



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 06:20 am GMT

PDB ID : 4DV5  
Title : Crystal structure of the *Thermus thermophilus* 30S ribosomal subunit with a 16S rRNA mutation, A914G, bound with streptomycin  
Authors : Demirci, H.; Murphy IV, F.; Murphy, E.; Gregory, S.T.; Dahlberg, A.E.; Jogl, G.  
Deposited on : 2012-02-22  
Resolution : 3.68 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

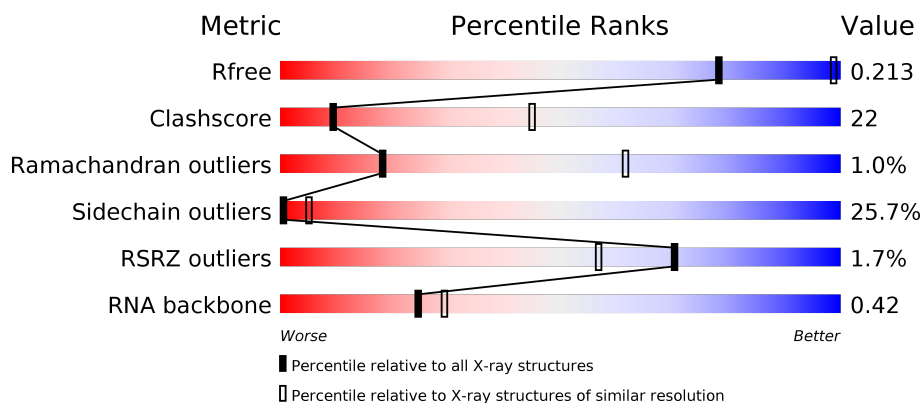
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.68 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.






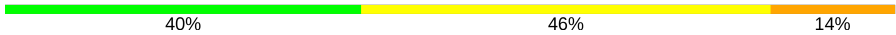
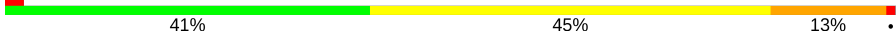
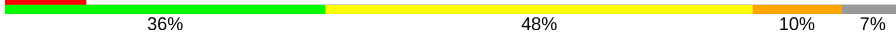
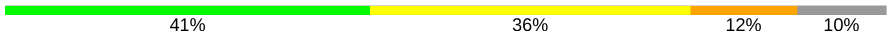
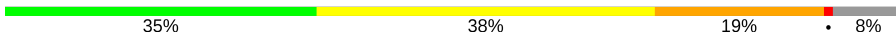
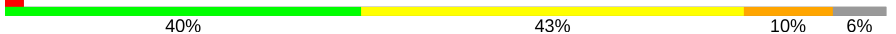
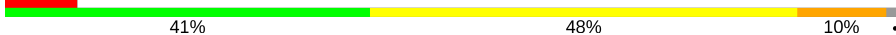
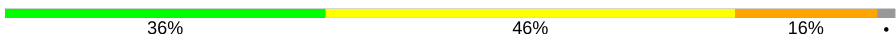
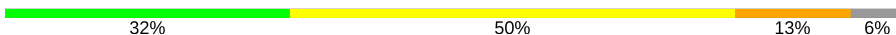
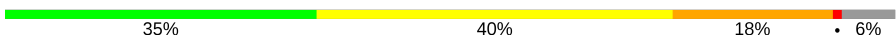
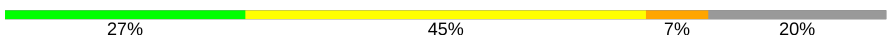
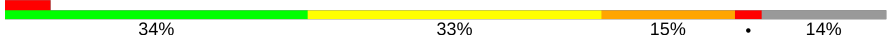


