N3	-6.73	114.49	119.20
2	I	425	DG	O4'-C1'-N9	6.70	112.69	108.00
2	I	421	DC	O4'-C1'-N1	6.68	112.68	108.00
2	L	424	DG	C8-N9-C1'	6.67	135.68	127.00
2	I	432	DC	N3-C4-N4	6.65	122.66	118.00
2	K	432	DC	C5-C6-N1	6.65	124.33	121.00
2	I	431	DG	C8-N9-C1'	6.64	135.63	127.00
1	E	410	DC	C5-C6-N1	6.64	124.32	121.00
1	E	413	DG	C8-N9-C1'	6.64	135.63	127.00
1	F	408	DT	O4'-C1'-N1	6.63	112.64	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	426	DA	O4'-C4'-C3'	-6.62	101.85	104.50
1	H	409	DC	C5-C6-N1	6.61	124.31	121.00
2	K	421	DC	O4'-C1'-N1	6.61	112.63	108.00
1	H	413	DG	N9-C4-C5	6.60	108.04	105.40
2	L	421	DC	N3-C4-N4	6.60	122.62	118.00
1	F	409	DC	C5-C6-N1	6.59	124.30	121.00
2	J	422	DC	P-O5'-C5'	-6.56	110.41	120.90
1	G	407	DC	N1-C2-N3	-6.56	114.61	119.20
2	K	428	DG	O4'-C1'-N9	-6.55	103.42	108.00
2	L	422	DC	O4'-C1'-N1	6.46	112.52	108.00
1	G	403	DC	N1-C2-O2	6.46	122.78	118.90
1	H	402	DG	N9-C4-C5	6.45	107.98	105.40
1	H	411	DT	O4'-C1'-N1	6.45	112.52	108.00
1	G	401	DG	O4'-C1'-N9	6.45	112.51	108.00
2	I	423	DA	O4'-C1'-N9	6.43	112.50	108.00
1	G	410	DC	C5-C6-N1	6.42	124.21	121.00
2	I	425	DG	N9-C4-C5	6.40	107.96	105.40
2	J	421	DC	N1-C2-O2	6.39	122.73	118.90
1	E	406	DC	C5-C6-N1	6.39	124.19	121.00
1	H	410	DC	O4'-C4'-C3'	-6.38	101.95	104.50
2	I	431	DG	C5-C6-O6	-6.36	124.78	128.60
1	E	404	DT	N1-C1'-C2'	6.34	124.65	112.60
1	F	411	DT	C5-C6-N1	-6.34	119.90	123.70
1	E	405	DT	O4'-C1'-N1	6.32	112.42	108.00
1	F	410	DC	C5-C6-N1	6.32	124.16	121.00
1	E	405	DT	C5-C6-N1	-6.30	119.92	123.70
2	K	424	DG	C8-N9-C1'	6.30	135.19	127.00
2	L	421	DC	C5-C6-N1	6.26	124.13	121.00
1	F	413	DG	C8-N9-C1'	6.25	135.13	127.00
2	J	423	DA	O4'-C4'-C3'	-6.25	102.00	104.50
1	G	402	DG	N9-C4-C5	6.25	107.90	105.40
2	J	431	DG	C8-N9-C1'	6.22	135.09	127.00
1	F	408	DT	N1-C2-N3	6.22	118.33	114.60
1	E	403	DC	C5-C6-N1	6.21	124.11	121.00
2	I	431	DG	N9-C4-C5	6.21	107.89	105.40
2	I	421	DC	N3-C4-N4	6.20	122.34	118.00
2	L	432	DC	N3-C2-O2	6.20	126.24	121.90
2	K	433	DC	N3-C4-N4	6.19	122.33	118.00
1	E	404	DT	O4'-C1'-N1	6.19	112.33	108.00
1	F	412	DG	N9-C4-C5	6.19	107.88	105.40
2	K	429	DA	C5-C6-N6	6.18	128.65	123.70
1	G	405	DT	N1-C2-N3	6.18	118.31	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	424	DG	C8-N9-C1'	6.18	135.04	127.00
1	G	413	DG	C8-N9-C1'	6.17	135.02	127.00
1	H	407	DC	N1-C2-N3	-6.16	114.89	119.20
2	L	424	DG	N9-C4-C5	6.14	107.86	105.40
1	E	406	DC	O4'-C1'-N1	6.13	112.29	108.00
1	G	409	DC	N3-C4-N4	6.12	122.28	118.00
1	G	412	DG	N9-C4-C5	6.08	107.83	105.40
2	J	430	DA	C4-C5-C6	6.05	120.03	117.00
2	J	424	DG	C8-N9-C1'	6.04	134.85	127.00
2	I	426	DA	N1-C2-N3	-6.03	126.28	129.30
2	I	422	DC	N3-C4-N4	6.03	122.22	118.00
