



# Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 03:29 AM GMT

PDB ID : 4DR7  
Title : Crystal structure of the *Thermus thermophilus* (HB8) 30S ribosomal subunit with codon, crystallographically disordered near-cognate transfer RNA anti-codon stem-loop mismatched at the second codon position, and streptomycin bound  
Authors : Demirci, H.; Murphy IV, F.; Murphy, E.; Gregory, S.T.; Dahlberg, A.E.; Jogle, G.  
Deposited on : 2012-02-16  
Resolution : 3.75 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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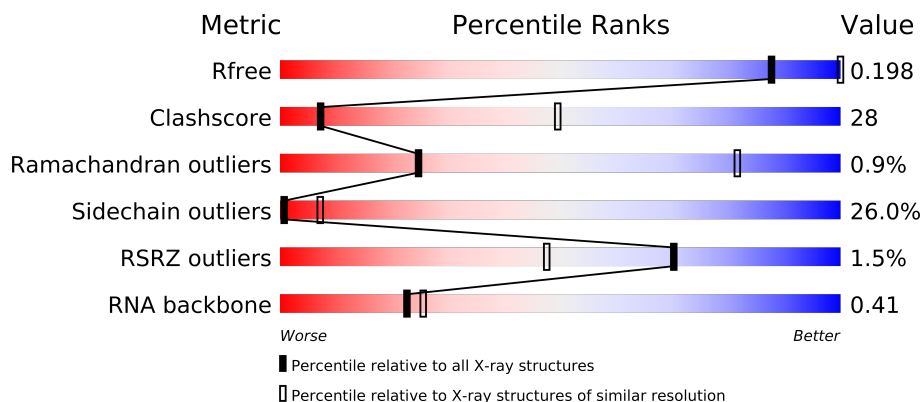
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.75 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.



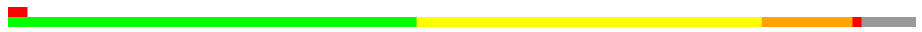
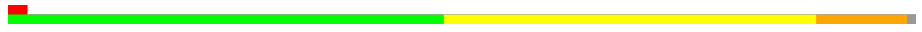

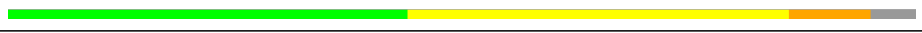
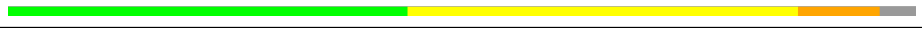
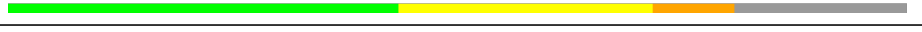
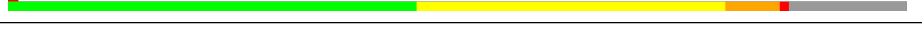



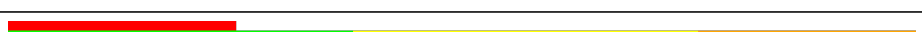
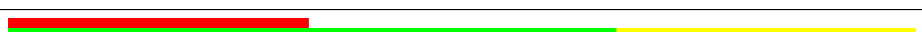

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1134 (4.12-3.40)
Clashscore	79885	1067 (4.02-3.50)
Ramachandran outliers	78287	1017 (4.02-3.50)
Sidechain outliers	78261	1010 (4.02-3.50)
RSRZ outliers	66119	1135 (4.12-3.40)
RNA backbone	1838	1008 (4.52-2.80)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	1522	
2	B	256	
3	C	239	
4	D	209	
5	E	162	
6	F	101	
7	G	156	
8	H	138	
9	I	128	
10	J	105	
11	K	129	
12	L	135	

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Mol	Chain	Length	Quality of chain
13	M	126	
14	N	61	
15	O	89	
16	P	88	
17	Q	105	
18	R	88	
19	S	93	
20	T	106	
21	U	27	
22	V	4	
23	W	11	
24	a	8	
25	b	3	

## 2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 53659 atoms, of which 0 are hydrogen and 0 are deuterium.

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 RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1513	Total	C	N	O	P	0	8	0
			32707	14570	6056	10561	1520			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1534	C	A	CONFLICT	GB M26923.1
A	1535	A	C	CONFLICT	GB M26923.1

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	236	Total	C	N	O	S	0	0	1
			1896	1211	337	343	5			

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	207	Total	C	N	O	S	0	0	1
			1613	1016	315	281	1			

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	151	Total	C	N	O	S	0	0	1
			1147	724	218	201	4			

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	127	Total	C	N	O	S	0	0	0
			1010	639	197	174				

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	99	Total	C	N	O	S	0	0	1
			793	498	157	137	1			

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	117	Total	C	N	O	S	0	0	0
			873	543	166	161	3			

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	125	Total	C	N	O	S	0	0	1
			973	612	196	163	2			

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	118	Total	C	N	O	S	0	0	0
			937	579	193	163	2			

- Molecule 14 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	100	Total	C	N	O	S	0	0	0
			834	534	156	142	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	96	GLN	GLU	CONFLICT	UNP Q5SHP7

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	R	71	Total	C	N	O		0	0	0
			585	373	116	96				

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	81	Total	C	N	O	S	0	0	1
			648	414	120	112	2			

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	T	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

- Molecule 21 is a protein called 30S ribosomal protein THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	U	25	Total	C	N	O	0	0	1
			209	128	51	30			

- Molecule 22 is a RNA chain called 5'-R(\*UP\*UP\*UP\*U)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	V	4	Total	C	N	O	P	0	0	0
			77	36	8	30	3			

- Molecule 23 is a RNA chain called 5'-R(\*GP\*CP\*CP\*UP\*GP\*GP\*AP\*AP\*AP\*GP\*(PSU))-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	W	11	Total	C	N	O	P	0	0	0
			235	106	45	74	10			

- Molecule 24 is a RNA chain called 5'-R(P\*UP\*GP\*GP\*AP\*AP\*AP\*GP\*(PSU))-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	a	8	Total	C	N	O	P	0	0	0
			175	78	34	55	8			

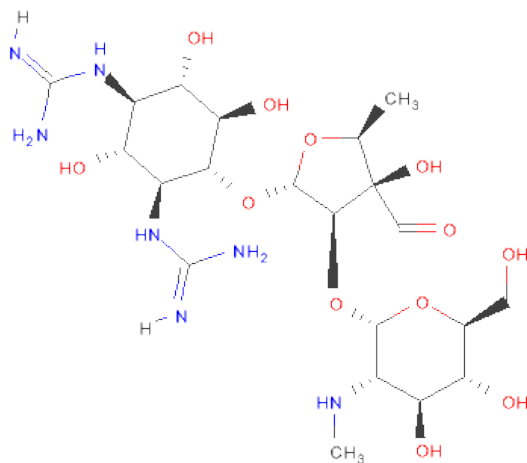
- Molecule 25 is a RNA chain called 5'-R(P\*UP\*UP\*U)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	b	3	Total	C	N	O	P	0	0	0
			60	27	6	24	3			

- Molecule 26 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
26	P	3	Total 3	Mg 3	0	0
26	G	1	Total 1	Mg 1	0	0
26	J	1	Total 1	Mg 1	0	0
26	Q	1	Total 1	Mg 1	0	0
26	D	3	Total 3	Mg 3	0	0
26	E	4	Total 4	Mg 4	0	0
26	H	1	Total 1	Mg 1	0	0
26	A	326	Total 326	Mg 326	0	0
26	N	1	Total 1	Mg 1	0	0
26	S	2	Total 2	Mg 2	0	0
26	F	1	Total 1	Mg 1	0	0

- Molecule 27 is STREPTOMYCIN (three-letter code: SRY) (formula:  $C_{21}H_{39}N_7O_{12}$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total 40	C 21	N 7	O 12	0	0



- Molecule 28 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	D	1	Total	Zn	0	0
			1	1		
28	N	1	Total	Zn	0	0
			1	1		

- Molecule 29 is water.

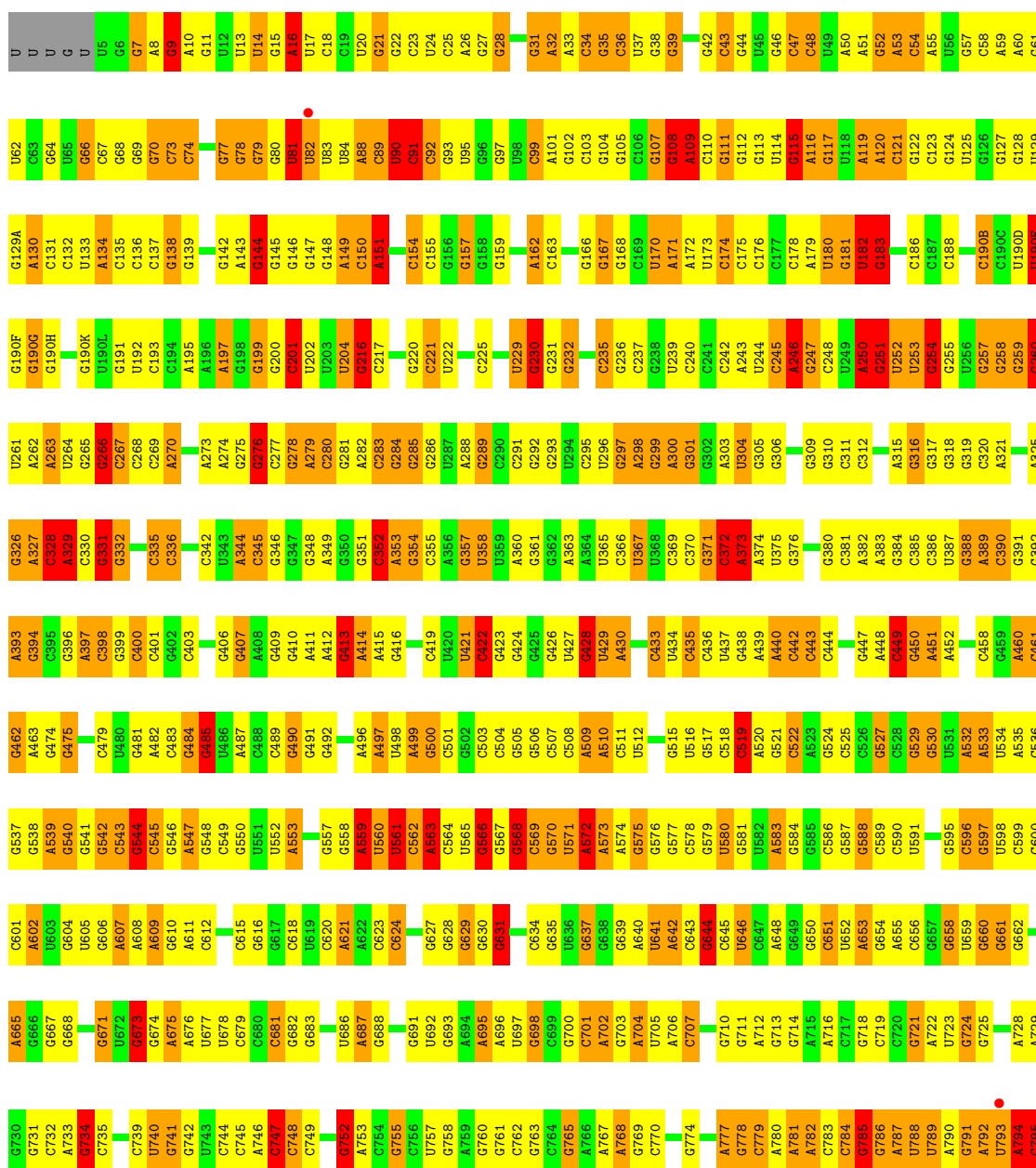
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	A	866	Total	O	0	0
			866	866		
29	C	1	Total	O	0	0
			1	1		
29	D	7	Total	O	0	0
			7	7		
29	E	5	Total	O	0	0
			5	5		
29	L	1	Total	O	0	0
			1	1		
29	N	1	Total	O	0	0
			1	1		
29	P	1	Total	O	0	0
			1	1		
29	Q	2	Total	O	0	0
			2	2		
29	T	3	Total	O	0	0
			3	3		
29	U	4	Total	O	0	0
			4	4		
29	W	1	Total	O	0	0
			1	1		

### 3 Residue-property plots

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

#### • Molecule 1: 16S rRNA

Chain A:

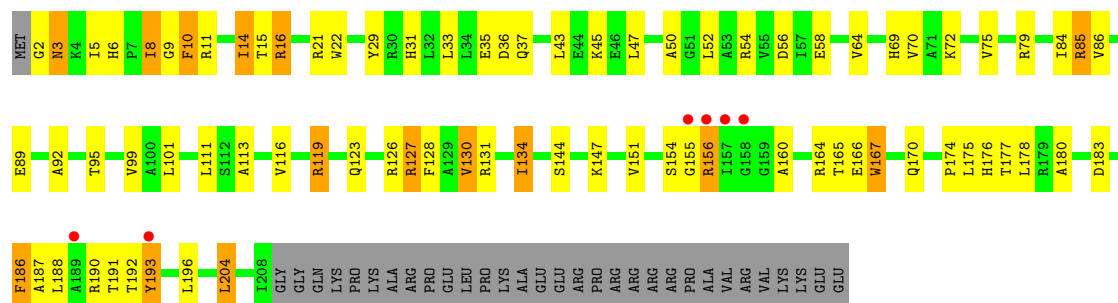




GLU  
SER  
GLU  
VAL  
GLU  
ALA

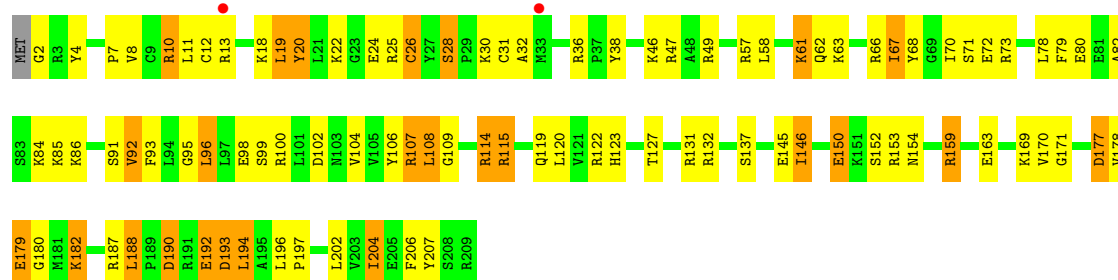
• Molecule 3: 30S ribosomal protein S3

Chain C:



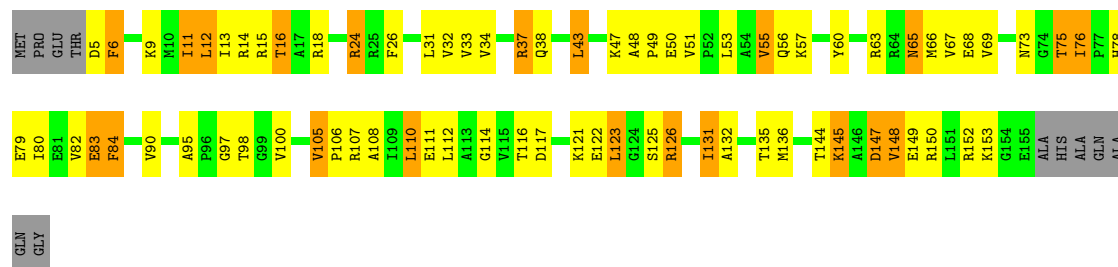
• Molecule 4: 30S ribosomal protein S4

Chain D:



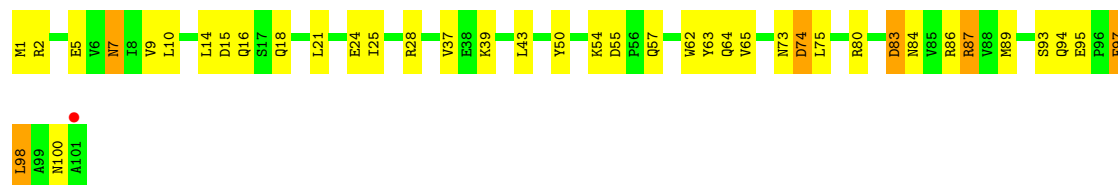
• Molecule 5: 30S ribosomal protein S5

Chain E:



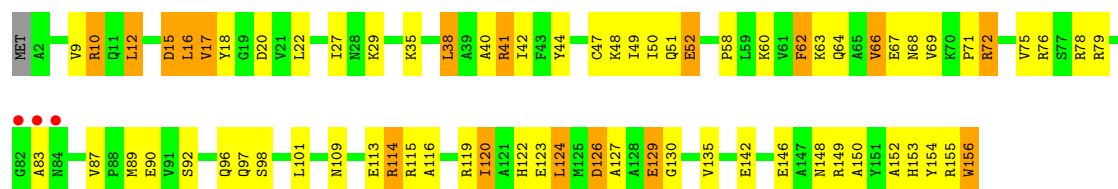
• Molecule 6: 30S ribosomal protein S6

Chain F:



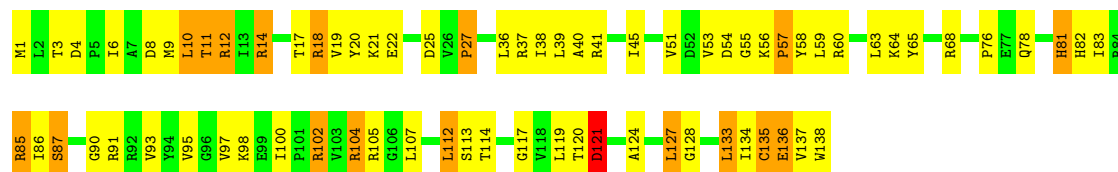
• Molecule 7: 30S ribosomal protein S7

Chain G:



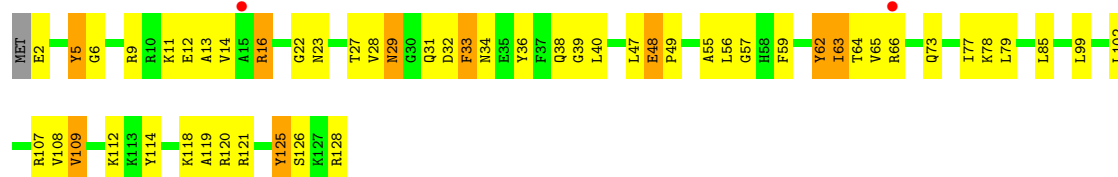
- Molecule 8: 30S ribosomal protein S8

Chain H:



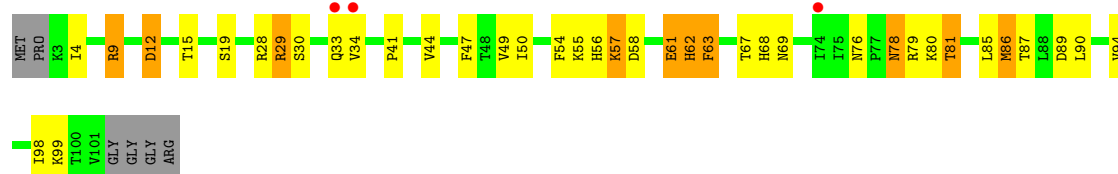
- Molecule 9: 30S ribosomal protein S9

Chain I:



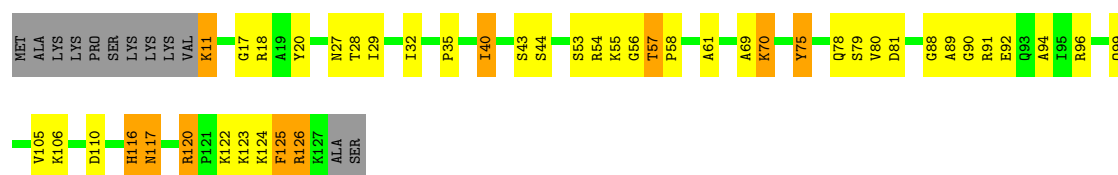
- Molecule 10: 30S ribosomal protein S10

Chain J:



- Molecule 11: 30S ribosomal protein S11

Chain K:

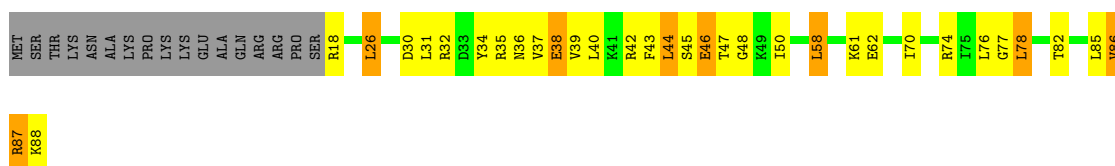


- Molecule 12: 30S ribosomal protein S12

Chain L:

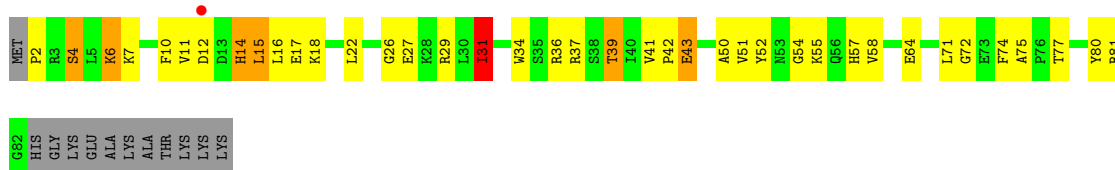






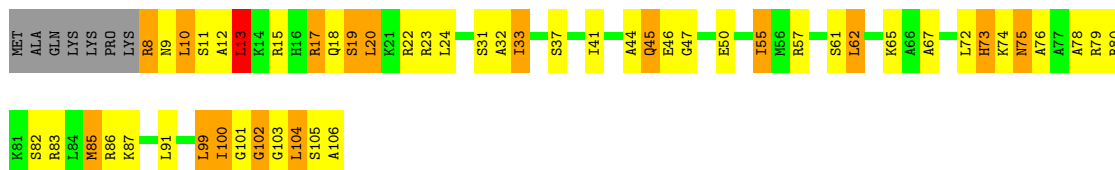
- Molecule 19: 30S ribosomal protein S19

Chain S:



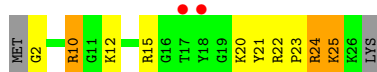
- Molecule 20: 30S ribosomal protein S20

Chain T:



- Molecule 21: 30S ribosomal protein THX

Chain U:



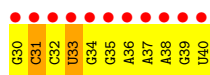
- Molecule 22: 5'-R(\*UP\*UP\*UP\*U)-3'

Chain V:



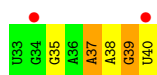
- Molecule 23: 5'-R(\*GP\*CP\*CP\*UP\*GP\*GP\*AP\*AP\*AP\*GP\*(PSU))-3'

Chain W:



- Molecule 24: 5'-R(P\*UP\*GP\*GP\*AP\*AP\*AP\*GP\*(PSU))-3'

Chain a:



- Molecule 25: 5'-R(P\*UP\*UP\*U)-3'

Chain b: 





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	402.49Å 402.49Å 174.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.91 – 3.75 49.65 – 3.75	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.91-3.75) 100.0 (49.65-3.75)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.41 (at 3.77Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_978)	Depositor
R, $R_{free}$	0.148 , 0.201 0.146 , 0.198	Depositor DCC
$R_{free}$ test set	7300 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	130.7	Xtriage
Anisotropy	0.226	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 89.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 146049 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	53659	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	146.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.65% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, M2G, MA6, 0TD, MG, 2MG, 5MC, UR3, 4OC, SRY, 7MG, PSU

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	A	1.21	135/36234 (0.4%)	1.90	1769/56547 (3.1%)
2	B	0.74	0/1931	0.93	2/2607 (0.1%)
3	C	0.62	0/1637	0.83	0/2207
4	D	0.73	1/1733 (0.1%)	0.93	4/2318 (0.2%)
5	E	1.04	1/1163 (0.1%)	1.17	3/1566 (0.2%)
6	F	0.65	0/856	0.86	0/1154
7	G	0.68	0/1276	0.87	0/1709
8	H	1.11	2/1136 (0.2%)	1.18	4/1527 (0.3%)
9	I	0.65	0/1029	0.88	2/1379 (0.1%)
10	J	0.71	1/806 (0.1%)	0.95	2/1084 (0.2%)
11	K	0.76	0/888	0.97	0/1198
12	L	0.90	0/978	1.08	3/1308 (0.2%)
13	M	0.68	0/947	0.94	0/1270
14	N	0.68	0/501	0.85	1/664 (0.2%)
15	O	0.86	0/745	1.02	3/992 (0.3%)
16	P	0.93	0/717	1.08	3/965 (0.3%)
17	Q	1.08	1/847 (0.1%)	1.25	4/1131 (0.4%)
18	R	0.76	0/590	1.00	1/782 (0.1%)
19	S	0.57	0/662	0.77	0/892
20	T	0.87	0/765	1.18	4/1007 (0.4%)
21	U	0.69	0/213	0.87	0/279
22	V	0.53	0/84	0.98	0/128
23	W	0.62	0/241	0.92	0/375
24	a	0.85	0/174	1.89	10/270 (3.7%)
25	b	0.76	0/65	1.31	2/98 (2.0%)
All	All	1.08	141/56218 (0.3%)	1.66	1817/83457 (2.2%)

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
2	B	0	3
3	C	0	2
4	D	0	1
8	H	0	2
9	I	0	1
10	J	0	2
12	L	0	2
16	P	0	1
19	S	0	1
20	T	0	2
21	U	0	1
All	All	0	18

All (141) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	828	A	N9-C4	-10.24	1.31	1.37
1	A	1513	A	N9-C4	-9.49	1.32	1.37
1	A	266	G	N7-C5	-9.34	1.33	1.39
1	A	573	A	N7-C5	-9.28	1.33	1.39
8	H	135	CYS	CB-SG	-9.04	1.66	1.82
1	A	1227	A	N9-C4	-8.41	1.32	1.37
1	A	1502	A	N3-C4	-8.37	1.29	1.34
1	A	860	A	N3-C4	-8.21	1.29	1.34
1	A	1502	A	N9-C4	-8.06	1.33	1.37
1	A	788	U	C2-N3	7.67	1.43	1.37
1	A	151	A	N9-C4	-7.36	1.33	1.37
1	A	868	C	N1-C6	-7.28	1.32	1.37
1	A	1509	C	N3-C4	-7.25	1.28	1.33
1	A	814	A	N9-C4	-7.15	1.33	1.37
1	A	1066	C	N1-C6	-7.12	1.32	1.37
1	A	787	A	N9-C4	-6.99	1.33	1.37
1	A	109	A	N9-C4	-6.97	1.33	1.37
1	A	130	A	N9-C4	-6.87	1.33	1.37
1	A	563	A	N3-C4	-6.87	1.30	1.34
1	A	366	C	N1-C2	6.81	1.47	1.40
1	A	1502	A	C5-C6	-6.80	1.34	1.41
1	A	1079	G	N7-C5	-6.78	1.35	1.39
1	A	920	U	C4-O4	6.69	1.28	1.23
1	A	868	C	C4-C5	-6.67	1.37	1.43
1	A	1080	A	N3-C4	-6.54	1.30	1.34
1	A	1525	G	C6-N1	-6.52	1.34	1.39
1	A	266	G	C5-C6	-6.52	1.35	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	882	C	N3-C4	-6.52	1.29	1.33
1	A	926	G	N9-C4	6.47	1.43	1.38
1	A	691	G	N7-C5	-6.45	1.35	1.39
1	A	298	A	N3-C4	-6.38	1.31	1.34
1	A	767	A	N3-C4	-6.38	1.31	1.34
1	A	26	A	N9-C4	-6.38	1.34	1.37
1	A	1076	C	N1-C6	-6.37	1.33	1.37
1	A	279	A	N9-C4	-6.36	1.34	1.37
1	A	780	A	N9-C4	-6.34	1.34	1.37
1	A	828	A	N7-C5	-6.34	1.35	1.39
1	A	798	G	C5-C4	-6.32	1.33	1.38
1	A	600	C	N1-C6	-6.28	1.33	1.37
1	A	858	G	C6-O6	6.28	1.29	1.24
1	A	26	A	N3-C4	-6.27	1.31	1.34
1	A	574	A	C5-C4	-6.22	1.34	1.38
1	A	1500	A	C6-N1	-6.16	1.31	1.35
1	A	892	A	N9-C4	-6.00	1.34	1.37
1	A	1487	G	N3-C4	-5.98	1.31	1.35
1	A	572	A	C5-C4	-5.97	1.34	1.38
1	A	938	A	N9-C4	-5.97	1.34	1.37
1	A	144	G	N1-C2	5.91	1.42	1.37
1	A	1340	A	N9-C4	-5.88	1.34	1.37
1	A	1239	A	N9-C4	-5.86	1.34	1.37
1	A	1513	A	N3-C4	-5.85	1.31	1.34
1	A	1500	A	N3-C4	-5.85	1.31	1.34
17	Q	9	VAL	CA-CB	-5.85	1.42	1.54
1	A	722	A	C5-C6	-5.84	1.35	1.41
1	A	242	C	N1-C6	-5.82	1.33	1.37
1	A	1528	U	C3'-O3'	5.81	1.50	1.42
1	A	934	C	C2-O2	5.79	1.29	1.24
1	A	644	G	N1-C2	-5.79	1.33	1.37
1	A	913	A	C3'-O3'	5.76	1.50	1.42
1	A	266	G	C3'-C2'	5.75	1.59	1.52
1	A	817	C	N1-C6	-5.75	1.33	1.37
1	A	1487	G	N7-C5	-5.75	1.35	1.39
1	A	1527	C	C4-C5	-5.73	1.38	1.43
1	A	1064	G	N3-C4	-5.73	1.31	1.35
1	A	807	A	N3-C4	-5.72	1.31	1.34
1	A	567	G	C5-C4	-5.71	1.34	1.38
1	A	572	A	C6-N1	-5.69	1.31	1.35
1	A	246	A	C5-C4	-5.67	1.34	1.38
4	D	12	CYS	CB-SG	5.67	1.91	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	569	C	N3-C4	-5.67	1.29	1.33
8	H	137	VAL	CB-CG2	-5.65	1.41	1.52
1	A	325	A	N3-C4	-5.62	1.31	1.34
1	A	698	G	N7-C5	-5.60	1.35	1.39
1	A	868	C	N3-C4	-5.57	1.30	1.33
1	A	1103	C	N1-C6	-5.57	1.33	1.37
1	A	863	U	N1-C2	-5.55	1.33	1.38
1	A	926	G	C5-C6	5.53	1.47	1.42
1	A	609	A	N9-C4	-5.52	1.34	1.37
1	A	298	A	N9-C4	-5.52	1.34	1.37
1	A	320	C	N1-C6	-5.50	1.33	1.37
1	A	915	A	N7-C5	-5.50	1.35	1.39
1	A	566	G	N7-C5	-5.47	1.35	1.39
1	A	577	G	N9-C4	-5.46	1.33	1.38
1	A	144	G	C5-C4	5.46	1.42	1.38
1	A	602	A	N3-C4	-5.46	1.31	1.34
1	A	1377	A	N9-C4	-5.43	1.34	1.37
1	A	107	G	C5-C6	-5.42	1.36	1.42
1	A	601	C	N1-C6	-5.42	1.33	1.37
1	A	1078	U	C4-O4	-5.42	1.19	1.23
1	A	642	A	N9-C4	-5.41	1.34	1.37
1	A	1530	G	C2-N3	-5.41	1.28	1.32
1	A	599	C	N1-C6	-5.41	1.33	1.37
1	A	81	U	N1-C2	5.40	1.43	1.38
1	A	611	A	N9-C4	-5.39	1.34	1.37
1	A	858	G	N3-C4	-5.36	1.31	1.35
1	A	1507	A	C6-N1	-5.34	1.31	1.35
1	A	881	G	N9-C8	-5.33	1.34	1.37
1	A	655	A	N9-C4	-5.33	1.34	1.37
1	A	1487	G	N9-C8	-5.31	1.34	1.37
1	A	1514	C	N3-C4	-5.29	1.30	1.33
5	E	90	VAL	CB-CG1	-5.29	1.41	1.52
1	A	574	A	C6-N1	-5.27	1.31	1.35
1	A	1512	U	C4-O4	5.26	1.27	1.23
1	A	1350	A	N7-C5	-5.25	1.36	1.39
1	A	926	G	C5-C4	5.23	1.42	1.38
1	A	1507	A	N3-C4	-5.22	1.31	1.34
1	A	1513	A	C5-C4	-5.22	1.35	1.38
1	A	266	G	C2-N3	5.22	1.36	1.32
1	A	811	C	N1-C6	-5.22	1.34	1.37
1	A	1502	A	N7-C5	-5.20	1.36	1.39
1	A	704	A	N3-C4	-5.19	1.31	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	162	A	N9-C4	5.18	1.41	1.37
1	A	327	A	C5-C6	-5.18	1.36	1.41
1	A	1053	G	N7-C5	5.15	1.42	1.39
1	A	574	A	N3-C4	-5.15	1.31	1.34
1	A	1080	A	C6-N1	-5.12	1.31	1.35
1	A	1375	A	C6-N6	-5.12	1.29	1.33
1	A	134	A	N3-C4	-5.12	1.31	1.34
1	A	1084	G	C5-C6	5.12	1.47	1.42
1	A	855	G	N3-C4	-5.12	1.31	1.35
1	A	819	A	N3-C4	-5.11	1.31	1.34
1	A	813	U	N1-C6	-5.10	1.33	1.38
1	A	325	A	N9-C4	-5.09	1.34	1.37
1	A	828	A	N3-C4	-5.08	1.31	1.34
1	A	853	G	N7-C5	-5.08	1.36	1.39
1	A	117	G	N1-C2	5.07	1.41	1.37
1	A	640	A	N3-C4	-5.05	1.31	1.34
1	A	823	G	N3-C4	-5.05	1.31	1.35
1	A	117	G	C5-C4	5.05	1.41	1.38
1	A	781	A	N7-C5	-5.05	1.36	1.39
1	A	926	G	C2-N3	5.04	1.36	1.32
1	A	741	G	N9-C4	-5.04	1.33	1.38
1	A	120	A	C6-N1	-5.02	1.32	1.35
1	A	568	G	P-O5'	-5.01	1.54	1.59
1	A	1488	G	N9-C8	-5.01	1.34	1.37
1	A	1350	A	C5-C6	-5.01	1.36	1.41
1	A	239	U	C4-O4	-5.00	1.19	1.23
1	A	640	A	C6-N1	-5.00	1.32	1.35
1	A	74	C	N1-C6	5.00	1.40	1.37
1	A	654	G	C6-N1	-5.00	1.36	1.39
10	J	57	LYS	CB-CG	5.00	1.66	1.52