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	1161 (3.86-3.50)
Clashscore	112137	1295 (3.86-3.50)
Ramachandran outliers	110173	1245 (3.86-3.50)
Sidechain outliers	110143	1242 (3.86-3.50)
RSRZ outliers	101464	1188 (3.86-3.50)
RNA backbone	2435	1005 (4.46-2.90)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1522	<div> <div>16%</div> <div>41%</div> <div>31%</div> <div>12%</div> <div>.</div> </div>
2	B	256	<div> <div>30%</div> <div>47%</div> <div>12%</div> <div>9%</div> </div>
3	C	239	<div> <div>4%</div> <div>35%</div> <div>37%</div> <div>14%</div> <div>14%</div> </div>
4	D	209	<div> <div>43%</div> <div>44%</div> <div>11%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
5	E	162	
6	F	101	
7	G	156	
8	H	138	
9	I	128	
10	J	105	
11	K	129	
12	L	135	
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	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	5MC	A	1404	-	-	X	-
23	MG	A	1606	-	-	-	X
23	MG	A	1609	-	-	-	X
23	MG	A	1637	-	-	-	X
23	MG	A	1640	-	-	-	X
23	MG	A	1700	-	-	-	X
23	MG	A	1701	-	-	-	X
23	MG	A	1711	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	MG	A	1724	-	-	-	X
23	MG	A	1725	-	-	-	X
23	MG	A	1728	-	-	-	X
23	MG	A	1738	-	-	-	X
23	MG	A	1743	-	-	-	X
23	MG	A	1760	-	-	-	X
23	MG	A	1766	-	-	-	X
23	MG	A	1771	-	-	-	X
23	MG	A	1784	-	-	-	X
23	MG	A	1786	-	-	-	X
23	MG	A	1810	-	-	-	X
23	MG	A	1830	-	-	-	X
23	MG	A	1846	-	-	-	X
23	MG	B	301	-	-	-	X
23	MG	H	203	-	-	-	X
23	MG	M	202	-	-	-	X
23	MG	T	202	-	-	-	X

## 2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 52300 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1512	Total	C	N	O	P	0	0	0
			32508	14477	6011	10508	1512			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	914	G	A	ENGINEERED MUTATION	GB M26923.1
A	1534	C	A	CONFLICT	GB M26923.1
A	1535	A	C	CONFLICT	GB M26923.1

- Molecule 2 is a protein called ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	234	Total	C	N	O	S	0	0	0
			1900	1213	341	341	5			

- Molecule 3 is a protein called ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			

- Molecule 4 is a protein called 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 ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	150	Total	C	N	O	S	0	0	0
			1146	724	217	201	4			

- Molecule 6 is a protein called 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 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 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 ribosomal protein S9.

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

- Molecule 10 is a protein called ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	98	Total	C	N	O	S	0	0	0
			792	498	156	137	1			

- Molecule 11 is a protein called ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	116	Total	C	N	O	S	0	0	0
			864	537	164	160	3			

- Molecule 12 is a protein called ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	124	Total	C	N	O	S	0	0	0
			972	612	195	163	2			

- Molecule 13 is a protein called 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 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 ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O	87	Total	C	N	O	S	0	0	0
			729	457	146	124	2			

- Molecule 16 is a protein called ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			

- Molecule 17 is a protein called ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	99	Total	C	N	O	S	0	0	0
			823	528	152	141	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 ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	R	70	Total	C	N	O	0	0	0
			574	367	112	95			

- Molecule 19 is a protein called ribosomal protein S19.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	S	80	Total	C	N	O	S	0	0
			647	414	119	112	2		

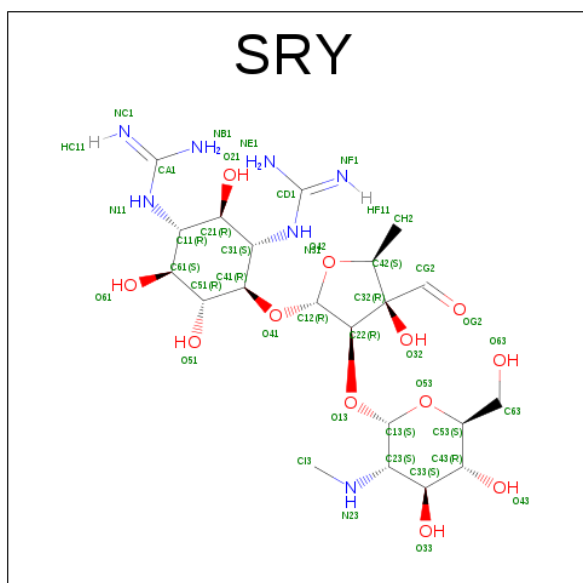
- Molecule 20 is a protein called ribosomal protein S20.