2	K	422	DC	P-O5'-C5'	-6.02	111.26	120.90
2	L	430	DA	N3-C4-C5	-6.02	122.59	126.80
1	H	412	DG	N9-C4-C5	6.01	107.80	105.40
1	H	410	DC	N3-C4-N4	6.01	122.21	118.00
1	E	409	DC	P-O5'-C5'	-6.00	111.30	120.90
1	F	409	DC	N3-C4-N4	6.00	122.20	118.00
3	A	28	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	E	407	DC	N1-C2-N3	-5.99	115.01	119.20
2	L	422	DC	C5-C6-N1	5.97	123.98	121.00
1	H	411	DT	N1-C2-N3	5.96	118.18	114.60
1	F	409	DC	N1-C2-N3	-5.96	115.03	119.20
2	K	422	DC	N1-C2-N3	-5.96	115.03	119.20
1	G	413	DG	N9-C4-C5	5.95	107.78	105.40
2	K	421	DC	N3-C4-N4	5.95	122.16	118.00
2	L	429	DA	O4'-C1'-C2'	-5.94	101.15	105.90
2	J	431	DG	O4'-C1'-N9	5.93	112.15	108.00
2	L	430	DA	C4-C5-C6	5.93	119.96	117.00
2	K	423	DA	C6-C5-N7	-5.92	128.16	132.30
1	G	403	DC	P-O5'-C5'	-5.92	111.44	120.90
2	L	428	DG	N9-C4-C5	5.90	107.76	105.40
2	L	425	DG	C8-N9-C1'	5.89	134.65	127.00
2	K	433	DC	O4'-C4'-C3'	-5.88	102.15	104.50
1	F	402	DG	N9-C4-C5	5.87	107.75	105.40
2	K	425	DG	N9-C4-C5	5.86	107.74	105.40
1	H	404	DT	C5-C6-N1	-5.85	120.19	123.70
2	I	423	DA	O4'-C4'-C3'	-5.84	102.16	104.50
2	J	433	DC	C5-C6-N1	5.84	123.92	121.00
2	L	433	DC	O4'-C1'-N1	5.82	112.08	108.00
1	F	406	DC	O4'-C1'-N1	5.80	112.06	108.00
2	J	429	DA	N1-C2-N3	-5.79	126.41	129.30
2	L	428	DG	C8-N9-C1'	5.77	134.50	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	401	DG	C8-N9-C1'	5.77	134.50	127.00
2	I	421	DC	N1-C2-N3	-5.75	115.17	119.20
2	I	422	DC	N1-C2-O2	5.75	122.35	118.90
1	G	404	DT	C5-C6-N1	-5.75	120.25	123.70
1	E	409	DC	C5-C6-N1	5.75	123.87	121.00
1	G	411	DT	C5-C6-N1	-5.75	120.25	123.70
2	J	426	DA	C6-C5-N7	-5.73	128.29	132.30
1	H	408	DT	C5-C6-N1	-5.73	120.26	123.70
2	I	430	DA	C6-C5-N7	-5.72	128.29	132.30
3	B	31	ARG	NE-CZ-NH1	-5.71	117.45	120.30
1	E	413	DG	N1-C2-N3	5.69	127.31	123.90
1	F	409	DC	P-O5'-C5'	-5.69	111.80	120.90
2	I	432	DC	N1-C2-N3	-5.67	115.23	119.20
3	B	31	ARG	CG-CD-NE	5.67	123.71	111.80
1	E	409	DC	N1-C2-N3	-5.66	115.24	119.20
2	J	424	DG	N9-C4-C5	5.66	107.66	105.40
2	J	432	DC	N1-C2-N3	-5.66	115.24	119.20
1	F	405	DT	O4'-C1'-N1	5.63	111.94	108.00
2	I	422	DC	N1-C2-N3	-5.62	115.27	119.20
1	G	410	DC	N1-C2-N3	-5.62	115.27	119.20
1	E	401	DG	C4-C5-N7	5.61	113.04	110.80
2	I	423	DA	P-O5'-C5'	-5.60	111.94	120.90
1	F	403	DC	N1-C1'-C2'	5.60	123.23	112.60
2	J	430	DA	C6-C5-N7	-5.60	128.38	132.30
2	I	433	DC	N1-C2-N3	-5.59	115.29	119.20
2	J	422	DC	N3-C4-N4	5.58	121.91	118.00
2	I	428	DG	C8-N9-C1'	5.57	134.24	127.00
2	K	428	DG	C8-N9-C1'	5.56	134.23	127.00
2	K	433	DC	N1-C2-N3	-5.56	115.31	119.20
1	G	401	DG	N9-C4-C5	5.55	107.62	105.40
2	I	422	DC	P-O5'-C5'	-5.52	112.06	120.90
2	K	431	DG	N1-C2-N3	5.52	127.21	123.90
1	E	413	DG	N3-C2-N2	-5.51	116.04	119.90