All (1817) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	266	G	C6-C5-N7	-19.86	118.48	130.40
1	A	366	C	N1-C2-O2	17.84	129.60	118.90
1	A	117	G	N1-C6-O6	15.21	129.03	119.90
1	A	1200	C	C2-N1-C1'	15.12	135.43	118.80
1	A	573	A	C8-N9-C4	-15.02	99.79	105.80
1	A	266	G	N1-C6-O6	14.91	128.85	119.90
1	A	1403	C	N3-C2-O2	14.11	131.78	121.90
1	A	1200	C	N1-C2-O2	14.05	127.33	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	858	G	C5-C6-N1	-13.71	104.64	111.50
1	A	366	C	N3-C2-O2	-13.36	112.55	121.90
1	A	1524	C	N3-C4-C5	-13.31	116.58	121.90
1	A	266	G	C5-C6-O6	-12.74	120.95	128.60
1	A	117	G	N9-C4-C5	-12.34	100.46	105.40
1	A	266	G	C4-C5-C6	12.10	126.06	118.80
1	A	1524	C	C6-N1-C2	-12.09	115.46	120.30
1	A	1092	A	N1-C6-N6	12.09	125.85	118.60
1	A	863	U	C2-N1-C1'	-12.03	103.27	117.70
1	A	1403	C	N1-C2-O2	-11.95	111.73	118.90
1	A	366	C	C2-N1-C1'	11.95	131.94	118.80
1	A	481	G	N1-C6-O6	11.95	127.07	119.90
1	A	1281	U	C5-C4-O4	11.94	133.06	125.90
1	A	624	C	C6-N1-C2	11.88	125.05	120.30
1	A	117	G	C6-C5-N7	-11.85	123.29	130.40
1	A	117	G	C2-N3-C4	-11.83	105.98	111.90
1	A	104	G	N1-C6-O6	11.73	126.94	119.90
1	A	144	G	N1-C6-O6	11.73	126.94	119.90
1	A	762	C	C6-N1-C2	11.70	124.98	120.30
1	A	579	G	N1-C6-O6	11.67	126.90	119.90
1	A	266	G	C4-C5-N7	11.64	115.45	110.80
1	A	873	A	C8-N9-C4	-11.51	101.20	105.80
1	A	1200	C	C5-C6-N1	11.48	126.74	121.00
1	A	1234	C	C6-N1-C2	11.42	124.87	120.30
1	A	1084	G	N3-C4-C5	-11.26	122.97	128.60
1	A	1079	G	C8-N9-C4	-11.20	101.92	106.40
1	A	1200	C	C6-N1-C1'	-11.19	107.38	120.80
1	A	586	C	C6-N1-C2	11.14	124.76	120.30
1	A	570	G	N3-C4-C5	-10.99	123.11	128.60
1	A	283	C	C2-N1-C1'	10.97	130.87	118.80
1	A	295	C	C6-N1-C2	10.96	124.68	120.30
1	A	117	G	C8-N9-C1'	-10.95	112.77	127.00
1	A	634	C	C6-N1-C2	-10.87	115.95	120.30
1	A	1084	G	C4-C5-N7	-10.80	106.48	110.80
1	A	788	U	N3-C4-O4	10.76	126.93	119.40
1	A	920	U	N3-C4-C5	-10.65	108.21	114.60
1	A	572	A	N1-C6-N6	-10.62	112.23	118.60
1	A	863	U	C5-C4-O4	10.58	132.25	125.90
1	A	868	C	N1-C2-O2	-10.58	112.55	118.90
1	A	732	C	N3-C4-C5	10.56	126.12	121.90
1	A	144	G	C5-C6-N1	-10.54	106.23	111.50
1	A	266	G	N7-C8-N9	10.54	118.37	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	572	A	C5-C6-N1	10.33	122.86	117.70
1	A	824	C	C6-N1-C2	10.31	124.42	120.30
1	A	449	C	C6-N1-C2	-10.25	116.20	120.30
1	A	572	A	N9-C4-C5	10.25	109.90	105.80
1	A	1502	A	C2-N3-C4	-10.24	105.48	110.60
1	A	248	C	C5-C6-N1	-10.22	115.89	121.00
1	A	644	G	C4-C5-N7	10.20	114.88	110.80
1	A	873	A	C2-N3-C4	10.20	115.70	110.60
1	A	863	U	C6-N1-C1'	10.18	135.45	121.20
1	A	248	C	C6-N1-C2	10.17	124.37	120.30
1	A	884	U	C5-C6-N1	-10.15	117.62	122.70
1	A	820	U	N1-C2-N3	10.05	120.93	114.90
1	A	1329	A	N1-C6-N6	10.02	124.61	118.60
1	A	860	A	C8-N9-C4	-10.00	101.80	105.80
1	A	703	G	C4-C5-N7	-9.97	106.81	110.80
1	A	176	C	C6-N1-C2	9.96	124.28	120.30
1	A	559	A	C6-N1-C2	-9.95	112.63	118.60
1	A	856	C	N1-C2-O2	-9.94	112.94	118.90
1	A	283	C	C5-C6-N1	9.94	125.97	121.00
1	A	1190	G	C4-N9-C1'	9.93	139.41	126.50
1	A	691	G	C8-N9-C4	-9.92	102.43	106.40
1	A	90	U	C5-C4-O4	9.90	131.84	125.90
1	A	117	G	C5-C6-N1	-9.90	106.55	111.50
1	A	770	C	C5-C6-N1	-9.90	116.05	121.00
1	A	648	A	C8-N9-C4	9.89	109.76	105.80
1	A	859	A	N1-C6-N6	9.89	124.53	118.60
1	A	266	G	C4-N9-C1'	9.87	139.33	126.50
1	A	729	A	N1-C6-N6	9.86	124.51	118.60
1	A	1530	G	N3-C4-C5	9.81	133.50	128.60
1	A	920	U	C5-C4-O4	9.76	131.75	125.90
1	A	866	C	C6-N1-C2	-9.75	116.40	120.30
1	A	1370	G	C8-N9-C4	-9.75	102.50	106.40
1	A	635	G	C2-N3-C4	-9.75	107.03	111.90
1	A	1381	U	N1-C2-O2	9.74	129.62	122.80
1	A	864	A	N1-C6-N6	-9.70	112.78	118.60
1	A	563	A	C8-N9-C4	-9.67	101.93	105.80
1	A	722	A	N1-C6-N6	9.67	124.40	118.60
1	A	825	G	C8-N9-C4	9.67	110.27	106.40
1	A	117	G	C8-N9-C4	9.66	110.26	106.40
1	A	1524	C	N1-C2-O2	-9.61	113.14	118.90
1	A	266	G	N3-C4-N9	9.58	131.75	126.00
1	A	146	G	N1-C6-O6	9.57	125.64	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	529	G	C4-C5-C6	9.54	124.52	118.80
1	A	139	G	C5-C6-N1	-9.53	106.74	111.50
1	A	232	G	C6-C5-N7	-9.51	124.69	130.40
1	A	1335	C	C6-N1-C2	9.51	124.10	120.30
1	A	563	A	N9-C4-C5	9.49	109.59	105.80
1	A	366	C	C6-N1-C1'	-9.48	109.43	120.80
1	A	1232	U	N1-C2-O2	-9.47	116.17	122.80
1	A	1066	C	C6-N1-C1'	-9.47	109.44	120.80
1	A	874	G	N1-C6-O6	9.47	125.58	119.90
1	A	703	G	C5-C6-O6	9.44	134.26	128.60
1	A	1528	U	C2-N1-C1'	9.43	129.02	117.70
1	A	91	C	C2-N1-C1'	9.43	129.17	118.80
1	A	481	G	C6-C5-N7	-9.43	124.75	130.40
1	A	266	G	C5-N7-C8	-9.42	99.59	104.30
1	A	768	A	C8-N9-C4	9.41	109.57	105.80
1	A	283	C	N1-C2-O2	9.40	124.54	118.90
1	A	328	C	N3-C4-N4	-9.38	111.44	118.00
1	A	732	C	C2-N3-C4	-9.36	115.22	119.90
1	A	621	A	C8-N9-C4	-9.32	102.07	105.80
1	A	815	A	C8-N9-C4	9.31	109.53	105.80
1	A	867	G	N1-C6-O6	9.31	125.49	119.90
1	A	1514	C	N1-C2-O2	-9.31	113.31	118.90
1	A	648	A	N7-C8-N9	-9.31	109.15	113.80
1	A	867	G	C8-N9-C1'	-9.30	114.90	127.00
1	A	698	G	C4-N9-C1'	9.29	138.58	126.50
1	A	795	C	N3-C2-O2	9.25	128.38	121.90
1	A	721	G	C6-C5-N7	-9.24	124.86	130.40
1	A	864	A	C5-C6-N6	9.21	131.07	123.70
1	A	90	U	N3-C4-O4	-9.20	112.96	119.40
1	A	1239	A	C8-N9-C4	9.20	109.48	105.80
1	A	529	G	N1-C6-O6	9.17	125.40	119.90
1	A	269	C	C5-C6-N1	-9.13	116.43	121.00
1	A	860	A	N9-C4-C5	9.13	109.45	105.80
1	A	722	A	C2-N3-C4	-9.10	106.05	110.60
1	A	1507	A	N1-C6-N6	-9.09	113.15	118.60
1	A	1200	C	C6-N1-C2	-9.08	116.67	120.30
1	A	559	A	C8-N9-C4	-9.08	102.17	105.80
1	A	644	G	C6-C5-N7	-9.06	124.96	130.40
1	A	577	G	C2-N3-C4	-9.06	107.37	111.90
1	A	940	C	C6-N1-C2	9.04	123.92	120.30
1	A	283	C	C2-N3-C4	9.02	124.41	119.90
1	A	818	G	N1-C6-O6	9.02	125.31	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	729	A	C5-N7-C8	-9.02	99.39	103.90
1	A	1381	U	N3-C2-O2	-9.00	115.90	122.20
1	A	635	G	C6-C5-N7	-8.99	125.00	130.40
1	A	481	G	C5-C6-N1	-8.98	107.01	111.50
1	A	1108	G	N3-C4-C5	-8.98	124.11	128.60
1	A	623	C	C6-N1-C2	8.97	123.89	120.30
1	A	1392	G	C6-C5-N7	-8.97	125.02	130.40
1	A	1107	C	C6-N1-C2	-8.96	116.72	120.30
1	A	881	G	C8-N9-C4	8.93	109.97	106.40
1	A	635	G	C5-C6-N1	-8.92	107.04	111.50
1	A	788	U	N3-C2-O2	8.91	128.44	122.20
1	A	975	A	N1-C6-N6	8.86	123.92	118.60
1	A	232	G	N1-C6-O6	8.86	125.22	119.90
1	A	284	G	N1-C6-O6	8.86	125.22	119.90
1	A	1186	G	N3-C4-C5	8.86	133.03	128.60
1	A	1068	G	C8-N9-C4	-8.84	102.86	106.40
1	A	1392	G	N1-C6-O6	8.83	125.20	119.90
1	A	91	C	C6-N1-C2	-8.82	116.77	120.30
1	A	783	C	C6-N1-C2	8.80	123.82	120.30
1	A	885	G	C2-N3-C4	-8.80	107.50	111.90
1	A	570	G	C8-N9-C4	-8.78	102.89	106.40
1	A	1524	C	C4-C5-C6	8.78	121.79	117.40
1	A	909	A	C5-C6-N6	-8.77	116.69	123.70
1	A	651	C	C6-N1-C2	8.73	123.79	120.30
1	A	698	G	C6-C5-N7	-8.73	125.16	130.40
1	A	529	G	C4-N9-C1'	8.73	137.85	126.50
1	A	621	A	N7-C8-N9	8.73	118.17	113.80
1	A	144	G	C2-N3-C4	-8.72	107.54	111.90
1	A	1053	G	C8-N9-C4	8.72	109.89	106.40
1	A	244	U	N1-C2-O2	8.72	128.90	122.80
1	A	91	C	N1-C2-O2	8.71	124.13	118.90
1	A	926	G	N3-C4-C5	-8.71	124.25	128.60
1	A	700	G	C4-C5-N7	8.70	114.28	110.80
1	A	700	G	N3-C4-N9	8.69	131.22	126.00
1	A	1066	C	C6-N1-C2	8.69	123.78	120.30
1	A	259	G	N1-C2-N3	8.68	129.11	123.90
1	A	1228	C	N1-C2-O2	8.68	124.11	118.90
1	A	741	G	N3-C4-N9	-8.68	120.80	126.00
1	A	814	A	C2-N3-C4	-8.67	106.27	110.60
1	A	1186	G	C2-N3-C4	-8.66	107.57	111.90
1	A	529	G	C8-N9-C1'	-8.64	115.77	127.00
1	A	50	A	C8-N9-C4	8.61	109.24	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	579	G	C5-C6-O6	-8.61	123.44	128.60
1	A	277	C	C6-N1-C2	8.60	123.74	120.30
1	A	1468	A	C8-N9-C4	8.59	109.24	105.80
1	A	795	C	N1-C2-O2	-8.58	113.75	118.90
1	A	1388	C	N3-C2-O2	8.55	127.89	121.90
1	A	266	G	C8-N9-C4	-8.55	102.98	106.40
1	A	868	C	C6-N1-C2	-8.55	116.88	120.30
1	A	618	C	C2-N1-C1'	-8.54	109.41	118.80
1	A	971	G	N1-C6-O6	8.53	125.02	119.90
1	A	909	A	N1-C6-N6	8.53	123.72	118.60
1	A	573	A	C4-C5-C6	8.52	121.26	117.00
1	A	1202	G	N1-C6-O6	-8.52	114.79	119.90
1	A	735	C	C6-N1-C2	8.52	123.71	120.30
1	A	858	G	N1-C6-O6	8.51	125.00	119.90
1	A	525	C	C6-N1-C2	8.50	123.70	120.30
1	A	127	G	C8-N9-C4	8.47	109.79	106.40
1	A	928	G	N1-C6-O6	8.47	124.98	119.90
1	A	232	G	C4-C5-N7	8.46	114.18	110.80
1	A	283	C	C6-N1-C2	-8.46	116.92	120.30
1	A	884	U	C4-C5-C6	8.46	124.77	119.70
1	A	1200	C	N3-C2-O2	-8.45	115.98	121.90
1	A	650	G	C8-N9-C4	8.45	109.78	106.40
1	A	780	A	C8-N9-C4	8.44	109.17	105.80
1	A	1080	A	N1-C6-N6	-8.43	113.54	118.60
1	A	382	A	C8-N9-C4	-8.42	102.43	105.80
1	A	656	C	C6-N1-C2	8.41	123.67	120.30
1	A	268	C	N1-C2-O2	8.40	123.94	118.90
1	A	519	C	N1-C2-O2	8.39	123.94	118.90
1	A	182	U	N3-C2-O2	-8.39	116.33	122.20
1	A	1083	U	N3-C2-O2	8.38	128.07	122.20
1	A	701	C	N1-C2-O2	8.37	123.92	118.90
1	A	721	G	N3-C4-N9	8.37	131.02	126.00
1	A	788	U	C5-C6-N1	8.37	126.88	122.70
1	A	872	A	C2-N3-C4	-8.36	106.42	110.60
1	A	572	A	C8-N9-C4	-8.36	102.46	105.80
1	A	874	G	C8-N9-C4	8.35	109.74	106.40
1	A	1527	C	C5-C4-N4	-8.34	114.36	120.20
1	A	111	G	N3-C4-N9	-8.34	121.00	126.00
1	A	763	G	C8-N9-C4	8.33	109.73	106.40
1	A	1202	G	C5-C6-O6	8.32	133.59	128.60
1	A	573	A	N7-C8-N9	8.32	117.96	113.80
1	A	1058	G	C8-N9-C4	8.31	109.72	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	716	A	N1-C6-N6	-8.29	113.63	118.60
1	A	8	A	C8-N9-C4	-8.28	102.49	105.80
1	A	175	C	C6-N1-C2	8.26	123.60	120.30
1	A	634	C	N3-C4-C5	-8.26	118.60	121.90
1	A	440	A	C2-N3-C4	-8.23	106.48	110.60
1	A	721	G	C4-C5-C6	8.23	123.74	118.80
1	A	810	C	N3-C4-N4	8.23	123.76	118.00
1	A	259	G	N1-C2-N2	-8.22	108.80	116.20
1	A	874	G	N9-C4-C5	-8.22	102.11	105.40
1	A	914	A	C8-N9-C4	-8.20	102.52	105.80
1	A	398	C	C6-N1-C2	8.19	123.58	120.30
1	A	559	A	N3-C4-C5	-8.18	121.08	126.80
1	A	814	A	N1-C2-N3	8.18	133.39	129.30
1	A	871	U	N1-C2-O2	8.18	128.53	122.80
1	A	1365	G	C8-N9-C4	-8.18	103.13	106.40
1	A	1054	C	N1-C2-O2	8.18	123.81	118.90
1	A	965	A	C8-N9-C4	8.17	109.07	105.80
1	A	721	G	C4-N9-C1'	8.16	137.11	126.50
1	A	132	C	C2-N3-C4	-8.15	115.82	119.90
1	A	283	C	N3-C4-C5	-8.14	118.64	121.90
1	A	867	G	C6-C5-N7	-8.12	125.53	130.40
1	A	1390	U	N3-C4-C5	-8.11	109.73	114.60
1	A	829	G	C8-N9-C4	8.11	109.64	106.40
1	A	1186	G	C5-C6-N1	-8.10	107.45	111.50
1	A	1392	G	C5-C6-N1	-8.10	107.45	111.50
1	A	266	G	C8-N9-C1'	-8.09	116.48	127.00
1	A	864	A	N9-C4-C5	8.08	109.03	105.80
1	A	1502	A	C5-N7-C8	-8.07	99.86	103.90
1	A	1512	U	N3-C4-C5	-8.07	109.76	114.60
1	A	873	A	C5-C6-N1	8.07	121.73	117.70
1	A	1190	G	N7-C8-N9	8.06	117.13	113.10
1	A	1530	G	N3-C4-N9	-8.05	121.17	126.00
1	A	816	A	N1-C6-N6	-8.05	113.77	118.60
1	A	1186	G	N3-C4-N9	-8.05	121.17	126.00
1	A	1452	C	N1-C2-O2	8.04	123.72	118.90
1	A	659	U	C5-C6-N1	-8.03	118.68	122.70
1	A	278	G	C4-C5-N7	-8.02	107.59	110.80
1	A	1083	U	C5-C4-O4	-8.02	121.09	125.90
1	A	32	A	C6-N1-C2	-8.01	113.80	118.60
1	A	1500	A	N1-C6-N6	-8.00	113.80	118.60
1	A	288	A	C2-N3-C4	-8.00	106.60	110.60
1	A	867	G	C4-N9-C1'	7.99	136.89	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1227	A	N1-C6-N6	7.99	123.39	118.60
1	A	788	U	N3-C4-C5	-7.99	109.81	114.60
1	A	481	G	C4-C5-C6	7.98	123.59	118.80
1	A	1279	A	C8-N9-C4	-7.98	102.61	105.80
1	A	91	C	N3-C2-O2	-7.97	116.32	121.90
1	A	940	C	C5-C6-N1	-7.97	117.02	121.00
1	A	807	A	N1-C2-N3	7.96	133.28	129.30
1	A	1092	A	N9-C4-C5	-7.96	102.62	105.80
1	A	1190	G	C8-N9-C1'	-7.96	116.66	127.00
1	A	479	C	N3-C4-C5	-7.95	118.72	121.90
1	A	820	U	N1-C2-O2	-7.95	117.23	122.80
1	A	885	G	N3-C4-C5	7.94	132.57	128.60
1	A	944	G	C5-C6-O6	7.94	133.36	128.60
1	A	1488	G	C8-N9-C4	7.94	109.58	106.40
1	A	265	G	N1-C2-N2	-7.93	109.06	116.20
1	A	1507	A	N9-C4-C5	7.93	108.97	105.80
1	A	1235	U	N1-C2-N3	7.93	119.66	114.90
1	A	704	A	C8-N9-C4	-7.93	102.63	105.80
1	A	609	A	C2-N3-C4	-7.92	106.64	110.60
1	A	815	A	N7-C8-N9	-7.92	109.84	113.80
1	A	853	G	C6-C5-N7	-7.92	125.65	130.40
1	A	1322	C	C2-N1-C1'	7.92	127.51	118.80
1	A	674	G	C8-N9-C4	7.92	109.57	106.40
1	A	970	C	N1-C2-O2	7.92	123.65	118.90
1	A	43	C	C6-N1-C2	7.91	123.47	120.30
1	A	299	G	N1-C6-O6	7.91	124.65	119.90
1	A	1528	U	C6-N1-C1'	-7.91	110.13	121.20
1	A	732	C	C5-C6-N1	-7.91	117.05	121.00
1	A	628	G	N3-C4-N9	7.91	130.74	126.00
1	A	721	G	C8-N9-C1'	-7.90	116.73	127.00
1	A	1064	G	N9-C4-C5	7.90	108.56	105.40
1	A	232	G	N9-C4-C5	-7.88	102.25	105.40
1	A	117	G	C4-N9-C1'	7.88	136.74	126.50
9	I	39	GLY	N-CA-C	-7.88	93.41	113.10
1	A	729	A	C5-C6-N6	-7.87	117.40	123.70
1	A	874	G	C5-C6-O6	-7.87	123.88	128.60
1	A	117	G	C4-C5-C6	7.87	123.52	118.80
1	A	852	G	N1-C6-O6	7.85	124.61	119.90
1	A	104	G	C6-C5-N7	-7.85	125.69	130.40
1	A	1344	C	C6-N1-C2	7.85	123.44	120.30
1	A	1493[A]	A	C5-N7-C8	-7.84	99.98	103.90
1	A	1493[B]	A	C5-N7-C8	-7.84	99.98	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1488	G	N7-C8-N9	-7.84	109.18	113.10
1	A	559	A	C5-C6-N1	7.84	121.62	117.70
1	A	813	U	C2-N1-C1'	7.84	127.10	117.70
24	a	39	G	N1-C6-O6	7.83	124.60	119.90
1	A	487	A	C8-N9-C4	7.83	108.93	105.80
1	A	522	C	C5-C6-N1	-7.83	117.09	121.00
20	T	20	LEU	CA-CB-CG	-7.83	97.30	115.30
1	A	266	G	N3-C4-C5	-7.82	124.69	128.60
1	A	1222	G	C5-C6-N1	-7.81	107.60	111.50
1	A	635	G	N1-C6-O6	7.80	124.58	119.90
1	A	858	G	C4-C5-C6	7.79	123.47	118.80
1	A	529	G	C5-C6-N1	-7.78	107.61	111.50
1	A	819	A	C4-C5-C6	7.78	120.89	117.00
1	A	596	C	C6-N1-C2	7.77	123.41	120.30
1	A	963	G	N1-C6-O6	7.75	124.55	119.90
1	A	135	C	N3-C4-C5	-7.75	118.80	121.90
1	A	383	A	N1-C6-N6	-7.74	113.96	118.60
1	A	580	U	N3-C4-C5	-7.74	109.96	114.60
1	A	570	G	C4-N9-C1'	7.74	136.56	126.50
1	A	400	C	N3-C4-C5	7.73	124.99	121.90
1	A	918	A	N1-C2-N3	7.73	133.16	129.30
1	A	1528	U	P-O3'-C3'	7.73	128.97	119.70
1	A	1092	A	C6-C5-N7	-7.72	126.89	132.30
1	A	190(G)	G	C5-C6-N1	-7.71	107.65	111.50
1	A	1414	U	N3-C2-O2	-7.71	116.81	122.20
1	A	1074	G	C5-C6-N1	-7.71	107.65	111.50
1	A	867	G	N3-C4-N9	7.70	130.62	126.00
1	A	522	C	C2-N1-C1'	-7.70	110.33	118.80
1	A	783	C	N3-C4-C5	7.69	124.98	121.90
1	A	1277	C	C6-N1-C2	-7.69	117.22	120.30
1	A	1099	G	N9-C4-C5	7.69	108.47	105.40
1	A	109	A	C2-N3-C4	-7.68	106.76	110.60
1	A	753	A	N9-C4-C5	7.68	108.87	105.80
1	A	813	U	C5-C4-O4	-7.67	121.30	125.90
1	A	1394	A	C5-C6-N6	-7.67	117.56	123.70
1	A	570	G	C2-N3-C4	7.67	115.74	111.90
1	A	128	G	N1-C6-O6	7.66	124.49	119.90
1	A	805	C	N3-C4-C5	7.66	124.96	121.90
1	A	770	C	C6-N1-C2	7.66	123.36	120.30
1	A	1108	G	C8-N9-C4	-7.66	103.34	106.40
1	A	783	C	N3-C4-N4	-7.65	112.64	118.00
1	A	55	A	N1-C6-N6	-7.63	114.02	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	21	G	C8-N9-C4	7.62	109.45	106.40
1	A	700	G	C6-C5-N7	-7.61	125.83	130.40
1	A	779	C	N1-C2-O2	-7.61	114.34	118.90
1	A	1230	C	N3-C4-N4	7.61	123.32	118.00
1	A	946	A	C6-N1-C2	-7.60	114.04	118.60
1	A	1390	U	N1-C2-N3	7.60	119.46	114.90
1	A	529	G	C6-C5-N7	-7.60	125.84	130.40
1	A	591	U	C5-C6-N1	-7.60	118.90	122.70
1	A	1496	C	N3-C4-C5	-7.60	118.86	121.90
1	A	697	U	C5-C6-N1	-7.59	118.90	122.70
1	A	1525	G	N1-C6-O6	-7.59	115.34	119.90
1	A	722	A	C6-C5-N7	-7.59	126.99	132.30
1	A	1353	G	N3-C4-C5	-7.59	124.81	128.60
1	A	1240	U	C5-C4-O4	7.58	130.45	125.90
1	A	1053	G	N7-C8-N9	-7.58	109.31	113.10
1	A	242	C	C4-C5-C6	7.58	121.19	117.40
1	A	326	G	C5-C6-N1	-7.57	107.72	111.50
1	A	858	G	N3-C2-N2	-7.57	114.60	119.90
1	A	32	A	C4-N9-C1'	7.57	139.92	126.30
1	A	572	A	C2-N3-C4	7.57	114.38	110.60
1	A	782	A	C8-N9-C4	-7.56	102.78	105.80
1	A	618	C	N3-C2-O2	7.56	127.19	121.90
1	A	297	G	N3-C4-C5	-7.55	124.82	128.60
1	A	1190	G	C8-N9-C4	-7.54	103.38	106.40
1	A	1403	C	N3-C4-N4	7.53	123.27	118.00
1	A	981	U	N3-C4-O4	7.52	124.67	119.40
1	A	1525	G	C5-C6-N1	7.52	115.26	111.50
1	A	579	G	C4-C5-N7	7.52	113.81	110.80
1	A	782	A	N9-C4-C5	7.52	108.81	105.80
1	A	400	C	N1-C2-O2	7.52	123.41	118.90
1	A	693	G	N1-C6-O6	7.52	124.41	119.90
1	A	1487	G	N3-C4-C5	-7.51	124.84	128.60
1	A	667	G	C2-N3-C4	-7.51	108.15	111.90
1	A	784	C	N3-C2-O2	-7.51	116.65	121.90
1	A	107	G	C4-C5-N7	7.49	113.80	110.80
1	A	928	G	C5-C6-O6	-7.49	124.10	128.60
1	A	1084	G	C5-N7-C8	7.49	108.05	104.30
1	A	1202	G	C4-C5-N7	-7.49	107.80	110.80
1	A	874	G	C8-N9-C1'	-7.49	117.26	127.00
1	A	698	G	C8-N9-C1'	-7.48	117.27	127.00
1	A	16	A	C8-N9-C4	7.48	108.79	105.80
1	A	1055	A	N1-C6-N6	-7.48	114.11	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	36	C	C6-N1-C2	-7.47	117.31	120.30
1	A	648	A	C5-N7-C8	7.46	107.63	103.90
1	A	27	G	C5-C6-O6	-7.46	124.13	128.60
1	A	893	C	N1-C2-O2	7.45	123.37	118.90
1	A	230	G	C8-N9-C1'	-7.45	117.32	127.00
1	A	859	A	C5-C6-N6	-7.44	117.75	123.70
1	A	881	G	C8-N9-C1'	-7.44	117.33	127.00
1	A	332	G	C5-C6-O6	-7.43	124.14	128.60
1	A	1281	U	N3-C4-O4	-7.42	114.20	119.40
1	A	781	A	C8-N9-C4	-7.42	102.83	105.80
1	A	923	A	C2-N3-C4	-7.42	106.89	110.60
1	A	920	U	C4-C5-C6	7.42	124.15	119.70
1	A	382	A	N9-C4-C5	7.40	108.76	105.80
1	A	628	G	N3-C4-C5	-7.40	124.90	128.60
1	A	637	G	C5-C6-N1	-7.39	107.80	111.50
1	A	698	G	N3-C4-C5	-7.39	124.91	128.60
1	A	1232	U	N3-C2-O2	7.38	127.37	122.20
1	A	760	G	C8-N9-C1'	-7.36	117.43	127.00
1	A	573	A	N9-C4-C5	7.36	108.75	105.80
1	A	1305	G	C5-C6-N1	-7.36	107.82	111.50
1	A	328	C	C5-C4-N4	7.36	125.35	120.20
1	A	1092	A	C5-C6-N6	-7.36	117.81	123.70
1	A	852	G	C5-C6-N1	-7.35	107.82	111.50
1	A	134	A	N1-C2-N3	7.33	132.97	129.30
1	A	745	C	C6-N1-C2	7.33	123.23	120.30
1	A	1094	G	C4-C5-N7	7.33	113.73	110.80
1	A	816	A	C5-C6-N6	7.33	129.56	123.70
1	A	946	A	N1-C6-N6	-7.32	114.21	118.60
1	A	436	C	C6-N1-C2	7.32	123.23	120.30
1	A	1068	G	N7-C8-N9	7.32	116.76	113.10
1	A	1199	U	N3-C2-O2	-7.31	117.08	122.20
1	A	251	G	N1-C2-N2	-7.31	109.62	116.20
1	A	447	G	N3-C4-N9	7.31	130.38	126.00
1	A	1370	G	N7-C8-N9	7.30	116.75	113.10
1	A	1084	G	N1-C6-O6	-7.30	115.52	119.90
1	A	635	G	N1-C2-N3	7.29	128.28	123.90
1	A	1092	A	C4-C5-N7	7.29	114.34	110.70
1	A	139	G	N1-C6-O6	7.29	124.27	119.90
1	A	38	G	N3-C4-N9	-7.28	121.63	126.00
1	A	1193	G	C5-C6-N1	-7.28	107.86	111.50
1	A	27	G	C8-N9-C4	-7.28	103.49	106.40
1	A	1080	A	N9-C4-C5	7.28	108.71	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	312	C	N3-C4-C5	7.27	124.81	121.90
1	A	823	G	C2-N3-C4	-7.27	108.26	111.90
1	A	1353	G	C8-N9-C4	-7.27	103.49	106.40
1	A	787	A	C5-N7-C8	-7.27	100.27	103.90
1	A	597	G	N3-C4-N9	7.26	130.36	126.00
1	A	1301	U	C6-N1-C2	-7.26	116.64	121.00
1	A	250	A	C5-C6-N1	-7.25	114.08	117.70
1	A	1205	U	N3-C2-O2	-7.24	117.13	122.20
1	A	1447	G	N1-C6-O6	7.24	124.25	119.90
1	A	1350	A	C5-N7-C8	-7.24	100.28	103.90
1	A	830	G	C2-N3-C4	-7.23	108.28	111.90
1	A	1143	G	N1-C6-O6	7.22	124.23	119.90
1	A	7	G	N9-C4-C5	-7.22	102.51	105.40
15	O	67	LEU	CA-CB-CG	-7.22	98.70	115.30
1	A	635	G	C4-C5-C6	7.20	123.12	118.80
1	A	577	G	N3-C4-C5	7.19	132.20	128.60
1	A	867	G	C4-C5-C6	7.19	123.11	118.80
1	A	1403	C	C6-N1-C2	7.19	123.18	120.30
1	A	254	G	C2-N3-C4	-7.19	108.31	111.90
1	A	451	A	C2-N3-C4	-7.19	107.00	110.60
1	A	586	C	C2-N1-C1'	-7.19	110.89	118.80
1	A	929	G	N1-C6-O6	7.18	124.21	119.90
1	A	1231	G	C8-N9-C1'	-7.18	117.66	127.00
1	A	868	C	N3-C4-C5	-7.18	119.03	121.90
1	A	32	A	C8-N9-C1'	-7.18	114.78	127.70
1	A	1530	G	C8-N9-C4	7.18	109.27	106.40
1	A	760	G	C6-C5-N7	-7.17	126.10	130.40
1	A	854	G	N1-C2-N2	-7.17	109.75	116.20
1	A	722	A	C4-C5-N7	7.16	114.28	110.70
1	A	197	A	N1-C6-N6	-7.16	114.30	118.60
1	A	1338	G	C5-C6-O6	7.16	132.90	128.60
1	A	109	A	N3-C4-N9	-7.16	121.67	127.40
1	A	522	C	C6-N1-C2	7.16	123.16	120.30
1	A	703	G	N9-C4-C5	7.16	108.26	105.40
1	A	732	C	C6-N1-C2	7.16	123.16	120.30
1	A	283	C	C6-N1-C1'	-7.15	112.22	120.80
1	A	20	U	C5-C6-N1	-7.15	119.12	122.70
1	A	783	C	C2-N1-C1'	-7.14	110.94	118.80
1	A	1399	C	C5-C4-N4	-7.14	115.20	120.20
1	A	183	G	C8-N9-C4	-7.14	103.54	106.40
1	A	583	A	N1-C6-N6	7.14	122.89	118.60
24	a	38	A	C5-C6-N1	-7.13	114.13	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	318	G	N1-C6-O6	7.13	124.18	119.90
1	A	718	G	N1-C6-O6	7.12	124.17	119.90
1	A	1230	C	C5-C4-N4	-7.11	115.22	120.20
1	A	813	U	N3-C4-O4	7.11	124.37	119.40
1	A	1227	A	C5-N7-C8	-7.10	100.35	103.90
1	A	365	U	C2-N1-C1'	7.10	126.22	117.70
1	A	1230	C	N3-C2-O2	7.10	126.87	121.90
1	A	50	A	N1-C2-N3	-7.10	125.75	129.30
1	A	1375	A	C5-C6-N1	7.10	121.25	117.70
1	A	729	A	C4-C5-N7	7.09	114.25	110.70
1	A	1310	G	C8-N9-C1'	-7.09	117.78	127.00
1	A	1276	G	N1-C6-O6	7.09	124.15	119.90
1	A	68	G	C8-N9-C4	7.08	109.23	106.40
1	A	91	C	C5-C6-N1	7.08	124.54	121.00
1	A	371	G	N1-C6-O6	-7.08	115.65	119.90
1	A	934	C	N1-C2-N3	-7.08	114.25	119.20
1	A	828	A	C2-N3-C4	-7.08	107.06	110.60
1	A	701	C	N3-C2-O2	-7.07	116.95	121.90
1	A	8	A	N9-C4-C5	7.07	108.63	105.80
1	A	856	C	N3-C4-C5	-7.07	119.07	121.90
1	A	698	G	N3-C4-N9	7.07	130.24	126.00
1	A	1190	G	C6-C5-N7	-7.07	126.16	130.40
1	A	120	A	N1-C6-N6	-7.06	114.36	118.60
1	A	895	G	C8-N9-C4	-7.06	103.58	106.40
1	A	945	G	C5-C6-N1	7.06	115.03	111.50
1	A	36	C	N3-C2-O2	-7.06	116.96	121.90
1	A	1388	C	C6-N1-C2	7.06	123.12	120.30
1	A	1507	A	C8-N9-C4	-7.05	102.98	105.80
1	A	365	U	N3-C4-O4	7.05	124.34	119.40
1	A	259	G	C2-N3-C4	-7.05	108.38	111.90
1	A	912	C	N3-C4-C5	7.05	124.72	121.90
1	A	1061	G	C2-N3-C4	-7.04	108.38	111.90
1	A	1380	U	N3-C2-O2	-7.04	117.27	122.20
1	A	269	C	C2-N3-C4	-7.04	116.38	119.90
1	A	1341	U	C5-C4-O4	7.04	130.12	125.90
1	A	799	G	N1-C6-O6	7.03	124.12	119.90
1	A	700	G	C5-C6-O6	-7.03	124.38	128.60
1	A	621	A	C5-N7-C8	-7.02	100.39	103.90
1	A	975	A	C4-C5-N7	7.01	114.21	110.70
1	A	681	C	C6-N1-C2	-7.01	117.50	120.30
1	A	190(G)	G	N1-C6-O6	7.01	124.11	119.90
1	A	104	G	C5-C6-N1	-7.01	108.00	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	7	G	C8-N9-C4	7.01	109.20	106.40
1	A	1322	C	N3-C4-C5	-7.01	119.10	121.90
1	A	250	A	C2-N3-C4	-7.00	107.10	110.60
1	A	1061	G	C5-C6-N1	-7.00	108.00	111.50
1	A	181	G	C4-N9-C1'	6.99	135.59	126.50
1	A	774	G	N1-C6-O6	6.99	124.09	119.90
1	A	940	C	C2-N3-C4	-6.99	116.41	119.90
1	A	552	U	C2-N3-C4	-6.98	122.81	127.00
1	A	1438	G	N1-C6-O6	6.98	124.09	119.90
1	A	1047	G	C8-N9-C4	6.98	109.19	106.40
1	A	117	G	C5-C6-O6	-6.98	124.41	128.60
1	A	316	G	N1-C6-O6	-6.98	115.71	119.90
1	A	329	A	C2-N3-C4	-6.98	107.11	110.60
1	A	1399	C	N3-C4-N4	6.97	122.88	118.00
1	A	674	G	N9-C4-C5	-6.97	102.61	105.40
1	A	278	G	N9-C4-C5	6.96	108.19	105.40
1	A	590	C	C6-N1-C2	6.96	123.09	120.30
1	A	817	C	C6-N1-C1'	-6.96	112.44	120.80
1	A	753	A	N1-C6-N6	-6.96	114.42	118.60
1	A	1403	C	C5-C4-N4	-6.96	115.33	120.20
1	A	552	U	N3-C2-O2	-6.96	117.33	122.20
1	A	854	G	C8-N9-C1'	-6.96	117.95	127.00
1	A	127	G	N1-C6-O6	6.96	124.07	119.90
1	A	447	G	C8-N9-C1'	-6.95	117.96	127.00
1	A	580	U	C5-C4-O4	6.95	130.07	125.90
1	A	722	A	C5-N7-C8	-6.95	100.42	103.90
1	A	1493[A]	A	N7-C8-N9	6.95	117.28	113.80
1	A	1493[B]	A	N7-C8-N9	6.95	117.28	113.80
1	A	27	G	C4-C5-N7	6.95	113.58	110.80
4	D	202	LEU	CA-CB-CG	-6.94	99.34	115.30
1	A	703	G	N1-C6-O6	-6.94	115.74	119.90
1	A	1421	G	C8-N9-C4	-6.94	103.62	106.40
1	A	686	U	C5-C4-O4	6.93	130.06	125.90
1	A	235	C	C6-N1-C2	6.93	123.07	120.30
1	A	946	A	C8-N9-C4	-6.93	103.03	105.80
1	A	1373	G	N9-C4-C5	6.93	108.17	105.40
1	A	295	C	C5-C6-N1	-6.92	117.54	121.00
1	A	755	G	C5-C6-O6	-6.92	124.45	128.60
10	J	58	ASP	CB-CG-OD2	-6.92	112.08	118.30
1	A	182	U	N1-C2-O2	6.91	127.64	122.80
1	A	824	C	N3-C4-C5	6.91	124.66	121.90
1	A	549	C	C6-N1-C2	6.91	123.06	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	863	U	N3-C4-O4	-6.91	114.57	119.40
1	A	260	G	C5-C6-N1	-6.90	108.05	111.50
1	A	1442	G	C8-N9-C1'	-6.89	118.04	127.00
1	A	1525	G	N9-C4-C5	6.89	108.16	105.40
1	A	635	G	C8-N9-C1'	-6.89	118.04	127.00
1	A	1228	C	C2-N1-C1'	6.89	126.38	118.80
1	A	246	A	C2-N3-C4	6.88	114.04	110.60
1	A	975	A	C5-N7-C8	-6.88	100.46	103.90
1	A	1530	G	N7-C8-N9	-6.88	109.66	113.10
1	A	487	A	N7-C8-N9	-6.88	110.36	113.80
1	A	113	G	N1-C6-O6	6.87	124.02	119.90
1	A	758	G	C2-N3-C4	-6.87	108.46	111.90
1	A	1066	C	N1-C2-O2	6.86	123.02	118.90
1	A	919	A	N1-C6-N6	6.86	122.71	118.60
1	A	1323	G	C2-N3-C4	-6.86	108.47	111.90
1	A	167	G	C5-C6-N1	6.85	114.92	111.50
1	A	90	U	C2-N1-C1'	-6.85	109.48	117.70
1	A	700	G	N3-C2-N2	6.85	124.69	119.90
1	A	830	G	N1-C2-N3	6.85	128.01	123.90
1	A	787	A	C2-N3-C4	-6.85	107.18	110.60
1	A	1336	C	N3-C4-C5	-6.84	119.16	121.90
1	A	357	G	C4-C5-N7	-6.84	108.06	110.80
1	A	741	G	C4-N9-C1'	-6.84	117.61	126.50
1	A	852	G	C2-N3-C4	-6.84	108.48	111.90
24	a	39	G	C5-C6-O6	-6.84	124.50	128.60
1	A	729	A	C6-C5-N7	-6.83	127.52	132.30
1	A	884	U	N3-C2-O2	-6.83	117.42	122.20
1	A	1202	G	N3-C4-C5	-6.83	125.19	128.60
1	A	874	G	C6-C5-N7	-6.83	126.31	130.40
1	A	857	C	C6-N1-C2	6.82	123.03	120.30
1	A	881	G	N9-C4-C5	-6.82	102.67	105.40
1	A	104	G	C2-N3-C4	-6.82	108.49	111.90
1	A	188	C	N3-C4-C5	-6.82	119.17	121.90
1	A	1178	G	C8-N9-C4	-6.81	103.68	106.40
1	A	398	C	N3-C4-C5	6.81	124.62	121.90
1	A	1200	C	C2-N3-C4	6.80	123.30	119.90
1	A	1337	G	C5-C6-N1	-6.80	108.10	111.50
1	A	1338	G	N1-C6-O6	-6.79	115.83	119.90
1	A	193	C	C5-C6-N1	-6.78	117.61	121.00
25	b	3	U	N1-C2-O2	6.78	127.55	122.80
1	A	644	G	N3-C2-N2	6.78	124.64	119.90
1	A	1292	U	N3-C2-O2	6.78	126.94	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	39	G	N9-C4-C5	-6.78	102.69	105.40
1	A	947	G	C4-C5-N7	6.77	113.51	110.80
1	A	788	U	N1-C2-O2	-6.77	118.06	122.80
1	A	1310	G	N3-C4-N9	6.77	130.06	126.00
1	A	1343	G	C6-C5-N7	-6.77	126.34	130.40
1	A	1447	G	C4-C5-N7	6.77	113.51	110.80
1	A	677	U	N1-C2-N3	6.76	118.96	114.90
1	A	168	G	C5-C6-N1	-6.76	108.12	111.50
1	A	765	G	N1-C6-O6	6.75	123.95	119.90
1	A	285	G	N3-C4-C5	6.75	131.98	128.60
1	A	706	A	C2-N3-C4	-6.75	107.22	110.60
1	A	1195	C	N3-C4-N4	6.75	122.72	118.00
1	A	1249	C	C6-N1-C2	-6.75	117.60	120.30
1	A	133	U	C5-C4-O4	6.75	129.95	125.90
1	A	1202	G	N9-C4-C5	6.75	108.10	105.40
1	A	677	U	N3-C2-O2	-6.74	117.48	122.20
1	A	973	G	C8-N9-C4	6.74	109.10	106.40
1	A	1054	C	C2-N3-C4	6.74	123.27	119.90
1	A	32	A	N3-C4-C5	-6.73	122.09	126.80
1	A	563	A	N1-C6-N6	-6.73	114.56	118.60
1	A	27	G	C5-N7-C8	-6.73	100.94	104.30
1	A	1338	G	N9-C4-C5	6.72	108.09	105.40
1	A	383	A	N9-C4-C5	6.72	108.49	105.80
1	A	1329	A	C5-C6-N6	-6.71	118.33	123.70
1	A	400	C	N3-C4-N4	-6.71	113.30	118.00
1	A	662	G	N1-C6-O6	6.71	123.92	119.90
17	Q	63	ARG	NE-CZ-NH1	-6.71	116.95	120.30
1	A	73	C	C5-C6-N1	6.70	124.35	121.00
1	A	644	G	N1-C2-N2	-6.70	110.17	116.20
1	A	964	A	C8-N9-C4	-6.70	103.12	105.80
1	A	1066	C	N1-C2-N3	-6.70	114.51	119.20
1	A	623	C	C5-C6-N1	-6.70	117.65	121.00
1	A	157	G	N1-C6-O6	6.69	123.92	119.90
1	A	615	C	C6-N1-C2	-6.69	117.62	120.30
1	A	824	C	C5-C6-N1	-6.68	117.66	121.00
1	A	1442	G	C4-N9-C1'	6.68	135.18	126.50
1	A	762	C	N3-C4-C5	6.68	124.57	121.90
1	A	64	G	N1-C6-O6	6.67	123.91	119.90
1	A	885	G	N1-C6-O6	6.67	123.90	119.90
1	A	275	G	N9-C4-C5	-6.67	102.73	105.40
24	a	39	G	C4-C5-N7	6.67	113.47	110.80
1	A	1447	G	C5-C6-O6	-6.67	124.60	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	27	G	N7-C8-N9	6.66	116.43	113.10
1	A	747	C	C6-N1-C2	6.66	122.96	120.30
1	A	975	A	N9-C4-C5	-6.66	103.14	105.80
1	A	285	G	C2-N3-C4	-6.66	108.57	111.90
1	A	586	C	C5-C6-N1	-6.66	117.67	121.00
1	A	687	A	P-O3'-C3'	6.66	127.69	119.70
1	A	1077	G	C6-C5-N7	-6.66	126.41	130.40
1	A	28	G	N9-C4-C5	6.65	108.06	105.40
1	A	1405	G	N3-C4-C5	6.65	131.93	128.60
1	A	729	A	N7-C8-N9	6.65	117.12	113.80
1	A	16	A	C2-N3-C4	-6.64	107.28	110.60
1	A	1234	C	N1-C2-N3	-6.64	114.55	119.20
1	A	14	U	C6-N1-C2	-6.64	117.02	121.00
1	A	275	G	C8-N9-C1'	-6.64	118.37	127.00
1	A	795	C	N3-C4-C5	-6.64	119.24	121.90
1	A	782	A	N1-C2-N3	6.64	132.62	129.30
1	A	18	C	C6-N1-C2	6.64	122.95	120.30
1	A	109	A	N9-C4-C5	6.64	108.45	105.80
1	A	828	A	C5-N7-C8	-6.64	100.58	103.90
1	A	1282	C	C6-N1-C2	-6.63	117.65	120.30
1	A	171	A	N1-C6-N6	-6.62	114.63	118.60
1	A	873	A	N7-C8-N9	6.62	117.11	113.80
1	A	247	G	C8-N9-C4	6.62	109.05	106.40
1	A	873	A	N3-C4-C5	-6.62	122.17	126.80
1	A	117	G	N1-C2-N3	6.61	127.87	123.90
1	A	529	G	N3-C4-N9	6.61	129.97	126.00
1	A	1483	A	N1-C6-N6	-6.61	114.63	118.60
17	Q	9	VAL	CB-CA-C	-6.61	98.85	111.40
1	A	275	G	C8-N9-C4	6.60	109.04	106.40
1	A	47	C	N3-C4-C5	6.59	124.54	121.90
1	A	700	G	N9-C4-C5	-6.59	102.76	105.40
1	A	1073	U	C5-C6-N1	-6.59	119.41	122.70
1	A	1107	C	C5-C6-N1	6.59	124.29	121.00
1	A	818	G	N3-C2-N2	-6.58	115.29	119.90
1	A	1226	C	C6-N1-C2	6.58	122.93	120.30
1	A	529	G	N3-C4-C5	-6.58	125.31	128.60
1	A	934	C	N1-C2-O2	6.58	122.85	118.90
1	A	784	C	C6-N1-C2	-6.58	117.67	120.30
1	A	824	C	C2-N1-C1'	-6.57	111.57	118.80
1	A	130	A	C2-N3-C4	-6.57	107.31	110.60
1	A	620	C	N1-C2-O2	6.57	122.84	118.90
1	A	1322	C	N3-C4-N4	6.57	122.60	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	111	G	N1-C2-N2	6.57	122.11	116.20
1	A	1079	G	N7-C8-N9	6.57	116.38	113.10
1	A	449	C	N3-C4-N4	6.56	122.59	118.00
1	A	543	C	C6-N1-C2	-6.56	117.67	120.30
1	A	644	G	C5-N7-C8	-6.56	101.02	104.30
1	A	7	G	N3-C4-N9	6.56	129.94	126.00
1	A	818	G	C5-C6-N1	-6.56	108.22	111.50
1	A	559	A	N1-C2-N3	6.56	132.58	129.30
1	A	563	A	C2-N3-C4	6.56	113.88	110.60
1	A	1227	A	C4-C5-N7	6.56	113.98	110.70
1	A	1227	A	C2-N3-C4	-6.56	107.32	110.60
1	A	521	G	N1-C6-O6	-6.56	115.97	119.90
1	A	784	C	N3-C4-C5	-6.56	119.28	121.90
1	A	1524	C	N3-C4-N4	6.55	122.59	118.00
1	A	734	G	N1-C6-O6	6.55	123.83	119.90
1	A	365	U	C5-C4-O4	-6.55	121.97	125.90
1	A	251	G	N3-C4-N9	6.55	129.93	126.00
1	A	676	A	C8-N9-C4	6.55	108.42	105.80
1	A	525	C	N3-C2-O2	6.55	126.48	121.90
1	A	1094	G	N9-C4-C5	-6.55	102.78	105.40
1	A	170	U	C5-C6-N1	-6.54	119.43	122.70
1	A	265	G	C2-N3-C4	-6.54	108.63	111.90
1	A	1033	G	C8-N9-C4	-6.54	103.78	106.40
1	A	1414	U	C5-C6-N1	-6.54	119.43	122.70
1	A	403	C	C5-C6-N1	-6.54	117.73	121.00
1	A	1500	A	N9-C4-C5	6.54	108.42	105.80
1	A	620	C	C6-N1-C2	6.53	122.91	120.30
1	A	854	G	C6-C5-N7	-6.53	126.48	130.40
1	A	1249	C	N3-C4-C5	-6.53	119.29	121.90
1	A	1341	U	C2-N1-C1'	-6.53	109.86	117.70
1	A	372	C	C6-N1-C1'	-6.53	112.97	120.80
1	A	1058	G	N7-C8-N9	-6.53	109.84	113.10
1	A	971	G	C5-C6-N1	-6.52	108.24	111.50
1	A	32	A	N3-C4-N9	6.52	132.62	127.40
1	A	770	C	C2-N3-C4	-6.52	116.64	119.90
1	A	742	G	N3-C4-N9	-6.52	122.09	126.00
1	A	859	A	N9-C4-C5	-6.51	103.19	105.80
1	A	1060	C	C2-N1-C1'	6.51	125.97	118.80
1	A	745	C	N3-C4-C5	6.51	124.50	121.90
1	A	1502	A	C4-C5-N7	6.51	113.96	110.70
1	A	885	G	C5-C6-N1	-6.51	108.25	111.50
1	A	365	U	C6-N1-C1'	-6.51	112.09	121.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	151	A	C5-N7-C8	-6.51	100.65	103.90
1	A	651	C	N3-C2-O2	6.51	126.45	121.90
1	A	889	A	N1-C2-N3	6.50	132.55	129.30
1	A	918	A	C6-N1-C2	-6.50	114.70	118.60
1	A	698	G	C4-C5-C6	6.50	122.70	118.80
1	A	229	U	N1-C2-O2	-6.50	118.25	122.80
1	A	1084	G	C6-N1-C2	-6.49	121.20	125.10
1	A	1051	C	N3-C4-C5	-6.49	119.30	121.90
1	A	1390	U	C4-C5-C6	6.48	123.59	119.70
1	A	963	G	C5-C6-N1	-6.48	108.26	111.50
1	A	268	C	C6-N1-C2	6.48	122.89	120.30
1	A	1053	G	C5-N7-C8	6.47	107.54	104.30
1	A	534	U	N3-C2-O2	6.47	126.73	122.20
1	A	760	G	C4-N9-C1'	6.47	134.91	126.50
1	A	111	G	N3-C4-C5	6.46	131.83	128.60
1	A	774	G	N9-C4-C5	-6.46	102.81	105.40
1	A	13	U	N3-C4-O4	6.46	123.92	119.40
1	A	181	G	N3-C4-C5	-6.46	125.37	128.60
1	A	276	G	N1-C6-O6	-6.46	116.03	119.90
1	A	1341	U	N3-C4-O4	-6.46	114.88	119.40
1	A	725	G	C5-C6-N1	6.45	114.73	111.50
1	A	693	G	C5-C6-O6	-6.45	124.73	128.60
1	A	1301	U	N3-C4-C5	-6.45	110.73	114.60
1	A	597	G	N1-C2-N2	-6.44	110.40	116.20
1	A	108	G	N1-C6-O6	6.44	123.76	119.90
1	A	258	G	N1-C6-O6	6.44	123.76	119.90
1	A	644	G	C4-N9-C1'	6.43	134.87	126.50
1	A	77	G	N3-C4-N9	6.43	129.86	126.00
1	A	761	G	C2-N3-C4	-6.43	108.69	111.90
1	A	867	G	N9-C4-C5	-6.42	102.83	105.40
1	A	867	G	N1-C2-N3	6.42	127.75	123.90
1	A	654	G	N1-C2-N2	-6.42	110.42	116.20
1	A	798	G	N1-C2-N2	6.42	121.98	116.20
1	A	825	G	N7-C8-N9	-6.42	109.89	113.10
1	A	561	U	N3-C4-O4	6.42	123.89	119.40
1	A	789	U	C5-C6-N1	6.42	125.91	122.70
1	A	248	C	C2-N3-C4	-6.41	116.69	119.90
1	A	1350	A	C8-N9-C4	-6.41	103.23	105.80
1	A	204	U	C2-N1-C1'	6.41	125.39	117.70
1	A	522	C	N3-C4-N4	-6.41	113.51	118.00
1	A	15	G	N1-C6-O6	6.41	123.74	119.90
1	A	1199	U	C6-N1-C2	-6.40	117.16	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1390	U	C6-N1-C2	-6.40	117.16	121.00
1	A	92	C	C6-N1-C1'	-6.39	113.13	120.80
1	A	1433	A	N1-C2-N3	6.39	132.50	129.30
1	A	635	G	N9-C4-C5	-6.39	102.84	105.40
1	A	807	A	N7-C8-N9	-6.39	110.61	113.80
1	A	1092	A	C5-N7-C8	-6.39	100.71	103.90
1	A	868	C	N3-C4-N4	6.39	122.47	118.00
1	A	870	U	C5-C6-N1	-6.38	119.51	122.70
1	A	721	G	N1-C2-N2	-6.38	110.46	116.20
1	A	1183	A	N1-C6-N6	6.38	122.43	118.60
1	A	390	C	N3-C4-N4	6.38	122.47	118.00
1	A	1099	G	C4-C5-N7	-6.38	108.25	110.80
1	A	32	A	C4-C5-C6	6.38	120.19	117.00
1	A	90	U	C6-N1-C1'	6.38	130.13	121.20
1	A	679	C	N1-C2-O2	-6.38	115.07	118.90
1	A	297	G	C8-N9-C4	-6.38	103.85	106.40
1	A	866	C	N1-C2-N3	6.37	123.66	119.20
1	A	1340	A	C2-N3-C4	-6.37	107.42	110.60
1	A	123	C	N3-C4-C5	-6.37	119.35	121.90
1	A	928	G	C6-C5-N7	-6.37	126.58	130.40
1	A	9	G	C4-C5-N7	6.36	113.34	110.80
1	A	129	U	N1-C2-N3	6.36	118.72	114.90
1	A	618	C	C6-N1-C2	6.36	122.84	120.30
1	A	946	A	N9-C4-C5	6.36	108.34	105.80
1	A	1073	U	C6-N1-C2	6.36	124.82	121.00
1	A	1107	C	N3-C4-C5	-6.36	119.36	121.90
1	A	447	G	N9-C4-C5	-6.36	102.86	105.40
1	A	77	G	C4-C5-N7	6.36	113.34	110.80
1	A	524	G	C5-C6-N1	-6.36	108.32	111.50
1	A	789	U	C6-N1-C2	-6.35	117.19	121.00
1	A	902	G	C8-N9-C4	6.35	108.94	106.40
1	A	639	G	C5-C6-O6	-6.35	124.79	128.60
1	A	269	C	C4-C5-C6	6.34	120.57	117.40
1	A	703	G	C5-N7-C8	6.34	107.47	104.30
1	A	230	G	C4-N9-C1'	6.34	134.74	126.50
1	A	1237	C	C4-C5-C6	6.33	120.57	117.40
1	A	960	U	N1-C2-O2	6.33	127.23	122.80
1	A	28	G	C4-C5-N7	-6.33	108.27	110.80
1	A	671	G	C5-C6-N1	-6.33	108.34	111.50
1	A	839	U	N1-C2-O2	6.33	127.23	122.80
1	A	579	G	C5-N7-C8	-6.32	101.14	104.30
1	A	874	G	C4-C5-N7	6.32	113.33	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	194	LEU	CA-CB-CG	6.32	129.84	115.30
1	A	721	G	C5-C6-N1	-6.32	108.34	111.50
9	I	47	LEU	CA-CB-CG	-6.32	100.77	115.30
1	A	924	C	N3-C2-O2	6.32	126.32	121.90
1	A	407	G	C2-N3-C4	-6.31	108.75	111.90
1	A	962	C	C6-N1-C2	6.31	122.82	120.30
1	A	616	G	C5-C6-N1	-6.31	108.35	111.50
1	A	741	G	N3-C4-C5	6.31	131.75	128.60
1	A	154	C	C5-C4-N4	-6.30	115.79	120.20
1	A	830	G	N1-C6-O6	6.30	123.68	119.90
1	A	881	G	N3-C4-N9	6.30	129.78	126.00
1	A	1487	G	C8-N9-C4	-6.30	103.88	106.40
1	A	1497	G	N3-C4-N9	6.29	129.78	126.00
1	A	372	C	C6-N1-C2	6.29	122.82	120.30
1	A	428	G	C8-N9-C4	-6.29	103.88	106.40
1	A	91	C	N3-C4-N4	6.29	122.40	118.00
1	A	342	C	C6-N1-C2	-6.29	117.79	120.30
1	A	1279	A	N7-C8-N9	6.29	116.94	113.80
1	A	1205	U	C2-N1-C1'	6.28	125.24	117.70
1	A	597	G	C6-C5-N7	-6.28	126.63	130.40
1	A	1530	G	C5-C6-N1	-6.28	108.36	111.50
1	A	77	G	N9-C4-C5	-6.28	102.89	105.40
1	A	557	G	N9-C4-C5	6.28	107.91	105.40
1	A	810	C	C5-C4-N4	-6.28	115.81	120.20
1	A	1389	C	C6-N1-C2	6.28	122.81	120.30
1	A	1350	A	N7-C8-N9	6.27	116.94	113.80
1	A	250	A	C8-N9-C4	6.27	108.31	105.80
1	A	297	G	C4-N9-C1'	6.27	134.65	126.50
1	A	721	G	N3-C4-C5	-6.27	125.46	128.60
1	A	774	G	C4-C5-N7	6.27	113.31	110.80
1	A	1074	G	C2-N3-C4	-6.27	108.77	111.90
1	A	1362	C	C6-N1-C2	-6.27	117.79	120.30
1	A	91	C	C5-C4-N4	-6.26	115.81	120.20
1	A	691	G	N7-C8-N9	6.26	116.23	113.10
1	A	788	U	C2-N3-C4	6.26	130.76	127.00
1	A	927	G	N1-C6-O6	6.26	123.66	119.90
1	A	285	G	C5-C6-N1	-6.26	108.37	111.50
1	A	246	A	N1-C2-N3	-6.26	126.17	129.30
1	A	1342	C	N1-C2-O2	-6.26	115.15	118.90
1	A	125	U	N1-C2-N3	6.25	118.65	114.90
1	A	1531	A	N7-C8-N9	6.25	116.92	113.80
1	A	637	G	N1-C6-O6	6.25	123.65	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	92	C	C2-N1-C1'	6.24	125.67	118.80
1	A	795	C	C6-N1-C2	6.24	122.80	120.30
1	A	252	U	C5-C6-N1	-6.24	119.58	122.70
1	A	1327	C	C4-C5-C6	6.24	120.52	117.40
1	A	32	A	C5-C6-N6	-6.23	118.71	123.70
1	A	947	G	N9-C4-C5	-6.23	102.91	105.40
1	A	1068	G	N3-C4-C5	-6.23	125.49	128.60
1	A	1281	U	N1-C2-N3	6.23	118.64	114.90
1	A	981	U	C5-C6-N1	6.22	125.81	122.70
1	A	665	A	C5-N7-C8	-6.22	100.79	103.90
1	A	969	A	N1-C6-N6	6.22	122.33	118.60
1	A	1310	G	C4-N9-C1'	6.22	134.59	126.50
1	A	598	U	N1-C2-O2	-6.22	118.45	122.80
1	A	260	G	N1-C2-N3	6.22	127.63	123.90
1	A	928	G	C4-C5-N7	6.21	113.28	110.80
1	A	1329	A	C6-C5-N7	-6.21	127.95	132.30
1	A	162	A	C8-N9-C4	-6.21	103.32	105.80
1	A	1157	A	C5-C6-N6	6.21	128.67	123.70
1	A	1228	C	C6-N1-C1'	-6.21	113.35	120.80
1	A	1338	G	C4-C5-N7	-6.21	108.32	110.80
1	A	199	G	C2-N3-C4	-6.20	108.80	111.90
1	A	828	A	N1-C6-N6	6.20	122.32	118.60
1	A	1178	G	N9-C4-C5	6.20	107.88	105.40
1	A	1512	U	C4-C5-C6	6.19	123.42	119.70
1	A	201	C	C2-N1-C1'	6.19	125.61	118.80
1	A	1157	A	N1-C6-N6	-6.19	114.89	118.60
1	A	232	G	C5-N7-C8	-6.18	101.21	104.30
1	A	400	C	N3-C2-O2	-6.18	117.57	121.90
1	A	7	G	C8-N9-C1'	-6.18	118.97	127.00
1	A	242	C	C5-C6-N1	-6.18	117.91	121.00
1	A	246	A	N7-C8-N9	-6.18	110.71	113.80
1	A	50	A	C4-C5-C6	-6.18	113.91	117.00
1	A	640	A	N1-C2-N3	6.17	132.39	129.30
1	A	884	U	N1-C2-O2	6.17	127.12	122.80
1	A	558	G	C4-C5-N7	6.16	113.27	110.80
1	A	887	G	N1-C2-N3	6.16	127.60	123.90
1	A	1066	C	C2-N1-C1'	6.16	125.58	118.80
1	A	859	A	C8-N9-C4	6.16	108.27	105.80
1	A	862	C	N3-C4-C5	6.16	124.36	121.90
1	A	673	G	C5-C6-O6	-6.16	124.90	128.60
1	A	1209	C	C6-N1-C2	-6.16	117.84	120.30
1	A	912	C	C4-C5-C6	-6.15	114.32	117.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	190(E)	U	C2-N3-C4	-6.15	123.31	127.00
1	A	1064	G	N3-C2-N2	-6.15	115.59	119.90
1	A	1231	G	N3-C4-N9	6.15	129.69	126.00
24	a	39	G	C8-N9-C4	6.15	108.86	106.40
1	A	284	G	C6-C5-N7	-6.15	126.71	130.40
1	A	1235	U	N1-C2-O2	-6.15	118.50	122.80
1	A	898	G	N1-C2-N3	6.14	127.59	123.90
1	A	848	C	C5-C6-N1	6.14	124.07	121.00
1	A	1442	G	N3-C4-C5	-6.14	125.53	128.60
1	A	285	G	N1-C6-O6	6.14	123.58	119.90
1	A	897	C	N3-C4-C5	6.13	124.35	121.90
1	A	1103	C	C5-C6-N1	-6.13	117.93	121.00
1	A	1487	G	N9-C4-C5	6.13	107.85	105.40
1	A	109	A	C8-N9-C4	-6.13	103.35	105.80
1	A	181	G	C4-C5-C6	6.13	122.48	118.80
1	A	755	G	N1-C6-O6	6.13	123.58	119.90
1	A	900	A	C2-N3-C4	-6.13	107.54	110.60
1	A	257	G	C8-N9-C4	6.12	108.85	106.40
1	A	1493[A]	A	C3'-C2'-C1'	-6.12	96.60	101.50