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

- Molecule 21 is a protein called ribosomal protein THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	U	24	Total	C	N	O	0	0	0
			208	128	50	30			

- Molecule 22 is STREPTOMYCIN (three-letter code: SRY) (formula:  $C_{21}H_{39}N_7O_{12}$ ).



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



- Molecule 23 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	P	3	Total 3	Mg 3	0	0
23	J	2	Total 2	Mg 2	0	0
23	Q	1	Total 1	Mg 1	0	0
23	D	1	Total 1	Mg 1	0	0
23	E	1	Total 1	Mg 1	0	0
23	H	4	Total 4	Mg 4	0	0
23	B	2	Total 2	Mg 2	0	0
23	A	253	Total 253	Mg 253	0	0
23	T	2	Total 2	Mg 2	0	0
23	N	1	Total 1	Mg 1	0	0
23	S	1	Total 1	Mg 1	0	0
23	M	2	Total 2	Mg 2	0	0

- Molecule 24 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 25 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	A	374	Total 374	O 374	0	0
25	B	1	Total 1	O 1	0	0
25	D	1	Total 1	O 1	0	0

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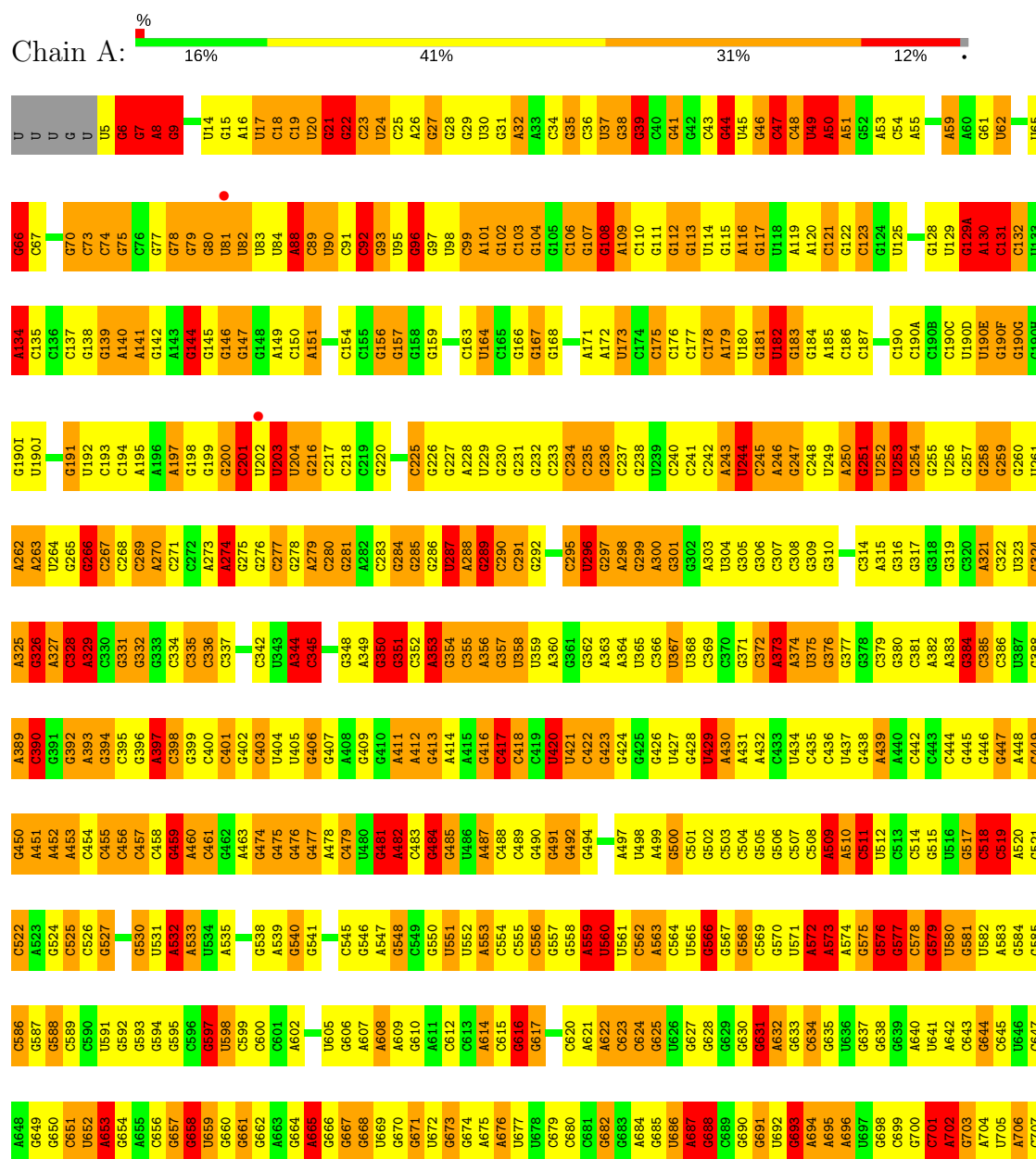
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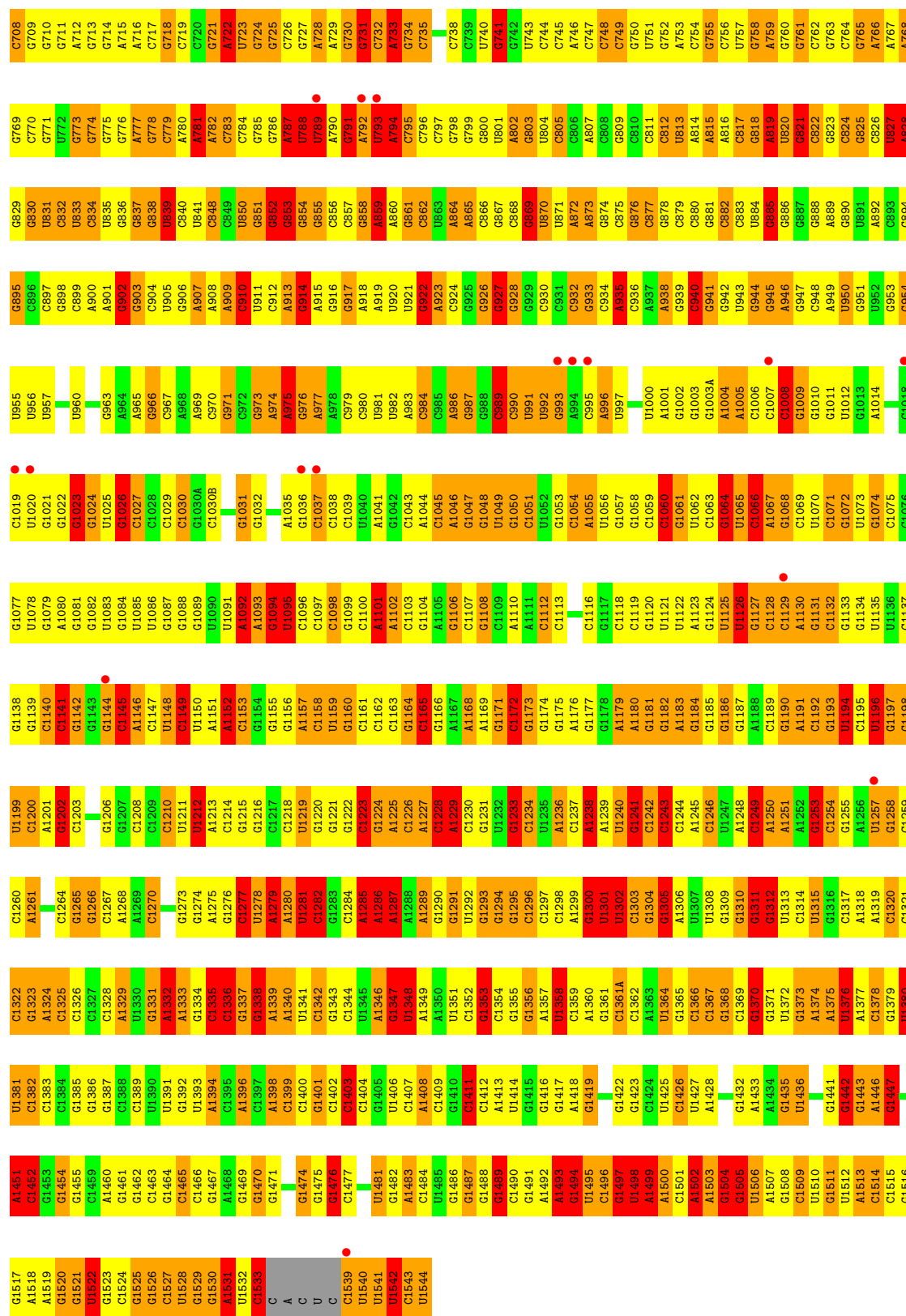
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	E	7	Total	O	0	0
			7	7		
25	L	1	Total	O	0	0
			1	1		
25	N	1	Total	O	0	0
			1	1		
25	P	2	Total	O	0	0
			2	2		
25	T	2	Total	O	0	0
			2	2		