1	H	405	DT	C5-C6-N1	-5.50	120.40	123.70
1	E	406	DC	N1-C2-N3	-5.50	115.35	119.20
2	I	426	DA	O4'-C1'-N9	5.50	111.85	108.00
1	H	407	DC	O4'-C1'-N1	5.49	111.84	108.00
2	J	422	DC	O4'-C1'-N1	5.49	111.84	108.00
2	K	430	DA	C4-C5-C6	5.48	119.74	117.00
2	L	426	DA	O4'-C1'-N9	5.46	111.82	108.00
1	F	403	DC	C6-N1-C2	-5.46	118.12	120.30
2	I	430	DA	C4-C5-C6	5.44	119.72	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	429	DA	O4'-C1'-C2'	-5.44	101.55	105.90
1	F	405	DT	C5-C6-N1	-5.42	120.44	123.70
2	J	426	DA	C4-C5-C6	5.42	119.71	117.00
2	K	429	DA	O4'-C1'-C2'	-5.42	101.56	105.90
2	J	429	DA	OP1-P-OP2	-5.39	111.51	119.60
1	E	407	DC	N3-C4-N4	5.39	121.77	118.00
2	L	423	DA	C4-C5-C6	5.39	119.69	117.00
1	E	410	DC	O4'-C1'-N1	5.38	111.76	108.00
1	E	402	DG	N9-C4-C5	5.36	107.55	105.40
2	J	429	DA	C2-N3-C4	5.36	113.28	110.60
2	I	433	DC	C5-C6-N1	5.35	123.67	121.00
2	J	428	DG	N9-C4-C5	5.35	107.54	105.40
2	J	421	DC	O4'-C1'-N1	5.35	111.74	108.00
2	J	425	DG	C8-N9-C1'	5.33	133.93	127.00
2	I	433	DC	O4'-C1'-N1	5.33	111.73	108.00
2	K	429	DA	N1-C2-N3	-5.32	126.64	129.30
2	J	430	DA	C2-N3-C4	5.32	113.26	110.60
1	G	403	DC	N1-C2-N3	-5.31	115.48	119.20
2	I	422	DC	C6-N1-C2	-5.31	118.18	120.30
1	H	409	DC	P-O5'-C5'	-5.31	112.41	120.90
2	I	423	DA	C2-N3-C4	5.30	113.25	110.60
1	H	413	DG	N1-C2-N3	5.29	127.08	123.90
1	H	407	DC	N3-C4-N4	5.29	121.70	118.00
2	L	425	DG	O4'-C4'-C3'	-5.28	102.39	104.50
2	K	430	DA	C2-N3-C4	5.27	113.24	110.60
2	L	433	DC	N1-C2-O2	5.27	122.06	118.90
2	L	431	DG	C4-C5-N7	5.26	112.91	110.80
2	J	422	DC	C4'-C3'-C2'	-5.26	98.37	103.10
1	F	407	DC	N1-C2-N3	-5.25	115.52	119.20
1	H	401	DG	N9-C4-C5	5.25	107.50	105.40
2	I	430	DA	N3-C4-C5	-5.25	123.13	126.80
2	I	426	DA	C4-C5-C6	5.24	119.62	117.00
1	H	410	DC	C4'-C3'-C2'	-5.24	98.39	103.10
1	F	406	DC	N3-C2-O2	5.24	125.56	121.90
2	I	425	DG	C8-N9-C1'	5.23	133.80	127.00
1	G	405	DT	O4'-C1'-C2'	5.23	110.08	105.90
1	H	410	DC	N3-C2-O2	5.23	125.56	121.90
1	H	408	DT	O4'-C1'-N1	5.22	111.66	108.00
2	L	421	DC	N1-C2-N3	-5.22	115.55	119.20
2	I	421	DC	N1-C2-O2	5.21	122.03	118.90
1	H	409	DC	N1-C2-N3	-5.21	115.55	119.20
2	L	429	DA	OP1-P-O3'	5.21	116.66	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	423	DA	C4-C5-C6	5.20	119.60	117.00
1	G	410	DC	P-O3'-C3'	-5.20	113.46	119.70
2	J	424	DG	O4'-C1'-N9	5.19	111.64	108.00
2	L	431	DG	C8-N9-C1'	5.19	133.75	127.00
2	I	430	DA	C2-N3-C4	5.19	113.20	110.60
2	J	426	DA	P-O5'-C5'	-5.18	112.61	120.90
1	F	402	DG	O4'-C1'-N9	5.17	111.62	108.00
1	G	406	DC	N1-C2-N3	-5.17	115.58	119.20
2	K	433	DC	O4'-C1'-N1	5.16	111.61	108.00
2	J	426	DA	C5-C6-N1	-5.15	115.13	117.70
1	E	403	DC	C6-N1-C2	-5.13	118.25	120.30