1	A	1493[B]	A	C3'-C2'-C1'	-6.12	96.60	101.50
1	A	265	G	N9-C4-C5	-6.12	102.95	105.40
1	A	926	G	N3-C4-N9	6.12	129.67	126.00
1	A	970	C	N3-C2-O2	-6.12	117.62	121.90
1	A	1391	U	C5-C6-N1	-6.12	119.64	122.70
1	A	1500	A	C6-N1-C2	-6.12	114.93	118.60
1	A	524	G	N1-C6-O6	6.11	123.57	119.90
1	A	35	G	N1-C6-O6	6.11	123.56	119.90
1	A	1253	G	C6-C5-N7	-6.11	126.74	130.40
1	A	1300	G	N9-C4-C5	6.10	107.84	105.40
1	A	1487	G	C6-N1-C2	-6.10	121.44	125.10
1	A	540	G	N1-C6-O6	6.10	123.56	119.90
1	A	230	G	N1-C2-N2	-6.10	110.71	116.20
1	A	373	A	C5-C6-N6	6.10	128.58	123.70
1	A	1058	G	C6-C5-N7	6.10	134.06	130.40
1	A	1483	A	C5-N7-C8	6.09	106.95	103.90
1	A	782	A	N1-C6-N6	-6.09	114.94	118.60
1	A	130	A	C5-N7-C8	-6.09	100.86	103.90
1	A	976	G	C2-N3-C4	-6.09	108.86	111.90
1	A	910	C	C2-N3-C4	-6.08	116.86	119.90
1	A	1531	A	C5-C6-N6	-6.08	118.83	123.70
1	A	144	G	C6-C5-N7	-6.08	126.75	130.40
1	A	335	C	C5-C6-N1	-6.08	117.96	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	277	C	N3-C4-C5	6.07	124.33	121.90
1	A	768	A	N7-C8-N9	-6.07	110.77	113.80
8	H	38	ILE	CB-CA-C	-6.07	99.46	111.60
1	A	115	G	C5-C6-N1	6.07	114.53	111.50
1	A	654	G	N1-C2-N3	6.07	127.54	123.90
1	A	174	C	C5-C4-N4	-6.06	115.95	120.20
1	A	733	A	C2-N3-C4	-6.06	107.57	110.60
1	A	833	U	N3-C2-O2	-6.05	117.96	122.20
1	A	812	C	C6-N1-C2	-6.05	117.88	120.30
1	A	1488	G	C5-N7-C8	6.05	107.32	104.30
1	A	127	G	N3-C4-C5	6.04	131.62	128.60
1	A	741	G	C4-C5-N7	-6.04	108.38	110.80
1	A	631	G	C4-N9-C1'	6.04	134.35	126.50
1	A	586	C	N3-C4-C5	6.03	124.31	121.90
1	A	1502	A	C6-C5-N7	-6.03	128.08	132.30
1	A	1237	C	N3-C4-C5	-6.03	119.49	121.90
1	A	742	G	N1-C2-N2	6.03	121.63	116.20
1	A	1079	G	N9-C4-C5	6.03	107.81	105.40
1	A	263	A	N1-C6-N6	-6.03	114.98	118.60
1	A	78	G	N1-C6-O6	6.03	123.52	119.90
1	A	1029	C	C6-N1-C2	-6.03	117.89	120.30
8	H	12	ARG	NE-CZ-NH1	-6.03	117.29	120.30
1	A	300	A	C4-C5-C6	6.02	120.01	117.00
1	A	868	C	N3-C2-O2	6.02	126.12	121.90
1	A	260	G	C4-C5-C6	6.02	122.41	118.80
1	A	363	A	C2-N3-C4	-6.02	107.59	110.60
1	A	1487	G	C4-N9-C1'	6.02	134.32	126.50
1	A	572	A	C6-N1-C2	-6.01	114.99	118.60
1	A	1505	G	N3-C2-N2	-6.01	115.69	119.90
1	A	1399	C	C6-N1-C2	-6.00	117.90	120.30
1	A	447	G	C6-C5-N7	-6.00	126.80	130.40
1	A	570	G	N9-C4-C5	6.00	107.80	105.40
1	A	1497	G	C8-N9-C1'	-6.00	119.20	127.00
1	A	852	G	C8-N9-C4	6.00	108.80	106.40
1	A	1337	G	N1-C6-O6	5.99	123.50	119.90
1	A	854	G	C2-N3-C4	-5.99	108.91	111.90
1	A	873	A	N9-C4-C5	5.99	108.19	105.80
1	A	1084	G	C5-C6-O6	5.98	132.19	128.60
1	A	79	G	N7-C8-N9	5.98	116.09	113.10
1	A	145	G	N1-C6-O6	5.97	123.48	119.90
1	A	21	G	N3-C4-N9	5.97	129.58	126.00
1	A	607	A	C5-C6-N1	-5.97	114.71	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	893	C	C2-N3-C4	5.97	122.89	119.90
1	A	896	C	C6-N1-C2	-5.97	117.91	120.30
1	A	1491	G	N3-C2-N2	-5.97	115.72	119.90
1	A	374	A	C8-N9-C4	5.97	108.19	105.80
1	A	1074	G	C4-C5-C6	5.97	122.38	118.80
1	A	1530	G	N3-C2-N2	-5.97	115.72	119.90
1	A	1325	C	C6-N1-C2	-5.97	117.91	120.30
1	A	1353	G	C2-N3-C4	5.96	114.88	111.90
1	A	117	G	C4-C5-N7	5.96	113.19	110.80
1	A	944	G	N1-C6-O6	-5.96	116.32	119.90
1	A	259	G	C4-C5-C6	5.96	122.38	118.80
1	A	786	G	N1-C6-O6	5.96	123.47	119.90
1	A	1531	A	C8-N9-C4	-5.96	103.42	105.80
1	A	768	A	N1-C6-N6	5.96	122.17	118.60
1	A	774	G	C5-C6-O6	-5.95	125.03	128.60
1	A	856	C	C4-C5-C6	5.95	120.38	117.40
1	A	1094	G	C6-C5-N7	-5.95	126.83	130.40
1	A	349	A	N1-C6-N6	-5.95	115.03	118.60
1	A	651	C	N3-C4-C5	5.95	124.28	121.90
1	A	712	A	N1-C2-N3	5.95	132.27	129.30
1	A	767	A	N9-C4-C5	5.95	108.18	105.80
1	A	946	A	C5-C6-N1	5.95	120.67	117.70
1	A	1531	A	C5-N7-C8	-5.95	100.93	103.90
1	A	38	G	C8-N9-C1'	5.94	134.72	127.00
1	A	170	U	N1-C2-O2	-5.94	118.64	122.80
1	A	1089	G	C8-N9-C4	-5.94	104.03	106.40
1	A	1439	C	N3-C4-C5	-5.94	119.53	121.90
1	A	1307	U	N1-C2-O2	5.94	126.95	122.80
17	Q	31	LEU	CA-CB-CG	-5.94	101.65	115.30
1	A	15	G	N9-C4-C5	-5.93	103.03	105.40
1	A	250	A	N1-C6-N6	5.93	122.16	118.60
1	A	654	G	C2-N3-C4	-5.93	108.93	111.90
1	A	853	G	N3-C4-N9	5.93	129.56	126.00
1	A	807	A	C8-N9-C4	5.93	108.17	105.80
8	H	135	CYS	CA-CB-SG	-5.93	103.32	114.00
1	A	1234	C	N3-C4-C5	5.93	124.27	121.90
1	A	265	G	C6-C5-N7	-5.93	126.84	130.40
1	A	898	G	C2-N3-C4	-5.93	108.94	111.90
1	A	190(K)	G	C8-N9-C4	5.92	108.77	106.40
1	A	542	G	N1-C6-O6	-5.92	116.35	119.90
1	A	774	G	C6-C5-N7	-5.92	126.85	130.40
1	A	791	G	C5-C6-N1	-5.92	108.54	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	718	G	C5-C6-O6	-5.92	125.05	128.60
1	A	920	U	N1-C2-N3	5.92	118.45	114.90
1	A	618	C	N3-C4-N4	-5.92	113.86	118.00
1	A	674	G	C2-N3-C4	-5.92	108.94	111.90
1	A	1529	G	N3-C2-N2	-5.91	115.76	119.90
1	A	711	G	C2-N3-C4	-5.91	108.94	111.90
1	A	1084	G	N1-C2-N3	5.91	127.45	123.90
1	A	136	C	C6-N1-C2	-5.91	117.94	120.30
1	A	931	C	C5-C6-N1	-5.91	118.05	121.00
1	A	1335	C	N1-C2-N3	-5.91	115.06	119.20
1	A	1507	A	N1-C2-N3	5.91	132.25	129.30
1	A	38	G	C4-N9-C1'	-5.91	118.82	126.50
1	A	144	G	N3-C2-N2	-5.91	115.77	119.90
1	A	553	A	C8-N9-C4	5.91	108.16	105.80
1	A	1300	G	C4-C5-N7	-5.91	108.44	110.80
1	A	328	C	P-O3'-C3'	5.90	126.78	119.70
1	A	317	G	C2-N3-C4	-5.90	108.95	111.90
1	A	1529	G	N1-C2-N3	5.90	127.44	123.90
1	A	1530	G	N1-C2-N2	5.90	121.51	116.20
24	a	37	A	C2-N3-C4	-5.90	107.65	110.60
2	B	7	VAL	N-CA-C	5.90	126.93	111.00
1	A	447	G	C4-N9-C1'	5.90	134.17	126.50
1	A	610	G	N1-C6-O6	-5.90	116.36	119.90
1	A	799	G	C4-C5-N7	5.90	113.16	110.80
1	A	1301	U	N3-C4-O4	5.90	123.53	119.40
1	A	924	C	N3-C4-C5	-5.89	119.54	121.90
1	A	104	G	C5-C6-O6	-5.89	125.06	128.60
1	A	854	G	C4-N9-C1'	5.89	134.15	126.50
1	A	1214	C	C2-N1-C1'	5.88	125.27	118.80
24	a	37	A	C5-C6-N1	-5.88	114.76	117.70
1	A	1099	G	C8-N9-C4	-5.88	104.05	106.40
8	H	136	GLU	N-CA-C	-5.88	95.13	111.00
1	A	284	G	C2-N3-C4	-5.88	108.96	111.90
1	A	686	U	C5-C6-N1	-5.88	119.76	122.70
1	A	1534	C	N1-C2-O2	5.88	122.42	118.90
1	A	1530	G	C4-N9-C1'	-5.87	118.86	126.50
1	A	650	G	N1-C6-O6	5.87	123.42	119.90
1	A	963	G	C6-C5-N7	-5.87	126.88	130.40
1	A	1253	G	N1-C6-O6	5.87	123.42	119.90
1	A	1467	G	C8-N9-C4	-5.87	104.05	106.40
1	A	90	U	N3-C2-O2	-5.87	118.09	122.20
1	A	1502	A	N3-C4-C5	5.87	130.91	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	122	G	N1-C6-O6	5.86	123.42	119.90
1	A	400	C	C6-N1-C2	5.86	122.65	120.30
1	A	53	A	C6-N1-C2	-5.86	115.08	118.60
1	A	449	C	C2-N1-C1'	5.86	125.25	118.80
1	A	599	C	C2-N3-C4	-5.86	116.97	119.90
1	A	875	C	C2-N3-C4	-5.86	116.97	119.90
1	A	552	U	N3-C4-O4	-5.86	115.30	119.40
1	A	880	C	C6-N1-C2	5.85	122.64	120.30
1	A	1062	U	C5-C4-O4	5.85	129.41	125.90
1	A	1452	C	C6-N1-C2	5.85	122.64	120.30
1	A	658	G	N1-C2-N3	5.85	127.41	123.90
1	A	1310	G	N1-C2-N2	-5.85	110.93	116.20
1	A	1064	G	C6-N1-C2	-5.85	121.59	125.10
1	A	251	G	N3-C4-C5	-5.85	125.68	128.60
1	A	1414	U	C4-C5-C6	5.85	123.21	119.70
1	A	607	A	C6-N1-C2	5.84	122.11	118.60
1	A	1108	G	C4-N9-C1'	5.84	134.10	126.50
1	A	1527	C	N3-C4-N4	5.84	122.09	118.00
1	A	579	G	C6-C5-N7	-5.84	126.89	130.40
1	A	975	A	C6-N1-C2	5.84	122.10	118.60
1	A	796	C	C4-C5-C6	5.84	120.32	117.40
1	A	481	G	C4-N9-C1'	5.84	134.09	126.50
1	A	741	G	C6-C5-N7	5.84	133.90	130.40
1	A	1335	C	C5-C4-N4	-5.84	116.11	120.20
1	A	1483	A	C2-N3-C4	5.84	113.52	110.60
20	T	13	LEU	CB-CA-C	-5.84	99.11	110.20
1	A	1438	G	C8-N9-C4	5.83	108.73	106.40
1	A	1523	G	N3-C2-N2	-5.83	115.82	119.90
1	A	1487	G	C4-C5-C6	5.83	122.30	118.80
1	A	1190	G	C4-C5-C6	5.82	122.30	118.80
1	A	864	A	C4-C5-N7	-5.82	107.79	110.70
1	A	656	C	N3-C4-C5	5.82	124.23	121.90
1	A	852	G	N9-C4-C5	-5.82	103.07	105.40
1	A	190(G)	G	C4-C5-C6	5.82	122.29	118.80
1	A	679	C	C5-C6-N1	-5.82	118.09	121.00
1	A	1249	C	C5-C6-N1	5.82	123.91	121.00
1	A	1482	G	C8-N9-C1'	-5.82	119.44	127.00
1	A	1510	U	N1-C2-O2	5.82	126.87	122.80
1	A	129	U	C5-C4-O4	5.82	129.39	125.90
1	A	865	A	C5-C6-N1	5.82	120.61	117.70
1	A	344	A	N7-C8-N9	5.81	116.71	113.80
1	A	693	G	C6-C5-N7	-5.81	126.91	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	127	G	N9-C4-C5	-5.81	103.08	105.40
1	A	854	G	N1-C2-N3	5.81	127.39	123.90
1	A	297	G	C5-C6-O6	5.80	132.08	128.60
1	A	707	C	C2-N1-C1'	-5.80	112.42	118.80
1	A	38	G	N3-C4-C5	5.80	131.50	128.60
1	A	235	C	C5-C6-N1	-5.80	118.10	121.00
1	A	242	C	C6-N1-C2	5.80	122.62	120.30
1	A	259	G	C5-C6-N1	-5.80	108.60	111.50
1	A	565	U	C6-N1-C2	5.80	124.48	121.00
1	A	676	A	N7-C8-N9	-5.80	110.90	113.80
1	A	925	G	N3-C4-C5	-5.80	125.70	128.60
1	A	860	A	N1-C2-N3	5.79	132.20	129.30
1	A	1200	C	N3-C4-N4	5.79	122.06	118.00
1	A	142	G	N3-C4-C5	-5.79	125.70	128.60
1	A	251	G	C8-N9-C1'	-5.79	119.47	127.00
1	A	1303	C	N3-C4-N4	-5.79	113.95	118.00
1	A	925	G	N3-C4-N9	5.79	129.47	126.00
1	A	519	C	C6-N1-C2	5.78	122.61	120.30
1	A	944	G	N9-C4-C5	5.78	107.71	105.40
1	A	1281	U	C6-N1-C1'	5.78	129.29	121.20
1	A	597	G	C8-N9-C1'	-5.78	119.49	127.00
1	A	760	G	C4-C5-C6	5.78	122.27	118.80
1	A	258	G	C2-N3-C4	-5.78	109.01	111.90
1	A	332	G	C4-C5-N7	5.78	113.11	110.80
1	A	566	G	N3-C4-N9	5.78	129.47	126.00
1	A	552	U	N1-C2-N3	5.77	118.36	114.90
1	A	644	G	N7-C8-N9	5.77	115.99	113.10
1	A	831	U	C5-C4-O4	5.77	129.36	125.90
1	A	629	G	N3-C4-C5	-5.77	125.72	128.60
1	A	716	A	C5-C6-N1	5.77	120.58	117.70
1	A	779	C	C2-N3-C4	-5.77	117.02	119.90
1	A	945	G	C4-C5-C6	-5.77	115.34	118.80
1	A	1153	C	C6-N1-C2	5.77	122.61	120.30
1	A	910	C	C5-C6-N1	-5.76	118.12	121.00
1	A	180	U	C5-C4-O4	-5.76	122.44	125.90
1	A	259	G	C8-N9-C4	-5.76	104.10	106.40
1	A	68	G	N7-C8-N9	-5.76	110.22	113.10
1	A	752	G	N1-C6-O6	5.76	123.35	119.90
1	A	1231	G	C4-N9-C1'	5.75	133.98	126.50
1	A	73	C	C2-N3-C4	5.75	122.78	119.90
1	A	618	C	C6-N1-C1'	5.75	127.70	120.80
1	A	414	A	N1-C2-N3	5.75	132.17	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	799	G	C5-C6-O6	-5.74	125.15	128.60
1	A	1227	A	N3-C4-C5	5.74	130.82	126.80
1	A	15	G	C8-N9-C4	5.74	108.70	106.40
1	A	1129	C	C5-C6-N1	5.74	123.87	121.00
1	A	130	A	N1-C6-N6	5.74	122.04	118.60
1	A	181	G	C8-N9-C1'	-5.74	119.54	127.00
1	A	292	G	N1-C6-O6	5.74	123.34	119.90
1	A	725	G	C5-C6-O6	-5.73	125.16	128.60
1	A	251	G	N3-C2-N2	5.73	123.91	119.90
1	A	1373	G	C8-N9-C4	-5.73	104.11	106.40
1	A	265	G	C8-N9-C1'	-5.73	119.55	127.00
1	A	637	G	C8-N9-C1'	-5.73	119.55	127.00
1	A	1055	A	C2-N3-C4	5.73	113.46	110.60
1	A	50	A	N7-C8-N9	-5.73	110.94	113.80
1	A	911	U	C2-N1-C1'	-5.73	110.83	117.70
1	A	635	G	N1-C2-N2	-5.72	111.05	116.20
1	A	875	C	C5-C6-N1	-5.72	118.14	121.00
1	A	905	U	C4-C5-C6	5.72	123.13	119.70
1	A	154	C	C6-N1-C1'	-5.72	113.94	120.80
1	A	558	G	C6-C5-N7	-5.72	126.97	130.40
1	A	693	G	N9-C4-C5	-5.72	103.11	105.40
1	A	745	C	C2-N3-C4	-5.72	117.04	119.90
1	A	326	G	N3-C4-N9	-5.72	122.57	126.00
1	A	21	G	C8-N9-C1'	-5.71	119.57	127.00
1	A	125	U	N3-C2-O2	-5.71	118.20	122.20
1	A	32	A	C6-C5-N7	-5.71	128.30	132.30
1	A	373	A	N1-C6-N6	-5.71	115.17	118.60
1	A	674	G	N1-C6-O6	5.71	123.32	119.90
1	A	698	G	C8-N9-C4	-5.71	104.12	106.40
1	A	1221	G	C5-C6-N1	-5.71	108.65	111.50
1	A	1531	A	C4-C5-N7	5.71	113.55	110.70
1	A	711	G	C5-N7-C8	-5.70	101.45	104.30
1	A	540	G	C5-C6-O6	-5.70	125.18	128.60
1	A	127	G	C5-C6-O6	-5.70	125.18	128.60
1	A	704	A	N7-C8-N9	5.70	116.65	113.80
1	A	963	G	N7-C8-N9	5.70	115.95	113.10
1	A	631	G	N7-C8-N9	5.70	115.95	113.10
1	A	779	C	C6-N1-C2	5.70	122.58	120.30
1	A	407	G	N3-C4-C5	5.70	131.45	128.60
1	A	1134	G	C8-N9-C4	-5.70	104.12	106.40
1	A	144	G	N3-C4-C5	5.70	131.45	128.60
1	A	232	G	C8-N9-C1'	-5.70	119.59	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	677	U	C6-N1-C2	-5.69	117.58	121.00
1	A	920	U	C6-N1-C2	-5.69	117.58	121.00
1	A	240	C	C6-N1-C2	5.69	122.58	120.30
1	A	279	A	C2-N3-C4	-5.69	107.75	110.60
1	A	1415	G	C8-N9-C4	5.69	108.68	106.40
1	A	1062	U	C6-N1-C2	-5.69	117.59	121.00
1	A	673	G	C4-C5-N7	5.68	113.07	110.80
1	A	856	C	N1-C2-N3	5.68	123.18	119.20
1	A	440	A	N1-C2-N3	5.68	132.14	129.30
1	A	1092	A	C8-N9-C1'	-5.68	117.48	127.70
1	A	91	C	C6-N1-C1'	-5.67	113.99	120.80
1	A	1084	G	N9-C4-C5	5.67	107.67	105.40
1	A	1329	A	N9-C4-C5	-5.67	103.53	105.80
1	A	1504	G	N3-C4-N9	5.67	129.40	126.00
1	A	753	A	C4-C5-N7	-5.67	107.86	110.70
1	A	858	G	C4-C5-N7	-5.67	108.53	110.80
1	A	1364	U	C6-N1-C2	5.67	124.40	121.00
1	A	1310	G	C6-C5-N7	-5.66	127.00	130.40
1	A	1381	U	C2-N1-C1'	5.66	124.50	117.70
1	A	204	U	C5-C6-N1	5.66	125.53	122.70
1	A	121	C	C6-N1-C2	5.66	122.56	120.30
1	A	1074	G	N1-C6-O6	5.66	123.30	119.90
15	O	77	ARG	NE-CZ-NH2	5.66	123.13	120.30
1	A	1388	C	N1-C2-O2	-5.66	115.51	118.90
1	A	597	G	C4-N9-C1'	5.66	133.85	126.50
1	A	1074	G	C6-C5-N7	-5.66	127.01	130.40
1	A	1524	C	N1-C2-N3	5.66	123.16	119.20
1	A	1058	G	C4-C5-N7	-5.65	108.54	110.80
1	A	637	G	C6-C5-N7	-5.65	127.01	130.40
1	A	971	G	C2-N3-C4	-5.65	109.08	111.90
1	A	1143	G	C4-C5-N7	5.65	113.06	110.80
1	A	830	G	N3-C2-N2	-5.65	115.95	119.90
1	A	21	G	N9-C4-C5	-5.65	103.14	105.40
1	A	330	C	N1-C2-O2	-5.65	115.51	118.90
1	A	1394	A	C5-C6-N1	5.64	120.52	117.70
1	A	1433	A	C6-N1-C2	-5.64	115.21	118.60
5	E	63	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	A	1442	G	N3-C4-N9	5.64	129.38	126.00
1	A	1505	G	C4-C5-N7	-5.64	108.55	110.80
1	A	902	G	N7-C8-N9	-5.64	110.28	113.10
1	A	1120	G	N3-C4-C5	-5.64	125.78	128.60
1	A	1286	A	C8-N9-C4	-5.63	103.55	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1438	G	C5-C6-O6	-5.63	125.22	128.60
1	A	111	G	C8-N9-C1'	5.63	134.32	127.00
1	A	393	A	C2-N3-C4	-5.62	107.79	110.60
1	A	1190	G	N3-C4-C5	-5.62	125.79	128.60
1	A	125	U	C4-C5-C6	5.62	123.07	119.70
1	A	435	C	N3-C4-C5	-5.62	119.65	121.90
1	A	933	G	C6-C5-N7	-5.62	127.03	130.40
1	A	1301	U	N1-C2-N3	5.62	118.27	114.90
1	A	1527	C	C2-N1-C1'	5.62	124.98	118.80
1	A	383	A	C8-N9-C4	-5.62	103.55	105.80
1	A	497	A	N1-C6-N6	-5.62	115.23	118.60
1	A	656	C	C5-C4-N4	-5.62	116.27	120.20
1	A	216	G	N1-C6-O6	-5.62	116.53	119.90
1	A	1077	G	C4-C5-C6	5.61	122.17	118.80
1	A	162	A	N1-C6-N6	-5.61	115.23	118.60
1	A	816	A	N7-C8-N9	-5.61	111.00	113.80
1	A	1531	A	C5-C6-N1	5.61	120.50	117.70
1	A	270	A	N1-C6-N6	5.61	121.96	118.60
1	A	190(G)	G	C6-C5-N7	-5.60	127.04	130.40
1	A	787	A	N7-C8-N9	5.60	116.60	113.80
1	A	588	G	C8-N9-C4	5.60	108.64	106.40
1	A	816	A	N3-C4-N9	-5.60	122.92	127.40
1	A	559	A	N7-C8-N9	5.60	116.60	113.80
1	A	1220	G	N1-C6-O6	5.60	123.26	119.90
1	A	1392	G	C4-C5-N7	5.60	113.04	110.80
1	A	21	G	N7-C8-N9	-5.59	110.30	113.10
1	A	120	A	N7-C8-N9	-5.59	111.00	113.80
1	A	1392	G	C4-N9-C1'	5.59	133.77	126.50
1	A	1343	G	C4-C5-N7	5.59	113.04	110.80
1	A	204	U	C6-N1-C1'	-5.59	113.38	121.20
24	a	39	G	N3-C4-C5	5.59	131.40	128.60
1	A	38	G	C5-C6-N1	-5.59	108.71	111.50
1	A	831	U	N3-C2-O2	-5.59	118.29	122.20
1	A	122	G	C2-N3-C4	-5.59	109.11	111.90
1	A	497	A	C4-C5-N7	-5.59	107.91	110.70
1	A	675	A	C2-N3-C4	-5.59	107.81	110.60
1	A	767	A	N1-C6-N6	-5.58	115.25	118.60
1	A	113	G	C6-C5-N7	-5.58	127.05	130.40
1	A	146	G	C5-C6-O6	-5.58	125.25	128.60
1	A	741	G	C8-N9-C1'	5.58	134.26	127.00
1	A	1186	G	N1-C6-O6	5.58	123.25	119.90
1	A	634	C	C5-C4-N4	5.58	124.11	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	297	G	C4-C5-C6	5.58	122.15	118.80
1	A	190(B)	C	C6-N1-C2	-5.58	118.07	120.30
17	Q	99	SER	N-CA-C	5.58	126.06	111.00
1	A	1075	C	C6-N1-C2	5.57	122.53	120.30
1	A	761	G	C6-C5-N7	-5.57	127.06	130.40
1	A	644	G	N3-C4-N9	5.57	129.34	126.00
1	A	696	A	N1-C6-N6	5.57	121.94	118.60
1	A	1112	C	N3-C2-O2	-5.57	118.00	121.90
1	A	79	G	C8-N9-C4	-5.56	104.17	106.40
1	A	265	G	N1-C2-N3	5.56	127.24	123.90
1	A	1253	G	C8-N9-C4	-5.56	104.18	106.40
1	A	332	G	N3-C2-N2	-5.56	116.01	119.90
1	A	373	A	N1-C2-N3	5.56	132.08	129.30
1	A	1425	U	C5-C4-O4	5.56	129.23	125.90
1	A	252	U	C4-C5-C6	5.55	123.03	119.70
1	A	1068	G	C6-C5-N7	-5.55	127.07	130.40
1	A	863	U	N1-C2-O2	-5.55	118.92	122.80
1	A	931	C	C2-N3-C4	-5.55	117.12	119.90
1	A	201	C	N1-C2-O2	5.55	122.23	118.90
1	A	52	G	N1-C2-N2	-5.55	111.21	116.20
1	A	55	A	C6-N1-C2	-5.55	115.27	118.60
1	A	580	U	C4-C5-C6	5.55	123.03	119.70
1	A	1500	A	C8-N9-C4	-5.54	103.58	105.80
1	A	389	A	C4-C5-C6	5.54	119.77	117.00
1	A	577	G	C8-N9-C4	5.54	108.62	106.40
1	A	811	C	C6-N1-C1'	-5.54	114.15	120.80
1	A	881	G	N7-C8-N9	-5.54	110.33	113.10
20	T	13	LEU	CB-CG-CD1	5.54	120.42	111.00
1	A	1415	G	C8-N9-C1'	-5.54	119.80	127.00
1	A	747	C	N1-C2-O2	-5.54	115.58	118.90
1	A	1322	C	C6-N1-C2	-5.54	118.08	120.30
1	A	9	G	N9-C4-C5	-5.54	103.19	105.40
1	A	422	C	N1-C2-N3	-5.54	115.32	119.20
1	A	1322	C	C6-N1-C1'	-5.54	114.16	120.80
1	A	232	G	N3-C4-N9	5.54	129.32	126.00
1	A	893	C	N1-C2-N3	-5.54	115.33	119.20
1	A	190(B)	C	C5-C6-N1	5.53	123.77	121.00
1	A	650	G	N7-C8-N9	-5.53	110.33	113.10
1	A	811	C	C5-C4-N4	-5.53	116.33	120.20
1	A	1293	G	N3-C4-N9	-5.53	122.68	126.00
1	A	924	C	C2-N3-C4	5.53	122.67	119.90
1	A	1529	G	C4-N9-C1'	5.53	133.69	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	451	A	N1-C2-N3	5.53	132.06	129.30
1	A	926	G	C4-C5-N7	-5.53	108.59	110.80
1	A	829	G	N9-C4-C5	-5.53	103.19	105.40
1	A	1157	A	N9-C4-C5	5.53	108.01	105.80
1	A	27	G	N1-C6-O6	5.53	123.22	119.90
1	A	135	C	C2-N1-C1'	-5.53	112.72	118.80
1	A	889	A	C8-N9-C4	-5.53	103.59	105.80
1	A	1394	A	N1-C6-N6	5.53	121.92	118.60
1	A	1084	G	N3-C4-N9	5.52	129.31	126.00
1	A	628	G	C4-N9-C1'	5.52	133.68	126.50
1	A	283	C	N3-C4-N4	5.52	121.86	118.00
1	A	357	G	C5-C6-O6	5.52	131.91	128.60
1	A	650	G	C2-N3-C4	-5.52	109.14	111.90
1	A	711	G	C8-N9-C4	-5.52	104.19	106.40
1	A	864	A	C8-N9-C4	-5.52	103.59	105.80
1	A	867	G	C5-C6-N1	-5.51	108.74	111.50
1	A	245	C	C5-C4-N4	-5.51	116.34	120.20
1	A	761	G	N1-C2-N3	5.51	127.21	123.90
1	A	962	C	N3-C4-C5	5.51	124.10	121.90
1	A	969	A	C6-C5-N7	-5.51	128.44	132.30
1	A	281	G	C4-C5-N7	5.51	113.00	110.80
1	A	778	G	N1-C2-N3	-5.51	120.60	123.90
1	A	1249	C	N3-C4-N4	5.51	121.85	118.00
1	A	142	G	C5-C6-N1	5.50	114.25	111.50
1	A	767	A	C5-C6-N6	5.50	128.10	123.70
1	A	1280	A	N9-C4-C5	5.50	108.00	105.80
1	A	117	G	N3-C4-N9	5.50	129.30	126.00
16	P	58	TYR	CB-CA-C	-5.50	99.40	110.40
1	A	145	G	C5-C6-N1	-5.50	108.75	111.50
1	A	973	G	N7-C8-N9	-5.50	110.35	113.10
1	A	264	U	C5-C4-O4	5.50	129.20	125.90
1	A	1392	G	C8-N9-C1'	-5.49	119.86	127.00
1	A	1140	C	C6-N1-C2	-5.49	118.10	120.30
1	A	107	G	N1-C6-O6	5.49	123.19	119.90
1	A	583	A	C8-N9-C4	5.49	108.00	105.80
1	A	583	A	C2-N3-C4	-5.49	107.85	110.60
1	A	175	C	C5-C6-N1	-5.49	118.26	121.00
1	A	1083	U	C6-N1-C2	5.49	124.29	121.00
1	A	372	C	N3-C4-N4	5.49	121.84	118.00
1	A	1322	C	C5-C6-N1	5.49	123.74	121.00
1	A	976	G	N3-C4-N9	-5.49	122.71	126.00
1	A	1417	G	N3-C4-C5	-5.49	125.86	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	675	A	C5-C6-N6	5.48	128.09	123.70
1	A	77	G	C5-C6-O6	-5.48	125.31	128.60
1	A	279	A	N1-C2-N3	5.48	132.04	129.30
1	A	301	G	C4-N9-C1'	5.48	133.62	126.50
1	A	20	U	C4-C5-C6	5.48	122.99	119.70
1	A	1373	G	C4-C5-N7	-5.48	108.61	110.80
1	A	1083	U	N3-C4-O4	5.47	123.23	119.40
1	A	73	C	N3-C2-O2	5.47	125.73	121.90
1	A	1235	U	C6-N1-C2	-5.47	117.72	121.00
1	A	1374	A	C8-N9-C4	-5.47	103.61	105.80
1	A	570	G	C6-N1-C2	-5.47	121.82	125.10
1	A	686	U	C4-C5-C6	5.47	122.98	119.70
1	A	260	G	C2-N3-C4	-5.47	109.17	111.90
1	A	678	U	C5-C4-O4	-5.47	122.62	125.90
1	A	132	C	C5-C6-N1	-5.46	118.27	121.00
1	A	1199	U	N1-C2-N3	5.46	118.18	114.90
1	A	300	A	C8-N9-C4	-5.46	103.61	105.80
1	A	745	C	C5-C6-N1	-5.46	118.27	121.00
1	A	816	A	C2-N3-C4	-5.46	107.87	110.60
1	A	860	A	C4-C5-C6	5.46	119.73	117.00
1	A	335	C	C6-N1-C2	5.46	122.48	120.30
1	A	734	G	N7-C8-N9	5.46	115.83	113.10
1	A	59	A	C5-C6-N1	5.46	120.43	117.70
1	A	419	C	C6-N1-C2	5.45	122.48	120.30
1	A	1368	G	N3-C4-C5	-5.45	125.87	128.60
1	A	174	C	C2-N1-C1'	5.45	124.80	118.80
1	A	180	U	C6-N1-C1'	-5.45	113.57	121.20
1	A	366	C	C6-N1-C2	-5.45	118.12	120.30
1	A	853	G	C4-N9-C1'	5.45	133.59	126.50
4	D	12	CYS	CA-CB-SG	5.45	123.81	114.00
1	A	34	C	N1-C2-O2	-5.45	115.63	118.90
1	A	43	C	C5-C6-N1	-5.45	118.28	121.00
1	A	1434	A	C8-N9-C4	5.45	107.98	105.80
1	A	32	A	N1-C6-N6	5.45	121.87	118.60
1	A	232	G	C4-N9-C1'	5.45	133.58	126.50
1	A	280	C	N3-C4-N4	-5.45	114.19	118.00
1	A	1098	C	C6-N1-C2	5.45	122.48	120.30
1	A	1240	U	N3-C2-O2	-5.45	118.39	122.20
1	A	1354	C	C6-N1-C2	-5.45	118.12	120.30
1	A	1494	G	N3-C4-N9	5.45	129.27	126.00
1	A	70	G	N3-C4-C5	5.45	131.32	128.60
1	A	394	G	C5-C6-O6	5.44	131.87	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	953	G	N9-C4-C5	-5.44	103.22	105.40
1	A	1323	G	C5-C6-N1	-5.44	108.78	111.50
1	A	1506	U	C5-C4-O4	-5.44	122.64	125.90
1	A	26	A	N1-C2-N3	5.44	132.02	129.30
1	A	265	G	N3-C2-N2	5.43	123.70	119.90
1	A	1055	A	N9-C4-C5	5.43	107.97	105.80
1	A	1527	C	C6-N1-C1'	-5.43	114.28	120.80
1	A	111	G	N3-C2-N2	-5.43	116.10	119.90
1	A	1493[A]	A	C4-C5-N7	5.43	113.41	110.70
1	A	1493[B]	A	C4-C5-N7	5.43	113.41	110.70
1	A	552	U	N3-C4-C5	5.43	117.86	114.60
1	A	250	A	N9-C4-C5	-5.42	103.63	105.80
1	A	278	G	C5-C6-O6	5.42	131.85	128.60
1	A	1502	A	N3-C4-N9	-5.42	123.06	127.40
1	A	608	A	C2-N3-C4	-5.42	107.89	110.60
1	A	648	A	C6-N1-C2	-5.42	115.35	118.60
1	A	724	G	N1-C6-O6	5.42	123.15	119.90
1	A	924	C	N1-C2-O2	-5.42	115.65	118.90
1	A	120	A	C5-N7-C8	5.42	106.61	103.90
1	A	317	G	N3-C4-C5	5.42	131.31	128.60
1	A	628	G	C8-N9-C1'	-5.42	119.96	127.00
1	A	675	A	C5-C6-N1	-5.42	114.99	117.70
1	A	230	G	N3-C4-N9	5.42	129.25	126.00
1	A	530	G	N1-C6-O6	-5.42	116.65	119.90
1	A	1343	G	N7-C8-N9	5.42	115.81	113.10
1	A	1405	G	N3-C4-N9	-5.42	122.75	126.00
1	A	107	G	C6-C5-N7	-5.42	127.15	130.40
18	R	76	LEU	CA-CB-CG	-5.41	102.85	115.30
1	A	259	G	C4-N9-C1'	5.41	133.53	126.50
1	A	874	G	C2-N3-C4	-5.41	109.19	111.90
1	A	881	G	N1-C6-O6	5.41	123.15	119.90
1	A	400	C	C5-C6-N1	-5.41	118.30	121.00
1	A	671	G	N1-C6-O6	5.41	123.14	119.90
1	A	1125	U	N3-C2-O2	5.41	125.99	122.20
1	A	107	G	N9-C4-C5	-5.41	103.24	105.40
1	A	283	C	N3-C2-O2	-5.41	118.12	121.90
1	A	817	C	C2-N1-C1'	5.41	124.75	118.80
1	A	589	C	C2-N3-C4	-5.40	117.20	119.90
1	A	1242	C	N3-C4-C5	5.40	124.06	121.90
1	A	304	U	C5-C6-N1	-5.40	120.00	122.70
1	A	16	A	N7-C8-N9	-5.39	111.10	113.80
1	A	124	G	N1-C2-N3	5.39	127.14	123.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1202	G	C8-N9-C4	-5.39	104.24	106.40
1	A	641	U	N1-C2-N3	5.38	118.13	114.90
1	A	826	C	N3-C4-N4	5.38	121.77	118.00
1	A	20	U	C2-N3-C4	-5.38	123.77	127.00
1	A	1143	G	C5-C6-O6	-5.38	125.37	128.60
1	A	1276	G	C6-C5-N7	-5.38	127.17	130.40
1	A	1395	C	N1-C2-O2	-5.38	115.67	118.90
1	A	1413	A	N1-C2-N3	5.38	131.99	129.30
1	A	1231	G	N9-C4-C5	-5.38	103.25	105.40
16	P	60	LEU	CA-CB-CG	-5.38	102.93	115.30
1	A	631	G	C8-N9-C4	-5.37	104.25	106.40
1	A	1375	A	N1-C6-N6	-5.37	115.38	118.60
1	A	197	A	C5-C6-N6	5.37	128.00	123.70
1	A	264	U	N1-C2-N3	5.37	118.12	114.90
1	A	413	G	C4-C5-N7	-5.37	108.65	110.80
1	A	490	G	C5-C6-O6	-5.37	125.38	128.60
5	E	69	VAL	CB-CA-C	-5.37	101.20	111.40
1	A	931	C	N3-C4-C5	5.37	124.05	121.90
1	A	1023	G	N3-C4-C5	-5.37	125.92	128.60
1	A	1332	A	C5-C6-N6	5.37	127.99	123.70
1	A	1053	G	C4-C5-N7	-5.37	108.65	110.80
1	A	1108	G	N3-C4-N9	5.37	129.22	126.00
1	A	92	C	C5-C4-N4	-5.36	116.44	120.20
1	A	279	A	C4-C5-C6	5.36	119.68	117.00
1	A	497	A	N9-C4-C5	5.36	107.95	105.80
1	A	1054	C	C5-C6-N1	5.36	123.68	121.00
1	A	1206	G	C5-C6-N1	-5.36	108.82	111.50
1	A	1350	A	C4-C5-N7	5.36	113.38	110.70
1	A	566	G	C6-C5-N7	-5.36	127.19	130.40
1	A	200	G	C5-C6-N1	-5.36	108.82	111.50
1	A	800	G	C4-N9-C1'	5.36	133.46	126.50
1	A	854	G	N9-C4-C5	-5.35	103.26	105.40
1	A	524	G	N3-C2-N2	-5.35	116.15	119.90
1	A	779	C	C5-C6-N1	-5.35	118.32	121.00
1	A	1304	G	C8-N9-C4	-5.35	104.26	106.40
1	A	1338	G	N1-C2-N3	5.35	127.11	123.90
1	A	1460	A	N1-C6-N6	5.35	121.81	118.60
1	A	10	A	N1-C2-N3	5.35	131.97	129.30
1	A	358	U	N1-C2-N3	5.35	118.11	114.90
1	A	1165	C	C6-N1-C2	-5.35	118.16	120.30
1	A	1399	C	N1-C2-O2	-5.35	115.69	118.90
1	A	204	U	N1-C2-N3	-5.35	111.69	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	934	C	C2-N3-C4	5.35	122.57	119.90
1	A	1125	U	C5-C4-O4	-5.35	122.69	125.90
1	A	1080	A	C5-C6-N6	5.35	127.98	123.70
1	A	558	G	N1-C6-O6	5.34	123.11	119.90
4	D	188	LEU	CB-CG-CD1	5.34	120.08	111.00
1	A	77	G	C6-C5-N7	-5.34	127.19	130.40
1	A	277	C	C5-C6-N1	-5.34	118.33	121.00
1	A	291	C	N3-C4-C5	5.34	124.04	121.90
1	A	1068	G	C4-N9-C1'	5.34	133.44	126.50
1	A	1433	A	N1-C6-N6	-5.34	115.39	118.60
1	A	786	G	C5-C6-N1	-5.34	108.83	111.50
1	A	1530	G	N1-C6-O6	5.34	123.10	119.90
1	A	483	C	C2-N1-C1'	-5.34	112.93	118.80
1	A	644	G	C8-N9-C1'	-5.34	120.06	127.00
1	A	1246	C	C2-N1-C1'	-5.34	112.93	118.80
1	A	55	A	C5-C6-N1	5.33	120.37	117.70
1	A	281	G	C5-N7-C8	-5.33	101.64	104.30
1	A	767	A	C4-C5-N7	-5.33	108.03	110.70
1	A	871	U	N3-C2-O2	-5.33	118.47	122.20
1	A	1167	A	C8-N9-C4	-5.33	103.67	105.80
20	T	102	GLY	N-CA-C	-5.33	99.78	113.10
1	A	635	G	C4-N9-C1'	5.33	133.43	126.50
1	A	557	G	C4-C5-N7	-5.33	108.67	110.80
1	A	351	G	N1-C2-N3	5.32	127.09	123.90
1	A	403	C	C4-C5-C6	5.32	120.06	117.40
1	A	288	A	N1-C6-N6	5.32	121.79	118.60
1	A	1055	A	C5-C6-N1	5.32	120.36	117.70
1	A	1286	A	N7-C8-N9	5.32	116.46	113.80
1	A	780	A	N7-C8-N9	-5.32	111.14	113.80
1	A	1092	A	C4-N9-C1'	5.32	135.87	126.30
1	A	317	G	N1-C6-O6	5.31	123.09	119.90
1	A	1324	A	C8-N9-C4	-5.31	103.67	105.80
1	A	423	G	N3-C4-N9	5.31	129.19	126.00
1	A	479	C	C2-N3-C4	5.31	122.55	119.90
1	A	876	G	C5-N7-C8	-5.31	101.64	104.30
1	A	1480	G	C5-C6-N1	-5.31	108.84	111.50
1	A	980	C	C5-C4-N4	-5.31	116.48	120.20
1	A	936	C	C5-C6-N1	-5.30	118.35	121.00
1	A	1481	U	C5-C4-O4	5.30	129.08	125.90
2	B	25	ASN	C-N-CD	5.30	139.54	128.40
1	A	17	U	N1-C2-N3	5.30	118.08	114.90
1	A	70	G	N1-C6-O6	5.29	123.08	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	783	C	C5-C6-N1	-5.29	118.35	121.00
1	A	895	G	N7-C8-N9	5.29	115.75	113.10
1	A	963	G	C8-N9-C4	-5.29	104.28	106.40
1	A	1415	G	N9-C4-C5	-5.29	103.28	105.40
1	A	607	A	N1-C6-N6	5.29	121.77	118.60
1	A	69	G	C8-N9-C4	5.29	108.52	106.40
1	A	389	A	N1-C2-N3	5.29	131.94	129.30
1	A	732	C	N3-C2-O2	-5.29	118.20	121.90
1	A	752	G	C8-N9-C4	5.29	108.52	106.40
1	A	822	C	C2-N3-C4	-5.29	117.26	119.90
1	A	947	G	C6-C5-N7	-5.29	127.23	130.40
1	A	1091	U	N3-C4-C5	-5.29	111.43	114.60
1	A	534	U	C6-N1-C2	5.29	124.17	121.00
1	A	820	U	C6-N1-C1'	5.29	128.60	121.20
1	A	947	G	N3-C2-N2	5.29	123.60	119.90
1	A	705	U	C5-C6-N1	-5.28	120.06	122.70
1	A	1295	G	C8-N9-C4	-5.28	104.29	106.40
1	A	861	G	C5-C6-N1	5.28	114.14	111.50
1	A	920	U	C6-N1-C1'	5.28	128.59	121.20
1	A	1201	A	N3-C4-C5	-5.28	123.11	126.80
1	A	259	G	C6-C5-N7	-5.27	127.24	130.40
14	N	10	ALA	N-CA-C	-5.27	96.76	111.00
1	A	577	G	N1-C2-N3	5.27	127.06	123.90
1	A	721	G	N3-C2-N2	5.27	123.59	119.90
1	A	1350	A	C6-C5-N7	-5.27	128.61	132.30
1	A	820	U	C2-N3-C4	-5.27	123.84	127.00
1	A	934	C	C6-N1-C2	5.27	122.41	120.30
1	A	827	U	C2-N1-C1'	5.27	124.02	117.70
1	A	54	C	C2-N3-C4	-5.26	117.27	119.90
1	A	635	G	C8-N9-C4	5.26	108.51	106.40
1	A	644	G	N9-C4-C5	-5.26	103.29	105.40
1	A	800	G	C6-C5-N7	-5.26	127.24	130.40
1	A	819	A	N1-C2-N3	5.26	131.93	129.30
12	L	66	VAL	CB-CA-C	-5.26	101.40	111.40
1	A	919	A	C5-C6-N6	-5.26	119.49	123.70
1	A	1077	G	N1-C2-N2	-5.26	111.46	116.20
1	A	1380	U	C5-C4-O4	5.26	129.06	125.90
10	J	58	ASP	CB-CG-OD1	5.26	123.03	118.30
1	A	1033	G	N9-C4-C5	5.26	107.50	105.40
1	A	1281	U	N3-C2-O2	-5.26	118.52	122.20
1	A	221	C	C5-C6-N1	-5.25	118.37	121.00
1	A	565	U	N1-C2-N3	-5.25	111.75	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	964	A	C2-N3-C4	-5.25	107.97	110.60
1	A	1505	G	N9-C4-C5	5.25	107.50	105.40
1	A	1512	U	N1-C2-N3	5.25	118.05	114.90
1	A	1487	G	N3-C2-N2	-5.25	116.22	119.90
1	A	1494	G	C6-C5-N7	-5.25	127.25	130.40
1	A	248	C	C4-C5-C6	5.25	120.03	117.40
1	A	1249	C	C2-N1-C1'	5.25	124.58	118.80
1	A	112	G	C8-N9-C4	5.25	108.50	106.40
1	A	119	A	N1-C6-N6	5.25	121.75	118.60
1	A	244	U	N1-C2-N3	-5.24	111.75	114.90
1	A	1058	G	N3-C4-C5	5.24	131.22	128.60
15	O	45	VAL	CB-CA-C	-5.24	101.44	111.40
1	A	573	A	C6-C5-N7	-5.24	128.63	132.30
1	A	1392	G	C4-C5-C6	5.24	121.94	118.80
1	A	711	G	N7-C8-N9	5.24	115.72	113.10
1	A	740	U	C5-C6-N1	-5.24	120.08	122.70
1	A	1099	G	N3-C4-N9	-5.24	122.86	126.00
1	A	440	A	C5-C6-N1	-5.23	115.08	117.70
1	A	1200	C	C5-C4-N4	-5.23	116.54	120.20
1	A	801	U	N3-C4-C5	5.23	117.74	114.60
1	A	831	U	N1-C2-N3	5.23	118.04	114.90
1	A	946	A	N1-C2-N3	5.23	131.92	129.30
1	A	149	A	N1-C6-N6	-5.23	115.46	118.60
1	A	650	G	N3-C2-N2	-5.23	116.24	119.90
1	A	668	G	C8-N9-C4	5.23	108.49	106.40
1	A	489	C	C6-N1-C2	5.23	122.39	120.30
1	A	1497	G	N3-C4-C5	-5.22	125.99	128.60
1	A	309	G	C4-C5-N7	5.22	112.89	110.80
1	A	544	G	N3-C4-C5	-5.22	125.99	128.60
1	A	816	A	N3-C4-C5	5.22	130.46	126.80
1	A	122	G	N3-C4-C5	5.22	131.21	128.60
1	A	352	C	N1-C2-O2	-5.22	115.77	118.90
1	A	965	A	N9-C4-C5	-5.22	103.71	105.80
1	A	1096	C	C6-N1-C2	-5.22	118.21	120.30
1	A	975	A	C2-N3-C4	-5.22	107.99	110.60
1	A	1305	G	C4-C5-C6	5.22	121.93	118.80
1	A	641	U	C2-N3-C4	-5.21	123.87	127.00
1	A	1027	C	N3-C4-C5	-5.21	119.81	121.90
1	A	1525	G	C6-N1-C2	-5.21	121.97	125.10
1	A	744	C	C5-C6-N1	-5.21	118.39	121.00
1	A	823	G	N1-C2-N3	5.21	127.03	123.90
1	A	190(E)	U	N1-C2-N3	5.21	118.03	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	931	C	N3-C4-N4	-5.21	114.35	118.00
1	A	1507	A	C5-C6-N6	5.21	127.87	123.70
1	A	1134	G	N9-C4-C5	5.21	107.48	105.40
1	A	331	G	C8-N9-C1'	-5.21	120.23	127.00
1	A	1484	C	N1-C2-O2	-5.21	115.78	118.90
1	A	15	G	C4-C5-N7	5.20	112.88	110.80
1	A	781	A	N7-C8-N9	5.20	116.40	113.80
1	A	781	A	C4-C5-C6	5.20	119.60	117.00
1	A	782	A	C5-C6-N6	5.20	127.86	123.70
1	A	953	G	N1-C6-O6	5.20	123.02	119.90
1	A	1421	G	N7-C8-N9	5.20	115.70	113.10
1	A	900	A	N1-C2-N3	5.20	131.90	129.30
1	A	679	C	C6-N1-C2	5.20	122.38	120.30
1	A	964	A	N7-C8-N9	5.19	116.40	113.80
1	A	436	C	C2-N1-C1'	-5.19	113.09	118.80
1	A	830	G	C5-C6-N1	-5.19	108.90	111.50
1	A	1049	U	C2-N1-C1'	5.19	123.93	117.70
12	L	17	LYS	CD-CE-NZ	5.19	123.64	111.70
1	A	25	C	C6-N1-C2	5.19	122.38	120.30
1	A	104	G	C4-C5-C6	5.19	121.91	118.80
1	A	481	G	C8-N9-C1'	-5.19	120.25	127.00
1	A	1108	G	C4-C5-C6	5.19	121.91	118.80
1	A	540	G	C4-C5-N7	5.19	112.88	110.80
1	A	804	U	C4-C5-C6	5.19	122.81	119.70
1	A	1037	C	C6-N1-C2	-5.18	118.23	120.30
1	A	882	C	N1-C2-N3	5.18	122.83	119.20
5	E	63	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	A	760	G	N9-C4-C5	-5.18	103.33	105.40
1	A	497	A	C5-C6-N6	5.18	127.84	123.70
1	A	1322	C	C2-N3-C4	5.18	122.49	119.90
1	A	1293	G	N3-C4-C5	5.18	131.19	128.60
1	A	1272	G	N3-C4-C5	-5.18	126.01	128.60
1	A	232	G	C5-C6-N1	-5.17	108.91	111.50
1	A	691	G	C6-C5-N7	-5.17	127.30	130.40
1	A	311	C	C5-C6-N1	-5.17	118.42	121.00
1	A	969	A	C5-N7-C8	-5.17	101.31	103.90
1	A	1030(C)	G	C8-N9-C4	-5.17	104.33	106.40
1	A	816	A	C6-C5-N7	5.17	135.92	132.30
1	A	558	G	C5-N7-C8	-5.17	101.72	104.30
1	A	811	C	C2-N3-C4	-5.17	117.32	119.90
1	A	816	A	C8-N9-C4	5.17	107.87	105.80
1	A	134	A	C2-N3-C4	-5.16	108.02	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	299	G	C5-C6-O6	-5.16	125.50	128.60
1	A	190(H)	G	C4-C5-N7	-5.16	108.74	110.80
1	A	648	A	C4-C5-N7	-5.16	108.12	110.70
1	A	1253	G	C4-N9-C1'	5.16	133.21	126.50
1	A	700	G	N3-C4-C5	-5.16	126.02	128.60
1	A	1493[A]	A	N1-C6-N6	5.16	121.69	118.60
1	A	1493[B]	A	N1-C6-N6	5.16	121.69	118.60
1	A	824	C	C2-N3-C4	-5.16	117.32	119.90
1	A	190(B)	C	C2-N1-C1'	5.16	124.47	118.80
1	A	667	G	N3-C4-C5	5.16	131.18	128.60
1	A	566	G	N3-C4-C5	-5.15	126.02	128.60
1	A	280	C	C5-C6-N1	-5.15	118.42	121.00
1	A	701	C	N3-C4-N4	-5.15	114.39	118.00
1	A	705	U	N1-C2-N3	5.15	117.99	114.90
1	A	976	G	N3-C2-N2	-5.15	116.30	119.90
1	A	1390	U	C5-C4-O4	5.15	128.99	125.90
1	A	97	G	C8-N9-C4	-5.15	104.34	106.40
1	A	596	C	N3-C2-O2	5.15	125.50	121.90
1	A	193	C	C6-N1-C2	5.15	122.36	120.30
1	A	1052	U	C6-N1-C2	-5.14	117.91	121.00
1	A	596	C	C2-N1-C1'	-5.14	113.14	118.80
1	A	220	G	N1-C6-O6	5.14	122.98	119.90
1	A	306	G	N3-C4-C5	5.14	131.17	128.60
1	A	785	G	C8-N9-C4	5.14	108.46	106.40
1	A	1377	A	N1-C6-N6	-5.14	115.52	118.60
1	A	1395	C	C5-C4-N4	5.14	123.80	120.20
1	A	612	C	C5-C6-N1	-5.14	118.43	121.00
1	A	1484	C	N3-C2-O2	5.14	125.50	121.90
1	A	109	A	C5-C6-N6	5.13	127.81	123.70
1	A	357	G	N9-C4-C5	5.13	107.45	105.40
1	A	246	A	C8-N9-C4	5.13	107.85	105.80
1	A	881	G	C6-C5-N7	-5.13	127.32	130.40
1	A	558	G	C5-C6-O6	-5.13	125.52	128.60
1	A	796	C	C5-C6-N1	-5.13	118.44	121.00
1	A	1186	G	N3-C2-N2	-5.13	116.31	119.90
1	A	618	C	C5-C4-N4	5.13	123.79	120.20
1	A	120	A	C5-C6-N6	5.13	127.80	123.70
1	A	435	C	C6-N1-C2	-5.13	118.25	120.30
1	A	805	C	C4-C5-C6	-5.13	114.84	117.40
12	L	52	LEU	CA-CB-CG	5.13	127.09	115.30
1	A	683	G	C8-N9-C4	-5.12	104.35	106.40
1	A	390	C	N3-C4-C5	-5.12	119.85	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	758	G	N1-C2-N3	5.12	126.97	123.90
1	A	1030(C)	G	N3-C4-C5	-5.12	126.04	128.60
1	A	1365	G	N9-C4-C5	5.12	107.45	105.40
1	A	201	C	C6-N1-C1'	-5.12	114.65	120.80
1	A	539	A	C2-N3-C4	5.12	113.16	110.60
1	A	570	G	N3-C4-N9	5.12	129.07	126.00
1	A	812	C	N3-C2-O2	-5.12	118.31	121.90
1	A	889	A	C4-C5-C6	5.12	119.56	117.00
1	A	1332	A	C8-N9-C4	-5.12	103.75	105.80
1	A	1077	G	N1-C2-N3	5.12	126.97	123.90
1	A	828	A	C6-C5-N7	-5.12	128.72	132.30
1	A	109	A	N1-C2-N3	5.12	131.86	129.30
1	A	1139	G	N3-C4-C5	-5.12	126.04	128.60
1	A	317	G	C4-C5-N7	5.11	112.84	110.80
1	A	621	A	C6-C5-N7	-5.11	128.72	132.30
1	A	910	C	N1-C2-N3	5.11	122.78	119.20
1	A	919	A	C4-C5-N7	5.11	113.26	110.70
1	A	1370	G	C4-N9-C1'	5.11	133.14	126.50
1	A	47	C	C6-N1-C2	5.11	122.34	120.30
1	A	316	G	C6-C5-N7	5.11	133.46	130.40
1	A	803	G	N1-C2-N2	-5.11	111.60	116.20
1	A	823	G	C6-C5-N7	-5.11	127.33	130.40
1	A	10	A	N1-C6-N6	-5.11	115.54	118.60
1	A	530	G	N3-C2-N2	5.11	123.47	119.90
1	A	120	A	C4-C5-N7	-5.10	108.15	110.70
1	A	266	G	N9-C4-C5	-5.10	103.36	105.40
1	A	284	G	C5-C6-N1	-5.10	108.95	111.50
1	A	521	G	C6-C5-N7	5.10	133.46	130.40
1	A	660	G	N9-C4-C5	-5.10	103.36	105.40
1	A	1344	C	C5-C6-N1	-5.10	118.45	121.00
1	A	181	G	N3-C4-N9	5.10	129.06	126.00
1	A	66	G	C2-N3-C4	-5.10	109.35	111.90
1	A	485	G	C5-C6-N1	-5.10	108.95	111.50
1	A	741	G	N9-C4-C5	5.10	107.44	105.40
1	A	1341	U	C6-N1-C1'	5.10	128.34	121.20
1	A	757	U	N1-C2-O2	-5.10	119.23	122.80
1	A	253	U	N1-C2-O2	-5.09	119.23	122.80
1	A	930	C	C2-N3-C4	-5.09	117.35	119.90
1	A	1084	G	C4-C5-C6	5.09	121.86	118.80
1	A	1504	G	N9-C4-C5	-5.09	103.36	105.40
1	A	190(F)	G	C4-C5-N7	-5.09	108.76	110.80
1	A	259	G	N7-C8-N9	5.09	115.64	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	570	G	C8-N9-C1'	-5.09	120.39	127.00
1	A	1078	U	C4-C5-C6	-5.09	116.65	119.70
1	A	1222	G	N1-C6-O6	5.09	122.95	119.90
1	A	796	C	N3-C4-C5	-5.09	119.86	121.90
1	A	306	G	N1-C6-O6	5.09	122.95	119.90
1	A	853	G	N7-C8-N9	5.09	115.64	113.10
1	A	909	A	C4-C5-N7	5.09	113.24	110.70
1	A	1277	C	N3-C2-O2	-5.09	118.34	121.90
1	A	1012	U	C6-N1-C2	-5.08	117.95	121.00
1	A	947	G	N1-C2-N2	-5.08	111.62	116.20
1	A	1310	G	N9-C4-C5	-5.08	103.37	105.40
24	a	37	A	N1-C2-N3	5.08	131.84	129.30
1	A	336	C	N3-C4-N4	5.08	121.56	118.00
1	A	903	G	N9-C4-C5	5.08	107.43	105.40
1	A	1195	C	C5-C4-N4	-5.08	116.64	120.20
1	A	1236	A	C5-C6-N6	-5.08	119.64	123.70
1	A	393	A	N1-C6-N6	5.08	121.65	118.60
1	A	814	A	C8-N9-C4	5.07	107.83	105.80
1	A	597	G	N1-C2-N3	5.07	126.94	123.90
1	A	933	G	C4-C5-N7	5.07	112.83	110.80
1	A	977	A	N3-C4-C5	-5.07	123.25	126.80
1	A	1405	G	C4-N9-C1'	-5.07	119.91	126.50
1	A	1494	G	C4-C5-N7	5.07	112.83	110.80
1	A	92	C	N1-C2-O2	5.07	121.94	118.90
1	A	344	A	C5-N7-C8	-5.07	101.37	103.90
1	A	183	G	N7-C8-N9	5.06	115.63	113.10
1	A	544	G	C4-N9-C1'	5.06	133.08	126.50
1	A	579	G	N3-C4-C5	5.06	131.13	128.60
1	A	190(D)	U	N3-C2-O2	-5.06	118.66	122.20
1	A	292	G	C8-N9-C4	5.06	108.42	106.40
1	A	794	A	N1-C2-N3	-5.06	126.77	129.30
1	A	795	C	C2-N1-C1'	-5.06	113.23	118.80
1	A	1127	G	N1-C6-O6	-5.06	116.86	119.90
1	A	858	G	C4-N9-C1'	5.06	133.08	126.50
1	A	886	G	C5-C6-N1	-5.06	108.97	111.50
1	A	433	C	N3-C2-O2	-5.05	118.36	121.90
1	A	50	A	C6-N1-C2	5.05	121.63	118.60
1	A	149	A	N1-C2-N3	5.05	131.83	129.30
1	A	642	A	N1-C2-N3	5.05	131.83	129.30
1	A	600	C	C4-C5-C6	5.05	119.92	117.40
1	A	658	G	N1-C2-N2	-5.05	111.66	116.20
1	A	1356	G	C8-N9-C4	-5.05	104.38	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	24	U	C2-N3-C4	-5.05	123.97	127.00
1	A	903	G	N1-C6-O6	-5.05	116.87	119.90
1	A	1324	A	N1-C6-N6	5.05	121.63	118.60
1	A	403	C	C2-N1-C1'	-5.04	113.25	118.80
1	A	1232	U	C2-N3-C4	-5.04	123.97	127.00
1	A	16	A	C5-C6-N1	-5.04	115.18	117.70
1	A	288	A	N3-C4-C5	5.04	130.33	126.80
1	A	447	G	N3-C2-N2	5.04	123.43	119.90
1	A	910	C	C4-C5-C6	5.04	119.92	117.40
1	A	1279	A	C4-C5-C6	5.04	119.52	117.00
1	A	637	G	C4-N9-C1'	5.04	133.05	126.50
1	A	1434	A	C5-C6-N6	-5.04	119.67	123.70
1	A	1476	G	C8-N9-C4	-5.04	104.38	106.40
1	A	521	G	C4-C5-N7	-5.03	108.79	110.80
1	A	964	A	N9-C4-C5	5.03	107.81	105.80
25	b	3	U	N3-C2-O2	-5.03	118.68	122.20
1	A	64	G	C6-C5-N7	-5.03	127.38	130.40
1	A	646	U	C5-C4-O4	5.03	128.92	125.90
1	A	330	C	N3-C4-C5	-5.03	119.89	121.90
1	A	800	G	N1-C6-O6	5.03	122.92	119.90
1	A	899	C	C2-N1-C1'	5.03	124.33	118.80
1	A	250	A	C6-N1-C2	5.03	121.62	118.60
1	A	558	G	C8-N9-C4	-5.03	104.39	106.40
1	A	1488	G	C4-C5-N7	-5.03	108.79	110.80
1	A	142	G	C2-N3-C4	5.03	114.41	111.90
1	A	826	C	C2-N1-C1'	5.03	124.33	118.80
1	A	135	C	C6-N1-C1'	5.02	126.83	120.80
1	A	1055	A	C4-C5-N7	-5.02	108.19	110.70
1	A	828	A	C4-C5-N7	5.02	113.21	110.70
1	A	1099	G	N3-C2-N2	-5.02	116.39	119.90
1	A	1303	C	N3-C4-C5	5.02	123.91	121.90
1	A	712	A	C2-N3-C4	-5.02	108.09	110.60
1	A	651	C	N1-C2-O2	-5.02	115.89	118.90
1	A	859	A	N3-C4-N9	5.02	131.41	127.40
1	A	357	G	N1-C6-O6	-5.02	116.89	119.90
1	A	21	G	N3-C2-N2	5.01	123.41	119.90
16	P	5	ARG	NE-CZ-NH2	-5.01	117.79	120.30
1	A	276	G	C5-C6-O6	5.01	131.60	128.60
1	A	611	A	N1-C6-N6	5.01	121.61	118.60
1	A	786	G	N3-C4-C5	5.01	131.10	128.60
1	A	125	U	C5-C6-N1	-5.01	120.20	122.70
1	A	673	G	N1-C6-O6	5.01	122.90	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1303	C	C6-N1-C2	5.00	122.30	120.30
1	A	266	G	P-O3'-C3'	5.00	125.70	119.70
1	A	1179	A	N1-C6-N6	-5.00	115.60	118.60