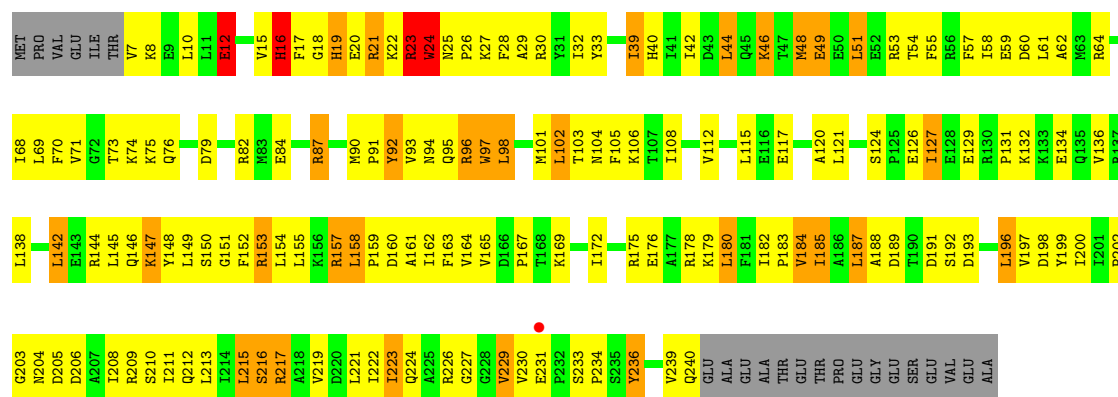
### 3 Residue-property plots

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

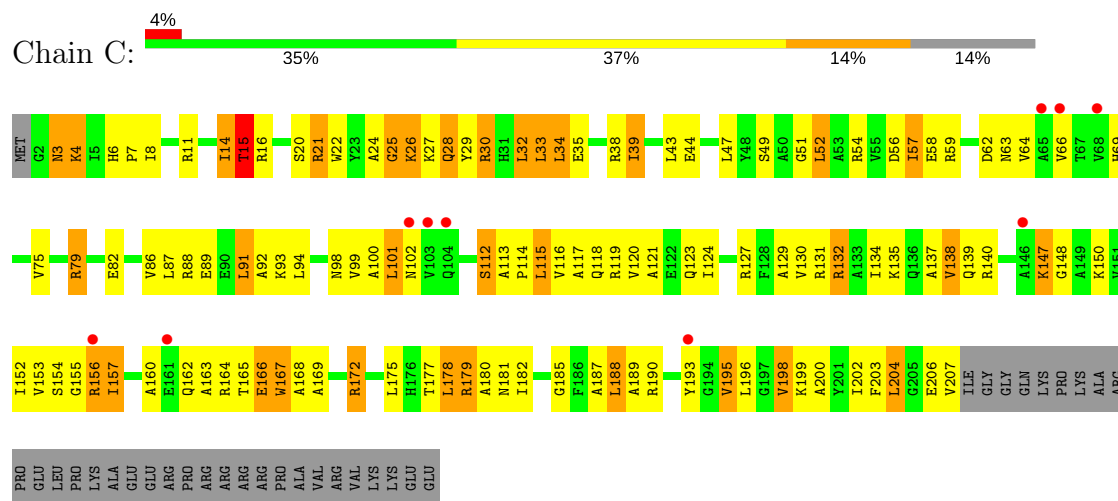
#### • Molecule 1: 16S rRNA



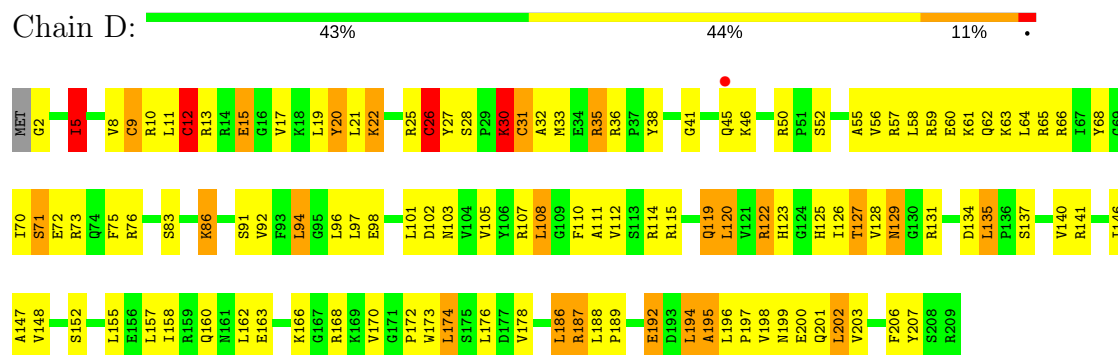




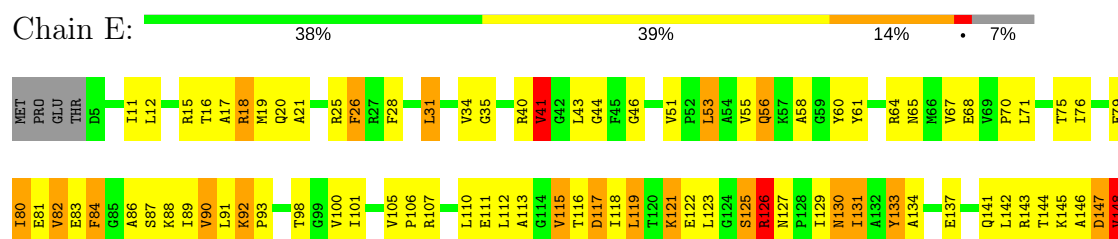