1	F	408	DT	C5-C6-N1	-5.12	120.63	123.70
2	K	428	DG	N9-C4-C5	5.12	107.45	105.40
2	J	428	DG	C8-N9-C1'	5.10	133.63	127.00
1	H	407	DC	N3-C2-O2	5.10	125.47	121.90
2	I	432	DC	N3-C2-O2	5.10	125.47	121.90
2	K	423	DA	N3-C4-C5	-5.09	123.23	126.80
1	H	406	DC	O4'-C1'-N1	5.09	111.56	108.00
2	K	430	DA	P-O5'-C5'	-5.09	112.76	120.90
1	E	408	DT	O4'-C1'-N1	5.08	111.56	108.00
2	K	430	DA	N3-C4-C5	-5.08	123.24	126.80
1	G	410	DC	P-O5'-C5'	-5.08	112.78	120.90
1	F	410	DC	O4'-C1'-N1	5.08	111.55	108.00
2	K	421	DC	OP1-P-O3'	5.06	116.32	105.20
1	F	409	DC	N1-C2-O2	5.05	121.93	118.90
2	L	423	DA	C2-N3-C4	5.05	113.13	110.60
1	H	412	DG	N1-C2-N3	5.05	126.93	123.90
1	H	411	DT	C5-C6-N1	-5.05	120.67	123.70
2	J	421	DC	OP1-P-O3'	5.03	116.27	105.20
2	J	424	DG	N1-C2-N3	5.03	126.92	123.90
2	L	422	DC	C6-N1-C2	-5.02	118.29	120.30
2	L	426	DA	C2-N3-C4	5.02	113.11	110.60
1	G	401	DG	N1-C2-N3	5.01	126.90	123.90
2	I	424	DG	N1-C2-N3	5.00	126.90	123.90

There are no chirality outliers.

There are no planarity outliers.

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	260	0	149	9	0
1	F	260	0	149	5	0
1	G	260	0	149	2	0
1	H	260	0	149	9	0
2	I	256	0	142	6	0
2	J	256	0	142	5	0
2	K	256	0	142	3	0
2	L	256	0	142	6	0
3	A	2038	0	2058	42	0
3	B	2030	0	2048	53	0
3	C	2042	0	2062	53	0
3	D	2039	0	2059	40	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	93	0	0	1	0
5	B	82	0	0	2	0
5	C	77	0	0	1	0
5	D	92	0	0	1	0
5	E	15	0	0	0	0
5	F	16	0	0	0	0
5	G	18	0	0	1	0
5	H	18	0	0	0	0
5	I	23	0	0	0	0
5	J	24	0	0	0	0
5	K	20	0	0	1	0
5	L	21	0	0	1	0
All	All	10716	0	9391	229	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (229) 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)
3:C:122:HIS:ND1	3:C:123:ASN:O	1.76	1.16
3:D:211:GLN:OE1	3:D:232:GLU:OE2	1.76	1.03
3:A:80:LEU:HD13	3:A:84:LEU:HD23	1.45	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:122:HIS:CE1	3:C:123:ASN:O	2.17	0.98
3:D:122:HIS:O	3:D:126:THR:OG1	1.82	0.96
3:C:123:ASN:O	3:C:124:VAL:HG13	1.68	0.94
3:D:122:HIS:C	3:D:126:THR:OG1	2.07	0.92
3:C:181:HIS:HD2	3:C:183:ASP:H	1.22	0.84
3:B:169:ILE:HD11	3:B:216:LEU:HD11	1.58	0.83
3:D:122:HIS:C	3:D:126:THR:HG1	1.80	0.82
3:B:122:HIS:CE1	3:B:124:VAL:HG22	2.17	0.80
3:D:169:ILE:HD11	3:D:216:LEU:HD11	1.62	0.80
3:C:240:GLY:O	3:C:249:PRO:HB3	1.84	0.77
3:B:122:HIS:O	3:B:123:ASN:HB2	1.85	0.75
3:B:154:LYS:HE3	3:B:260:THR:HB	1.71	0.72
3:D:228:TYR:O	3:D:231:GLN:HG2	1.90	0.71
3:B:240:GLY:O	3:B:249:PRO:HB3	1.90	0.71
3:C:190:SER:OG	3:C:193:GLU:HG3	1.90	0.70
3:C:154:LYS:HZ2	3:C:260:THR:HG22	1.56	0.70
2:K:422:DC:H2''	2:K:423:DA:N7	2.07	0.69
3:C:216:LEU:HD21	3:C:236:TYR:HE2	1.56	0.69
2:J:421:DC:H4'	2:J:422:DC:OP1	1.93	0.69
3:D:154:LYS:HZ1	3:D:260:THR:HG22	1.57	0.69