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	14	GLY	Peptide
2	B	75	LYS	Peptide
2	B	89	GLY	Peptide
3	C	166	GLU	Peptide
3	C	2	GLY	Peptide
4	D	154	ASN	Peptide
8	H	27	PRO	Peptide
8	H	90	GLY	Peptide
9	I	38	GLN	Peptide
10	J	61	GLU	Peptide
10	J	85	LEU	Peptide
12	L	46	LYS	Peptide
12	L	91	LYS	Peptide
16	P	82	GLN	Peptide
19	S	4	SER	Peptide
20	T	12	ALA	Peptide
20	T	8	ARG	Peptide
21	U	24	ARG	Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32707	0	0	870	1
2	B	1896	0	6	51	0
3	C	1613	0	0	45	0
4	D	1703	0	0	61	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	1147	0	0	36	1
6	F	843	0	0	17	0
7	G	1257	0	0	41	0
8	H	1116	0	0	41	0
9	I	1010	0	0	29	0
10	J	793	0	0	25	0
11	K	873	0	12	27	0
12	L	973	0	0	35	0
13	M	937	0	0	37	0
14	N	492	0	0	21	0
15	O	734	0	2	28	0
16	P	701	0	0	22	0
17	Q	834	0	12	32	0
18	R	585	0	12	29	0
19	S	648	0	0	25	0
20	T	763	0	0	31	0
21	U	209	0	0	11	0
22	V	77	0	0	1	0
23	W	235	0	23	23	0
24	a	175	0	0	0	0
25	b	60	0	11	0	0
26	A	326	0	0	0	0
26	D	3	0	0	0	0
26	E	4	0	0	0	0
26	F	1	0	0	0	0
26	G	1	0	0	0	0
26	H	1	0	0	0	0
26	J	1	0	0	0	0
26	N	1	0	0	0	0
26	P	3	0	0	0	0
26	Q	1	0	0	0	0
26	S	2	0	0	0	0
27	A	40	0	38	12	0
28	D	1	0	0	0	0
28	N	1	0	0	0	0
29	A	866	0	0	91	0
29	C	1	0	0	0	0
29	D	7	0	0	0	0
29	E	5	0	0	0	0
29	L	1	0	0	0	0
29	N	1	0	0	0	0
29	P	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	Q	2	0	0	0	0
29	T	3	0	0	0	0
29	U	4	0	0	0	0
29	W	1	0	0	0	0
All	All	53659	0	116	1421	2