### • Molecule 3: ribosomal protein S3



### • Molecule 4: ribosomal protein S4



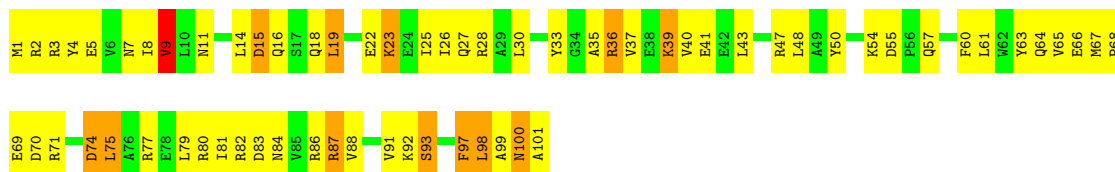
### • Molecule 5: ribosomal protein S5





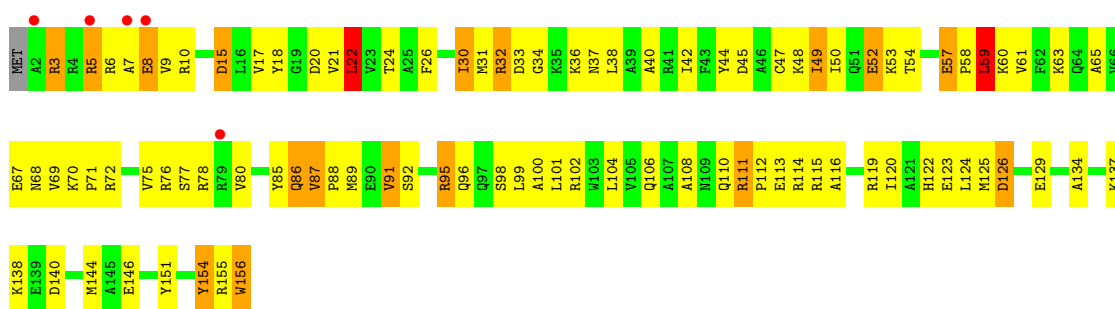
• Molecule 6: ribosomal protein S6

Chain F: 35% 52% 12% .