3:B:184:ARG:HD3	3:B:268:LYS:O	1.93	0.68
3:D:154:LYS:HE3	3:D:260:THR:HB	1.74	0.68
3:A:154:LYS:HE3	3:A:260:THR:HB	1.75	0.68
2:I:423:DA:H1'	2:I:424:DG:H5'	1.76	0.67
3:A:80:LEU:HD11	3:A:103:ARG:HD2	1.74	0.67
3:B:154:LYS:HZ1	3:B:260:THR:HG22	1.59	0.67
3:C:154:LYS:HE3	3:C:260:THR:HB	1.77	0.67
3:B:255:HIS:ND1	3:B:260:THR:HG21	2.10	0.66
3:D:255:HIS:ND1	3:D:260:THR:HG21	2.10	0.66
3:C:215:THR:OG1	3:C:226:PRO:HB3	1.95	0.66
3:B:238:ARG:O	3:B:250:ILE:HB	1.96	0.65
3:C:169:ILE:HD11	3:C:216:LEU:HD11	1.79	0.65
3:C:255:HIS:ND1	3:C:260:THR:HG21	2.12	0.65
2:L:422:DC:H2''	2:L:423:DA:H5'	1.78	0.65
3:B:149:LYS:HE2	3:B:156:TRP:CD2	2.33	0.64
3:C:123:ASN:C	3:C:124:VAL:HG13	2.18	0.64
3:B:37:SER:OG	3:B:114:LEU:HA	1.98	0.63
3:C:95:VAL:HA	3:C:101:VAL:HG22	1.78	0.63
1:E:409:DC:H2''	1:E:410:DC:O5'	1.99	0.63
3:A:215:THR:OG1	3:A:226:PRO:HB3	1.98	0.63
3:B:84:LEU:HG	3:B:85:PRO:HD2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:409:DC:H2''	1:G:410:DC:O5'	1.99	0.63
3:D:122:HIS:CA	3:D:126:THR:OG1	2.47	0.62
3:C:178:ALA:HB2	3:C:200:VAL:HG21	1.81	0.62
3:A:154:LYS:HZ2	3:A:260:THR:HG22	1.64	0.61
1:H:412:DG:H2''	1:H:413:DG:O4'	2.00	0.60
3:A:255:HIS:ND1	3:A:260:THR:HG21	2.16	0.60
3:B:178:ALA:HB2	3:B:200:VAL:HG21	1.83	0.60
1:E:413:DG:H1	2:I:421:DC:H42	1.51	0.59
3:C:46:GLN:HB3	3:C:62:LEU:HD13	1.83	0.59
3:C:122:HIS:O	3:C:126:THR:OG1	2.16	0.58
1:F:411:DT:H4'	1:F:412:DG:OP1	2.02	0.58
3:D:62:LEU:HD12	3:D:115:TRP:HZ3	1.68	0.58
3:C:123:ASN:O	3:C:124:VAL:CG1	2.49	0.58
3:D:122:HIS:HA	3:D:126:THR:OG1	2.04	0.58
1:E:411:DT:H2''	1:E:412:DG:N7	2.19	0.58
3:A:98:ASN:ND2	3:A:100:LYS:HD2	2.19	0.58
3:A:149:LYS:HE2	3:A:156:TRP:CD2	2.39	0.58
3:B:208:SER:OG	3:B:213:GLY:HA2	2.03	0.58
3:D:62:LEU:HD12	3:D:115:TRP:CZ3	2.39	0.58
1:H:412:DG:H2'	1:H:413:DG:C8	2.39	0.57
2:K:422:DC:H2''	2:K:423:DA:C5	2.39	0.57
2:L:422:DC:C2'	2:L:423:DA:H5'	2.34	0.57
1:E:413:DG:H1	2:I:421:DC:N4	2.02	0.57
3:C:181:HIS:CD2	3:C:182:PRO:HD2	2.39	0.57
1:H:412:DG:H2''	1:H:413:DG:O5'	2.05	0.56
3:B:122:HIS:HE1	3:B:124:VAL:HG22	1.67	0.56
1:H:412:DG:H4'	1:H:412:DG:OP1	2.01	0.56
3:C:88:LYS:HD2	3:C:89:HIS:CE1	2.40	0.56
2:I:423:DA:C1'	2:I:424:DG:H5'	2.35	0.56
3:A:181:HIS:HB3	3:A:184:ARG:HG2	1.87	0.56
3:B:122:HIS:CE1	3:B:124:VAL:H	2.24	0.56
3:B:215:THR:HG21	3:B:226:PRO:HB3	1.87	0.56
3:A:178:ALA:HB2	3:A:200:VAL:HG21	1.88	0.55
3:C:169:ILE:HG12	3:C:236:TYR:CD2	2.42	0.55
1:H:411:DT:H2''	1:H:412:DG:O4'	2.06	0.55
2:L:423:DA:H2''	2:L:424:DG:N7	2.21	0.55
3:B:134:SER:OG	3:B:136:ASP:HB2	2.06	0.55
3:D:65:GLY:HA3	3:D:115:TRP:CZ2	2.42	0.55
3:D:64:GLU:HA	3:D:64:GLU:OE1	2.07	0.55
3:A:169:ILE:HD11	3:A:216:LEU:HD11	1.88	0.55