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 28.

All (1421) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:451:A:O2'	29:A:2729:HOH:O	1.59	1.20
1:A:692:U:OP1	11:K:124:LYS:NZ	1.82	1.10
1:A:266:G:O2'	1:A:267:C:OP2	1.72	1.08
1:A:328:C:O2'	1:A:329:A:OP2	1.72	1.07
1:A:61:G:O2'	29:A:2002:HOH:O	1.76	1.04
1:A:89:C:C5	1:A:90:U:N3	2.25	1.02
7:G:152:ALA:O	7:G:155:ARG:NH1	1.93	1.01
18:R:37:VAL:O	18:R:40:LEU:N	1.92	1.00
1:A:103:C:OP1	20:T:17:ARG:NH1	1.93	1.00
4:D:150:GLU:N	4:D:150:GLU:OE2	1.92	1.00
1:A:1328:C:OP1	21:U:20:LYS:NZ	1.96	0.99
13:M:16:ASP:OD2	13:M:17:VAL:N	1.95	0.99
1:A:1316:G:N2	1:A:1319:A:OP2	1.96	0.99
1:A:1026:G:O2'	1:A:1027:C:OP1	1.80	0.98
27:A:1928:SRY:HI32	27:A:1928:SRY:H22	1.46	0.97
1:A:914:A:P	27:A:1928:SRY:HI33	2.06	0.95
1:A:1305:G:OP2	21:U:2:GLY:N	1.99	0.95
1:A:1299:A:C5	1:A:1301:U:O2	2.20	0.94
1:A:1068:G:P	29:A:2218:HOH:O	2.25	0.94
1:A:372:C:O2'	29:A:2721:HOH:O	1.84	0.94
8:H:54:ASP:OD2	8:H:55:GLY:N	2.02	0.93
1:A:279:A:OP2	17:Q:95:TYR:OH	1.86	0.91
1:A:1381:U:C5	1:A:1382:C:C5	2.58	0.91
1:A:991:U:O2'	1:A:992:U:O5'	1.90	0.89
1:A:1442:G:C6	1:A:1446:A:N6	2.41	0.88
1:A:484:G:O2'	1:A:485:G:OP2	1.90	0.88
1:A:500:G:C5	1:A:546:G:N2	2.42	0.88
12:L:117:ARG:O	12:L:120:TYR:N	2.06	0.88
1:A:353:A:OP1	29:A:2224:HOH:O	1.91	0.87
1:A:974:A:OP2	14:N:41:ARG:NH1	2.09	0.86
1:A:1493[A]:A:C8	1:A:1493[A]:A:C3'	2.59	0.86

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:54:C:C4	1:A:352:C:C5	2.65	0.85
1:A:328:C:O2	1:A:328:C:C2'	2.22	0.85
4:D:192:GLU:N	4:D:192:GLU:OE2	2.10	0.85
1:A:393:A:C2	1:A:394:G:C8	2.64	0.85
12:L:127:GLU:CG	12:L:128:ALA:N	2.40	0.84
1:A:509:A:O2'	1:A:510:A:OP1	1.93	0.84
1:A:304:U:O4	29:A:2495:HOH:O	1.94	0.84
18:R:38:GLU:OE2	18:R:38:GLU:N	2.12	0.83
1:A:1300:G:O2'	1:A:1301:U:P	2.37	0.83
9:I:32:ASP:OD1	9:I:33:PHE:N	2.12	0.83
2:B:130:ARG:NH1	2:B:134:GLU:OE1	2.12	0.82
1:A:1399:C:O2	1:A:1401:G:C5	2.32	0.82
15:O:26:GLU:OE2	15:O:77:ARG:NH1	2.12	0.82
1:A:512:U:O2	1:A:540:G:N2	2.13	0.81
5:E:144:THR:O	5:E:148:VAL:CG2	2.28	0.81
1:A:1532:U:C4	1:A:1533:C:N4	2.48	0.81
19:S:10:PHE:O	19:S:39:THR:OG1	1.98	0.81
1:A:1515[B]:C:N4	1:A:1520[B]:G:O6	2.14	0.81
1:A:1054:C:C3'	1:A:1054:C:O2	2.28	0.81
1:A:1152:A:OP1	10:J:68:HIS:ND1	2.14	0.81
1:A:117:G:OP2	29:A:2018:HOH:O	1.98	0.81
1:A:1005:A:N7	1:A:1026:G:N1	2.30	0.81
1:A:1399:C:C6	1:A:1502:A:N6	2.48	0.81
1:A:1300:G:O2'	1:A:1301:U:O5'	1.99	0.80
1:A:303:A:N6	29:A:2495:HOH:O	2.15	0.80
21:U:10:ARG:NH1	21:U:10:ARG:CB	2.45	0.80
1:A:1412:C:OP1	12:L:57:LYS:NZ	2.15	0.80
13:M:19:LEU:O	13:M:22:ILE:CG1	2.30	0.79
1:A:512:U:OP1	4:D:46:LYS:NZ	2.15	0.79
8:H:4:ASP:OD2	8:H:85:ARG:NE	2.15	0.79
1:A:777:A:OP1	29:A:2536:HOH:O	2.00	0.79
1:A:542:G:OP1	4:D:10:ARG:NH2	2.16	0.79
1:A:1272:G:N7	29:A:2695:HOH:O	2.16	0.78
1:A:527:7MG:OP2	27:A:1928:SRY:O32	2.01	0.78
1:A:1346:A:C4	7:G:10:ARG:NH1	2.51	0.78
1:A:1482:G:N1	29:A:2362:HOH:O	2.16	0.78
20:T:67:ALA:O	20:T:73:HIS:ND1	2.16	0.78
1:A:352:C:O2'	1:A:354:G:OP1	2.02	0.78
4:D:8:VAL:O	4:D:11:LEU:N	2.17	0.78
1:A:965:A:C2	1:A:969:A:C2	2.72	0.78
1:A:1347:G:O2'	1:A:1348:U:P	2.41	0.78
1:A:768:A:OP2	29:A:2052:HOH:O	2.02	0.77