3:C:26:VAL:HG11	3:C:28:ARG:NH1	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:131:GLU:HB3	5:C:641:HOH:O	2.08	0.54
3:A:94:LEU:HB2	3:A:102:LEU:HB3	1.90	0.54
1:E:410:DC:H4'	1:E:410:DC:OP1	2.08	0.54
3:D:214:THR:HG23	3:D:230:ALA:HB2	1.89	0.54
3:B:241:GLU:O	3:B:249:PRO:HA	2.08	0.53
3:A:77:LEU:HD22	3:A:102:LEU:HD11	1.91	0.53
3:A:94:LEU:HD22	3:A:102:LEU:HD23	1.90	0.53
5:L:744:HOH:O	3:D:128:LEU:HD21	2.07	0.53
3:C:26:VAL:HG11	3:C:28:ARG:HH11	1.73	0.53
3:D:84:LEU:HG	3:D:85:PRO:HD2	1.90	0.53
3:A:200:VAL:O	3:A:204:VAL:HG23	2.08	0.53
3:C:64:GLU:HA	3:C:64:GLU:OE1	2.09	0.53
3:B:149:LYS:HE2	3:B:156:TRP:CE3	2.44	0.53
3:A:3:LEU:HB3	3:A:4:PRO:HD3	1.91	0.52
3:C:123:ASN:O	3:C:124:VAL:HG22	2.09	0.52
3:B:180:ILE:HA	3:B:268:LYS:OXT	2.09	0.52
3:D:122:HIS:O	3:D:123:ASN:HB2	2.10	0.52
3:D:3:LEU:HB3	3:D:4:PRO:HD3	1.90	0.52
3:A:79:ILE:HA	3:A:101:VAL:O	2.10	0.52
3:D:139:GLY:HA3	3:D:195:GLU:HG2	1.91	0.52
1:H:410:DC:OP1	1:H:410:DC:H4'	2.09	0.52
2:J:421:DC:H2''	2:J:422:DC:C5	2.45	0.52
3:B:215:THR:CB	3:B:226:PRO:HB3	2.40	0.51
3:C:241:GLU:O	3:C:249:PRO:HA	2.10	0.51
1:H:411:DT:H2''	1:H:412:DG:H5''	1.92	0.51
3:D:154:LYS:NZ	3:D:260:THR:HG22	2.24	0.51
2:I:422:DC:H2''	2:I:423:DA:N7	2.25	0.51
3:D:141:TYR:CE1	3:D:145:LYS:HE2	2.46	0.51
3:D:169:ILE:CD1	3:D:216:LEU:HD11	2.37	0.51
1:H:412:DG:H2''	1:H:413:DG:C5'	2.40	0.51
3:C:140:GLU:HG3	3:C:144:GLN:NE2	2.24	0.51
2:L:421:DC:H2'	2:L:422:DC:C6	2.46	0.51
3:C:215:THR:CB	3:C:226:PRO:HB3	2.41	0.51
3:A:149:LYS:HE2	3:A:156:TRP:CE3	2.47	0.50
3:B:215:THR:OG1	3:B:226:PRO:HB3	2.12	0.50
5:G:649:HOH:O	3:C:151:THR:HB	2.09	0.50
3:C:139:GLY:HA3	3:C:195:GLU:HG3	1.94	0.50
3:D:80:LEU:HD11	3:D:103:ARG:HD2	1.92	0.50
3:B:246:CYS:HB2	3:B:265:GLN:NE2	2.27	0.50
5:K:707:HOH:O	3:D:161:LYS:HE2	2.11	0.50
3:D:181:HIS:HB3	3:D:184:ARG:HG2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:411:DT:H4'	1:E:412:DG:OP1	2.12	0.50
3:A:125:LEU:HA	3:A:128:LEU:CD1	2.42	0.50
3:C:180:ILE:HA	3:C:268:LYS:OXT	2.12	0.50
3:A:96:MET:HB2	3:A:98:ASN:OD1	2.12	0.49
3:C:134:SER:OG	3:C:136:ASP:HB2	2.12	0.49
3:C:216:LEU:HD21	3:C:236:TYR:CE2	2.41	0.49
3:D:95:VAL:HG22	3:D:101:VAL:HG22	1.94	0.49
3:A:65:GLY:HA3	3:A:115:TRP:CZ2	2.47	0.49
1:F:409:DC:H2''	1:F:410:DC:O5'	2.13	0.49
3:A:23:LEU:HD21	3:A:97:SER:HB3	1.95	0.49
3:A:225:LYS:O	3:A:226:PRO:O	2.32	0.48
1:G:411:DT:H2''	1:G:412:DG:N7	2.28	0.48
1:H:410:DC:H2''	1:H:411:DT:C6	2.49	0.48
3:C:28:ARG:NH2	3:C:86:PRO:HB3	2.28	0.48
3:A:215:THR:HG22	3:A:215:THR:O	2.13	0.48
3:B:84:LEU:HG	3:B:85:PRO:CD	2.43	0.48
3:C:181:HIS:CD2	3:C:183:ASP:HB2	2.49	0.48
3:C:211:GLN:NE2	3:C:232:GLU:OE2	2.47	0.48
3:B:3:LEU:HB3	3:B:4:PRO:HD3	1.94	0.47
3:C:32:LEU:HB3	3:C:111:GLY:O	2.14	0.47
3:B:122:HIS:HE1	3:B:124:VAL:HG13	1.79	0.47
3:C:3:LEU:HB3	3:C:4:PRO:HD3	1.95	0.47
2:K:423:DA:H2''	2:K:424:DG:OP2	2.13	0.47
3:C:181:HIS:CD2	3:C:183:ASP:H	2.14	0.47
3:B:131:GLU:HG2	5:B:611:HOH:O	2.15	0.47
3:B:262:TYR:HB2	3:B:267:GLN:OE1	2.15	0.47
3:A:139:GLY:HA3	3:A:195:GLU:HG2	1.98	0.46
3:B:141:TYR:CE1	3:B:145:LYS:HE3	2.50	0.46
3:A:122:HIS:O	3:A:126:THR:OG1	2.28	0.46
3:C:21:THR:HA	3:C:47:PRO:HA	1.97	0.46
2:J:424:DG:H2''	2:J:425:DG:OP2	2.16	0.46
3:B:181:HIS:CE1	3:B:183:ASP:HB2	2.50	0.46
3:B:214:THR:HG23	3:B:230:ALA:HB2	1.97	0.46
3:A:240:GLY:O	3:A:249:PRO:HB3	2.16	0.46
3:D:178:ALA:HB2	3:D:200:VAL:HG21	1.98	0.45
2:I:423:DA:H2''	2:I:424:DG:OP2	2.15	0.45
2:L:423:DA:H4'	2:L:424:DG:OP1	2.14	0.45
3:B:81:PRO:HA	3:B:100:LYS:HG2	1.98	0.45
3:B:200:VAL:O	3:B:204:VAL:HG23	2.17	0.45
3:A:131:GLU:HB3	5:A:512:HOH:O	2.16	0.45
3:A:211:GLN:NE2	3:A:232:GLU:OE2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:120:GLU:HG2	3:C:120:GLU:H	1.43	0.45
1:F:410:DC:OP1	1:F:410:DC:H4'	2.17	0.45
2:J:422:DC:H2''	2:J:423:DA:N7	2.32	0.45
3:B:228:TYR:O	3:B:231:GLN:HG2	2.16	0.45
3:C:183:ASP:OD1	3:C:255:HIS:NE2	2.50	0.45
3:A:10:ARG:HB2	3:A:58:LEU:CD2	2.47	0.45
3:A:228:TYR:HA	3:A:231:GLN:HE22	1.82	0.45
3:B:95:VAL:HA	3:B:101:VAL:HG22	1.99	0.45
3:B:131:GLU:HB3	5:B:578:HOH:O	2.17	0.44
3:C:33:ARG:HD3	3:C:34:TRP:CH2	2.51	0.44
3:D:61:GLU:HG3	3:D:66:TRP:CH2	2.52	0.44
1:E:410:DC:H2'	1:E:411:DT:H72	2.00	0.44
3:A:238:ARG:HD2	3:A:244:ARG:HH21	1.83	0.44
3:B:80:LEU:O	3:B:100:LYS:HB3	2.17	0.44
3:D:46:GLN:HB3	3:D:62:LEU:HD13	2.00	0.44
2:L:424:DG:H1'	2:L:425:DG:H5''	2.00	0.44
3:C:38:GLU:OE2	3:C:42:ARG:NE	2.50	0.44
3:A:238:ARG:O	3:A:250:ILE:HB	2.18	0.44
3:B:210:GLU:HG3	3:B:210:GLU:O	2.18	0.44
3:C:80:LEU:HD11	3:C:103:ARG:HD2	2.00	0.44
3:D:27:VAL:HG11	3:D:41:TYR:CZ	2.54	0.43
3:B:61:GLU:OE1	3:D:61:GLU:OE1	2.37	0.43
3:A:23:LEU:HD21	3:A:97:SER:HA	2.00	0.43
3:B:169:ILE:HG12	3:B:236:TYR:CE2	2.52	0.43
3:C:234:GLN:OE1	3:C:244:ARG:HD2	2.19	0.43
3:D:122:HIS:CD2	3:D:126:THR:HG21	2.53	0.43
3:D:61:GLU:HG3	3:D:66:TRP:CZ2	2.54	0.43
3:C:207:ARG:NH1	3:C:210:GLU:HG2	2.33	0.43
3:B:207:ARG:NH1	3:B:210:GLU:HG2	2.34	0.43
3:B:199:ARG:HG2	3:B:199:ARG:HH11	1.84	0.43
1:F:412:DG:O5'	1:F:412:DG:H2'	2.19	0.43
3:B:198:ALA:O	3:B:202:LYS:HG3	2.19	0.42
3:B:248:THR:HA	3:B:249:PRO:HD3	1.95	0.42
3:C:123:ASN:C	3:C:124:VAL:CG1	2.88	0.42
3:D:131:GLU:HB3	5:D:704:HOH:O	2.19	0.42
3:C:80:LEU:HA	3:C:81:PRO:HD3	1.91	0.42
3:C:262:TYR:HB2	3:C:267:GLN:OE1	2.20	0.42
3:D:106:ASP:OD2	3:D:109:ARG:HA	2.19	0.42
1:E:412:DG:H2''	1:E:413:DG:C8	2.54	0.42
3:D:75:GLY:HA2	3:D:105:THR:O	2.20	0.42
3:A:262:TYR:HB2	3:A:267:GLN:OE1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:134:SER:OG	3:D:136:ASP:HB2	2.20	0.42