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1534:C:N3	1:A:1535:A:C2	2.53	0.77
19:S:80:TYR:CD1	19:S:81:ARG:N	2.53	0.77
1:A:89:C:C2'	1:A:90:U:O5'	2.33	0.77
27:A:1928:SRV:HI32	27:A:1928:SRV:C22	2.16	0.76
4:D:32:ALA:O	4:D:36:ARG:N	2.17	0.76
1:A:1245:A:C2	1:A:1293:G:C2	2.74	0.76
1:A:1047:G:N7	29:A:2425:HOH:O	2.19	0.76
1:A:266:G:C8	1:A:266:G:C5'	2.69	0.76
7:G:64:GLN:O	7:G:68:ASN:ND2	2.18	0.76
1:A:1268:A:OP1	29:A:2314:HOH:O	2.02	0.76
3:C:11:ARG:NH1	3:C:177:THR:O	2.19	0.76
1:A:1200:C:O2	1:A:1205:U:N3	2.19	0.76
1:A:1493[A]:A:O2'	1:A:1494:G:OP1	2.04	0.75
1:A:1003(A):G:N2	1:A:1038:C:O2	2.19	0.75
10:J:76:ASN:O	10:J:78:ASN:N	2.19	0.75
1:A:461:C:OP2	29:A:2254:HOH:O	2.04	0.75
12:L:117:ARG:O	12:L:119:LYS:N	2.20	0.75
1:A:73:C:N4	1:A:74:C:N4	2.34	0.75
1:A:1256:A:N6	1:A:1277:C:C5	2.54	0.75
1:A:1054:C:OP1	1:A:1197:G:OP2	2.04	0.75
2:B:97:TRP:CE3	2:B:98:LEU:O	2.40	0.75
11:K:18:ARG:NH1	11:K:35:PRO:O	2.19	0.75
1:A:9:G:OP2	5:E:121:LYS:NZ	2.20	0.74
1:A:427:U:OP1	4:D:13:ARG:NH2	2.20	0.74
9:I:118:LYS:O	9:I:120:ARG:N	2.20	0.74
23:W:39:G:N2	23:W:40:PSU:O4	2.21	0.74
10:J:78:ASN:OD1	10:J:79:ARG:NH1	2.21	0.74
2:B:103:THR:N	2:B:176:GLU:OE1	2.20	0.74
1:A:297:G:N7	29:A:2519:HOH:O	2.19	0.74
1:A:348:G:N7	29:A:2636:HOH:O	2.21	0.74
1:A:583:A:OP2	29:A:2103:HOH:O	2.05	0.74
1:A:413:G:O2'	1:A:428:G:N2	2.20	0.74
1:A:331:G:OP2	29:A:2266:HOH:O	2.06	0.74
1:A:949:A:C2	1:A:1233:G:N3	2.56	0.74
1:A:924:C:O2'	1:A:1399:C:C6	2.41	0.73
1:A:289:G:OP2	29:A:2015:HOH:O	2.04	0.73
10:J:55:LYS:CG	10:J:56:HIS:N	2.51	0.73
1:A:1133:G:N2	1:A:1141:C:N3	2.36	0.73
1:A:1361(A):C:O2'	1:A:1362:C:O5'	2.05	0.73
1:A:52:G:O6	29:A:2441:HOH:O	2.06	0.73
1:A:243:A:C2	1:A:246:A:C8	2.76	0.73
1:A:500:G:C6	1:A:501:C:N4	2.58	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:F:74:ASP:OD2	6:F:74:ASP:N	2.19	0.72
1:A:427:U:OP2	1:A:428:G:O2'	2.07	0.72
1:A:421:U:OP2	1:A:422:C:N4	2.22	0.72
1:A:995:C:O2	14:N:4:LYS:NZ	2.23	0.72
1:A:1067:A:O2'	1:A:1093:A:O2'	2.07	0.72
4:D:22:LYS:CB	4:D:26:CYS:SG	2.78	0.72
1:A:928:G:O2'	1:A:1533:C:OP1	2.08	0.72
13:M:19:LEU:O	13:M:22:ILE:CD1	2.37	0.72
1:A:914:A:O5'	27:A:1928:SRV:HI33	1.88	0.72
1:A:1385:G:N7	29:A:2670:HOH:O	2.23	0.72
1:A:1347:G:O2'	1:A:1348:U:OP2	2.08	0.71
3:C:174:PRO:O	3:C:177:THR:N	2.23	0.71
2:B:97:TRP:CZ3	2:B:98:LEU:O	2.43	0.71
10:J:41:PRO:O	10:J:69:ASN:ND2	2.23	0.71
18:R:87:ARG:CG	18:R:87:ARG:NH2	2.53	0.71
1:A:89:C:O2'	1:A:90:U:P	2.49	0.71
1:A:835:U:O4	29:A:2788:HOH:O	2.06	0.71
7:G:120:ILE:N	7:G:120:ILE:CD1	2.52	0.71
1:A:951:G:OP2	13:M:102:ARG:NH2	2.24	0.71
8:H:82:HIS:ND1	8:H:138:TRP:NE1	2.38	0.71
1:A:77:G:C4	1:A:93:G:N2	2.59	0.70
12:L:27:LEU:C	12:L:29:GLY:N	2.45	0.70
1:A:1533:C:O2'	1:A:1534:C:OP1	2.09	0.70
1:A:782:A:OP1	29:A:2280:HOH:O	2.09	0.70
1:A:1534:C:C4	1:A:1535:A:N1	2.59	0.70
1:A:1270:C:OP2	21:U:24:ARG:NH2	2.25	0.70
1:A:1110:A:OP2	29:A:2142:HOH:O	2.09	0.70
1:A:597:G:N2	1:A:643:C:N3	2.40	0.70
1:A:1286:A:C2	21:U:22:ARG:NH2	2.60	0.70
1:A:298:A:N6	29:A:2215:HOH:O	2.25	0.70
1:A:88:A:N7	1:A:89:C:N4	2.39	0.69
4:D:146:ILE:N	4:D:146:ILE:CD1	2.56	0.69
7:G:71:PRO:O	7:G:96:GLN:NE2	2.24	0.69
1:A:606:G:N1	29:A:2550:HOH:O	2.25	0.69
1:A:1454:G:N7	29:A:2825:HOH:O	2.25	0.69
1:A:1130:A:OP1	1:A:1131:G:OP2	2.11	0.69
1:A:1206:G:C6	1:A:1207:2MG:C5	2.81	0.69
4:D:4:TYR:O	4:D:4:TYR:CD2	2.45	0.69
9:I:28:VAL:O	9:I:31:GLN:N	2.25	0.69
1:A:316:G:O2'	29:A:2463:HOH:O	2.10	0.69
1:A:1057:G:C4	1:A:1204:A:C2	2.81	0.69
1:A:1003:G:C2	1:A:1003(A):G:C6	2.81	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
14:N:15:LYS:O	14:N:16:PHE:CD2	2.46	0.69
1:A:79:G:C2	1:A:80:G:C8	2.81	0.69
1:A:119:A:OP2	29:A:2559:HOH:O	2.11	0.69
1:A:117:G:OP2	29:A:2016:HOH:O	2.11	0.68
1:A:1419:G:C6	1:A:1420:C:C4	2.81	0.68
1:A:1249:C:O2'	9:I:73:GLN:NE2	2.27	0.68
2:B:25:ASN:ND2	2:B:193:ASP:CB	2.55	0.68
1:A:1501:C:N4	1:A:1504:G:N3	2.42	0.68
7:G:148:ASN:O	7:G:150:ALA:N	2.25	0.68
6:F:95:GLU:O	18:R:32:ARG:NH1	2.27	0.68
23:W:37:A:N1	23:W:38:A:C2	2.61	0.68
1:A:357:G:N7	29:A:2433:HOH:O	2.27	0.68
1:A:1067:A:O3'	29:A:2218:HOH:O	2.11	0.68
4:D:79:PHE:O	4:D:82:ALA:N	2.27	0.68
3:C:54:ARG:NH1	3:C:56:ASP:OD1	2.27	0.68
27:A:1928:SRY:OG2	12:L:91:LYS:NZ	2.27	0.67
1:A:1003:G:N2	1:A:1039:C:C2	2.61	0.67
4:D:206:PHE:CD2	4:D:207:TYR:CE2	2.81	0.67
1:A:1014:A:N7	1:A:1015:A:C6	2.63	0.67
1:A:1347:G:C2'	1:A:1348:U:OP2	2.41	0.67
1:A:109:A:C6	1:A:326:G:C6	2.83	0.67
1:A:606:G:O6	29:A:2549:HOH:O	2.11	0.67
1:A:1124:G:N7	1:A:1145:C:O2'	2.28	0.67
1:A:1125:U:O2'	1:A:1126:U:OP2	2.13	0.67
1:A:182:U:OP1	29:A:2183:HOH:O	2.11	0.67
1:A:1299:A:C6	1:A:1301:U:O2	2.48	0.67
15:O:88:ARG:CA	15:O:88:ARG:NE	2.57	0.67
17:Q:51:TYR:CE1	17:Q:73:VAL:CG1	2.78	0.66
20:T:44:ALA:O	20:T:47:GLY:N	2.28	0.66
1:A:407:G:OP1	4:D:115:ARG:NH2	2.28	0.66
13:M:16:ASP:O	13:M:19:LEU:N	2.28	0.66
1:A:1068:G:C8	1:A:1068:G:OP2	2.48	0.66
1:A:1328:C:OP1	21:U:21:TYR:OH	2.13	0.66
1:A:1015:A:N6	1:A:1016:A:C6	2.63	0.66
1:A:509:A:O3'	29:A:2165:HOH:O	2.14	0.66
1:A:174:C:OP1	29:A:2211:HOH:O	2.14	0.66
1:A:458:C:OP2	29:A:2257:HOH:O	2.13	0.66
3:C:186:PHE:CD2	3:C:187:ALA:N	2.64	0.66
5:E:13:ILE:CG2	5:E:14:ARG:N	2.59	0.66
1:A:276:G:OP1	17:Q:12:SER:OG	2.14	0.66
1:A:944:G:OP1	29:A:2285:HOH:O	2.14	0.66
4:D:106:TYR:O	4:D:109:GLY:N	2.29	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:191:THR:OG1	3:C:193:TYR:CE1	2.49	0.65
11:K:117:ASN:N	11:K:117:ASN:OD1	2.26	0.65
1:A:1197:G:OP1	29:A:2229:HOH:O	2.14	0.65
1:A:1407:5MC:C4	1:A:1408:A:N7	2.64	0.65
9:I:5:TYR:CD1	9:I:6:GLY:N	2.64	0.65
1:A:858:G:O2'	1:A:859:A:C5'	2.44	0.65
4:D:204:ILE:N	4:D:204:ILE:CD1	2.60	0.65
1:A:913:A:O3'	27:A:1928:SRY:CI3	2.45	0.65
1:A:1294:G:N7	29:A:2265:HOH:O	2.30	0.65
1:A:661:G:N7	29:A:2819:HOH:O	2.30	0.65
12:L:78:GLN:N	12:L:81:SER:OG	2.29	0.65
1:A:1222:G:OP2	1:A:1322:C:N4	2.30	0.65
6:F:5:GLU:OE1	18:R:34:TYR:OH	2.15	0.65
20:T:55:ILE:N	20:T:55:ILE:CD1	2.61	0.65
11:K:27:ASN:OD1	11:K:28:THR:N	2.30	0.64
21:U:10:ARG:NH1	21:U:10:ARG:CG	2.59	0.64
1:A:1129:C:OP1	9:I:62:TYR:OH	2.15	0.64
1:A:976:G:OP2	1:A:1358:U:O2'	2.15	0.64
15:O:14:GLU:CG	15:O:15:PHE:CD1	2.80	0.64
1:A:584:G:OP2	17:Q:87:LYS:NZ	2.31	0.64
6:F:97:PHE:C	6:F:97:PHE:CD2	2.70	0.64
2:B:201:ILE:O	2:B:203:GLY:N	2.31	0.64
3:C:131:ARG:NH1	5:E:50:GLU:OE1	2.31	0.64
1:A:89:C:C5	1:A:90:U:C4	2.84	0.64
1:A:1314:C:OP2	19:S:6:LYS:CD	2.46	0.64
9:I:31:GLN:NE2	9:I:36:TYR:CD1	2.66	0.64
1:A:580:U:OP2	29:A:2740:HOH:O	2.15	0.64
1:A:1330:U:OP1	13:M:23:TYR:O	2.16	0.63
14:N:27:CYS:SG	14:N:29:ARG:CB	2.86	0.63
1:A:1081:G:OP1	5:E:16:THR:OG1	2.16	0.63
1:A:1256:A:C8	1:A:1258:G:N1	2.66	0.63
16:P:58:TYR:CD1	16:P:58:TYR:C	2.72	0.63
1:A:790:A:C8	1:A:791:G:N7	2.67	0.63
1:A:500:G:C6	1:A:546:G:N2	2.66	0.63
1:A:54:C:N3	1:A:352:C:C5	2.67	0.63
3:C:16:ARG:NH2	3:C:183:ASP:OD2	2.32	0.63
1:A:627:G:O6	29:A:2664:HOH:O	2.14	0.63
20:T:61:SER:O	20:T:62:LEU:C	2.37	0.63
1:A:1204:A:OP2	29:A:2248:HOH:O	2.15	0.63
1:A:1130:A:OP1	1:A:1131:G:P	2.56	0.63
1:A:1125:U:O2'	1:A:1126:U:P	2.57	0.63
1:A:1281:U:C4'	1:A:1282:C:OP2	2.47	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
19:S:36:ARG:NH2	19:S:75:ALA:O	2.32	0.63
13:M:59:TYR:CD2	13:M:59:TYR:C	2.69	0.63
1:A:1003(A):G:N1	1:A:1038:C:N3	2.46	0.63
1:A:235:C:N4	29:A:2113:HOH:O	2.31	0.63
1:A:890:G:O2'	1:A:906:G:O6	2.16	0.63
1:A:1003:G:N1	1:A:1003(A):G:O6	2.31	0.62
1:A:837:G:C2	1:A:850:U:O2	2.51	0.62
1:A:1026:G:C8	1:A:1027:C:N3	2.68	0.62
1:A:1057:G:C5	1:A:1204:A:C2	2.87	0.62
23:W:37:A:N6	23:W:38:A:N1	2.47	0.62
1:A:1160:G:O6	1:A:1181:G:O6	2.16	0.62
7:G:17:VAL:CG1	7:G:18:TYR:N	2.62	0.62
1:A:506:G:C5	1:A:507:C:C5	2.87	0.62
1:A:35:G:C6	1:A:36:C:N4	2.68	0.62
1:A:984:C:N3	1:A:1221:G:N2	2.47	0.62
4:D:31:CYS:SG	4:D:31:CYS:O	2.57	0.62
1:A:544:G:C5	1:A:545:C:C5	2.88	0.62
1:A:792:A:C4'	1:A:793:U:OP1	2.48	0.62
2:B:178:ARG:NH1	2:B:198:ASP:OD1	2.33	0.62
1:A:414:A:C2	1:A:415:A:N9	2.68	0.62
1:A:415:A:C4	1:A:416:G:C8	2.88	0.62
9:I:125:TYR:CD2	9:I:125:TYR:N	2.67	0.62
1:A:88:A:C5	1:A:89:C:N3	2.68	0.61
2:B:193:ASP:C	2:B:193:ASP:OD1	2.38	0.61
10:J:47:PHE:CZ	14:N:37:PHE:CE1	2.88	0.61
11:K:125:PHE:N	11:K:125:PHE:CD2	2.68	0.61
6:F:83:ASP:N	6:F:83:ASP:OD1	2.32	0.61
1:A:986:A:C2	1:A:1220:G:C2	2.88	0.61
4:D:36:ARG:CB	4:D:38:TYR:CE2	2.83	0.61
1:A:1385:G:C5	29:A:2670:HOH:O	2.52	0.61
8:H:104:ARG:CZ	8:H:138:TRP:CZ2	2.82	0.61
1:A:1536:C:C5	1:A:1537:U:C2	2.87	0.61
1:A:544:G:C6	1:A:545:C:C5	2.89	0.61
1:A:1498:UR3:C4'	1:A:1519[A]:MA6:C2	2.78	0.61
1:A:892:A:C2	1:A:907:A:C4	2.89	0.61
1:A:914:A:P	27:A:1928:SRY:CI3	2.87	0.61
1:A:544:G:C4	1:A:545:C:C6	2.89	0.61
1:A:304:U:C4	29:A:2495:HOH:O	2.48	0.61
20:T:22:ARG:O	20:T:23:ARG:C	2.38	0.61
11:K:79:SER:OG	11:K:106:LYS:NZ	2.34	0.61
1:A:191:G:N3	20:T:103:GLY:O	2.34	0.61
5:E:95:ALA:O	5:E:98:THR:OG1	2.17	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:543:C:C2'	1:A:544:G:C5'	2.79	0.61
1:A:53:A:C6	1:A:54:C:C5	2.89	0.61
1:A:289:G:P	29:A:2015:HOH:O	2.57	0.61
14:N:15:LYS:O	14:N:16:PHE:CG	2.53	0.61
23:W:32:C:O2'	23:W:33:U:O4'	2.17	0.61
17:Q:29:HIS:C	17:Q:29:HIS:ND1	2.54	0.61
20:T:10:LEU:CD2	20:T:13:LEU:N	2.64	0.61
1:A:1399:C:O2	1:A:1401:G:C4	2.54	0.61
1:A:1035:A:N6	1:A:1036:G:O6	2.33	0.61
1:A:182:U:C5	1:A:183:G:N9	2.69	0.61
8:H:112:LEU:CD2	8:H:112:LEU:N	2.64	0.61
17:Q:83:ASP:OD1	17:Q:84:LEU:N	2.34	0.60
1:A:1015:A:C6	1:A:1016:A:C6	2.89	0.60
17:Q:40:LYS:CD	17:Q:42:TYR:CE1	2.83	0.60
1:A:386:C:O2'	29:A:2002:HOH:O	2.15	0.60
1:A:644:G:C5	1:A:645:C:C5	2.89	0.60
1:A:1454:G:O6	29:A:2826:HOH:O	2.16	0.60
9:I:27:THR:OG1	9:I:31:GLN:O	2.19	0.60
1:A:1065:U:O2'	1:A:1066:C:OP2	2.19	0.60
1:A:1279:A:C4'	1:A:1280:A:OP1	2.50	0.60
8:H:102:ARG:N	8:H:102:ARG:CD	2.64	0.60
4:D:150:GLU:O	4:D:153:ARG:N	2.34	0.60
1:A:1027:C:C5	1:A:1035:A:N1	2.69	0.60
1:A:28:G:O2'	1:A:296:U:OP1	2.20	0.60
7:G:12:LEU:N	7:G:12:LEU:CD1	2.64	0.60
1:A:14:U:O2	1:A:16:A:C8	2.54	0.60
1:A:1500:A:OP2	1:A:1505:G:OP1	2.19	0.60
1:A:875:C:O2'	8:H:14:ARG:NH1	2.35	0.60
1:A:44:G:N2	1:A:399:G:C4	2.70	0.60
10:J:63:PHE:CD1	10:J:63:PHE:N	2.68	0.60
4:D:79:PHE:CD2	4:D:79:PHE:C	2.75	0.60
1:A:1126:U:C4	1:A:1127:G:C2	2.89	0.60
1:A:31:G:N2	1:A:48:C:OP1	2.34	0.60
11:K:91:ARG:O	11:K:94:ALA:N	2.35	0.60
2:B:240:GLN:O	2:B:240:GLN:CG	2.50	0.60
3:C:14:ILE:O	3:C:16:ARG:N	2.35	0.60
1:A:1004:A:N7	1:A:1037:C:N3	2.49	0.60
23:W:37:A:C6	23:W:38:A:C2	2.89	0.60
1:A:1049:U:C4'	1:A:1050:G:O5'	2.50	0.60
1:A:499:A:C4'	1:A:500:G:OP1	2.49	0.60
1:A:254:G:OP1	17:Q:67:LYS:O	2.20	0.60
5:E:126:ARG:CG	5:E:126:ARG:NH1	2.65	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1503:A:C4	1:A:1531:A:C2	2.90	0.59
13:M:78:ILE:O	13:M:81:LEU:N	2.34	0.59
1:A:1060:C:O2	1:A:1198:G:C2	2.55	0.59
19:S:34:TRP:CZ2	19:S:57:HIS:CE1	2.90	0.59
1:A:1027:C:O4'	1:A:1027:C:O2	2.17	0.59
1:A:182:U:C5	1:A:183:G:C1'	2.85	0.59
1:A:1060:C:C2	1:A:1198:G:N1	2.70	0.59
1:A:89:C:O2'	1:A:90:U:O5'	2.19	0.59
7:G:52:GLU:N	7:G:52:GLU:OE1	2.35	0.59
1:A:1026:G:N7	1:A:1027:C:N3	2.50	0.59
1:A:1130:A:P	1:A:1131:G:OP2	2.60	0.59
1:A:399:G:OP1	29:A:2086:HOH:O	2.17	0.59
1:A:1399:C:O2	1:A:1401:G:C8	2.55	0.59
16:P:82:GLN:O	16:P:84:ALA:N	2.35	0.59
1:A:380:G:N7	29:A:2680:HOH:O	2.35	0.59
1:A:504:C:OP1	29:A:2163:HOH:O	2.17	0.59
10:J:49:VAL:O	10:J:61:GLU:N	2.36	0.59
19:S:22:LEU:O	19:S:26:GLY:O	2.21	0.59
1:A:500:G:C6	1:A:501:C:C4	2.91	0.59
1:A:994:A:C2	1:A:995:C:C6	2.90	0.59
2:B:105:PHE:O	2:B:109:SER:OG	2.20	0.59
1:A:1256:A:N6	1:A:1277:C:C6	2.71	0.59
1:A:1126:U:O4	1:A:1127:G:N2	2.35	0.59
1:A:923:A:O4'	1:A:1398:A:C2	2.56	0.58
19:S:12:ASP:O	19:S:15:LEU:CD1	2.51	0.58
5:E:15:ARG:NH1	5:E:26:PHE:CE2	2.71	0.58
1:A:35:G:O2'	12:L:118:SER:O	2.20	0.58
1:A:510:A:O2'	1:A:542:G:O2'	2.20	0.58
1:A:1332:A:C2	1:A:1333:A:C4	2.91	0.58
1:A:345:C:C6	1:A:345:C:OP2	2.56	0.58
3:C:186:PHE:CD2	3:C:186:PHE:C	2.76	0.58
1:A:11:G:O6	29:A:2647:HOH:O	2.16	0.58
9:I:55:ALA:O	9:I:56:LEU:C	2.42	0.58
1:A:1147:C:O2	9:I:16:ARG:NH2	2.37	0.58
15:O:62:GLN:O	15:O:63:ARG:C	2.39	0.58
1:A:1371:G:C5	1:A:1372:U:C5	2.90	0.58
1:A:1035:A:C6	1:A:1036:G:O6	2.57	0.58
1:A:922:G:O2'	1:A:1398:A:N1	2.37	0.58
1:A:1003:G:N1	1:A:1003(A):G:C6	2.71	0.58
13:M:86:CYS:SG	13:M:87:TYR:N	2.77	0.58
1:A:1424:C:C4	1:A:1425:U:C5	2.91	0.58
1:A:1407:5MC:N3	1:A:1494:G:N2	2.52	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1054:C:O2'	1:A:1055:A:O5'	2.22	0.58
1:A:1124:G:O2'	1:A:1145:C:N4	2.36	0.58
1:A:409:G:OP1	4:D:24:GLU:O	2.21	0.58
1:A:1501:C:C4	1:A:1504:G:C4	2.92	0.58
1:A:201:C:N3	1:A:216:G:N2	2.52	0.58
3:C:151:VAL:O	3:C:167:TRP:O	2.20	0.58
1:A:150:C:C2'	1:A:151:A:O5'	2.51	0.58
1:A:1250:A:C2	1:A:1287:A:C2	2.91	0.58
1:A:297:G:N2	1:A:300:A:OP2	2.37	0.57
1:A:115:G:O2'	1:A:116:A:OP2	2.22	0.57
1:A:1005:A:C6	1:A:1026:G:N2	2.73	0.57
1:A:1501:C:N4	1:A:1504:G:C2	2.72	0.57
1:A:540:G:C6	1:A:541:G:C5	2.92	0.57
1:A:409:G:N2	1:A:434:U:C5	2.72	0.57
1:A:909:A:C8	1:A:910:C:C6	2.91	0.57
4:D:150:GLU:N	4:D:150:GLU:CD	2.57	0.57
1:A:53:A:N6	1:A:54:C:C4	2.73	0.57
1:A:1347:G:C3'	9:I:108:VAL:O	2.52	0.57
1:A:1212:U:C1'	1:A:1213:A:OP2	2.52	0.57
1:A:1193:G:C2	1:A:1194:U:C5	2.92	0.57
1:A:1419:G:O6	1:A:1420:C:N4	2.38	0.57
5:E:9:LYS:NZ	5:E:111:GLU:OE1	2.38	0.57
1:A:839:U:C2'	1:A:839:U:O2	2.52	0.57
12:L:92:0TD:N	12:L:92:0TD:OD1	2.36	0.57
7:G:38:LEU:O	7:G:42:ILE:CG1	2.52	0.57
1:A:293:G:C4	1:A:305:G:N2	2.72	0.57
1:A:571:U:C5'	1:A:572:A:OP2	2.52	0.57
9:I:28:VAL:N	9:I:31:GLN:O	2.38	0.57
16:P:67:THR:CG2	16:P:68:ASP:N	2.63	0.57
3:C:10:PHE:C	3:C:10:PHE:CD1	2.77	0.57
1:A:315:A:OP1	29:A:2576:HOH:O	2.17	0.57
1:A:1533:C:O2'	1:A:1534:C:P	2.63	0.57
1:A:1494:G:N3	1:A:1495:U:C6	2.73	0.57
1:A:540:G:C4	1:A:541:G:C8	2.92	0.57
4:D:79:PHE:CD2	4:D:80:GLU:N	2.73	0.57
1:A:1124:G:O2'	1:A:1145:C:C5	2.58	0.57
13:M:87:TYR:C	13:M:87:TYR:CD1	2.77	0.57
5:E:65:ASN:ND2	5:E:65:ASN:O	2.38	0.57
2:B:170:GLU:O	2:B:173:ALA:N	2.38	0.57
1:A:975:A:C5'	1:A:975:A:C8	2.87	0.57
12:L:53:ARG:NH1	12:L:92:0TD:OD2	2.38	0.57
1:A:910:C:OP2	12:L:21:LYS:NZ	2.38	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:H:17:THR:O	8:H:78:GLN:NE2	2.38	0.57
1:A:1128:C:O2'	1:A:1130:A:C8	2.58	0.56
13:M:87:TYR:O	13:M:90:LEU:N	2.38	0.56
5:E:117:ASP:OD2	5:E:117:ASP:N	2.37	0.56
13:M:4:ILE:CG2	13:M:5:ALA:N	2.68	0.56
16:P:23:ASP:OD1	16:P:24:ALA:N	2.39	0.56
1:A:1054:C:N3	23:W:34:G:C5'	2.68	0.56
3:C:174:PRO:O	3:C:176:HIS:N	2.38	0.56
1:A:994:A:C2	1:A:995:C:C5	2.92	0.56
1:A:1126:U:O4	1:A:1127:G:C2	2.58	0.56
1:A:1507:A:C8	1:A:1530:G:N2	2.73	0.56
9:I:108:VAL:CG1	9:I:109:VAL:N	2.68	0.56
1:A:9:G:OP1	5:E:122:GLU:CG	2.53	0.56
23:W:39:G:C2	23:W:40:PSU:N3	2.74	0.56
13:M:87:TYR:CE1	13:M:91:ARG:CD	2.88	0.56
17:Q:100:LYS:CB	17:Q:101:ARG:HH11	2.18	0.56
1:A:563:A:O2'	1:A:566:G:O2'	2.24	0.56
1:A:854:G:N2	1:A:855:G:C4	2.74	0.56
1:A:1534:C:C2	1:A:1535:A:C2	2.93	0.56
1:A:1005:A:C8	1:A:1026:G:N1	2.73	0.56
1:A:1404:5MC:C1'	1:A:1499:A:C2	2.89	0.56
1:A:945:G:N1	1:A:1337:G:C2	2.73	0.56
1:A:1499:A:OP1	1:A:1519[A]:MA6:N1	2.38	0.56
10:J:76:ASN:C	10:J:78:ASN:N	2.59	0.56
2:B:97:TRP:CH2	2:B:176:GLU:OE2	2.58	0.56
1:A:182:U:C5	1:A:183:G:C4	2.94	0.56
16:P:57:ARG:O	16:P:58:TYR:C	2.40	0.56
1:A:102:G:O2'	1:A:151:A:N3	2.39	0.56
1:A:1250:A:C2	1:A:1287:A:N1	2.74	0.56
1:A:609:A:N6	29:A:2320:HOH:O	2.39	0.56
12:L:47:LYS:N	12:L:48:PRO:CD	2.68	0.56
11:K:122:LYS:O	11:K:124:LYS:N	2.39	0.56
1:A:89:C:O2'	1:A:90:U:OP1	2.23	0.56
1:A:427:U:C4	1:A:428:G:C6	2.94	0.56
1:A:1014:A:N7	1:A:1015:A:N6	2.54	0.56
1:A:908:A:C2	1:A:909:A:C4	2.94	0.56
11:K:110:ASP:N	18:R:85:LEU:O	2.39	0.56
1:A:1407:5MC:C2	1:A:1408:A:C8	2.94	0.56
15:O:12:ILE:C	15:O:14:GLU:N	2.57	0.56
1:A:1536:C:C5	1:A:1537:U:N3	2.74	0.56
1:A:559:A:OP1	5:E:126:ARG:NH2	2.39	0.56
1:A:186:C:O2'	20:T:85:MET:SD	2.63	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
18:R:37:VAL:O	18:R:39:VAL:N	2.39	0.56
1:A:273:A:N6	1:A:274:A:C6	2.73	0.56
1:A:137:C:C2'	1:A:138:G:C5'	2.84	0.56
1:A:500:G:O6	1:A:501:C:N4	2.39	0.55
9:I:27:THR:OG1	9:I:28:VAL:N	2.39	0.55
8:H:124:ALA:O	8:H:128:GLY:N	2.38	0.55
1:A:190(E):U:C5	17:Q:72:ARG:NH2	2.74	0.55
15:O:17:ARG:NH1	15:O:17:ARG:CG	2.69	0.55
1:A:1399:C:O2	1:A:1401:G:N7	2.38	0.55
1:A:1436:U:C2	1:A:1437:C:C6	2.93	0.55
1:A:21:G:P	29:A:2044:HOH:O	2.65	0.55
13:M:99:ARG:NH2	19:S:2:PRO:CG	2.70	0.55
8:H:36:LEU:O	8:H:37:ARG:C	2.44	0.55
5:E:11:ILE:CG2	5:E:12:LEU:N	2.68	0.55
3:C:8:ILE:CG2	3:C:9:GLY:N	2.70	0.55
1:A:1131:G:C8	1:A:1131:G:OP2	2.59	0.55
1:A:414:A:C2	1:A:415:A:C4	2.93	0.55
1:A:1360:A:C2'	1:A:1361:G:O5'	2.54	0.55
1:A:1027:C:O2'	1:A:1034:G:N2	2.40	0.55
2:B:8:LYS:C	2:B:10:LEU:N	2.58	0.55
1:A:547:A:OP2	4:D:2:GLY:CA	2.55	0.55
1:A:836:G:OP1	18:R:61:LYS:NZ	2.40	0.55
1:A:255:G:O6	1:A:266:G:O6	2.25	0.55
1:A:1256:A:C8	1:A:1258:G:C2	2.94	0.55
1:A:261:U:O2	1:A:263:A:C8	2.60	0.55
1:A:746:A:C2'	1:A:747:C:C5'	2.85	0.55
1:A:838:G:N2	1:A:849:C:C2	2.75	0.55
1:A:581:G:O3'	15:O:64:ARG:NH2	2.39	0.55
8:H:57:PRO:CG	8:H:57:PRO:O	2.53	0.55
1:A:1139:G:N2	1:A:1143:G:N2	2.54	0.55
1:A:1028:C:N3	1:A:1034:G:C2	2.75	0.55
1:A:103:C:O2'	1:A:172:A:N1	2.40	0.55
1:A:545:C:O2	1:A:546:G:O4'	2.25	0.55
1:A:1027:C:C5	1:A:1035:A:C2	2.95	0.55
1:A:1206:G:C6	1:A:1207:2MG:C6	2.94	0.55
1:A:1376:U:OP1	7:G:98:SER:OG	2.25	0.55
1:A:357:G:C2	1:A:358:U:C5	2.95	0.55
1:A:421:U:O2	1:A:421:U:O4'	2.25	0.54
1:A:1160:G:O6	1:A:1181:G:C6	2.60	0.54
18:R:45:SER:OG	18:R:46:GLU:N	2.38	0.54
12:L:76:ASN:O	12:L:76:ASN:CG	2.45	0.54
1:A:1515[A]:C:N3	1:A:1520[A]:G:N2	2.55	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1346:A:C5	7:G:10:ARG:NH1	2.75	0.54
3:C:130:VAL:O	3:C:134:ILE:CD1	2.56	0.54
1:A:1500:A:P	1:A:1505:G:OP1	2.65	0.54
1:A:1030(A):G:C4	1:A:1030(C):G:OP2	2.60	0.54
1:A:860:A:OP2	29:A:2124:HOH:O	2.18	0.54
1:A:1381:U:C6	1:A:1382:C:C5	2.96	0.54
1:A:1497:G:C2'	1:A:1498:UR3:C5'	2.85	0.54
1:A:568:G:N2	1:A:883:C:C2	2.75	0.54
10:J:29:ARG:CD	10:J:29:ARG:N	2.70	0.54
1:A:529:G:C8	1:A:529:G:C3'	2.89	0.54
5:E:144:THR:CG2	5:E:145:LYS:N	2.70	0.54
1:A:22:G:C6	1:A:23:C:C4	2.96	0.54
1:A:22:G:C5	1:A:23:C:C5	2.96	0.54
4:D:63:LYS:NZ	4:D:197:PRO:O	2.40	0.54
12:L:52:LEU:O	12:L:54:LYS:NZ	2.41	0.54
1:A:1108:G:O6	29:A:2136:HOH:O	2.16	0.54
3:C:127:ARG:NE	3:C:127:ARG:CA	2.69	0.54
1:A:53:A:C6	1:A:54:C:C4	2.96	0.54
1:A:380:G:C8	29:A:2680:HOH:O	2.54	0.54
1:A:991:U:O2'	1:A:992:U:P	2.66	0.54
8:H:4:ASP:OD1	8:H:6:ILE:N	2.40	0.54
20:T:82:SER:O	20:T:83:ARG:C	2.44	0.54
1:A:989:C:O2	1:A:1216:G:N2	2.40	0.54
17:Q:90:ILE:O	17:Q:91:ARG:C	2.46	0.54
1:A:89:C:C6	1:A:90:U:N3	2.75	0.54
1:A:1006:C:N3	1:A:1023:G:N2	2.56	0.54
1:A:119:A:P	29:A:2559:HOH:O	2.64	0.54
3:C:54:ARG:O	3:C:69:HIS:N	2.41	0.54
1:A:1147:C:O2'	9:I:5:TYR:OH	2.26	0.54
17:Q:81:ARG:NE	17:Q:84:LEU:CD1	2.71	0.54
1:A:1279:A:C5'	1:A:1280:A:OP1	2.56	0.54
1:A:1327:C:OP2	21:U:12:LYS:NZ	2.41	0.54
1:A:257:G:C2	1:A:270:A:C2	2.94	0.54
5:E:107:ARG:O	5:E:108:ALA:C	2.46	0.54
3:C:3:ASN:N	3:C:3:ASN:OD1	2.40	0.54
9:I:121:ARG:CG	9:I:121:ARG:NH1	2.69	0.54
1:A:500:G:C6	1:A:546:G:C2	2.96	0.54
1:A:1055:A:C8	1:A:1206:G:N2	2.76	0.54
1:A:983:A:OP1	14:N:3:ARG:NH2	2.41	0.54
14:N:9:LYS:O	14:N:11:LYS:N	2.40	0.54
1:A:507:C:OP2	1:A:508:C:O2'	2.25	0.54
1:A:1004:A:C5'	29:A:2327:HOH:O	2.55	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1206:G:C4	1:A:1207:2MG:C8	2.96	0.53
1:A:1190:G:C5'	1:A:1190:G:C8	2.91	0.53
3:C:86:VAL:O	3:C:89:GLU:CB	2.57	0.53
19:S:31:ILE:O	19:S:50:ALA:CB	2.56	0.53
6:F:98:LEU:N	6:F:98:LEU:CD1	2.71	0.53
8:H:54:ASP:CG	8:H:55:GLY:N	2.61	0.53
1:A:1502:A:C2'	1:A:1502:A:N3	2.70	0.53
1:A:602:A:C2	1:A:637:G:C2	2.96	0.53
17:Q:59:ILE:CG2	17:Q:71:PHE:CD1	2.90	0.53
1:A:1054:C:N4	23:W:34:G:C8	2.76	0.53
23:W:31:C:N4	23:W:39:G:N1	2.49	0.53
11:K:56:GLY:O	11:K:57:THR:C	2.45	0.53
2:B:170:GLU:CA	2:B:170:GLU:OE2	2.54	0.53
6:F:50:TYR:CE1	18:R:77:GLY:CA	2.91	0.53
1:A:1055:A:C8	1:A:1206:G:C2	2.96	0.53
1:A:1413:A:C2	1:A:1414:U:C2	2.97	0.53
1:A:1133:G:N2	1:A:1141:C:C2	2.77	0.53
2:B:16:HIS:CD2	2:B:17:PHE:CD2	2.96	0.53
7:G:62:PHE:CD1	7:G:62:PHE:C	2.79	0.53
1:A:1026:G:C8	1:A:1027:C:C2	2.96	0.53
1:A:392:G:N3	1:A:393:A:C8	2.77	0.53
1:A:1148:U:C2'	1:A:1149:C:O4'	2.57	0.53
23:W:35:G:N3	23:W:36:A:C8	2.76	0.53
4:D:28:SER:O	4:D:30:LYS:N	2.41	0.53
12:L:70:ILE:CG2	12:L:75:HIS:CD2	2.92	0.53
1:A:1026:G:C8	1:A:1027:C:O2	2.62	0.53
1:A:1303:C:N4	1:A:1304:G:C6	2.77	0.53
1:A:1407:5MC:N3	1:A:1408:A:C8	2.77	0.53
1:A:922:G:C6	1:A:923:A:C6	2.97	0.53
2:B:100:GLY:CA	2:B:176:GLU:OE2	2.55	0.53
17:Q:18:THR:OG1	17:Q:69:LYS:NZ	2.42	0.53
1:A:1035:A:C4	1:A:1036:G:N7	2.76	0.53
1:A:1077:G:N2	1:A:1081:G:C4	2.77	0.53
1:A:1004:A:O2'	1:A:1005:A:OP1	2.27	0.53
1:A:279:A:OP1	1:A:280:C:O2'	2.27	0.53
10:J:61:GLU:CG	10:J:61:GLU:O	2.57	0.53
1:A:781:A:C5	1:A:802:A:C2	2.97	0.53
20:T:105:SER:O	20:T:106:ALA:OXT	2.27	0.53
1:A:643:C:C2'	1:A:644:G:C5'	2.87	0.52
1:A:978:A:O2'	1:A:1322:C:O2	2.27	0.52
4:D:177:ASP:OD1	4:D:180:GLY:N	2.42	0.52
1:A:437:U:OP2	29:A:2795:HOH:O	2.19	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:375:U:C4	1:A:376:G:N7	2.77	0.52
11:K:40:ILE:CG2	11:K:75:TYR:CD1	2.92	0.52
1:A:1054:C:N4	23:W:34:G:OP1	2.41	0.52
5:E:152:ARG:O	8:H:64:LYS:NZ	2.42	0.52
11:K:120:ARG:CG	11:K:120:ARG:NH1	2.72	0.52
1:A:229:U:C2'	1:A:230:G:C5'	2.87	0.52
1:A:35:G:C5	1:A:36:C:C5	2.97	0.52
1:A:1005:A:OP2	1:A:1006:C:C5	2.62	0.52
1:A:1054:C:C4	23:W:34:G:OP1	2.63	0.52
1:A:1003(A):G:N1	1:A:1038:C:C2	2.77	0.52
11:K:32:ILE:O	11:K:40:ILE:N	2.42	0.52
1:A:1350:A:C5	1:A:1351:U:C5	2.97	0.52
2:B:204:ASN:C	2:B:204:ASN:OD1	2.47	0.52
1:A:837:G:N2	1:A:850:U:O2	2.42	0.52
3:C:123:GLN:O	3:C:128:PHE:CB	2.58	0.52
2:B:212:GLN:NE2	2:B:235:SER:CB	2.72	0.52
1:A:259:G:C2'	1:A:260:G:O5'	2.58	0.52
1:A:1085:U:C6	1:A:1094:G:N1	2.78	0.52
1:A:509:A:C3'	1:A:509:A:C8	2.92	0.52
1:A:191:G:O2'	20:T:101:GLY:O	2.28	0.52
1:A:171:A:P	29:A:2844:HOH:O	2.68	0.52
1:A:1190:G:O2'	1:A:1191:A:O5'	2.27	0.52
1:A:440:A:C5'	1:A:442:C:OP2	2.58	0.52
7:G:89:MET:SD	7:G:156:TRP:CZ3	3.03	0.52
1:A:35:G:C4	1:A:36:C:C5	2.98	0.52
1:A:1494:G:C2	1:A:1495:U:C6	2.98	0.52
1:A:512:U:O2	1:A:540:G:C2	2.62	0.52
1:A:414:A:C2	1:A:415:A:C8	2.98	0.52
1:A:1288:A:N6	1:A:1289:A:N6	2.57	0.52
1:A:909:A:C8	1:A:910:C:C5	2.98	0.52
1:A:504:C:C2	1:A:542:G:N2	2.78	0.52
1:A:60:A:OP1	1:A:331:G:N1	2.43	0.52
1:A:1124:G:C8	1:A:1145:C:C6	2.98	0.52
1:A:443:C:N3	1:A:491:G:N2	2.58	0.52
5:E:55:VAL:O	5:E:56:GLN:C	2.47	0.51
1:A:1009:G:N2	1:A:1010:G:C4	2.78	0.51
1:A:1206:G:C5	1:A:1207:2MG:N7	2.78	0.51
1:A:1103:C:OP1	2:B:96:ARG:NH1	2.43	0.51
1:A:1031:G:N2	1:A:1032:G:C4	2.78	0.51
1:A:328:C:C2'	1:A:329:A:OP2	2.58	0.51
1:A:988:G:C2	1:A:1218:C:O2	2.64	0.51
10:J:47:PHE:CD2	14:N:34:TYR:CD2	2.99	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:747:C:C2'	1:A:748:C:O5'	2.58	0.51
11:K:122:LYS:O	11:K:123:LYS:C	2.47	0.51
1:A:1407:5MC:N3	1:A:1408:A:N7	2.58	0.51
1:A:1061:G:C6	1:A:1062:U:N3	2.78	0.51
14:N:24:CYS:SG	14:N:40:CYS:N	2.83	0.51
13:M:65:LYS:NZ	13:M:73:GLU:OE2	2.43	0.51
1:A:1408:A:C4	1:A:1409:C:C5	2.99	0.51
1:A:1152:A:OP1	10:J:68:HIS:CE1	2.63	0.51
23:W:35:G:C4	23:W:36:A:N7	2.79	0.51
1:A:658:G:C2	1:A:749:C:N3	2.79	0.51
1:A:1060:C:OP1	14:N:45:ARG:NH2	2.44	0.51
1:A:23:C:N4	29:A:2650:HOH:O	2.43	0.51
15:O:9:GLN:CA	15:O:9:GLN:OE1	2.58	0.51
9:I:29:ASN:ND2	9:I:29:ASN:O	2.44	0.51
1:A:429:U:O2	1:A:430:A:C8	2.64	0.51
1:A:1055:A:N7	1:A:1206:G:C2	2.79	0.51
1:A:278:G:OP2	17:Q:41:LYS:NZ	2.44	0.51
1:A:1148:U:C4	1:A:1149:C:C2	2.99	0.51
1:A:1163:C:C2	1:A:1174:G:N2	2.79	0.51
4:D:70:ILE:CG2	4:D:71:SER:O	2.59	0.51
1:A:1534:C:C4	1:A:1535:A:C2	2.99	0.51
23:W:39:G:C2	23:W:40:PSU:O4	2.64	0.51
1:A:1126:U:O4	1:A:1127:G:N1	2.44	0.51
1:A:191:G:N2	20:T:103:GLY:O	2.43	0.51
1:A:22:G:C4	1:A:23:C:C5	2.99	0.51
2:B:83:MET:SD	2:B:234:PRO:O	2.69	0.51
1:A:1392:G:C2'	1:A:1393:U:C5'	2.89	0.51
3:C:29:TYR:OH	14:N:54:PRO:O	2.29	0.51
1:A:1225:A:C5'	1:A:1226:C:OP2	2.58	0.51
1:A:352:C:C3'	1:A:352:C:C6	2.94	0.51
1:A:922:G:C2	1:A:1396:A:C6	2.98	0.51
1:A:1048:G:C6	1:A:1210:C:N4	2.79	0.51
4:D:61:LYS:CD	4:D:61:LYS:C	2.79	0.51
4:D:61:LYS:NZ	4:D:72:GLU:OE2	2.44	0.51
17:Q:11:VAL:CG1	17:Q:88:TYR:CD2	2.94	0.51
1:A:134:A:N6	16:P:25:ARG:NH2	2.59	0.51
7:G:127:ALA:O	7:G:130:GLY:N	2.44	0.50
4:D:92:VAL:O	4:D:93:PHE:C	2.47	0.50
1:A:475:G:O6	29:A:2600:HOH:O	2.20	0.50
1:A:928:G:C2	1:A:1390:U:O2	2.65	0.50
2:B:100:GLY:O	2:B:101:MET:C	2.49	0.50
3:C:113:ALA:N	3:C:183:ASP:OD1	2.44	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
17:Q:40:LYS:CD	17:Q:42:TYR:CZ	2.94	0.50
1:A:1375:A:C5	1:A:1376:U:C5	2.99	0.50
1:A:1297:C:O2'	1:A:1298:C:OP2	2.29	0.50
1:A:1136:U:C5'	1:A:1137:C:OP2	2.58	0.50
1:A:1110:A:N7	29:A:2140:HOH:O	2.35	0.50
1:A:976:G:C8	1:A:1358:U:C2	2.99	0.50
1:A:652:U:O4	1:A:752:G:O2'	2.29	0.50
9:I:9:ARG:CB	9:I:13:ALA:O	2.59	0.50
1:A:1052:U:C2'	1:A:1055:A:OP1	2.59	0.50
1:A:1349:A:C2	1:A:1374:A:C4	3.00	0.50
1:A:1073:U:O2	2:B:104:ASN:ND2	2.45	0.50
1:A:811:C:O2'	1:A:901:A:N1	2.45	0.50
8:H:18:ARG:NH2	8:H:81:HIS:O	2.45	0.50
1:A:821:G:C4'	29:A:2105:HOH:O	2.59	0.50
2:B:57:PHE:CG	2:B:199:TYR:CE1	2.99	0.50
18:R:37:VAL:O	18:R:38:GLU:C	2.49	0.50
1:A:1517[A]:G:C6	1:A:1518[A]:MA6:C5	2.95	0.50
4:D:4:TYR:OH	4:D:7:PRO:O	2.30	0.50
1:A:1438:G:C6	1:A:1439:C:C4	2.99	0.50
12:L:55:VAL:CG1	12:L:67:THR:OG1	2.59	0.50
2:B:238:LEU:CD2	2:B:238:LEU:O	2.60	0.50
1:A:768:A:C5	1:A:769:G:C8	2.99	0.50
1:A:83:U:C5	1:A:84:U:C6	3.00	0.50
1:A:53:A:OP2	29:A:2222:HOH:O	2.19	0.50
2:B:97:TRP:CZ3	2:B:176:GLU:OE2	2.65	0.50
14:N:13:THR:N	14:N:14:PRO:CD	2.75	0.50
23:W:35:G:C4	23:W:36:A:C8	2.99	0.50
1:A:491:G:C4	1:A:492:G:C8	3.00	0.50
8:H:87:SER:OG	8:H:93:VAL:N	2.44	0.50
17:Q:53:LEU:CD1	17:Q:54:GLY:N	2.74	0.50
1:A:653:A:OP1	8:H:56:LYS:NZ	2.45	0.50
5:E:37:ARG:CG	5:E:37:ARG:NH1	2.75	0.50
1:A:426:G:OP1	4:D:38:TYR:OH	2.29	0.50
7:G:48:LYS:O	7:G:52:GLU:OE2	2.30	0.50
13:M:4:ILE:O	13:M:6:GLY:O	2.30	0.50
16:P:1:MET:CG	16:P:1:MET:O	2.60	0.50
1:A:1057:G:C5'	3:C:154:SER:OG	2.60	0.49
1:A:1126:U:C2'	1:A:1127:G:O5'	2.59	0.49
1:A:1536:C:C5	1:A:1537:U:C4	3.00	0.49
4:D:180:GLY:O	4:D:182:LYS:CG	2.60	0.49
1:A:1368:G:OP2	9:I:114:TYR:N	2.45	0.49
2:B:195:ASP:O	8:H:68:ARG:NH2	2.45	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:540:G:C5	1:A:541:G:N7	2.80	0.49
1:A:1031:G:C2	1:A:1032:G:C5	3.00	0.49
1:A:561:U:O2'	1:A:562:C:OP1	2.30	0.49
23:W:30:G:N3	23:W:30:G:H2'	2.27	0.49
1:A:1090:U:C2	1:A:1091:U:C6	3.00	0.49
12:L:27:LEU:CG	12:L:28:LYS:N	2.75	0.49
4:D:61:LYS:CD	4:D:62:GLN:N	2.75	0.49
7:G:72:ARG:NH1	7:G:142:GLU:OE2	2.46	0.49
11:K:43:SER:OG	11:K:44:SER:N	2.45	0.49
5:E:24:ARG:CG	5:E:24:ARG:NH1	2.75	0.49
1:A:1026:G:C2'	1:A:1027:C:OP1	2.60	0.49
1:A:1300:G:C6	1:A:1335:C:C5	3.01	0.49
1:A:1441:G:O2'	1:A:1442:G:N2	2.45	0.49
1:A:1425:U:C2	1:A:1426:C:C5	3.00	0.49
1:A:854:G:N1	1:A:855:G:C5	2.80	0.49
1:A:491:G:N3	1:A:492:G:C8	2.80	0.49
1:A:1493[B]:A:O2'	1:A:1494:G:C8	2.66	0.49
8:H:21:LYS:O	8:H:65:TYR:OH	2.29	0.49
10:J:30:SER:CB	10:J:80:LYS:CB	2.91	0.49
15:O:56:LEU:C	15:O:56:LEU:CD1	2.80	0.49
2:B:28:PHE:CD2	2:B:28:PHE:O	2.66	0.49
1:A:544:G:C2	1:A:545:C:C6	3.00	0.49
1:A:1501:C:C5	1:A:1504:G:C4	3.00	0.49
13:M:59:TYR:CD2	13:M:59:TYR:O	2.66	0.49
1:A:1193:G:N3	1:A:1194:U:C6	2.80	0.49
1:A:836:G:C6	1:A:851:G:C5	3.00	0.49
4:D:98:GLU:OE2	4:D:107:ARG:CD	2.60	0.49
1:A:1166:G:C2	1:A:1171:G:C6	3.01	0.49
3:C:92:ALA:O	3:C:95:THR:O	2.30	0.49
1:A:89:C:O2'	1:A:90:U:C5'	2.61	0.49
1:A:1303:C:C2'	1:A:1303:C:O2	2.56	0.49
1:A:1090:U:C2	1:A:1091:U:C5	3.00	0.49
1:A:1403:C:O2'	1:A:1404:5MC:C5'	2.61	0.49
1:A:644:G:C8	1:A:644:G:C5'	2.95	0.49
1:A:1507:A:C5	1:A:1530:G:C2	3.00	0.49
1:A:1435:G:C2'	1:A:1436:U:C6	2.95	0.49
10:J:86:MET:CG	10:J:87:THR:N	2.75	0.49
1:A:1047:G:C5	29:A:2425:HOH:O	2.63	0.49
1:A:1233:G:N2	1:A:1234:C:C2	2.81	0.49
1:A:949:A:C2	1:A:1233:G:C4	3.01	0.49
1:A:1361(A):C:C2'	1:A:1362:C:O5'	2.60	0.49
1:A:1419:G:C6	1:A:1420:C:N4	2.81	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:443:C:C4	1:A:444:C:C5	3.01	0.49
1:A:490:G:C6	1:A:491:G:N7	2.81	0.49
15:O:4:THR:CG2	15:O:5:LYS:N	2.76	0.49
20:T:44:ALA:O	20:T:45:GLN:C	2.50	0.49
7:G:123:GLU:O	7:G:126:ASP:N	2.46	0.49
7:G:20:ASP:OD2	7:G:63:LYS:NZ	2.46	0.49
3:C:119:ARG:NH1	3:C:119:ARG:CG	2.76	0.49
1:A:1055:A:O2'	3:C:156:ARG:NH2	2.46	0.49
2:B:102:LEU:CD1	2:B:102:LEU:N	2.75	0.49
20:T:13:LEU:C	20:T:13:LEU:CD1	2.80	0.49
1:A:79:G:N3	1:A:80:G:C8	2.81	0.48
4:D:206:PHE:CE2	4:D:207:TYR:CE2	3.01	0.48
17:Q:17:LYS:N	17:Q:49:GLU:OE2	2.46	0.48
16:P:8:ARG:CB	16:P:28:ARG:NH1	2.75	0.48
1:A:39:G:C2'	1:A:39:G:N3	3.30	0.48
1:A:834:C:N4	29:A:2788:HOH:O	2.45	0.48
1:A:1248:A:C6	1:A:1249:C:C4	3.01	0.48
1:A:83:U:C5	1:A:84:U:C5	3.01	0.48
2:B:168:THR:O	2:B:169:LYS:C	2.51	0.48
6:F:62:TRP:CE2	18:R:35:ARG:NH2	2.81	0.48
1:A:570:G:C6	1:A:873:A:C2	3.01	0.48
3:C:35:GLU:O	3:C:36:ASP:C	2.51	0.48
1:A:1256:A:C4'	1:A:1257:U:O5'	2.61	0.48
1:A:254:G:C2	1:A:273:A:C2	3.01	0.48
1:A:923:A:C1'	1:A:1398:A:C2	2.96	0.48
1:A:1399:C:C2	1:A:1401:G:C4	3.02	0.48
2:B:212:GLN:O	2:B:213:LEU:C	2.51	0.48
20:T:18:GLN:O	20:T:19:SER:C	2.52	0.48
1:A:1229:A:C2	1:A:1230:C:C4	3.02	0.48
12:L:117:ARG:O	12:L:118:SER:C	2.52	0.48
1:A:923:A:O2'	1:A:1399:C:OP2	2.31	0.48
1:A:553:A:O2'	12:L:29:GLY:O	2.31	0.48
1:A:1248:A:N6	1:A:1249:C:N4	2.62	0.48
12:L:76:ASN:OD1	12:L:76:ASN:N	2.44	0.48
16:P:9:PHE:N	16:P:16:HIS:O	2.46	0.48
18:R:86:VAL:O	18:R:87:ARG:NH2	2.46	0.48
1:A:1330:U:OP1	13:M:25:ILE:O	2.31	0.48
1:A:926:G:C6	1:A:1505:G:C6	3.01	0.48
1:A:401:C:O2'	1:A:621:A:N3	2.47	0.48
1:A:867:G:C2'	1:A:868:C:C5'	2.92	0.48
27:A:1928:SRV:H12	27:A:1928:SRV:O53	2.13	0.48
1:A:1104:G:O5'	2:B:111:ARG:CD	2.61	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:H:27:PRO:CA	8:H:58:TYR:CD2	2.96	0.48
6:F:87:ARG:NH1	6:F:87:ARG:CG	2.76	0.48
2:B:70:PHE:O	2:B:93:VAL:N	2.47	0.48
1:A:109:A:C4	1:A:327:A:C2	3.01	0.48
6:F:7:ASN:ND2	18:R:34:TYR:CE1	2.82	0.48
8:H:14:ARG:CZ	8:H:14:ARG:CB	2.91	0.48
1:A:945:G:O6	1:A:1236:A:N1	2.47	0.48
1:A:516:PSU:O2'	1:A:519:C:N3	2.46	0.48
7:G:116:ALA:O	7:G:119:ARG:N	2.47	0.48
15:O:79:ARG:CG	15:O:79:ARG:NH1	2.76	0.48
16:P:40:ASP:OD1	16:P:44:THR:OG1	2.31	0.48
1:A:427:U:O2'	1:A:541:G:OP1	2.31	0.48
17:Q:29:HIS:ND1	17:Q:30:PRO:CD	2.76	0.48
13:M:99:ARG:NH2	19:S:2:PRO:CD	2.77	0.48
8:H:40:ALA:O	8:H:41:ARG:C	2.52	0.48
1:A:353:A:C8	1:A:353:A:C5'	2.96	0.48
1:A:1054:C:N3	23:W:34:G:O4'	2.47	0.48
1:A:782:A:P	29:A:2280:HOH:O	2.71	0.48
8:H:11:THR:O	8:H:12:ARG:C	2.53	0.48
1:A:1371:G:C6	1:A:1372:U:C4	3.01	0.48
1:A:114:U:C2'	1:A:115:G:C5'	2.92	0.48
5:E:97:GLY:N	5:E:117:ASP:OD1	2.47	0.48
1:A:707:C:C4'	11:K:20:TYR:CD1	2.97	0.48
6:F:7:ASN:OD1	6:F:7:ASN:N	2.47	0.47
1:A:433:C:C2	1:A:434:U:C5	3.02	0.47
12:L:75:HIS:ND1	12:L:75:HIS:C	2.67	0.47
1:A:1263:C:N4	1:A:1264:C:N4	2.62	0.47
7:G:90:GLU:CA	7:G:90:GLU:OE1	2.62	0.47
1:A:500:G:N7	1:A:546:G:N2	2.60	0.47
1:A:924:C:C4'	1:A:1399:C:OP2	2.62	0.47
1:A:1204:A:N7	1:A:1205:U:C5	2.82	0.47
1:A:1048:G:O6	1:A:1210:C:N4	2.47	0.47
1:A:1015:A:N6	1:A:1016:A:N6	2.61	0.47
1:A:802:A:O2'	29:A:2374:HOH:O	2.20	0.47
1:A:390:C:O3'	16:P:28:ARG:NH2	2.47	0.47
2:B:92:TYR:CD1	2:B:151:GLY:CA	2.97	0.47
14:N:36:PHE:CD1	14:N:36:PHE:C	2.87	0.47
1:A:1054:C:O2'	1:A:1056:U:OP2	2.32	0.47
1:A:1162:C:N3	1:A:1175:G:C2	2.83	0.47
10:J:54:PHE:CD2	10:J:54:PHE:C	2.87	0.47
13:M:20:THR:CG2	13:M:20:THR:O	2.62	0.47
1:A:90:U:O2'	1:A:91:C:O5'	2.33	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:981:U:C5'	14:N:21:TYR:CE1	2.97	0.47
13:M:39:ILE:CG2	13:M:40:ASN:O	2.62	0.47
1:A:1532:U:C2'	1:A:1533:C:C6	2.98	0.47
1:A:1381:U:C6	1:A:1382:C:C6	3.02	0.47
1:A:448:A:OP2	1:A:485:G:N1	2.48	0.47
1:A:645:C:C2	1:A:646:U:C6	3.02	0.47
1:A:892:A:C2	1:A:907:A:C5	3.02	0.47
8:H:121:ASP:OD1	8:H:121:ASP:N	2.47	0.47
11:K:11:LYS:N	11:K:75:TYR:CE2	2.82	0.47
1:A:503:C:OP2	12:L:116:SER:CB	2.63	0.47
1:A:147:G:C2	1:A:148:G:C8	3.03	0.47
13:M:82:MET:O	13:M:85:GLY:N	2.47	0.47
1:A:506:G:C6	1:A:507:C:C4	3.02	0.47
1:A:836:G:C6	1:A:851:G:C6	3.03	0.47
4:D:63:LYS:O	4:D:67:ILE:CD1	2.63	0.47
18:R:74:ARG:O	18:R:77:GLY:N	2.47	0.47
20:T:102:GLY:O	20:T:104:LEU:N	2.47	0.47
1:A:70:G:C2	1:A:99:C:O2	2.67	0.47
1:A:78:G:C6	1:A:79:G:N7	2.83	0.47
1:A:77:G:C6	1:A:93:G:N1	2.83	0.47
19:S:41:VAL:O	19:S:42:PRO:C	2.52	0.47
1:A:1148:U:C5	1:A:1149:C:C4	3.03	0.47
1:A:1503:A:C5	1:A:1531:A:C2	3.02	0.47
1:A:1060:C:C2	1:A:1198:G:C2	3.03	0.47
1:A:1435:G:C4	1:A:1436:U:C5	3.03	0.47
4:D:177:ASP:OD1	4:D:179:GLU:N	2.47	0.47
16:P:8:ARG:O	16:P:9:PHE:CD2	2.68	0.47
2:B:82:ARG:CA	2:B:92:TYR:CE2	2.97	0.47
9:I:48:GLU:N	9:I:49:PRO:CD	2.78	0.47
1:A:719:C:O2	18:R:50:ILE:N	2.48	0.47
1:A:284:G:N3	1:A:285:G:C8	2.82	0.47
1:A:1035:A:C6	1:A:1036:G:C6	3.02	0.47
20:T:75:ASN:O	20:T:76:ALA:C	2.53	0.47
1:A:644:G:C6	1:A:645:C:C5	3.01	0.47
12:L:76:ASN:O	12:L:77:LEU:CD2	2.63	0.47
7:G:153:HIS:CE1	7:G:154:TYR:CE2	3.03	0.47
4:D:102:ASP:OD1	4:D:102:ASP:N	2.48	0.47
1:A:262:A:C6	1:A:263:A:C6	3.03	0.47
1:A:1061:G:C2	1:A:1062:U:O2	2.67	0.47
7:G:123:GLU:O	7:G:124:LEU:C	2.53	0.47
1:A:868:C:C2'	1:A:869:G:O5'	2.63	0.47
4:D:104:VAL:O	4:D:108:LEU:N	2.48	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
12:L:33:ARG:O	12:L:85:ILE:N	2.48	0.47
17:Q:10:VAL:CG1	17:Q:52:LYS:O	2.63	0.47
1:A:826:C:C2	1:A:827:U:C5	3.02	0.47
1:A:913:A:O3'	27:A:1928:SRV:HI33	2.10	0.47
1:A:1054:C:N3	23:W:34:G:OP1	2.48	0.47
1:A:1206:G:O6	1:A:1207:2MG:C6	2.68	0.47
1:A:282:A:OP2	1:A:283:C:N4	2.48	0.47
18:R:47:THR:CG2	18:R:48:GLY:N	2.76	0.47
1:A:77:G:N2	1:A:92:C:O2	2.48	0.46
1:A:1538:C:C2'	1:A:1539:C:O4'	2.64	0.46
1:A:1181:G:C2	1:A:1182:G:N2	2.83	0.46
17:Q:40:LYS:CG	17:Q:41:LYS:N	2.78	0.46
19:S:18:LYS:O	19:S:22:LEU:CG	2.63	0.46
1:A:22:G:C6	1:A:23:C:N4	2.83	0.46
15:O:70:LEU:CD2	15:O:78:TYR:CB	2.94	0.46
2:B:236:TYR:O	2:B:239:VAL:CG2	2.63	0.46
18:R:39:VAL:CG1	18:R:40:LEU:N	2.79	0.46
12:L:90:VAL:O	12:L:91:LYS:C	2.53	0.46
16:P:48:TRP:CD1	16:P:48:TRP:N	2.81	0.46
7:G:69:VAL:CG1	7:G:69:VAL:O	2.63	0.46
1:A:1516[A]:G:N1	1:A:1519[A]:MA6:OP2	2.49	0.46
1:A:1054:C:C3'	1:A:1054:C:C2	2.98	0.46
1:A:44:G:C2	1:A:399:G:C4	3.04	0.46
1:A:853:G:C2	1:A:854:G:C8	3.02	0.46
1:A:1367:C:N3	1:A:1368:G:C8	2.84	0.46
18:R:44:LEU:CD2	18:R:44:LEU:N	2.78	0.46
8:H:10:LEU:N	8:H:10:LEU:CD2	2.71	0.46
1:A:918:A:OP2	29:A:2624:HOH:O	2.21	0.46
1:A:391:G:C6	1:A:392:G:C5	3.04	0.46
4:D:8:VAL:C	4:D:10:ARG:N	2.69	0.46
1:A:575:G:C8	1:A:881:G:N2	2.83	0.46
1:A:285:G:C2	1:A:286:G:C8	3.03	0.46
1:A:1109:C:OP2	3:C:176:HIS:ND1	2.48	0.46
1:A:1148:U:C5	1:A:1149:C:C5	3.03	0.46
1:A:491:G:C2	1:A:492:G:C4	3.04	0.46
1:A:1393:U:C6	1:A:1393:U:C3'	2.99	0.46
1:A:107:G:C2'	1:A:108:G:C5'	2.93	0.46
10:J:12:ASP:OD2	10:J:12:ASP:O	2.33	0.46
1:A:438:G:O6	29:A:2233:HOH:O	2.17	0.46
1:A:1300:G:O2'	1:A:1301:U:OP2	2.34	0.46
4:D:68:TYR:OH	4:D:98:GLU:OE1	2.34	0.46
15:O:5:LYS:CA	15:O:5:LYS:NZ	2.79	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:89:C:C6	1:A:90:U:C2	3.03	0.46
1:A:532:A:N6	1:A:1207:2MG:C5'	2.79	0.46
1:A:1148:U:C6	1:A:1149:C:C6	3.04	0.46
1:A:1370:G:C2	1:A:1371:G:C8	3.04	0.46
15:O:85:LEU:CD2	15:O:85:LEU:N	2.71	0.46
1:A:1502:A:C2	1:A:1504:G:C2	3.04	0.46
1:A:1519[B]:MA6:C9	1:A:1520[B]:G:N2	2.79	0.46
1:A:1064:G:N2	1:A:1190:G:C2'	2.79	0.46
4:D:107:ARG:NH1	4:D:114:ARG:NH2	2.64	0.46
1:A:538:G:C2	1:A:539:A:C4	3.04	0.46
1:A:460:A:C6	1:A:462:G:C6	3.04	0.46
3:C:47:LEU:O	3:C:50:ALA:N	2.49	0.46
1:A:335:C:O2'	1:A:1433:A:N3	2.49	0.46
1:A:1015:A:C5	1:A:1016:A:C5	3.04	0.46
17:Q:23:VAL:CG2	17:Q:42:TYR:CD1	2.98	0.46
1:A:144:G:N2	1:A:178:C:N3	2.64	0.46
1:A:630:G:C5'	1:A:631:G:OP2	2.64	0.46
1:A:66:G:C2	1:A:67:C:C6	3.03	0.46
19:S:51:VAL:CG2	19:S:51:VAL:O	2.64	0.46
18:R:36:ASN:OD1	18:R:39:VAL:CG1	2.64	0.46
1:A:510:A:P	29:A:2165:HOH:O	2.74	0.46
5:E:144:THR:N	5:E:147:ASP:OD1	2.49	0.46
1:A:1454:G:C5	29:A:2825:HOH:O	2.65	0.46
11:K:116:HIS:ND1	11:K:116:HIS:N	2.62	0.46
3:C:113:ALA:O	3:C:116:VAL:N	2.50	0.46
8:H:121:ASP:O	8:H:124:ALA:N	2.49	0.46
9:I:77:ILE:O	9:I:78:LYS:C	2.54	0.46
1:A:336:C:N4	29:A:2573:HOH:O	2.49	0.46
1:A:803:G:C6	1:A:804:U:C4	3.04	0.46
8:H:114:THR:OG1	8:H:117:GLY:O	2.34	0.46
1:A:545:C:C2'	1:A:545:C:O2	2.64	0.45
1:A:1304:G:C6	1:A:1305:G:N1	2.83	0.45
1:A:182:U:P	29:A:2183:HOH:O	2.73	0.45
1:A:192:U:C1'	20:T:103:GLY:CA	2.94	0.45
1:A:515:G:C6	1:A:516:PSU:C2	3.04	0.45
8:H:9:MET:O	8:H:10:LEU:C	2.54	0.45
1:A:642:A:C4	8:H:114:THR:O	2.70	0.45
1:A:1379:G:C6	1:A:1380:U:C5	3.04	0.45
1:A:89:C:C5	1:A:90:U:C2	3.03	0.45
1:A:1068:G:O4'	1:A:1068:G:OP2	2.33	0.45
1:A:373:A:C2	1:A:482:A:C6	3.04	0.45
3:C:16:ARG:NH1	3:C:16:ARG:CG	2.78	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:957:U:O2'	1:A:959:A:N7	2.49	0.45
1:A:1290:G:C6	1:A:1291:G:C6	3.04	0.45
15:O:46:HIS:C	15:O:48:LYS:N	2.70	0.45
4:D:159:ARG:NH1	4:D:159:ARG:CG	2.77	0.45
7:G:148:ASN:C	7:G:150:ALA:N	2.66	0.45
1:A:1503:A:C4	1:A:1531:A:N3	2.85	0.45
5:E:5:ASP:OD1	5:E:6:PHE:N	2.49	0.45
4:D:38:TYR:N	4:D:38:TYR:CD2	2.84	0.45
19:S:10:PHE:CD2	19:S:10:PHE:C	2.89	0.45
17:Q:81:ARG:CG	17:Q:81:ARG:O	2.65	0.45
1:A:101:A:N3	1:A:102:G:C8	2.85	0.45
1:A:1415:G:C6	1:A:1486:G:C6	3.04	0.45
1:A:1084:G:N2	29:A:2128:HOH:O	2.50	0.45
12:L:7:ILE:O	12:L:8:ASN:C	2.55	0.45
1:A:77:G:C2	1:A:93:G:C2	3.05	0.45
1:A:1005:A:C8	1:A:1026:G:O6	2.70	0.45
9:I:32:ASP:CG	9:I:33:PHE:N	2.69	0.45
1:A:1111:A:N1	3:C:177:THR:OG1	2.49	0.45
1:A:1233:G:C2	1:A:1234:C:C4	3.05	0.45
14:N:14:PRO:O	14:N:15:LYS:CB	2.64	0.45
7:G:148:ASN:O	7:G:149:ARG:C	2.55	0.45
11:K:116:HIS:C	11:K:117:ASN:OD1	2.54	0.45
1:A:1288:A:C6	1:A:1289:A:C6	3.04	0.45
4:D:177:ASP:C	4:D:177:ASP:OD1	2.54	0.45
20:T:31:SER:O	20:T:32:ALA:C	2.55	0.45
1:A:1004:A:C5'	29:A:2325:HOH:O	2.65	0.45
1:A:1494:G:C2	1:A:1495:U:C5	3.05	0.45
20:T:50:GLU:CA	20:T:99:LEU:CD1	2.95	0.45
1:A:1250:A:C6	1:A:1251:A:N1	2.84	0.45
4:D:92:VAL:O	4:D:95:GLY:N	2.49	0.45
5:E:112:LEU:C	5:E:114:GLY:N	2.70	0.45
1:A:428:G:C1'	1:A:429:U:OP2	2.65	0.45
1:A:62:U:OP1	1:A:385:C:O2'	2.35	0.45
20:T:57:ARG:NH2	20:T:100:ILE:CD1	2.79	0.45
3:C:5:ILE:C	3:C:5:ILE:CD1	2.85	0.45
1:A:1157:A:C4	1:A:1181:G:C2	3.05	0.45
19:S:52:TYR:CE2	19:S:54:GLY:CA	3.00	0.45
13:M:7:VAL:O	13:M:9:ILE:CD1	2.65	0.45
1:A:1166:G:N2	1:A:1171:G:C6	2.85	0.45
1:A:1345:U:P	29:A:2503:HOH:O	2.74	0.45
1:A:1162:C:C2	1:A:1175:G:C2	3.05	0.45
5:E:83:GLU:CG	5:E:83:GLU:O	2.65	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1090:U:N3	1:A:1091:U:C5	2.84	0.45
1:A:1442:G:N1	1:A:1446:A:N6	2.63	0.45
1:A:1059:C:N3	1:A:1198:G:O6	2.50	0.45
3:C:84:ILE:CG2	3:C:85:ARG:N	2.80	0.45
1:A:283:C:C2	1:A:284:G:C8	3.04	0.45
1:A:438:G:N2	1:A:496:A:C8	2.85	0.45
15:O:45:VAL:CB	15:O:46:HIS:ND1	2.79	0.45
5:E:48:ALA:CB	5:E:49:PRO:CD	2.95	0.45
1:A:533:A:OP1	29:A:2170:HOH:O	2.21	0.45
1:A:522:C:OP2	12:L:69:TYR:OH	2.35	0.45
1:A:964:A:O2'	10:J:55:LYS:NZ	2.50	0.45
1:A:1110:A:C8	29:A:2140:HOH:O	2.69	0.45
1:A:1248:A:C6	1:A:1249:C:N4	2.85	0.45
1:A:1015:A:N3	1:A:1218:C:O2'	2.50	0.45
17:Q:29:HIS:CE1	17:Q:32:TYR:N	2.85	0.45
16:P:53:VAL:O	16:P:54:GLU:C	2.53	0.45
1:A:895:G:C5	1:A:896:C:C5	3.05	0.45
1:A:713:G:N2	1:A:714:G:C2	2.85	0.45
1:A:1314:C:OP2	19:S:6:LYS:CG	2.65	0.44
2:B:57:PHE:CD1	2:B:199:TYR:CE1	3.05	0.44
17:Q:10:VAL:CG1	17:Q:10:VAL:O	2.65	0.44
5:E:106:PRO:O	5:E:110:LEU:CD1	2.65	0.44
1:A:355:C:C5'	1:A:389:A:OP2	2.65	0.44
19:S:41:VAL:CG2	19:S:43:GLU:OE2	2.65	0.44
1:A:1052:U:O4	1:A:1200:C:C2	2.70	0.44
1:A:1054:C:N3	23:W:34:G:P	2.91	0.44
23:W:39:G:N2	23:W:40:PSU:C4	2.86	0.44
18:R:87:ARG:NH2	18:R:87:ARG:CB	2.79	0.44
1:A:1507:A:C4	1:A:1530:G:C2	3.05	0.44
1:A:400:C:N4	1:A:401:C:N4	2.65	0.44
1:A:42:G:C2	1:A:43:C:C2	3.05	0.44
13:M:52:GLU:O	13:M:53:VAL:C	2.54	0.44
10:J:50:ILE:N	10:J:50:ILE:CD1	2.80	0.44
1:A:784:C:C2'	1:A:785:G:O5'	2.65	0.44
2:B:97:TRP:CH2	2:B:176:GLU:CD	2.90	0.44
13:M:11:ARG:CG	13:M:12:ASN:N	2.80	0.44
7:G:40:ALA:O	7:G:41:ARG:C	2.53	0.44
1:A:925:G:C1'	1:A:1502:A:C8	3.01	0.44
8:H:4:ASP:OD2	8:H:85:ARG:CZ	2.64	0.44
1:A:1014:A:C5	1:A:1015:A:C6	3.06	0.44
11:K:54:ARG:O	11:K:57:THR:OG1	2.35	0.44
14:N:40:CYS:O	14:N:44:LEU:N	2.51	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1225:A:N3	1:A:1225:A:C2'	2.80	0.44
1:A:681:C:C2	1:A:682:G:C8	3.06	0.44
11:K:88:GLY:O	11:K:89:ALA:C	2.56	0.44
1:A:448:A:C4	1:A:449:C:C5	3.05	0.44
1:A:1347:G:C6	9:I:107:ARG:NH1	2.85	0.44
8:H:11:THR:OG1	8:H:14:ARG:NH2	2.50	0.44
1:A:114:U:O2'	1:A:115:G:C5'	2.65	0.44
1:A:440:A:C8	1:A:442:C:C6	3.05	0.44
1:A:1346:A:N3	7:G:10:ARG:NH1	2.66	0.44
1:A:1245:A:C2	1:A:1293:G:N3	2.86	0.44
1:A:1350:A:C4	1:A:1351:U:C6	3.06	0.44
17:Q:11:VAL:CG1	17:Q:88:TYR:CE2	3.01	0.44
1:A:155:C:C2	1:A:167:G:C2	3.06	0.44
5:E:135:THR:O	5:E:136:MET:C	2.52	0.44
13:M:96:LEU:CD2	13:M:96:LEU:N	2.79	0.44
1:A:1347:G:O2'	1:A:1348:U:O5'	2.36	0.44
1:A:972:C:OP1	10:J:57:LYS:NZ	2.50	0.44
7:G:15:ASP:OD2	7:G:44:TYR:OH	2.35	0.44
1:A:595:G:C2	1:A:641:U:C2	3.05	0.44
8:H:127:LEU:CD2	8:H:127:LEU:O	2.65	0.44
15:O:53:HIS:O	15:O:54:ARG:C	2.54	0.44
5:E:84:PHE:CD2	5:E:84:PHE:C	2.90	0.44
17:Q:94:ASN:O	17:Q:97:SER:OG	2.35	0.44
1:A:653:A:OP1	8:H:56:LYS:CE	2.66	0.44
1:A:710:G:N7	29:A:2472:HOH:O	2.36	0.44
6:F:55:ASP:OD1	6:F:57:GLN:N	2.51	0.44
4:D:58:LEU:C	4:D:58:LEU:CD2	2.86	0.44
19:S:52:TYR:CE1	19:S:55:LYS:C	2.91	0.44
18:R:61:LYS:O	18:R:62:GLU:C	2.54	0.44
16:P:1:MET:O	16:P:2:VAL:C	2.56	0.44
2:B:92:TYR:CE1	2:B:151:GLY:CA	3.00	0.44
2:B:231:GLU:O	2:B:232:PRO:C	2.55	0.44
2:B:160:ASP:O	2:B:161:ALA:CB	2.66	0.44
15:O:21:ASP:OD1	15:O:24:SER:CB	2.66	0.44
13:M:68:GLY:C	13:M:70:LEU:N	2.70	0.44
21:U:21:TYR:N	21:U:21:TYR:CD1	2.86	0.43
1:A:922:G:N3	1:A:1398:A:C2	2.86	0.43
1:A:1401:G:C5	1:A:1402:4OC:C5	3.01	0.43
3:C:156:ARG:NE	3:C:160:ALA:O	2.51	0.43
1:A:1124:G:C2'	1:A:1145:C:C5	3.01	0.43
1:A:1222:G:OP1	19:S:77:THR:OG1	2.35	0.43
1:A:956:U:C2	1:A:1225:A:C2	3.06	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:285:G:O6	29:A:2039:HOH:O	2.20	0.43
5:E:33:VAL:CG1	5:E:34:VAL:N	2.80	0.43
15:O:23:GLY:O	15:O:28:GLN:NE2	2.51	0.43
7:G:16:LEU:CD2	7:G:16:LEU:N	2.82	0.43
1:A:310:G:OP2	16:P:27:LYS:NZ	2.51	0.43
18:R:38:GLU:CD	18:R:38:GLU:N	2.71	0.43
1:A:1004:A:N6	1:A:1037:C:N4	2.66	0.43
3:C:14:ILE:CD1	3:C:14:ILE:N	2.81	0.43
1:A:1465:C:C5	1:A:1466:C:C5	3.06	0.43
1:A:1255:G:C2	1:A:1283:G:C2	3.06	0.43
1:A:81:U:C5'	1:A:82:U:OP2	2.66	0.43
10:J:62:HIS:O	10:J:62:HIS:ND1	2.51	0.43
8:H:20:TYR:CE1	8:H:76:PRO:CD	3.00	0.43
1:A:1149:C:O2'	1:A:1280:A:N1	2.51	0.43
1:A:949:A:N1	1:A:1233:G:C4	2.86	0.43
1:A:644:G:C8	1:A:644:G:C4'	3.02	0.43
20:T:44:ALA:O	20:T:46:GLU:N	2.51	0.43
1:A:986:A:O2'	19:S:55:LYS:O	2.35	0.43
1:A:1332:A:C2	1:A:1333:A:N9	2.86	0.43
1:A:1163:C:C6	1:A:1163:C:C3'	3.02	0.43
1:A:537:G:C2	1:A:538:G:C5	3.06	0.43
5:E:75:THR:CG2	5:E:76:ILE:N	2.78	0.43
3:C:37:GLN:OE1	14:N:47:LEU:CD2	2.66	0.43
1:A:1515[B]:C:C4	1:A:1520[B]:G:O6	2.69	0.43
1:A:1412:C:C2'	1:A:1413:A:C8	3.01	0.43
1:A:778:G:C6	1:A:779:C:N3	2.87	0.43
1:A:1221:G:C4	1:A:1222:G:C8	3.06	0.43
7:G:127:ALA:C	7:G:129:GLU:N	2.71	0.43
1:A:1166:G:N2	1:A:1171:G:C5	2.86	0.43
1:A:231:G:C2	1:A:232:G:C8	3.06	0.43
1:A:1168:A:C6	1:A:1169:A:C6	3.07	0.43
1:A:90:U:C2'	1:A:91:C:O5'	2.66	0.43
1:A:448:A:C2	1:A:449:C:C5	3.06	0.43
1:A:484:G:C2'	1:A:485:G:OP2	2.66	0.43
1:A:925:G:C2	1:A:927:G:C8	3.07	0.43
1:A:1054:C:OP1	1:A:1197:G:P	2.76	0.43
1:A:1039:C:N3	1:A:1040:U:C4	2.86	0.43
1:A:1124:G:O2'	1:A:1145:C:C4	2.71	0.43
15:O:33:THR:CG2	15:O:63:ARG:NH1	2.81	0.43
11:K:89:ALA:O	11:K:90:GLY:C	2.56	0.43
9:I:126:SER:O	9:I:128:ARG:N	2.52	0.43
1:A:360:A:C6	1:A:361:G:C6	3.06	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:T:41:ILE:N	20:T:41:ILE:CD1	2.82	0.43
1:A:77:G:N2	1:A:78:G:C4	2.86	0.43
1:A:1501:C:C4	1:A:1504:G:C2	3.07	0.43
5:E:121:LYS:CG	5:E:123:LEU:CD2	2.96	0.43
1:A:596:C:N3	1:A:644:G:N2	2.67	0.43
4:D:24:GLU:O	4:D:25:ARG:CB	2.67	0.43
1:A:236:G:C6	1:A:237:C:C2	3.06	0.43
1:A:1521:G:C2	1:A:1522:U:C2	3.07	0.43
1:A:397:A:C6	1:A:548:G:C8	3.07	0.43
1:A:78:G:C6	1:A:79:G:C8	3.06	0.43
1:A:1126:U:C4	1:A:1127:G:N2	2.87	0.43
1:A:1224:G:O2'	1:A:1322:C:OP1	2.37	0.43
1:A:1032:G:C4	1:A:1033:G:C8	3.06	0.43
1:A:702:A:OP2	29:A:2798:HOH:O	2.21	0.43
1:A:1480:G:C4	1:A:1481:U:C5	3.07	0.43
1:A:988:G:N2	1:A:1218:C:O2	2.51	0.43
19:S:72:GLY:O	19:S:75:ALA:N	2.52	0.43
1:A:1287:A:C6	1:A:1288:A:C6	3.07	0.43
1:A:1298:C:OP2	7:G:114:ARG:NH2	2.51	0.43
8:H:20:TYR:CE1	8:H:76:PRO:CG	3.02	0.43
1:A:46:G:C2	1:A:396:G:C2	3.06	0.43
1:A:266:G:C4'	1:A:266:G:C8	3.01	0.43
1:A:77:G:C2'	1:A:78:G:O5'	2.67	0.43
2:B:100:GLY:N	2:B:176:GLU:OE2	2.52	0.43
9:I:118:LYS:C	9:I:120:ARG:N	2.72	0.43
1:A:1135:U:N3	1:A:1137:C:O2	2.52	0.43
1:A:284:G:C4	1:A:285:G:C8	3.07	0.43
15:O:78:TYR:CZ	15:O:82:ILE:CD1	3.01	0.43
1:A:355:C:O4'	1:A:388:G:O2'	2.37	0.43
1:A:57:G:C2	1:A:58:C:C2	3.07	0.43
2:B:74:LYS:C	2:B:76:GLN:N	2.72	0.43
1:A:958:A:N3	1:A:985:C:O2'	2.52	0.43
11:K:53:SER:O	11:K:55:LYS:N	2.51	0.43
1:A:1472:U:C2'	1:A:1473:A:O5'	2.67	0.43
1:A:110:C:N4	1:A:111:G:C6	2.87	0.43
12:L:93:LEU:O	12:L:94:PRO:C	2.56	0.43
18:R:78:LEU:N	18:R:78:LEU:CD2	2.79	0.43
4:D:150:GLU:C	4:D:152:SER:N	2.72	0.42
1:A:1005:A:C5	1:A:1026:G:N1	2.87	0.42
2:B:131:PRO:O	2:B:134:GLU:CB	2.67	0.42
1:A:1501:C:C4	1:A:1504:G:N3	2.87	0.42
1:A:1126:U:C6	1:A:1126:U:OP1	2.71	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:976:G:N7	1:A:1358:U:N3	2.67	0.42
1:A:1073:U:OP2	5:E:57:LYS:NZ	2.52	0.42
1:A:81:U:C6	1:A:81:U:C3'	3.02	0.42
1:A:942:G:C2	1:A:943:U:C6	3.07	0.42
1:A:596:C:C2	1:A:644:G:N2	2.88	0.42
23:W:37:A:C6	23:W:38:A:N1	2.87	0.42
1:A:1126:U:N3	1:A:1127:G:C2	2.87	0.42
3:C:6:HIS:O	3:C:10:PHE:N	2.52	0.42
5:E:43:LEU:O	5:E:65:ASN:ND2	2.52	0.42
17:Q:101:ARG:N	17:Q:101:ARG:HD3	2.34	0.42
14:N:9:LYS:CD	14:N:9:LYS:O	2.68	0.42
1:A:827:U:C5'	1:A:828:A:OP2	2.66	0.42
1:A:1508:G:C5	1:A:1509:C:C5	3.07	0.42
1:A:1052:U:O2'	1:A:1055:A:OP1	2.38	0.42
20:T:75:ASN:OD1	20:T:75:ASN:N	2.52	0.42
23:W:39:G:C2	23:W:40:PSU:C4	3.07	0.42
15:O:15:PHE:CD1	15:O:15:PHE:N	2.86	0.42
1:A:792:A:C6	1:A:794:A:C2	3.07	0.42
1:A:1321:C:C5'	13:M:87:TYR:CE2	3.02	0.42
1:A:1193:G:C4	1:A:1194:U:C5	3.08	0.42
1:A:1437:C:C2	1:A:1438:G:C8	3.07	0.42
1:A:1310:G:N2	1:A:1327:C:N3	2.68	0.42
1:A:245:C:C6	1:A:284:G:N2	2.87	0.42
1:A:1480:G:C5	1:A:1481:U:C5	3.07	0.42
16:P:12:LYS:O	16:P:13:HIS:CB	2.65	0.42
8:H:133:LEU:C	8:H:133:LEU:CD2	2.85	0.42
1:A:1092:A:C4'	1:A:1092:A:C8	3.02	0.42
4:D:192:GLU:CA	4:D:192:GLU:OE2	2.68	0.42
1:A:1400:5MC:C3'	1:A:1401:G:C5'	2.96	0.42
1:A:925:G:O4'	1:A:1502:A:C5	2.72	0.42
1:A:1221:G:C6	1:A:1222:G:N7	2.87	0.42
1:A:1367:C:C2	1:A:1368:G:C8	3.08	0.42
1:A:673:G:C5'	6:F:87:ARG:NH1	2.82	0.42
1:A:958:A:O2'	1:A:985:C:O2'	2.37	0.42
3:C:204:LEU:CD2	3:C:204:LEU:N	2.81	0.42
1:A:914:A:OP1	27:A:1928:SRV:HI33	2.19	0.42
1:A:1077:G:N2	1:A:1081:G:C5	2.88	0.42
20:T:99:LEU:O	20:T:101:GLY:N	2.52	0.42
15:O:8:LYS:O	15:O:9:GLN:C	2.55	0.42
1:A:1072:G:C5	1:A:1073:U:C4	3.07	0.42
1:A:1241:G:C4	1:A:1242:C:C5	3.07	0.42
1:A:1115:C:C4	1:A:1116:C:C5	3.08	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
14:N:61:TRP:O	14:N:61:TRP:CD1	2.73	0.42
18:R:26:LEU:N	18:R:26:LEU:CD1	2.82	0.42
18:R:58:LEU:N	18:R:58:LEU:CD2	2.82	0.42
1:A:448:A:N3	1:A:449:C:C6	2.87	0.42
1:A:1401:G:C5	1:A:1402:4OC:C6	3.03	0.42
12:L:46:LYS:N	12:L:92:0TD:O	2.53	0.42
1:A:53:A:C5	1:A:54:C:C5	3.08	0.42
19:S:39:THR:O	19:S:41:VAL:CG1	2.68	0.42
1:A:415:A:C5	1:A:416:G:C5	3.08	0.42
1:A:1505:G:C5'	1:A:1506:U:OP1	2.67	0.42
9:I:11:LYS:O	9:I:12:GLU:CB	2.66	0.42
7:G:47:CYS:O	7:G:50:ILE:N	2.53	0.42
19:S:14:HIS:N	19:S:14:HIS:ND1	2.68	0.42
12:L:105:TYR:N	12:L:105:TYR:CD2	2.83	0.42
13:M:16:ASP:O	13:M:17:VAL:C	2.58	0.42
1:A:1493[B]:A:C2'	1:A:1494:G:C8	3.03	0.42
4:D:8:VAL:O	4:D:10:ARG:N	2.53	0.42
20:T:61:SER:OG	20:T:65:LYS:CD	2.67	0.42
19:S:72:GLY:O	19:S:74:PHE:N	2.53	0.42
7:G:109:ASN:OD1	7:G:119:ARG:NH2	2.53	0.42
17:Q:4:LYS:CG	17:Q:6:LEU:CD2	2.97	0.42
13:M:54:VAL:CG1	13:M:55:ARG:N	2.83	0.42
9:I:22:GLY:O	9:I:57:GLY:O	2.38	0.42
10:J:9:ARG:CB	10:J:9:ARG:CZ	2.97	0.42
13:M:21:TYR:N	13:M:21:TYR:CD1	2.87	0.42
1:A:1250:A:N1	1:A:1287:A:C2	2.88	0.42
1:A:1379:G:C6	1:A:1380:U:C4	3.07	0.42
1:A:397:A:C6	1:A:548:G:N7	2.88	0.42
1:A:505:G:C5	1:A:535:A:C2	3.08	0.42
1:A:1381:U:C5	1:A:1382:C:C6	3.08	0.42
1:A:924:C:C3'	1:A:924:C:C6	3.03	0.42
1:A:1204:A:C5	1:A:1205:U:C6	3.08	0.42
1:A:1047:G:C2'	1:A:1048:G:C5'	2.97	0.42
3:C:131:ARG:O	3:C:134:ILE:CG1	2.68	0.42
1:A:415:A:C5	1:A:416:G:N7	2.88	0.42
1:A:804:U:C5'	1:A:805:C:OP2	2.68	0.42
15:O:52:SER:O	15:O:53:HIS:C	2.58	0.42
1:A:154:C:C6	1:A:154:C:C3'	3.03	0.42
4:D:19:LEU:CD2	4:D:19:LEU:N	2.83	0.42
1:A:973:G:C2'	1:A:974:A:OP1	2.68	0.41
1:A:1003(A):G:N2	1:A:1038:C:C2	2.86	0.41
1:A:316:G:C5	29:A:2572:HOH:O	2.72	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1222:G:N2	1:A:1223:C:C2	2.88	0.41
1:A:1536:C:C3'	1:A:1536:C:C6	3.03	0.41
1:A:1410:G:C4	1:A:1411:C:C5	3.08	0.41
13:M:49:THR:C	13:M:51:ALA:N	2.73	0.41
1:A:78:G:C2	1:A:79:G:C8	3.08	0.41
1:A:79:G:N3	1:A:91:C:O2	2.54	0.41
1:A:1532:U:C5	1:A:1533:C:N4	2.88	0.41
1:A:1502:A:C2	1:A:1504:G:N3	2.88	0.41
1:A:1190:G:C8	1:A:1190:G:C4'	3.02	0.41
3:C:10:PHE:CD1	3:C:10:PHE:O	2.73	0.41
1:A:1030(A):G:N2	1:A:1030(D):A:OP2	2.53	0.41
1:A:1241:G:OP1	7:G:35:LYS:NZ	2.53	0.41
3:C:155:GLY:CA	3:C:164:ARG:O	2.68	0.41
2:B:180:LEU:O	2:B:181:PHE:CB	2.68	0.41
21:U:23:PRO:C	21:U:25:LYS:N	2.74	0.41
7:G:66:VAL:CG1	7:G:67:GLU:N	2.83	0.41
7:G:79:ARG:CB	7:G:83:ALA:O	2.68	0.41
1:A:734:G:C8	1:A:734:G:O5'	2.73	0.41
1:A:243:A:C2	1:A:246:A:N7	2.88	0.41
1:A:1052:U:O2	1:A:1207:2MG:N2	2.54	0.41
22:V:1:U:N3	23:W:37:A:C2	2.88	0.41
1:A:101:A:C2	1:A:102:G:C8	3.08	0.41
20:T:105:SER:O	20:T:106:ALA:C	2.58	0.41
15:O:5:LYS:O	15:O:6:GLU:C	2.57	0.41
1:A:937:A:N6	1:A:1345:U:O4	2.53	0.41
5:E:105:VAL:O	5:E:106:PRO:C	2.56	0.41
4:D:190:ASP:CB	4:D:193:ASP:OD2	2.68	0.41
6:F:63:TYR:CD2	6:F:63:TYR:N	2.89	0.41
1:A:1026:G:C2'	1:A:1027:C:O2	2.68	0.41
1:A:1091:U:O2	1:A:1093:A:C8	2.74	0.41
17:Q:95:TYR:O	17:Q:97:SER:N	2.53	0.41
1:A:504:C:C2	1:A:542:G:C2	3.09	0.41
8:H:104:ARG:O	8:H:107:LEU:N	2.54	0.41
1:A:977:A:C2'	1:A:978:A:C5'	2.98	0.41
15:O:12:ILE:O	15:O:14:GLU:N	2.53	0.41
1:A:892:A:C6	1:A:907:A:C8	3.09	0.41
1:A:839:U:C5'	1:A:840:C:C5	3.04	0.41
1:A:505:G:C6	1:A:535:A:C2	3.07	0.41
1:A:250:A:C4'	1:A:251:G:O5'	2.69	0.41
1:A:370:C:C2	1:A:371:G:C8	3.09	0.41
1:A:88:A:N7	1:A:89:C:N3	2.68	0.41
1:A:1502:A:O2'	1:A:1502:A:N3	2.53	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:777:A:N6	1:A:778:G:C2	2.89	0.41
1:A:794:A:N6	1:A:795:C:N4	2.68	0.41
19:S:15:LEU:CD1	19:S:15:LEU:N	2.83	0.41
1:A:450:G:OP1	16:P:43:LYS:NZ	2.53	0.41
2:B:121:LEU:O	2:B:124:SER:OG	2.38	0.41
8:H:86:ILE:N	8:H:134:ILE:O	2.54	0.41
1:A:739:C:N4	1:A:740:U:C4	2.89	0.41
1:A:740:U:C4'	15:O:42:HIS:CD2	3.03	0.41
16:P:20:VAL:CG1	16:P:21:VAL:N	2.78	0.41
1:A:544:G:N3	1:A:545:C:C6	2.88	0.41
1:A:1022:G:C2	1:A:1023:G:C8	3.08	0.41
27:A:1928:SRV:O61	12:L:46:LYS:CD	2.69	0.41
1:A:1068:G:OP1	29:A:2218:HOH:O	2.20	0.41
1:A:21:G:C2	1:A:22:G:C6	3.09	0.41
1:A:22:G:C5	1:A:23:C:C4	3.09	0.41
4:D:100:ARG:NH1	4:D:137:SER:CA	2.83	0.41
16:P:78:GLY:C	16:P:80:PHE:N	2.69	0.41
1:A:536:C:OP2	29:A:2174:HOH:O	2.22	0.41
4:D:150:GLU:O	4:D:152:SER:N	2.54	0.41
1:A:357:G:C2	1:A:358:U:C6	3.09	0.41
1:A:922:G:N3	1:A:1396:A:C2	2.89	0.41
1:A:1497:G:O2'	1:A:1518[A]:MA6:N1	2.53	0.41
12:L:25:PRO:C	12:L:27:LEU:N	2.73	0.41
6:F:50:TYR:N	6:F:50:TYR:CD1	2.88	0.41
1:A:491:G:C2	1:A:492:G:C8	3.08	0.41
1:A:438:G:C4'	4:D:123:HIS:CD2	3.03	0.41
2:B:157:ARG:CG	2:B:158:LEU:N	2.83	0.41
5:E:131:ILE:CG2	5:E:132:ALA:N	2.78	0.41
16:P:32:TYR:CD1	16:P:32:TYR:N	2.88	0.41
1:A:1042:G:C6	1:A:1043:C:C4	3.08	0.41
1:A:695:A:C2	1:A:787:A:O2'	2.74	0.41
1:A:216:G:O2'	1:A:217:C:O4'	2.38	0.41
2:B:16:HIS:NE2	2:B:17:PHE:CD2	2.89	0.41
1:A:1010:G:C2	1:A:1020:U:O2	2.74	0.41
1:A:148:G:N2	1:A:149:A:C4	2.89	0.41
2:B:86:GLU:O	2:B:88:ALA:O	2.38	0.41
11:K:58:PRO:O	11:K:61:ALA:N	2.54	0.41
20:T:33:ILE:O	20:T:37:SER:N	2.53	0.41
1:A:1101:A:C4'	1:A:1102:A:O5'	2.68	0.41
12:L:117:ARG:C	12:L:119:LYS:N	2.70	0.41
1:A:500:G:C5	1:A:501:C:C4	3.09	0.41
1:A:36:C:O2'	1:A:501:C:OP1	2.38	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1035:A:C2'	1:A:1036:G:C8	3.03	0.41
1:A:392:G:C2	1:A:393:A:C8	3.09	0.41
1:A:1496:C:C2'	1:A:1497:G:C8	3.03	0.41
1:A:1405:G:O2'	1:A:1518[A]:MA6:O2'	2.39	0.41
1:A:791:G:N2	1:A:1518[A]:MA6:C9	2.84	0.41
10:J:78:ASN:O	10:J:81:THR:OG1	2.39	0.41
2:B:97:TRP:CZ2	2:B:102:LEU:CD1	3.04	0.41
1:A:1321:C:C4'	13:M:87:TYR:CE2	3.03	0.41
16:P:66:PRO:C	16:P:67:THR:O	2.59	0.41
3:C:6:HIS:C	3:C:6:HIS:CD2	2.94	0.41
3:C:85:ARG:O	3:C:86:VAL:C	2.60	0.41
1:A:652:U:O2'	1:A:752:G:N1	2.54	0.41
1:A:575:G:C6	1:A:821:G:N7	2.89	0.41
14:N:36:PHE:O	14:N:36:PHE:CD1	2.73	0.41
2:B:216:SER:OG	2:B:217:ARG:N	2.53	0.41
1:A:604:G:C2'	1:A:605:U:C5'	2.98	0.41
11:K:69:ALA:O	11:K:70:LYS:C	2.58	0.41
8:H:25:ASP:OD1	8:H:60:ARG:NE	2.54	0.41
3:C:178:LEU:C	3:C:180:ALA:N	2.73	0.41
13:M:108:ARG:NH2	13:M:114:ARG:CA	2.84	0.41
1:A:1038:C:C2	1:A:1039:C:C6	3.09	0.41
8:H:82:HIS:ND1	8:H:138:TRP:CE2	2.89	0.41
17:Q:86:GLU:O	17:Q:87:LYS:C	2.60	0.41
7:G:18:TYR:OH	7:G:58:PRO:CG	2.69	0.41
1:A:16:A:C2	1:A:920:U:O2	2.74	0.41
7:G:51:GLN:O	7:G:52:GLU:CG	2.69	0.41
1:A:1190:G:O2'	1:A:1191:A:P	2.79	0.41
1:A:853:G:C2'	1:A:854:G:C5'	2.99	0.41
11:K:120:ARG:NH2	11:K:126:ARG:NE	2.69	0.41
1:A:474:G:C2	1:A:475:G:C8	3.09	0.41
1:A:719:C:O2'	18:R:50:ILE:O	2.38	0.41
15:O:70:LEU:C	15:O:70:LEU:CD2	2.90	0.41
1:A:462:G:C5'	1:A:463:A:OP2	2.69	0.41
1:A:179:A:C4	1:A:180:U:C5	3.09	0.41
1:A:143:A:C2	1:A:221:C:O2	2.74	0.41
4:D:170:VAL:CG2	4:D:171:GLY:N	2.84	0.41
12:L:113:ARG:NH2	12:L:120:TYR:CE1	2.89	0.40
1:A:1005:A:C8	1:A:1026:G:C6	3.10	0.40
1:A:923:A:C8	1:A:923:A:O5'	2.75	0.40
1:A:1404:5MC:C2	1:A:1499:A:N1	2.89	0.40
1:A:559:A:O2'	1:A:560:U:OP2	2.39	0.40
7:G:51:GLN:CB	7:G:52:GLU:OE1	2.69	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
10:J:12:ASP:OD2	10:J:15:THR:OG1	2.39	0.40
1:A:1102:A:O2'	2:B:99:GLY:N	2.54	0.40
4:D:96:LEU:O	4:D:99:SER:N	2.54	0.40
1:A:411:A:C3'	1:A:411:A:C8	3.05	0.40
1:A:1305:G:P	21:U:2:GLY:N	2.94	0.40
1:A:427:U:O4	1:A:428:G:C6	2.74	0.40
1:A:1518[A]:MA6:C2	1:A:1519[A]:MA6:C5	2.99	0.40
18:R:30:ASP:OD1	18:R:32:ARG:N	2.54	0.40
13:M:6:GLY:O	13:M:7:VAL:C	2.59	0.40
6:F:15:ASP:OD2	6:F:18:GLN:NE2	2.54	0.40
1:A:367:U:O2	1:A:369:C:C6	2.73	0.40
1:A:79:G:N1	1:A:80:G:C5	2.89	0.40
1:A:1027:C:C6	1:A:1035:A:C2	3.10	0.40
1:A:246:A:C4	1:A:279:A:N6	2.90	0.40
1:A:393:A:N3	1:A:394:G:C8	2.89	0.40
1:A:777:A:C2'	1:A:777:A:N3	2.85	0.40
8:H:120:THR:O	8:H:121:ASP:C	2.59	0.40
1:A:660:G:C2	1:A:746:A:C2	3.10	0.40
1:A:838:G:C2	1:A:849:C:C2	3.10	0.40
1:A:166:G:C6	1:A:167:G:N7	2.89	0.40
1:A:848:C:C6	1:A:848:C:C3'	3.05	0.40
1:A:36:C:C2	1:A:37:U:C6	3.10	0.40
1:A:392:G:C4	1:A:393:A:C8	3.09	0.40
1:A:429:U:OP1	4:D:36:ARG:NH1	2.54	0.40
1:A:1244:C:C2	1:A:1294:G:N2	2.90	0.40
1:A:1158:C:C5	1:A:1160:G:C8	3.09	0.40
1:A:1425:U:O2	1:A:1426:C:C6	2.75	0.40
1:A:747:C:C6	1:A:747:C:C3'	3.04	0.40
18:R:43:PHE:C	18:R:44:LEU:CD2	2.90	0.40
9:I:63:ILE:O	9:I:63:ILE:CG2	2.63	0.40
20:T:78:ALA:O	20:T:79:ARG:C	2.59	0.40
4:D:18:LYS:CE	4:D:20:TYR:CE2	3.04	0.40
1:A:328:C:O2'	1:A:329:A:P	2.74	0.40
1:A:1519[A]:MA6:C3'	1:A:1520[A]:G:C5'	3.00	0.40
1:A:1057:G:C5'	3:C:154:SER:CB	3.00	0.40
20:T:73:HIS:O	20:T:76:ALA:CB	2.70	0.40
6:F:73:ASN:O	6:F:74:ASP:C	2.59	0.40
1:A:1157:A:C4'	1:A:1158:C:O5'	2.69	0.40
1:A:490:G:C4	1:A:491:G:C8	3.10	0.40
1:A:1378:C:O2	7:G:76:ARG:NH1	2.55	0.40
10:J:9:ARG:CB	10:J:9:ARG:NH1	2.85	0.40
1:A:765:G:C6	1:A:812:C:C2	3.09	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
11:K:17:GLY:O	11:K:81:ASP:N	2.55	0.40
1:A:948:C:C6	13:M:106:ASN:ND2	2.89	0.40
13:M:63:THR:CG2	13:M:64:TRP:N	2.84	0.40
12:L:20:LYS:N	12:L:20:LYS:CE	2.84	0.40