3:A:208:SER:OG	3:A:213:GLY:HA2	2.20	0.41
3:A:61:GLU:C	3:A:62:LEU:HD23	2.41	0.41
3:A:238:ARG:HD2	3:A:244:ARG:NH2	2.36	0.41
3:B:106:ASP:OD2	3:B:109:ARG:HA	2.20	0.41
3:B:215:THR:CG2	3:B:226:PRO:HB3	2.49	0.41
3:D:181:HIS:CE1	3:D:183:ASP:HB2	2.56	0.41
3:A:238:ARG:NE	3:A:244:ARG:NH2	2.68	0.41
3:B:122:HIS:CE1	3:B:124:VAL:HG13	2.55	0.41
3:A:62:LEU:HD23	3:A:62:LEU:N	2.36	0.41
3:B:40:ILE:O	3:B:43:LEU:HG	2.21	0.41
3:C:207:ARG:NE	3:C:232:GLU:OE2	2.54	0.41
1:F:410:DC:N4	2:J:423:DA:N6	2.69	0.40
3:A:125:LEU:HA	3:A:128:LEU:HD12	2.04	0.40
3:A:10:ARG:HB2	3:A:58:LEU:HD21	2.03	0.40
3:B:184:ARG:HH22	3:B:193:GLU:CD	2.25	0.40
3:B:225:LYS:HA	3:B:226:PRO:HD3	1.92	0.40
1:E:411:DT:H2"	1:E:412:DG:C8	2.56	0.40
3:B:208:SER:O	3:B:213:GLY:N	2.50	0.40
3:B:242:PRO:HA	3:B:249:PRO:HA	2.03	0.40
3:C:207:ARG:O	3:C:210:GLU:HB3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	256/268 (96%)	243 (95%)	10 (4%)	3 (1%)	13	8
3	B	256/268 (96%)	244 (95%)	11 (4%)	1 (0%)	34	32
3	C	256/268 (96%)	249 (97%)	5 (2%)	2 (1%)	19	15
3	D	256/268 (96%)	240 (94%)	15 (6%)	1 (0%)	34	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1024/1072 (96%)	976 (95%)	41 (4%)	7 (1%)	22	18

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	226	PRO
3	B	123	ASN
3	C	124	VAL
3	A	82	GLU
3	A	123	ASN
3	D	126	THR
3	C	226	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	218/230 (95%)	206 (94%)	12 (6%)	21	19
3	B	216/230 (94%)	204 (94%)	12 (6%)	21	18
3	C	219/230 (95%)	204 (93%)	15 (7%)	16	13
3	D	218/230 (95%)	210 (96%)	8 (4%)	34	35
All	All	871/920 (95%)	824 (95%)	47 (5%)	22	20

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	31	ARG
3	A	32	LEU
3	A	33	ARG
3	A	38	GLU
3	A	44	SER
3	A	94	LEU
3	A	122	HIS
3	A	210	GLU

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Mol	Chain	Res	Type
3	A	211	GLN
3	A	215	THR
3	A	260	THR
3	A	268	LYS
3	B	31	ARG
3	B	32	LEU
3	B	33	ARG
3	B	42	ARG
3	B	120	GLU
3	B	144	GLN
3	B	161	LYS
3	B	199	ARG
3	B	210	GLU
3	B	216	LEU
3	B	260	THR
3	B	268	LYS
3	C	31	ARG
3	C	32	LEU
3	C	38	GLU
3	C	82	GLU
3	C	84	LEU
3	C	88	LYS
3	C	120	GLU
3	C	124	VAL
3	C	144	GLN
3	C	207	ARG
3	C	210	GLU
3	C	215	THR
3	C	216	LEU
3	C	260	THR
3	C	265	GLN
3	D	32	LEU
3	D	33	ARG
3	D	38	GLU
3	D	88	LYS
3	D	122	HIS
3	D	127	HIS
3	D	260	THR
3	D	268	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	24	HIS
3	A	127	HIS
3	B	122	HIS
3	B	265	GLN
3	C	144	GLN
3	C	181	HIS
3	C	211	GLN
3	D	122	HIS
3	D	211	GLN

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](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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 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.