All (2) 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	Distance(Å)	Clash(Å)
1:A:82:U:O2	1:A:1400:5MC:N4[3_545]	2.15	0.05
5:E:73:ASN:N	5:E:149:GLU:OE1[7_555]	2.18	0.02

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	
2	B	234/256 (91%)	197 (84%)	34 (14%)	3 (1%)	18	76
3	C	205/239 (86%)	169 (82%)	35 (17%)	1 (0%)	38	88
4	D	206/209 (99%)	180 (87%)	25 (12%)	1 (0%)	38	88
5	E	149/162 (92%)	137 (92%)	11 (7%)	1 (1%)	30	84
6	F	99/101 (98%)	93 (94%)	6 (6%)	0	100	100
7	G	153/156 (98%)	132 (86%)	21 (14%)	0	100	100
8	H	136/138 (99%)	128 (94%)	7 (5%)	1 (1%)	30	84
9	I	125/128 (98%)	107 (86%)	17 (14%)	1 (1%)	27	83
10	J	97/105 (92%)	77 (79%)	17 (18%)	3 (3%)	7	59
11	K	115/129 (89%)	98 (85%)	17 (15%)	0	100	100
12	L	122/135 (90%)	110 (90%)	8 (7%)	4 (3%)	6	58
13	M	116/126 (92%)	99 (85%)	16 (14%)	1 (1%)	25	81
14	N	58/61 (95%)	50 (86%)	8 (14%)	0	100	100
15	O	86/89 (97%)	72 (84%)	14 (16%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	P	82/88 (93%)	74 (90%)	7 (8%)	1 (1%)	19	78
17	Q	98/105 (93%)	93 (95%)	5 (5%)	0	100	100
18	R	69/88 (78%)	60 (87%)	9 (13%)	0	100	100
19	S	79/93 (85%)	68 (86%)	9 (11%)	2 (2%)	9	63
20	T	97/106 (92%)	80 (82%)	16 (16%)	1 (1%)	22	81
21	U	23/27 (85%)	22 (96%)	1 (4%)	0	100	100
All	All	2349/2541 (92%)	2046 (87%)	283 (12%)	20 (1%)	25	81

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	15	THR
9	I	119	ALA
12	L	28	LYS
16	P	83	GLU
19	S	31	ILE
10	J	81	THR
10	J	86	MET
19	S	6	LYS
12	L	115	LYS
20	T	73	HIS
2	B	21	ARG
2	B	95	GLN
2	B	229	VAL
5	E	153	LYS
8	H	121	ASP
12	L	27	LEU
10	J	34	VAL
12	L	71	PRO
13	M	7	VAL
4	D	67	ILE

### 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	
2	B	201/220 (91%)	151 (75%)	50 (25%)	1	8
3	C	160/188 (85%)	119 (74%)	41 (26%)	1	8
4	D	180/181 (99%)	134 (74%)	46 (26%)	1	8
5	E	115/123 (94%)	75 (65%)	40 (35%)	0	3
6	F	90/90 (100%)	60 (67%)	30 (33%)	0	3
7	G	126/127 (99%)	92 (73%)	34 (27%)	1	6
8	H	119/119 (100%)	83 (70%)	36 (30%)	0	5
9	I	98/99 (99%)	75 (76%)	23 (24%)	1	9
10	J	87/92 (95%)	70 (80%)	17 (20%)	2	16
11	K	89/99 (90%)	72 (81%)	17 (19%)	2	16
12	L	103/110 (94%)	80 (78%)	23 (22%)	1	11
13	M	94/101 (93%)	64 (68%)	30 (32%)	0	4
14	N	49/50 (98%)	35 (71%)	14 (29%)	0	5
15	O	79/80 (99%)	60 (76%)	19 (24%)	1	8
16	P	72/74 (97%)	54 (75%)	18 (25%)	1	8
17	Q	95/97 (98%)	74 (78%)	21 (22%)	1	11
18	R	62/77 (80%)	48 (77%)	14 (23%)	1	10
19	S	71/80 (89%)	55 (78%)	16 (22%)	1	11
20	T	76/82 (93%)	51 (67%)	25 (33%)	0	4
21	U	19/22 (86%)	16 (84%)	3 (16%)	4	28
All	All	1985/2111 (94%)	1468 (74%)	517 (26%)	1	7

All (517) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	10	LEU
2	B	11	LEU
2	B	16	HIS
2	B	17	PHE
2	B	20	GLU
2	B	30	ARG
2	B	33	TYR
2	B	35	GLU
2	B	39	ILE
2	B	44	LEU
2	B	53	ARG

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Mol	Chain	Res	Type
2	B	61	LEU
2	B	63	MET
2	B	64	ARG
2	B	67	THR
2	B	69	LEU
2	B	92	TYR
2	B	97	TRP
2	B	101	MET
2	B	107	THR
2	B	109	SER
2	B	111	ARG
2	B	114	ARG
2	B	115	LEU
2	B	122	PHE
2	B	127	ILE
2	B	128	GLU
2	B	144	ARG
2	B	150	SER
2	B	153	ARG
2	B	162	ILE
2	B	163	PHE
2	B	169	LYS
2	B	172	ILE
2	B	182	ILE
2	B	187	LEU
2	B	189	ASP
2	B	193	ASP
2	B	196	LEU
2	B	200	ILE
2	B	204	ASN
2	B	209	ARG
2	B	210	SER
2	B	212	GLN
2	B	215	LEU
2	B	216	SER
2	B	221	LEU
2	B	226	ARG
2	B	236	TYR
2	B	240	GLN
3	C	3	ASN
3	C	8	ILE
3	C	10	PHE

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Mol	Chain	Res	Type
3	C	14	ILE
3	C	16	ARG
3	C	21	ARG
3	C	22	TRP
3	C	31	HIS
3	C	33	LEU
3	C	43	LEU
3	C	45	LYS
3	C	52	LEU
3	C	58	GLU
3	C	64	VAL
3	C	70	VAL
3	C	72	LYS
3	C	75	VAL
3	C	79	ARG
3	C	85	ARG
3	C	99	VAL
3	C	101	LEU
3	C	111	LEU
3	C	119	ARG
3	C	126	ARG
3	C	127	ARG
3	C	130	VAL
3	C	134	ILE
3	C	144	SER
3	C	147	LYS
3	C	156	ARG
3	C	165	THR
3	C	167	TRP
3	C	170	GLN
3	C	175	LEU
3	C	186	PHE
3	C	188	LEU
3	C	190	ARG
3	C	192	THR
3	C	193	TYR
3	C	196	LEU
3	C	204	LEU
4	D	10	ARG
4	D	19	LEU
4	D	20	TYR
4	D	26	CYS

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Mol	Chain	Res	Type
4	D	28	SER
4	D	47	ARG
4	D	49	ARG
4	D	57	ARG
4	D	61	LYS
4	D	66	ARG
4	D	73	ARG
4	D	78	LEU
4	D	84	LYS
4	D	85	LYS
4	D	86	LYS
4	D	91	SER
4	D	92	VAL
4	D	96	LEU
4	D	107	ARG
4	D	108	LEU
4	D	114	ARG
4	D	115	ARG
4	D	119	GLN
4	D	120	LEU
4	D	122	ARG
4	D	127	THR
4	D	131	ARG
4	D	132	ARG
4	D	145	GLU
4	D	146	ILE
4	D	150	GLU
4	D	159	ARG
4	D	163	GLU
4	D	169	LYS
4	D	177	ASP
4	D	178	VAL
4	D	179	GLU
4	D	182	LYS
4	D	187	ARG
4	D	188	LEU
4	D	190	ASP
4	D	192	GLU
4	D	193	ASP
4	D	194	LEU
4	D	196	LEU
4	D	204	ILE

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Mol	Chain	Res	Type
5	E	6	PHE
5	E	11	ILE
5	E	12	LEU
5	E	16	THR
5	E	18	ARG
5	E	24	ARG
5	E	31	LEU
5	E	32	VAL
5	E	37	ARG
5	E	38	GLN
5	E	43	LEU
5	E	47	LYS
5	E	51	VAL
5	E	53	LEU
5	E	55	VAL
5	E	60	TYR
5	E	65	ASN
5	E	66	MET
5	E	67	VAL
5	E	68	GLU
5	E	75	THR
5	E	76	ILE
5	E	78	HIS
5	E	79	GLU
5	E	80	ILE
5	E	82	VAL
5	E	83	GLU
5	E	84	PHE
5	E	100	VAL
5	E	105	VAL
5	E	110	LEU
5	E	116	THR
5	E	123	LEU
5	E	125	SER
5	E	126	ARG
5	E	131	ILE
5	E	145	LYS
5	E	147	ASP
5	E	148	VAL
5	E	150	ARG
6	F	1	MET
6	F	2	ARG

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Mol	Chain	Res	Type
6	F	7	ASN
6	F	9	VAL
6	F	10	LEU
6	F	14	LEU
6	F	16	GLN
6	F	21	LEU
6	F	24	GLU
6	F	25	ILE
6	F	28	ARG
6	F	37	VAL
6	F	39	LYS
6	F	43	LEU
6	F	54	LYS
6	F	64	GLN
6	F	65	VAL
6	F	74	ASP
6	F	75	LEU
6	F	80	ARG
6	F	83	ASP
6	F	84	ASN
6	F	86	ARG
6	F	87	ARG
6	F	89	MET
6	F	93	SER
6	F	94	GLN
6	F	97	PHE
6	F	98	LEU
6	F	100	ASN
7	G	9	VAL
7	G	10	ARG
7	G	12	LEU
7	G	15	ASP
7	G	16	LEU
7	G	17	VAL
7	G	22	LEU
7	G	27	ILE
7	G	29	LYS
7	G	38	LEU
7	G	41	ARG
7	G	49	ILE
7	G	52	GLU
7	G	60	LYS

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Mol	Chain	Res	Type
7	G	62	PHE
7	G	66	VAL
7	G	72	ARG
7	G	75	VAL
7	G	78	ARG
7	G	87	VAL
7	G	92	SER
7	G	97	GLN
7	G	101	LEU
7	G	113	GLU
7	G	114	ARG
7	G	115	ARG
7	G	120	ILE
7	G	122	HIS
7	G	124	LEU
7	G	126	ASP
7	G	129	GLU
7	G	135	VAL
7	G	146	GLU
7	G	156	TRP
8	H	1	MET
8	H	3	THR
8	H	8	ASP
8	H	10	LEU
8	H	11	THR
8	H	14	ARG
8	H	18	ARG
8	H	19	VAL
8	H	22	GLU
8	H	39	LEU
8	H	45	ILE
8	H	51	VAL
8	H	53	VAL
8	H	57	PRO
8	H	59	LEU
8	H	63	LEU
8	H	81	HIS
8	H	83	ILE
8	H	85	ARG
8	H	87	SER
8	H	91	ARG
8	H	95	VAL

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Mol	Chain	Res	Type
8	H	97	VAL
8	H	98	LYS
8	H	100	ILE
8	H	102	ARG
8	H	104	ARG
8	H	105	ARG
8	H	112	LEU
8	H	113	SER
8	H	119	LEU
8	H	121	ASP
8	H	127	LEU
8	H	133	LEU
8	H	135	CYS
8	H	136	GLU
9	I	2	GLU
9	I	5	TYR
9	I	14	VAL
9	I	16	ARG
9	I	23	ASN
9	I	29	ASN
9	I	33	PHE
9	I	34	ASN
9	I	40	LEU
9	I	48	GLU
9	I	59	PHE
9	I	62	TYR
9	I	63	ILE
9	I	64	THR
9	I	65	VAL
9	I	66	ARG
9	I	79	LEU
9	I	85	LEU
9	I	99	LEU
9	I	102	LEU
9	I	109	VAL
9	I	112	LYS
9	I	125	TYR
10	J	4	ILE
10	J	9	ARG
10	J	12	ASP
10	J	19	SER
10	J	28	ARG

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Mol	Chain	Res	Type
10	J	29	ARG
10	J	33	GLN
10	J	44	VAL
10	J	62	HIS
10	J	63	PHE
10	J	67	THR
10	J	78	ASN
10	J	89	ASP
10	J	90	LEU
10	J	94	VAL
10	J	98	ILE
10	J	99	LYS
11	K	11	LYS
11	K	29	ILE
11	K	40	ILE
11	K	57	THR
11	K	70	LYS
11	K	75	TYR
11	K	78	GLN
11	K	80	VAL
11	K	92	GLU
11	K	96	ARG
11	K	99	GLN
11	K	105	VAL
11	K	116	HIS
11	K	117	ASN
11	K	120	ARG
11	K	125	PHE
11	K	126	ARG
12	L	7	ILE
12	L	18	VAL
12	L	19	ARG
12	L	20	LYS
12	L	32	PHE
12	L	34	ARG
12	L	36	VAL
12	L	43	VAL
12	L	44	THR
12	L	50	SER
12	L	52	LEU
12	L	53	ARG
12	L	54	LYS

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Mol	Chain	Res	Type
12	L	60	LEU
12	L	75	HIS
12	L	81	SER
12	L	82	VAL
12	L	98	TYR
12	L	101	VAL
12	L	113	ARG
12	L	116	SER
12	L	122	THR
12	L	127	GLU
13	M	7	VAL
13	M	11	ARG
13	M	14	ARG
13	M	17	VAL
13	M	22	ILE
13	M	27	LYS
13	M	32	GLU
13	M	44	ARG
13	M	46	LYS
13	M	48	LEU
13	M	50	GLU
13	M	52	GLU
13	M	55	ARG
13	M	56	LEU
13	M	57	ARG
13	M	58	GLU
13	M	59	TYR
13	M	64	TRP
13	M	67	GLU
13	M	69	GLU
13	M	70	LEU
13	M	74	VAL
13	M	81	LEU
13	M	84	ILE
13	M	87	TYR
13	M	88	ARG
13	M	94	ARG
13	M	99	ARG
13	M	102	ARG
13	M	105	THR
14	N	3	ARG
14	N	6	LEU

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Mol	Chain	Res	Type
14	N	7	ILE
14	N	9	LYS
14	N	12	ARG
14	N	17	LYS
14	N	24	CYS
14	N	27	CYS
14	N	29	ARG
14	N	33	VAL
14	N	45	ARG
14	N	46	GLU
14	N	49	HIS
14	N	58	LYS
15	O	6	GLU
15	O	11	VAL
15	O	17	ARG
15	O	24	SER
15	O	26	GLU
15	O	31	LEU
15	O	38	ARG
15	O	39	LEU
15	O	40	SER
15	O	45	VAL
15	O	47	LYS
15	O	54	ARG
15	O	56	LEU
15	O	57	LEU
15	O	67	LEU
15	O	73	GLU
15	O	81	LEU
15	O	87	ILE
15	O	88	ARG
16	P	1	MET
16	P	8	ARG
16	P	11	SER
16	P	18	ARG
16	P	22	THR
16	P	25	ARG
16	P	42	ARG
16	P	45	THR
16	P	48	TRP
16	P	53	VAL
16	P	54	GLU

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Mol	Chain	Res	Type
16	P	55	ARG
16	P	62	VAL
16	P	69	THR
16	P	72	ARG
16	P	75	ARG
16	P	79	VAL
16	P	81	ARG
17	Q	10	VAL
17	Q	13	ASP
17	Q	23	VAL
17	Q	27	PHE
17	Q	29	HIS
17	Q	36	ILE
17	Q	40	LYS
17	Q	43	LEU
17	Q	50	LYS
17	Q	53	LEU
17	Q	59	ILE
17	Q	62	SER
17	Q	70	ARG
17	Q	72	ARG
17	Q	77	VAL
17	Q	85	VAL
17	Q	90	ILE
17	Q	91	ARG
17	Q	92	ARG
17	Q	93	GLN
17	Q	98	LEU
18	R	18	ARG
18	R	26	LEU
18	R	31	LEU
18	R	38	GLU
18	R	42	ARG
18	R	44	LEU
18	R	46	GLU
18	R	58	LEU
18	R	70	ILE
18	R	78	LEU
18	R	82	THR
18	R	86	VAL
18	R	87	ARG
18	R	88	LYS

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Mol	Chain	Res	Type
19	S	4	SER
19	S	7	LYS
19	S	11	VAL
19	S	14	HIS
19	S	15	LEU
19	S	16	LEU
19	S	17	GLU
19	S	27	GLU
19	S	29	ARG
19	S	31	ILE
19	S	37	ARG
19	S	39	THR
19	S	43	GLU
19	S	58	VAL
19	S	64	GLU
19	S	71	LEU
20	T	8	ARG
20	T	9	ASN
20	T	10	LEU
20	T	11	SER
20	T	13	LEU
20	T	15	ARG
20	T	17	ARG
20	T	19	SER
20	T	20	LEU
20	T	24	LEU
20	T	33	ILE
20	T	45	GLN
20	T	55	ILE
20	T	62	LEU
20	T	72	LEU
20	T	74	LYS
20	T	75	ASN
20	T	80	ARG
20	T	85	MET
20	T	86	ARG
20	T	87	LYS
20	T	91	LEU
20	T	99	LEU
20	T	100	ILE
20	T	104	LEU
21	U	10	ARG

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Mol	Chain	Res	Type
21	U	15	ARG
21	U	25	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1503/1522 (98%)	377 (25%)	48 (3%)
22	V	3/4 (75%)	1 (33%)	0
23	W	10/11 (90%)	2 (20%)	0
24	a	7/8 (87%)	4 (57%)	0
25	b	2/3 (66%)	0	0
All	All	1525/1548 (98%)	384 (25%)	48 (3%)

All (384) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	7	G
1	A	9	G
1	A	16	A
1	A	31	G
1	A	32	A
1	A	33	A
1	A	34	C
1	A	39	G
1	A	47	C
1	A	48	C
1	A	51	A
1	A	81	U
1	A	82	U
1	A	88	A
1	A	89	C
1	A	90	U
1	A	91	C
1	A	95	U
1	A	99	C
1	A	105	G
1	A	108	G
1	A	109	A

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Mol	Chain	Res	Type
1	A	115	G
1	A	116	A
1	A	120	A
1	A	121	C
1	A	129(A)	G
1	A	130	A
1	A	131	C
1	A	138	G
1	A	144	G
1	A	151	A
1	A	157	G
1	A	159	G
1	A	162	A
1	A	163	C
1	A	170	U
1	A	173	U
1	A	181	G
1	A	182	U
1	A	183	G
1	A	190(B)	C
1	A	190(E)	U
1	A	190(G)	G
1	A	195	A
1	A	197	A
1	A	199	G
1	A	201	C
1	A	202	U
1	A	216	G
1	A	222	U
1	A	225	C
1	A	230	G
1	A	246	A
1	A	247	G
1	A	250	A
1	A	251	G
1	A	252	U
1	A	253	U
1	A	254	G
1	A	258	G
1	A	260	G
1	A	266	G
1	A	267	C

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Mol	Chain	Res	Type
1	A	276	G
1	A	289	G
1	A	299	G
1	A	301	G
1	A	319	G
1	A	321	A
1	A	328	C
1	A	329	A
1	A	331	G
1	A	332	G
1	A	345	C
1	A	346	G
1	A	352	C
1	A	353	A
1	A	354	G
1	A	367	U
1	A	372	C
1	A	373	A
1	A	381	C
1	A	384	G
1	A	387	U
1	A	388	G
1	A	397	A
1	A	398	C
1	A	406	G
1	A	410	G
1	A	412	A
1	A	413	G
1	A	421	U
1	A	422	C
1	A	424	G
1	A	429	U
1	A	430	A
1	A	435	C
1	A	439	A
1	A	442	C
1	A	443	C
1	A	449	C
1	A	450	G
1	A	452	A
1	A	460	A
1	A	461	C

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Mol	Chain	Res	Type
1	A	462	G
1	A	475	G
1	A	485	G
1	A	497	A
1	A	498	U
1	A	500	G
1	A	509	A
1	A	510	A
1	A	511	C
1	A	517	G
1	A	518	C
1	A	519	C
1	A	520	A
1	A	527	7MG
1	A	530	G
1	A	532	A
1	A	533	A
1	A	544	G
1	A	545	C
1	A	547	A
1	A	550	G
1	A	559	A
1	A	560	U
1	A	561	U
1	A	562	C
1	A	563	A
1	A	564	C
1	A	566	G
1	A	568	G
1	A	569	C
1	A	571	U
1	A	572	A
1	A	573	A
1	A	575	G
1	A	576	G
1	A	578	C
1	A	587	G
1	A	588	G
1	A	607	A
1	A	624	C
1	A	629	G
1	A	631	G

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Mol	Chain	Res	Type
1	A	644	G
1	A	651	C
1	A	653	A
1	A	661	G
1	A	665	A
1	A	671	G
1	A	673	G
1	A	675	A
1	A	687	A
1	A	688	G
1	A	695	A
1	A	698	G
1	A	701	C
1	A	702	A
1	A	704	A
1	A	721	G
1	A	723	U
1	A	724	G
1	A	728	A
1	A	731	G
1	A	734	G
1	A	741	G
1	A	747	C
1	A	748	C
1	A	752	G
1	A	755	G
1	A	777	A
1	A	785	G
1	A	786	G
1	A	788	U
1	A	789	U
1	A	792	A
1	A	793	U
1	A	794	A
1	A	795	C
1	A	804	U
1	A	812	C
1	A	813	U
1	A	815	A
1	A	816	A
1	A	817	C
1	A	827	U

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Mol	Chain	Res	Type
1	A	828	A
1	A	829	G
1	A	839	U
1	A	840	C
1	A	841	U
1	A	848	C
1	A	851	G
1	A	866	C
1	A	867	G
1	A	868	C
1	A	869	G
1	A	873	A
1	A	889	A
1	A	902	G
1	A	905	U
1	A	914	A
1	A	922	G
1	A	926	G
1	A	927	G
1	A	933	G
1	A	934	C
1	A	935	A
1	A	944	G
1	A	950	U
1	A	954	G
1	A	961	U
1	A	966	M2G
1	A	967	5MC
1	A	968	A
1	A	969	A
1	A	971	G
1	A	974	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	978	A
1	A	984	C
1	A	985	C
1	A	992	U
1	A	993	G
1	A	1003(A)	G
1	A	1004	A

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Mol	Chain	Res	Type
1	A	1005	A
1	A	1006	C
1	A	1021	G
1	A	1025	U
1	A	1026	G
1	A	1027	C
1	A	1028	C
1	A	1030(B)	C
1	A	1030(C)	G
1	A	1045	C
1	A	1048	G
1	A	1050	G
1	A	1052	U
1	A	1053	G
1	A	1054	C
1	A	1055	A
1	A	1064	G
1	A	1065	U
1	A	1066	C
1	A	1068	G
1	A	1078	U
1	A	1079	G
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1104	G
1	A	1111	A
1	A	1122	U
1	A	1124	G
1	A	1125	U
1	A	1126	U
1	A	1127	G
1	A	1129	C
1	A	1130	A
1	A	1131	G
1	A	1137	C
1	A	1138	G
1	A	1139	G
1	A	1141	C
1	A	1142	G
1	A	1143	G
1	A	1159	U

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Mol	Chain	Res	Type
1	A	1162	C
1	A	1164	G
1	A	1171	G
1	A	1178	G
1	A	1181	G
1	A	1182	G
1	A	1183	A
1	A	1184	G
1	A	1190	G
1	A	1191	A
1	A	1193	G
1	A	1196	U
1	A	1198	G
1	A	1200	C
1	A	1201	A
1	A	1202	G
1	A	1206	G
1	A	1211	U
1	A	1212	U
1	A	1213	A
1	A	1214	C
1	A	1215	G
1	A	1225	A
1	A	1226	C
1	A	1227	A
1	A	1235	U
1	A	1238	A
1	A	1245	A
1	A	1249	C
1	A	1250	A
1	A	1251	A
1	A	1253	G
1	A	1256	A
1	A	1257	U
1	A	1258	G
1	A	1270	C
1	A	1273	G
1	A	1279	A
1	A	1280	A
1	A	1281	U
1	A	1282	C
1	A	1286	A

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Mol	Chain	Res	Type
1	A	1287	A
1	A	1288	A
1	A	1300	G
1	A	1301	U
1	A	1302	U
1	A	1303	C
1	A	1304	G
1	A	1305	G
1	A	1312	G
1	A	1313	U
1	A	1317	C
1	A	1318	A
1	A	1319	A
1	A	1320	C
1	A	1322	C
1	A	1328	C
1	A	1338	G
1	A	1348	U
1	A	1353	G
1	A	1356	G
1	A	1359	C
1	A	1360	A
1	A	1361	G
1	A	1362	C
1	A	1363	A
1	A	1370	G
1	A	1379	G
1	A	1381	U
1	A	1382	C
1	A	1393	U
1	A	1394	A
1	A	1397	C
1	A	1398	A
1	A	1399	C
1	A	1400	5MC
1	A	1401	G
1	A	1406	U
1	A	1407	5MC
1	A	1414	U
1	A	1418	A
1	A	1419	G
1	A	1420	C

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Mol	Chain	Res	Type
1	A	1442	G
1	A	1443	G
1	A	1447	G
1	A	1451	A
1	A	1455	G
1	A	1478	C
1	A	1487	G
1	A	1494	G
1	A	1497	G
1	A	1502	A
1	A	1504	G
1	A	1505	G
1	A	1506	U
1	A	1507	A
1	A	1526	G
1	A	1529	G
1	A	1530	G
1	A	1534	C
1	A	1538	C
22	V	2	U
23	W	31	C
23	W	33	U
24	a	35	G
24	a	37	A
24	a	39	G
24	a	40	PSU

All (48) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	7	G
1	A	89	C
1	A	115	G
1	A	129(A)	G
1	A	150	C
1	A	181	G
1	A	204	U
1	A	246	A
1	A	250	A
1	A	251	G
1	A	266	G
1	A	328	C

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Mol	Chain	Res	Type
1	A	344	A
1	A	428	G
1	A	429	U
1	A	484	G
1	A	499	A
1	A	509	A
1	A	544	G
1	A	559	A
1	A	560	U
1	A	587	G
1	A	687	A
1	A	701	C
1	A	812	C
1	A	913	A
1	A	960	U
1	A	991	U
1	A	1026	G
1	A	1049	U
1	A	1065	U
1	A	1067	A
1	A	1137	C
1	A	1182	G
1	A	1190	G
1	A	1201	A
1	A	1212	U
1	A	1256	A
1	A	1279	A
1	A	1281	U
1	A	1300	G
1	A	1319	A
1	A	1347	G
1	A	1360	A
1	A	1361(A)	C
1	A	1397	C
1	A	1528	U
1	A	1533	C

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

18 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	2MG	A	1207	1	24,26,27	2.16	8 (33%)	32,38,41	9.09	2 (6%)
1	5MC	A	1400	1	20,22,23	3.41	6 (30%)	26,32,35	1.47	2 (7%)
1	4OC	A	1402	1	21,23,24	1.78	4 (19%)	26,32,35	1.34	4 (15%)
1	5MC	A	1404	1	20,22,23	2.20	3 (15%)	26,32,35	1.68	4 (15%)
1	5MC	A	1407	1	20,22,23	2.81	4 (20%)	26,32,35	1.33	4 (15%)
1	UR3	A	1498	1	20,22,23	0.94	1 (5%)	23,32,35	0.96	2 (8%)
1	MA6	A	1518[A]	1	26,26,27	1.73	5 (19%)	37,38,41	1.17	4 (10%)
1	MA6	A	1518[B]	1	26,26,27	1.26	2 (7%)	37,38,41	0.98	2 (5%)
1	MA6	A	1519[A]	1	26,26,27	1.12	4 (15%)	37,38,41	1.16	3 (8%)
1	MA6	A	1519[B]	1	26,26,27	1.74	8 (30%)	37,38,41	1.00	3 (8%)
1	PSU	A	1540	1	19,21,22	1.17	1 (5%)	23,30,33	0.94	1 (4%)
1	PSU	A	516	1	19,21,22	1.45	2 (10%)	23,30,33	1.09	3 (13%)
1	7MG	A	527	1	24,26,27	4.46	9 (37%)	34,39,42	1.64	8 (23%)
1	M2G	A	966	1	25,27,28	1.15	3 (12%)	34,40,43	7.33	5 (14%)
1	5MC	A	967	1	20,22,23	1.12	1 (5%)	26,32,35	1.51	4 (15%)
12	0TD	L	92	12	9,9,10	7.57	2 (22%)	9,11,13	3.39	5 (55%)
23	PSU	W	40	23	19,21,22	1.00	1 (5%)	23,30,33	1.22	3 (13%)
24	PSU	a	40	24,1	19,21,22	1.31	1 (5%)	23,30,33	1.36	3 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	2MG	A	1207	1	-	0/10/27/28	0/1/3/3
1	5MC	A	1400	1	-	1/6/25/26	0/2/2/2
1	4OC	A	1402	1	-	2/10/29/30	0/2/2/2
1	5MC	A	1404	1	-	0/6/25/26	0/2/2/2
1	5MC	A	1407	1	-	0/6/25/26	0/2/2/2
1	UR3	A	1498	1	-	0/6/25/26	0/2/2/2
1	MA6	A	1518[A]	1	-	0/13/29/30	0/1/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MA6	A	1518[B]	1	-	0/13/29/30	0/1/3/3
1	MA6	A	1519[A]	1	-	0/13/29/30	0/1/3/3
1	MA6	A	1519[B]	1	-	1/13/29/30	0/1/3/3
1	PSU	A	1540	1	-	0/8/25/26	0/2/2/2
1	PSU	A	516	1	-	0/8/25/26	0/2/2/2
1	7MG	A	527	1	-	1/8/37/38	0/1/3/3
1	M2G	A	966	1	-	0/12/29/30	0/1/3/3
1	5MC	A	967	1	-	0/6/25/26	0/2/2/2
12	0TD	L	92	12	-	0/10/12/14	0/0/0/0
23	PSU	W	40	23	-	1/8/25/26	0/2/2/2
24	PSU	a	40	24,1	-	1/8/25/26	0/2/2/2

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	L	92	0TD	O-C	22.20	1.26	1.11
1	A	527	7MG	C8-N9	-17.77	1.32	1.46
1	A	1400	5MC	C2-N1	12.46	1.51	1.38
1	A	1407	5MC	C2-N1	8.99	1.48	1.38
1	A	1404	5MC	C2-N1	8.22	1.47	1.38
1	A	527	7MG	C2-N2	6.99	1.43	1.32
1	A	1407	5MC	C5-C4	5.95	1.50	1.41
1	A	1400	5MC	P-OP1	5.22	1.52	1.46
1	A	527	7MG	C6-C5	5.07	1.50	1.41
1	A	516	PSU	C6-N1	5.06	1.37	1.32
1	A	1518[A]	MA6	C8-N9	4.95	1.44	1.36
1	A	1207	2MG	C6-N1	4.94	1.45	1.37
1	A	1518[A]	MA6	C4-N9	4.77	1.44	1.37
1	A	527	7MG	C8-N7	-4.70	1.32	1.45
1	A	1402	4OC	C2-N1	4.45	1.43	1.38
24	a	40	PSU	C6-N1	4.37	1.36	1.32
1	A	1207	2MG	C8-N9	4.32	1.43	1.36
1	A	1540	PSU	C6-N1	4.30	1.36	1.32
1	A	1207	2MG	C6-C5	4.29	1.48	1.41
12	L	92	0TD	CA-C	4.28	1.56	1.48
1	A	1402	4OC	C2-N3	4.21	1.46	1.35
1	A	527	7MG	C4-N3	4.12	1.39	1.34
1	A	1518[B]	MA6	C8-N9	4.03	1.42	1.36
1	A	1519[B]	MA6	C2-N1	4.03	1.41	1.33
1	A	1407	5MC	P-OP1	3.96	1.51	1.46
1	A	1207	2MG	C2-N1	3.70	1.45	1.36
23	W	40	PSU	C6-N1	3.40	1.35	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1400	5MC	C2-N3	3.39	1.44	1.35
1	A	1519[B]	MA6	C8-N9	3.26	1.41	1.36
1	A	527	7MG	C5-N7	3.21	1.46	1.39
1	A	1400	5MC	C4-N3	3.16	1.37	1.32
1	A	1519[B]	MA6	C5-C4	3.14	1.47	1.40
1	A	527	7MG	CM7-N7	-3.13	1.41	1.46
1	A	1400	5MC	C5-C4	3.00	1.46	1.41
1	A	1519[B]	MA6	C2-N3	2.99	1.38	1.32
1	A	1404	5MC	P-OP1	2.95	1.50	1.46
1	A	1518[A]	MA6	C5-C4	2.92	1.47	1.40
1	A	1207	2MG	C2-N2	2.90	1.41	1.32
1	A	1407	5MC	C2-N3	2.88	1.43	1.35
1	A	1400	5MC	C4-N4	2.86	1.41	1.34
1	A	1519[B]	MA6	C6-N1	2.73	1.40	1.32
1	A	966	M2G	C8-N9	2.70	1.40	1.36
1	A	1518[A]	MA6	C2-N1	2.69	1.39	1.33
1	A	1498	UR3	P-OP1	2.66	1.49	1.46
1	A	1402	4OC	CM4-N4	2.62	1.50	1.45
1	A	1519[A]	MA6	C8-N9	2.62	1.40	1.36
1	A	1519[B]	MA6	C4-N3	2.62	1.39	1.35
1	A	1518[B]	MA6	C2-N1	2.61	1.39	1.33
1	A	1519[B]	MA6	C4-N9	2.60	1.41	1.37
1	A	1519[B]	MA6	C6-N6	2.57	1.44	1.37
1	A	527	7MG	P-OP1	2.47	1.49	1.46
1	A	527	7MG	C2-N1	-2.45	1.32	1.36
1	A	1207	2MG	P-OP1	2.40	1.49	1.46
1	A	1207	2MG	C5-C4	2.38	1.45	1.40
1	A	1207	2MG	O6-C6	2.36	1.29	1.24
1	A	1518[A]	MA6	C4-N3	2.34	1.39	1.35
1	A	1519[A]	MA6	C2-N1	2.30	1.38	1.33
1	A	1402	4OC	C4-N4	-2.24	1.31	1.36
1	A	966	M2G	C4-N9	2.20	1.40	1.37
1	A	1519[A]	MA6	C4-N9	2.19	1.40	1.37
1	A	966	M2G	C4-N3	2.13	1.39	1.35
1	A	967	5MC	O2-C2	-2.12	1.18	1.23
1	A	1404	5MC	C5-C4	2.09	1.44	1.41
1	A	516	PSU	P-OP1	2.04	1.49	1.46
1	A	1519[A]	MA6	C5-C4	2.02	1.45	1.40

All (62) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1207	2MG	C6-C5-N7	-51.19	127.25	134.14
1	A	966	M2G	C6-C5-N7	-42.22	128.46	134.14
12	L	92	0TD	CB-CA-N	-6.73	96.33	109.55
1	A	1404	5MC	C6-N1-C2	6.19	121.67	118.62
1	A	1400	5MC	C2-N3-C4	4.88	119.83	115.41
1	A	967	5MC	C6-N1-C2	4.75	120.96	118.62
1	A	527	7MG	C6-C5-N7	4.60	141.62	131.87
12	L	92	0TD	CSB-SB-CB	-4.57	93.56	101.48
24	a	40	PSU	C5-C1'-C2'	4.56	123.66	115.61
12	L	92	0TD	C-CA-N	-4.26	105.00	111.94
1	A	967	5MC	C2-N3-C4	3.86	118.91	115.41
1	A	1518[A]	MA6	C8-N9-C4	-3.69	104.08	106.90
1	A	1402	4OC	CM4-N4-C4	-3.67	119.52	122.80
1	A	1407	5MC	N4-C4-N3	-3.60	112.52	118.73
1	A	1400	5MC	C2-N1-C1'	3.60	123.92	119.03
1	A	966	M2G	C6-N1-C2	3.44	122.71	120.28
23	W	40	PSU	C5-C1'-C2'	-3.32	109.75	115.61
1	A	1402	4OC	C2-N1-C1'	3.29	123.50	119.03
1	A	527	7MG	N7-C8-N9	3.21	107.33	103.08
23	W	40	PSU	O4'-C1'-C5	-2.97	105.84	109.55
1	A	1407	5MC	C2-N3-C4	2.97	118.10	115.41
1	A	966	M2G	N1-C2-N2	-2.96	114.69	118.37
1	A	527	7MG	C5-C4-N3	-2.94	121.31	126.61
1	A	527	7MG	C2-N3-C4	2.92	121.76	117.61
1	A	1518[A]	MA6	N3-C2-N1	2.79	131.04	128.71
1	A	1518[B]	MA6	C2-N1-C6	2.74	117.48	111.53
24	a	40	PSU	C4-N3-C2	-2.72	119.85	125.36
1	A	1519[A]	MA6	N3-C2-N1	2.69	130.96	128.71
1	A	1404	5MC	N4-C4-N3	-2.67	114.13	118.73
1	A	1518[A]	MA6	C2-N1-C6	2.66	117.30	111.53
1	A	1404	5MC	C2-N3-C4	2.64	117.80	115.41
1	A	967	5MC	CM5-C5-C6	2.63	124.18	118.59
1	A	1519[A]	MA6	C2-N1-C6	2.60	117.16	111.53
1	A	1519[B]	MA6	C2-N1-C6	2.56	117.08	111.53
12	L	92	0TD	CA-CB-CG	-2.55	107.92	110.95
1	A	1540	PSU	C4-N3-C2	-2.54	120.22	125.36
23	W	40	PSU	C4-N3-C2	-2.52	120.25	125.36
1	A	1519[B]	MA6	N3-C2-N1	2.52	130.81	128.71
1	A	527	7MG	C4-C5-N7	-2.49	103.96	106.82
24	a	40	PSU	O4'-C1'-C5	2.45	112.60	109.55
1	A	967	5MC	N4-C4-N3	-2.42	114.56	118.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1498	UR3	C5-C4-N3	-2.36	112.57	117.61
1	A	1518[B]	MA6	N3-C2-N1	2.35	130.67	128.71
1	A	1518[A]	MA6	N3-C4-N9	2.30	129.58	125.43
1	A	1519[A]	MA6	C8-N9-C1'	2.26	130.84	126.38
1	A	516	PSU	C4-N3-C2	-2.24	120.82	125.36
12	L	92	0TD	OD1-CG-CB	-2.20	116.58	121.95
1	A	516	PSU	O4'-C1'-C2'	2.20	108.16	104.37
1	A	1402	4OC	C2-N3-C4	2.18	117.92	115.27
1	A	527	7MG	N2-C2-N3	-2.17	117.37	120.31
1	A	1407	5MC	C6-N1-C2	2.17	119.69	118.62
1	A	1404	5MC	C5-C4-N3	2.15	124.79	121.21
1	A	1519[B]	MA6	N3-C4-N9	2.15	129.31	125.43
1	A	527	7MG	N2-C2-N1	2.12	120.19	117.86
1	A	1402	4OC	C6-C5-C4	2.10	118.32	117.45
1	A	1407	5MC	CM5-C5-C4	2.08	123.53	121.43
1	A	516	PSU	O4'-C1'-C5	2.07	112.12	109.55
1	A	527	7MG	C5-C6-N1	2.06	121.09	115.25
1	A	1498	UR3	C3U-N3-C2	-2.06	115.08	119.51
1	A	966	M2G	C2-N3-C4	-2.03	112.27	115.14
1	A	1207	2MG	N3-C4-N9	2.02	129.87	126.91
1	A	966	M2G	C8-N9-C4	-2.01	105.36	106.90

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1402	4OC	N3-C4-N4-CM4
1	A	1402	4OC	OP2-P-O5'-C5'
1	A	527	7MG	OP2-P-O5'-C5'
1	A	1519[B]	MA6	OP2-P-O5'-C5'
24	a	40	PSU	OP2-P-O5'-C5'
1	A	1400	5MC	OP2-P-O5'-C5'
23	W	40	PSU	OP2-P-O5'-C5'

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 347 ligands modelled in this entry, 346 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	SRY	A	1928	-	42,42,42	2.22	9 (21%)	63,63,63	2.45	22 (34%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	SRY	A	1928	-	-	0/22/87/87	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	1928	SRY	CD1-N31	8.77	1.49	1.33
27	A	1928	SRY	CA1-N11	5.41	1.43	1.33
27	A	1928	SRY	C32-CG2	-4.47	1.47	1.52
27	A	1928	SRY	O53-C53	-3.49	1.35	1.44
27	A	1928	SRY	C23-N23	-3.12	1.42	1.47
27	A	1928	SRY	C11-N11	-2.40	1.41	1.45
27	A	1928	SRY	CD1-NE1	2.30	1.45	1.34
27	A	1928	SRY	C21-C11	-2.18	1.48	1.53
27	A	1928	SRY	CA1-NB1	2.16	1.44	1.34

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	1928	SRY	C43-C33-C23	-7.83	99.32	110.44
27	A	1928	SRY	C12-O42-C42	-5.95	98.71	108.25
27	A	1928	SRY	C61-C11-N11	-5.68	98.51	110.56
27	A	1928	SRY	C13-O13-C22	-5.46	106.79	116.28
27	A	1928	SRY	C42-C32-C22	-4.77	96.21	101.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	1928	SRY	O53-C13-C23	3.89	119.15	110.78
27	A	1928	SRY	O53-C53-C43	3.84	116.86	109.76
27	A	1928	SRY	O41-C41-C51	3.83	116.99	107.16
27	A	1928	SRY	O41-C12-C22	3.37	113.80	107.32
27	A	1928	SRY	C51-C61-C11	3.25	115.05	110.44
27	A	1928	SRY	O32-C32-C22	3.17	119.76	111.47
27	A	1928	SRY	O51-C51-C61	-3.05	103.52	110.35
27	A	1928	SRY	OG2-CG2-C32	-3.04	117.71	123.98
27	A	1928	SRY	O21-C21-C31	2.98	115.72	109.61
27	A	1928	SRY	CI3-N23-C23	-2.80	111.44	113.65
27	A	1928	SRY	O41-C41-C31	-2.71	101.88	108.77
27	A	1928	SRY	O53-C53-C63	-2.48	100.26	106.34
27	A	1928	SRY	O43-C43-C33	2.36	115.64	110.35
27	A	1928	SRY	O13-C22-C12	-2.35	107.81	111.78
27	A	1928	SRY	C63-C53-C43	-2.10	107.92	113.00
27	A	1928	SRY	O63-C63-C53	-2.07	104.24	111.36
27	A	1928	SRY	O51-C51-C41	2.05	114.63	109.85

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

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 ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	1512/1522 (99%)	-0.41	6 (0%) 90 79	80, 129, 232, 327	0
2	B	236/256 (92%)	0.14	0 100 100	62, 153, 220, 247	0
3	C	207/239 (86%)	0.09	6 (2%) 49 31	94, 191, 226, 244	0
4	D	208/209 (99%)	0.08	2 (0%) 79 58	105, 149, 198, 214	0
5	E	151/162 (93%)	-0.13	0 100 100	80, 114, 166, 193	0
6	F	101/101 (100%)	-0.17	1 (0%) 79 58	110, 150, 182, 226	0
7	G	155/156 (99%)	-0.09	3 (1%) 64 42	121, 160, 223, 238	0
8	H	138/138 (100%)	-0.04	0 100 100	75, 104, 138, 155	0
9	I	127/128 (99%)	0.32	2 (1%) 68 46	125, 184, 217, 240	0
10	J	99/105 (94%)	0.37	3 (3%) 48 30	81, 203, 272, 295	0
11	K	117/129 (90%)	-0.17	0 100 100	88, 130, 160, 167	0
12	L	124/135 (91%)	0.35	5 (4%) 36 24	97, 136, 168, 247	0
13	M	118/126 (93%)	0.29	2 (1%) 67 45	127, 158, 192, 211	0
14	N	60/61 (98%)	0.09	1 (1%) 67 45	144, 169, 210, 246	0
15	O	88/89 (98%)	0.33	2 (2%) 57 37	94, 127, 182, 225	0
16	P	84/88 (95%)	0.12	0 100 100	96, 126, 164, 239	0
17	Q	100/105 (95%)	0.09	0 100 100	83, 111, 150, 189	0
18	R	71/88 (80%)	0.04	0 100 100	95, 132, 178, 229	0
19	S	81/93 (87%)	0.41	1 (1%) 75 53	84, 184, 228, 234	0
20	T	99/106 (93%)	0.10	0 100 100	95, 126, 167, 212	0
21	U	25/27 (92%)	0.72	2 (8%) 12 11	77, 163, 192, 220	0
22	V	4/4 (100%)	3.70	4 (100%) 0 0	263, 267, 272, 275	0
23	W	11/11 (100%)	6.31	11 (100%) 0 0	234, 291, 345, 387	5 (45%)
24	a	8/8 (100%)	1.05	2 (25%) 1 2	200, 218, 290, 330	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	b	3/3 (100%)	1.25	1 (33%) 1 1	172, 172, 206, 218	0
All	All	3927/4089 (96%)	-0.07	54 (1%) 70 49	62, 140, 222, 387	5 (0%)

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
23	W	32	C	10.9
1	A	1498	UR3	9.1
23	W	31	C	8.4
23	W	38	A	7.2
23	W	33	U	7.2
23	W	35	G	7.1
23	W	30	G	7.0
15	O	89	GLY	6.6
12	L	129	ALA	6.6
1	A	1129	C	6.2
23	W	37	A	5.9
22	V	3	U	4.9
21	U	18	TYR	4.8
23	W	39	G	4.4
23	W	34	G	4.3
22	V	2	U	4.2
23	W	36	A	4.2
10	J	33	GLN	4.0
14	N	12	ARG	3.5
22	V	4	U	3.5
10	J	34	VAL	3.5
1	A	1519[A]	MA6	3.3
1	A	82	U	3.3
6	F	101	ALA	3.2
3	C	157	ILE	3.1
12	L	65	GLU	3.0
7	G	83	ALA	3.0
15	O	88	ARG	2.9
23	W	40	PSU	2.9
12	L	128	ALA	2.8
3	C	155	GLY	2.8
9	I	15	ALA	2.7
12	L	33	ARG	2.6
24	a	40	PSU	2.6
7	G	84	ASN	2.6
12	L	64	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
3	C	158	GLY	2.5
13	M	117	VAL	2.4
13	M	2	ALA	2.4
1	A	1540	PSU	2.3
10	J	74	ILE	2.3
4	D	33	MET	2.3
3	C	193	TYR	2.3
7	G	82	GLY	2.3
4	D	13	ARG	2.2
1	A	793	U	2.2
3	C	189	ALA	2.2
22	V	1	U	2.2
3	C	156	ARG	2.2
9	I	66	ARG	2.1
21	U	17	THR	2.1
25	b	2	U	2.1
24	a	34	G	2.0
19	S	12	ASP	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	5MC	A	967	21/22	0.16	-	117,131,145,146	0
1	5MC	A	1404	21/22	0.17	-	102,129,148,149	0
1	7MG	A	527	24/25	0.18	-	91,114,123,126	0
1	M2G	A	966	25/26	0.21	-	122,137,142,145	0
1	2MG	A	1207	24/25	0.14	-	154,167,200,202	0
1	UR3	A	1498	21/22	0.27	-	111,124,183,193	0
1	MA6	A	1518[A]	24/25	0.20	-	110,122,127,131	24
1	5MC	A	1407	21/22	0.12	-	127,152,158,162	0
12	0TD	L	92	10/11	0.19	-	113,121,127,289	0
23	PSU	W	40	20/21	0.39	-	291,301,325,326	0
1	PSU	A	516	20/21	0.10	-	123,147,168,168	0
1	4OC	A	1402	22/23	0.21	-	104,119,127,142	0
1	PSU	A	1540	20/21	0.35	-	253,269,289,293	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
1	MA6	A	1519[A]	24/25	0.29	-	100,115,125,126	24
1	MA6	A	1518[B]	24/25	0.20	-	107,122,137,148	24
1	MA6	A	1519[B]	24/25	0.29	-	101,116,129,130	24
24	PSU	a	40	20/21	0.37	-	208,236,258,262	0
1	5MC	A	1400	21/22	0.20	-	103,130,148,159	0

## 6.3 Carbohydrates

There are no carbohydrates in this entry.

## 6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
26	MG	A	1770	1/1	0.51	-	106,106,106,106	0
26	MG	A	1862	1/1	0.30	-	268,268,268,268	0
26	MG	A	1617	1/1	0.23	-	85,85,85,85	0
26	MG	A	1925	1/1	0.16	-	114,114,114,114	0
26	MG	A	1917	1/1	0.77	-	128,128,128,128	0
26	MG	A	1644	1/1	0.34	-	127,127,127,127	0
26	MG	A	1623	1/1	0.12	-	67,67,67,67	0
26	MG	A	1755	1/1	0.48	-	74,74,74,74	0
26	MG	A	1815	1/1	0.12	-	506,506,506,506	0
26	MG	A	1885	1/1	0.15	-	84,84,84,84	0
26	MG	A	1800	1/1	0.19	-	415,415,415,415	1
26	MG	P	103	1/1	0.49	-	96,96,96,96	0
26	MG	A	1859	1/1	0.17	-	427,427,427,427	0
28	ZN	N	101	1/1	0.15	-	164,164,164,164	0
26	MG	A	1871	1/1	0.24	-	392,392,392,392	0
26	MG	A	1832	1/1	0.09	-	278,278,278,278	0
26	MG	A	1669	1/1	0.12	-	123,123,123,123	0
26	MG	A	1905	1/1	0.24	-	105,105,105,105	0
26	MG	A	1756	1/1	0.08	-	126,126,126,126	0
26	MG	E	203	1/1	0.12	-	101,101,101,101	0
26	MG	A	1716	1/1	0.23	-	132,132,132,132	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
26	MG	A	1845	1/1	0.21	-	410,410,410,410	0
26	MG	A	1604	1/1	0.30	-	91,91,91,91	0
26	MG	A	1926	1/1	0.56	-	116,116,116,116	0
26	MG	A	1873	1/1	0.05	-	361,361,361,361	0
26	MG	A	1622	1/1	0.66	-	81,81,81,81	0
26	MG	A	1609	1/1	0.07	-	157,157,157,157	0
26	MG	A	1771	1/1	0.50	-	102,102,102,102	0
26	MG	A	1918	1/1	0.19	-	75,75,75,75	0
26	MG	A	1676	1/1	0.34	-	158,158,158,158	0
26	MG	A	1731	1/1	0.19	-	68,68,68,68	0
26	MG	A	1745	1/1	0.56	-	92,92,92,92	0
26	MG	A	1662	1/1	0.13	-	123,123,123,123	0
26	MG	A	1906	1/1	0.12	-	64,64,64,64	0
26	MG	A	1680	1/1	0.45	-	214,214,214,214	0
26	MG	A	1822	1/1	0.12	-	293,293,293,293	0
26	MG	A	1757	1/1	0.24	-	88,88,88,88	0
26	MG	A	1659	1/1	0.31	-	90,90,90,90	0
26	MG	A	1834	1/1	0.84	-	412,412,412,412	1
26	MG	A	1827	1/1	0.09	-	251,251,251,251	0
26	MG	A	1851	1/1	0.29	-	328,328,328,328	0
26	MG	A	1694	1/1	0.49	-	87,87,87,87	0
26	MG	A	1908	1/1	0.34	-	81,81,81,81	0
26	MG	A	1899	1/1	0.40	-	68,68,68,68	0
26	MG	A	1639	1/1	0.21	-	87,87,87,87	0
26	MG	A	1700	1/1	0.38	-	302,302,302,302	0
26	MG	A	1717	1/1	0.30	-	152,152,152,152	0
26	MG	A	1738	1/1	0.05	-	68,68,68,68	0
26	MG	A	1865	1/1	0.34	-	457,457,457,457	0
26	MG	A	1894	1/1	0.24	-	94,94,94,94	0
26	MG	A	1737	1/1	0.71	-	89,89,89,89	0
26	MG	A	1740	1/1	0.66	-	93,93,93,93	0
26	MG	A	1900	1/1	0.39	-	93,93,93,93	0
26	MG	A	1902	1/1	0.39	-	119,119,119,119	0
26	MG	A	1627	1/1	0.16	-	141,141,141,141	0
26	MG	A	1817	1/1	0.18	-	419,419,419,419	0
26	MG	A	1811	1/1	1.17	-	468,468,468,468	0
26	MG	A	1730	1/1	0.65	-	97,97,97,97	0
26	MG	A	1723	1/1	0.29	-	117,117,117,117	0
26	MG	A	1765	1/1	0.17	-	104,104,104,104	0
26	MG	A	1849	1/1	0.26	-	471,471,471,471	0
26	MG	A	1882	1/1	0.33	-	315,315,315,315	0
26	MG	A	1701	1/1	0.21	-	108,108,108,108	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
26	MG	A	1857	1/1	0.29	-	308,308,308,308	0
26	MG	A	1883	1/1	0.33	-	443,443,443,443	0
26	MG	A	1741	1/1	0.16	-	105,105,105,105	0
26	MG	A	1689	1/1	0.12	-	126,126,126,126	0
26	MG	A	1613	1/1	0.13	-	202,202,202,202	0
26	MG	A	1664	1/1	0.26	-	154,154,154,154	0
26	MG	A	1711	1/1	0.86	-	133,133,133,133	0
26	MG	A	1624	1/1	1.09	-	147,147,147,147	0
26	MG	Q	201	1/1	0.57	-	145,145,145,145	0
26	MG	A	1615	1/1	0.11	-	147,147,147,147	0
26	MG	A	1843	1/1	0.49	-	357,357,357,357	0
26	MG	A	1751	1/1	0.54	-	76,76,76,76	0
26	MG	A	1797	1/1	0.12	-	502,502,502,502	0
26	MG	A	1656	1/1	0.26	-	236,236,236,236	0
26	MG	A	1660	1/1	0.13	-	224,224,224,224	0
26	MG	A	1821	1/1	0.21	-	428,428,428,428	0
26	MG	A	1835	1/1	0.20	-	309,309,309,309	0
28	ZN	D	301	1/1	0.28	-	138,138,138,138	0
26	MG	A	1667	1/1	0.19	-	119,119,119,119	0
26	MG	G	201	1/1	0.84	-	117,117,117,117	0
26	MG	A	1640	1/1	0.26	-	172,172,172,172	0
26	MG	A	1907	1/1	0.32	-	120,120,120,120	0
26	MG	A	1632	1/1	0.38	-	248,248,248,248	0
26	MG	A	1606	1/1	0.40	-	87,87,87,87	0
26	MG	N	102	1/1	0.64	-	107,107,107,107	0
26	MG	A	1781	1/1	0.34	-	104,104,104,104	0
26	MG	A	1796	1/1	0.12	-	416,416,416,416	0
26	MG	A	1829	1/1	0.29	-	489,489,489,489	0
26	MG	A	1921	1/1	0.41	-	84,84,84,84	0
26	MG	A	1657	1/1	0.27	-	220,220,220,220	0
26	MG	A	1603	1/1	0.14	-	277,277,277,277	0
26	MG	A	1896	1/1	0.17	-	114,114,114,114	0
26	MG	A	1649	1/1	0.34	-	84,84,84,84	0
26	MG	A	1725	1/1	0.26	-	92,92,92,92	0
26	MG	A	1682	1/1	0.07	-	242,242,242,242	0
26	MG	A	1888	1/1	0.27	-	89,89,89,89	0
26	MG	A	1807	1/1	0.47	-	517,517,517,517	1
26	MG	A	1860	1/1	0.16	-	460,460,460,460	0
26	MG	A	1626	1/1	0.23	-	245,245,245,245	0
26	MG	A	1668	1/1	0.28	-	173,173,173,173	0
26	MG	A	1855	1/1	0.13	-	401,401,401,401	0
26	MG	A	1612	1/1	0.34	-	281,281,281,281	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
26	MG	A	1816	1/1	0.41	-	454,454,454,454	0
26	MG	A	1853	1/1	0.27	-	502,502,502,502	0
26	MG	A	1812	1/1	0.57	-	444,444,444,444	0
26	MG	A	1858	1/1	0.23	-	355,355,355,355	0
26	MG	A	1641	1/1	0.18	-	102,102,102,102	0
26	MG	A	1633	1/1	0.22	-	118,118,118,118	0
26	MG	A	1675	1/1	1.13	-	122,122,122,122	0
26	MG	A	1690	1/1	0.08	-	114,114,114,114	0
26	MG	A	1753	1/1	0.31	-	109,109,109,109	0
26	MG	A	1870	1/1	0.35	-	406,406,406,406	0
26	MG	H	201	1/1	0.36	-	67,67,67,67	0
26	MG	A	1743	1/1	0.44	-	105,105,105,105	0
26	MG	A	1780	1/1	0.31	-	119,119,119,119	0
26	MG	A	1910	1/1	0.29	-	120,120,120,120	0
26	MG	A	1914	1/1	1.00	-	99,99,99,99	0
26	MG	A	1608	1/1	0.24	-	73,73,73,73	0
26	MG	A	1650	1/1	0.18	-	151,151,151,151	0
26	MG	A	1848	1/1	0.29	-	407,407,407,407	0
26	MG	A	1763	1/1	0.18	-	120,120,120,120	0
26	MG	A	1801	1/1	0.17	-	464,464,464,464	0
26	MG	A	1838	1/1	0.57	-	538,538,538,538	0
26	MG	A	1688	1/1	0.53	-	186,186,186,186	0
26	MG	A	1824	1/1	0.14	-	503,503,503,503	0
26	MG	A	1788	1/1	0.12	-	285,285,285,285	0
26	MG	A	1864	1/1	0.18	-	393,393,393,393	0
26	MG	A	1878	1/1	0.17	-	346,346,346,346	0
26	MG	A	1779	1/1	0.27	-	102,102,102,102	0
26	MG	A	1830	1/1	0.17	-	480,480,480,480	0
26	MG	A	1729	1/1	0.88	-	101,101,101,101	0
26	MG	A	1791	1/1	0.17	-	283,283,283,283	0
26	MG	A	1844	1/1	0.07	-	420,420,420,420	0
26	MG	A	1739	1/1	0.12	-	78,78,78,78	0
26	MG	A	1746	1/1	0.15	-	104,104,104,104	0
26	MG	A	1880	1/1	0.45	-	508,508,508,508	0
26	MG	A	1708	1/1	0.24	-	152,152,152,152	0
26	MG	A	1715	1/1	0.21	-	229,229,229,229	0
26	MG	A	1724	1/1	0.62	-	117,117,117,117	0
26	MG	A	1911	1/1	0.10	-	100,100,100,100	0
26	MG	A	1607	1/1	0.15	-	154,154,154,154	0
26	MG	A	1786	1/1	0.06	-	109,109,109,109	0
26	MG	A	1634	1/1	0.10	-	107,107,107,107	0
26	MG	A	1679	1/1	0.14	-	369,369,369,369	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
26	MG	A	1698	1/1	0.20	-	124,124,124,124	0
26	MG	A	1666	1/1	0.09	-	149,149,149,149	0
26	MG	A	1852	1/1	0.31	-	450,450,450,450	0
26	MG	A	1794	1/1	0.24	-	518,518,518,518	0
26	MG	A	1828	1/1	0.15	-	432,432,432,432	0
26	MG	A	1923	1/1	0.81	-	86,86,86,86	0
26	MG	A	1727	1/1	0.61	-	84,84,84,84	0
26	MG	A	1768	1/1	0.40	-	107,107,107,107	0
26	MG	A	1819	1/1	0.46	-	493,493,493,493	0
26	MG	A	1793	1/1	0.14	-	483,483,483,483	0
26	MG	A	1774	1/1	0.52	-	109,109,109,109	0
26	MG	A	1890	1/1	0.14	-	112,112,112,112	0
26	MG	A	1814	1/1	0.10	-	440,440,440,440	0
26	MG	A	1803	1/1	0.17	-	345,345,345,345	0
26	MG	A	1776	1/1	0.12	-	96,96,96,96	0
26	MG	A	1920	1/1	0.08	-	138,138,138,138	0
26	MG	A	1671	1/1	0.24	-	96,96,96,96	0
26	MG	A	1636	1/1	0.52	-	88,88,88,88	0
26	MG	A	1898	1/1	0.53	-	89,89,89,89	0
26	MG	A	1887	1/1	0.48	-	102,102,102,102	0
26	MG	A	1837	1/1	0.15	-	469,469,469,469	0
26	MG	A	1823	1/1	0.10	-	422,422,422,422	0
26	MG	A	1658	1/1	0.18	-	115,115,115,115	0
26	MG	A	1904	1/1	0.75	-	97,97,97,97	0
26	MG	A	1642	1/1	0.29	-	78,78,78,78	0
26	MG	S	101	1/1	0.12	-	115,115,115,115	0
26	MG	A	1621	1/1	0.20	-	131,131,131,131	0
26	MG	A	1678	1/1	0.11	-	217,217,217,217	0
26	MG	A	1736	1/1	0.15	-	123,123,123,123	0
26	MG	A	1638	1/1	0.12	-	86,86,86,86	0
26	MG	A	1866	1/1	0.20	-	434,434,434,434	0
26	MG	A	1901	1/1	0.31	-	101,101,101,101	0
26	MG	A	1661	1/1	0.21	-	244,244,244,244	0
26	MG	A	1804	1/1	0.38	-	447,447,447,447	0
26	MG	A	1919	1/1	0.20	-	78,78,78,78	0
26	MG	A	1767	1/1	0.28	-	111,111,111,111	0
26	MG	A	1783	1/1	0.12	-	110,110,110,110	0
26	MG	A	1663	1/1	0.18	-	160,160,160,160	0
26	MG	A	1686	1/1	0.28	-	184,184,184,184	0
26	MG	A	1778	1/1	0.10	-	119,119,119,119	1
26	MG	J	201	1/1	0.34	-	109,109,109,109	0
26	MG	A	1839	1/1	0.08	-	467,467,467,467	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
26	MG	A	1712	1/1	0.19	-	170,170,170,170	0
26	MG	A	1808	1/1	0.56	-	498,498,498,498	0
26	MG	A	1775	1/1	0.10	-	79,79,79,79	0
26	MG	A	1710	1/1	0.13	-	253,253,253,253	0
26	MG	A	1630	1/1	0.26	-	158,158,158,158	0
26	MG	A	1876	1/1	0.37	-	463,463,463,463	1
26	MG	A	1720	1/1	0.29	-	74,74,74,74	0
26	MG	A	1881	1/1	0.13	-	414,414,414,414	0
26	MG	A	1696	1/1	0.25	-	263,263,263,263	0
26	MG	A	1611	1/1	0.09	-	113,113,113,113	0
26	MG	F	601	1/1	0.07	-	102,102,102,102	0
26	MG	A	1785	1/1	0.14	-	108,108,108,108	0
26	MG	A	1836	1/1	0.21	-	416,416,416,416	1
26	MG	A	1893	1/1	0.69	-	114,114,114,114	0
26	MG	A	1648	1/1	0.28	-	93,93,93,93	0
26	MG	P	101	1/1	0.35	-	58,58,58,58	0
26	MG	A	1699	1/1	0.08	-	414,414,414,414	0
26	MG	A	1818	1/1	0.12	-	189,189,189,189	0
26	MG	A	1895	1/1	0.12	-	106,106,106,106	0
26	MG	A	1748	1/1	0.23	-	110,110,110,110	0
26	MG	A	1750	1/1	0.11	-	74,74,74,74	0
26	MG	A	1897	1/1	0.49	-	114,114,114,114	0
26	MG	A	1916	1/1	0.14	-	119,119,119,119	0
26	MG	A	1654	1/1	0.09	-	161,161,161,161	0
26	MG	A	1773	1/1	0.10	-	103,103,103,103	0
26	MG	A	1787	1/1	0.14	-	496,496,496,496	0
26	MG	A	1820	1/1	0.14	-	373,373,373,373	0
26	MG	E	201	1/1	0.42	-	95,95,95,95	0
26	MG	A	1868	1/1	0.42	-	380,380,380,380	0
26	MG	A	1702	1/1	0.13	-	279,279,279,279	0
26	MG	A	1637	1/1	0.27	-	228,228,228,228	0
26	MG	A	1628	1/1	0.33	-	152,152,152,152	0
26	MG	A	1806	1/1	0.20	-	505,505,505,505	0
26	MG	A	1915	1/1	0.57	-	117,117,117,117	0
26	MG	A	1863	1/1	0.21	-	409,409,409,409	0
26	MG	A	1912	1/1	0.67	-	104,104,104,104	0
26	MG	A	1616	1/1	0.18	-	63,63,63,63	0
26	MG	A	1693	1/1	0.10	-	108,108,108,108	0
26	MG	A	1742	1/1	0.44	-	97,97,97,97	0
26	MG	A	1685	1/1	0.49	-	126,126,126,126	0
26	MG	E	204	1/1	0.22	-	128,128,128,128	0
26	MG	A	1674	1/1	0.04	-	260,260,260,260	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
26	MG	A	1728	1/1	0.97	-	114,114,114,114	0
26	MG	A	1872	1/1	0.25	-	359,359,359,359	0
26	MG	A	1869	1/1	0.20	-	431,431,431,431	0
26	MG	A	1809	1/1	0.22	-	494,494,494,494	0
26	MG	A	1846	1/1	0.21	-	449,449,449,449	0
26	MG	E	202	1/1	0.12	-	124,124,124,124	0
26	MG	A	1605	1/1	0.09	-	254,254,254,254	0
26	MG	A	1886	1/1	1.04	-	121,121,121,121	0
26	MG	A	1647	1/1	0.26	-	104,104,104,104	0
26	MG	A	1619	1/1	0.13	-	64,64,64,64	0
26	MG	A	1602	1/1	0.41	-	66,66,66,66	1
26	MG	A	1782	1/1	0.69	-	87,87,87,87	0
26	MG	A	1762	1/1	0.43	-	82,82,82,82	0
26	MG	A	1645	1/1	0.44	-	227,227,227,227	0
26	MG	D	304	1/1	0.43	-	455,455,455,455	0
26	MG	A	1620	1/1	0.27	-	166,166,166,166	0
27	SRY	A	1928	40/40	0.16	-	70,100,124,130	0
26	MG	A	1610	1/1	0.24	-	81,81,81,81	0
26	MG	D	303	1/1	0.20	-	104,104,104,104	0
26	MG	P	102	1/1	0.34	-	101,101,101,101	0
26	MG	A	1913	1/1	0.81	-	108,108,108,108	0
26	MG	A	1695	1/1	0.04	-	176,176,176,176	0
26	MG	A	1922	1/1	0.41	-	110,110,110,110	0
26	MG	A	1927	1/1	0.24	-	112,112,112,112	0
26	MG	A	1760	1/1	0.68	-	88,88,88,88	0
26	MG	A	1726	1/1	0.14	-	98,98,98,98	0
26	MG	A	1677	1/1	0.23	-	235,235,235,235	0
26	MG	A	1722	1/1	0.64	-	95,95,95,95	0
26	MG	A	1772	1/1	0.12	-	93,93,93,93	0
26	MG	A	1826	1/1	0.05	-	395,395,395,395	0
26	MG	A	1810	1/1	0.21	-	474,474,474,474	0
26	MG	A	1879	1/1	0.22	-	438,438,438,438	0
26	MG	A	1850	1/1	0.04	-	236,236,236,236	0
26	MG	A	1861	1/1	0.14	-	443,443,443,443	0
26	MG	A	1643	1/1	0.10	-	71,71,71,71	0
26	MG	A	1789	1/1	0.09	-	378,378,378,378	0
26	MG	A	1733	1/1	0.19	-	70,70,70,70	0
26	MG	A	1875	1/1	0.15	-	460,460,460,460	0
26	MG	A	1735	1/1	0.15	-	106,106,106,106	0
26	MG	A	1795	1/1	1.02	-	359,359,359,359	0
26	MG	A	1874	1/1	0.08	-	467,467,467,467	0
26	MG	A	1909	1/1	0.27	-	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
26	MG	A	1704	1/1	0.15	-	104,104,104,104	0
26	MG	A	1665	1/1	0.72	-	117,117,117,117	0
26	MG	A	1749	1/1	0.13	-	84,84,84,84	0
26	MG	A	1672	1/1	0.09	-	166,166,166,166	0
26	MG	A	1618	1/1	0.48	-	130,130,130,130	0
26	MG	A	1758	1/1	0.49	-	101,101,101,101	0
26	MG	A	1651	1/1	0.17	-	110,110,110,110	0
26	MG	A	1798	1/1	0.05	-	464,464,464,464	0
26	MG	A	1847	1/1	0.17	-	441,441,441,441	0
26	MG	A	1805	1/1	0.05	-	331,331,331,331	0
26	MG	A	1714	1/1	0.21	-	108,108,108,108	0
26	MG	A	1840	1/1	0.31	-	467,467,467,467	1
26	MG	A	1683	1/1	0.06	-	154,154,154,154	0
26	MG	A	1703	1/1	0.15	-	97,97,97,97	0
26	MG	A	1625	1/1	0.07	-	113,113,113,113	0
26	MG	A	1614	1/1	0.21	-	285,285,285,285	0
26	MG	A	1856	1/1	0.06	-	478,478,478,478	0
26	MG	A	1867	1/1	0.61	-	413,413,413,413	1
26	MG	A	1747	1/1	0.13	-	115,115,115,115	0
26	MG	S	102	1/1	0.16	-	106,106,106,106	0
26	MG	A	1707	1/1	0.40	-	135,135,135,135	0
26	MG	A	1718	1/1	0.20	-	326,326,326,326	0
26	MG	A	1631	1/1	0.09	-	158,158,158,158	0
26	MG	A	1713	1/1	0.15	-	211,211,211,211	0
26	MG	A	1877	1/1	0.27	-	456,456,456,456	1
26	MG	A	1684	1/1	0.14	-	109,109,109,109	0
26	MG	A	1924	1/1	0.16	-	131,131,131,131	0
26	MG	A	1635	1/1	0.13	-	74,74,74,74	0
26	MG	A	1697	1/1	0.19	-	135,135,135,135	0
26	MG	A	1744	1/1	0.32	-	82,82,82,82	0
26	MG	A	1792	1/1	0.13	-	415,415,415,415	0
26	MG	D	302	1/1	0.39	-	104,104,104,104	0
26	MG	A	1759	1/1	0.86	-	86,86,86,86	0
26	MG	A	1691	1/1	0.16	-	186,186,186,186	0
26	MG	A	1646	1/1	0.18	-	136,136,136,136	0
26	MG	A	1784	1/1	0.19	-	122,122,122,122	0
26	MG	A	1802	1/1	0.12	-	355,355,355,355	0
26	MG	A	1709	1/1	0.23	-	245,245,245,245	0
26	MG	A	1734	1/1	0.60	-	124,124,124,124	0
26	MG	A	1889	1/1	0.29	-	95,95,95,95	0
26	MG	A	1761	1/1	0.49	-	105,105,105,105	0
26	MG	A	1673	1/1	0.88	-	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
26	MG	A	1777	1/1	0.15	-	94,94,94,94	0
26	MG	A	1681	1/1	0.04	-	256,256,256,256	0
26	MG	A	1903	1/1	0.17	-	78,78,78,78	0
26	MG	A	1732	1/1	0.24	-	100,100,100,100	0
26	MG	A	1721	1/1	0.24	-	92,92,92,92	0
26	MG	A	1825	1/1	0.17	-	436,436,436,436	0
26	MG	A	1653	1/1	0.21	-	96,96,96,96	0
26	MG	A	1752	1/1	0.25	-	91,91,91,91	0
26	MG	A	1841	1/1	0.18	-	496,496,496,496	0
26	MG	A	1670	1/1	0.28	-	234,234,234,234	0
26	MG	A	1754	1/1	0.16	-	85,85,85,85	0
26	MG	A	1813	1/1	0.30	-	471,471,471,471	0
26	MG	A	1692	1/1	0.20	-	182,182,182,182	0
26	MG	A	1884	1/1	1.43	-	119,119,119,119	0
26	MG	A	1764	1/1	0.34	-	78,78,78,78	0
26	MG	A	1706	1/1	0.17	-	190,190,190,190	0
26	MG	A	1719	1/1	0.07	-	262,262,262,262	0
26	MG	A	1705	1/1	0.13	-	74,74,74,74	0
26	MG	A	1766	1/1	0.59	-	105,105,105,105	0
26	MG	A	1842	1/1	0.59	-	488,488,488,488	0
26	MG	A	1655	1/1	0.38	-	125,125,125,125	0
26	MG	A	1892	1/1	0.55	-	92,92,92,92	0
26	MG	A	1854	1/1	0.33	-	418,418,418,418	0
26	MG	A	1769	1/1	0.62	-	127,127,127,127	0
26	MG	A	1891	1/1	0.16	-	127,127,127,127	0
26	MG	A	1833	1/1	0.12	-	335,335,335,335	0
26	MG	A	1652	1/1	0.09	-	72,72,72,72	0
26	MG	A	1687	1/1	0.14	-	106,106,106,106	0
26	MG	A	1831	1/1	0.22	-	395,395,395,395	0
26	MG	A	1799	1/1	0.23	-	426,426,426,426	0
26	MG	A	1790	1/1	0.15	-	444,444,444,444	0
26	MG	A	1629	1/1	0.39	-	223,223,223,223	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.