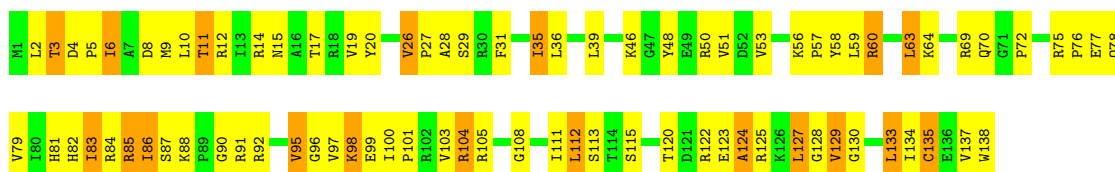
• Molecule 7: ribosomal protein S7

Chain G: 3% 39% 48% 11% ..



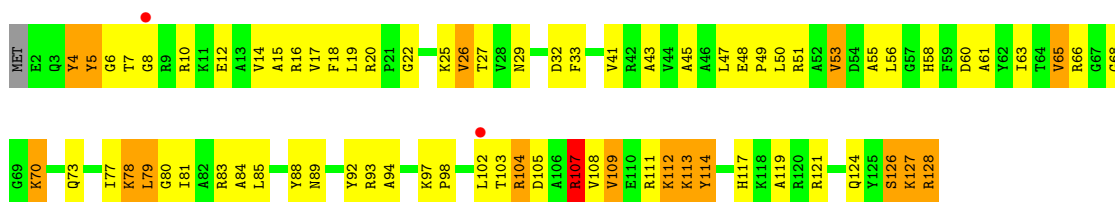
• Molecule 8: ribosomal protein S8

Chain H: 40% 46% 14%



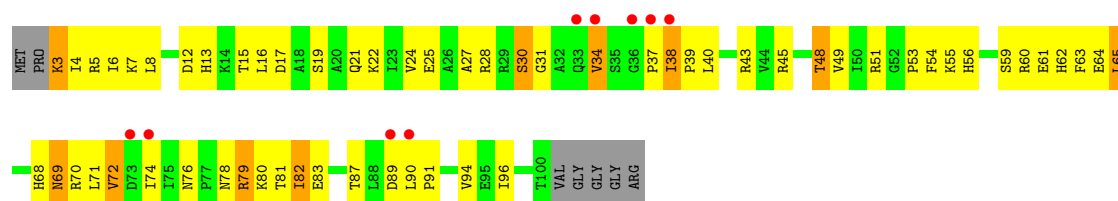
• Molecule 9: ribosomal protein S9

Chain I: 2% 41% 45% 13% ..



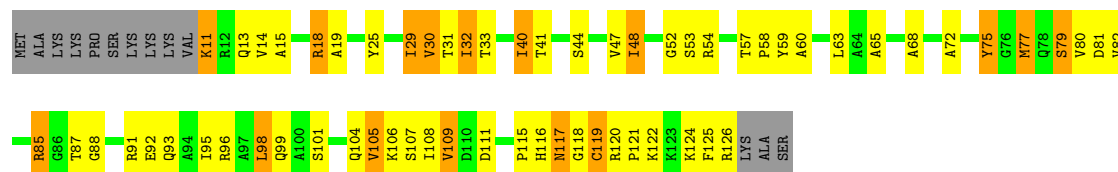
• Molecule 10: ribosomal protein S10

Chain J: 9% 36% 48% 10% 7%



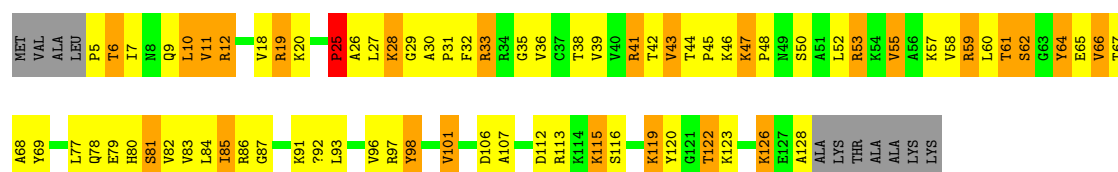
• Molecule 11: ribosomal protein S11

Chain K: 41% 36% 12% 10%



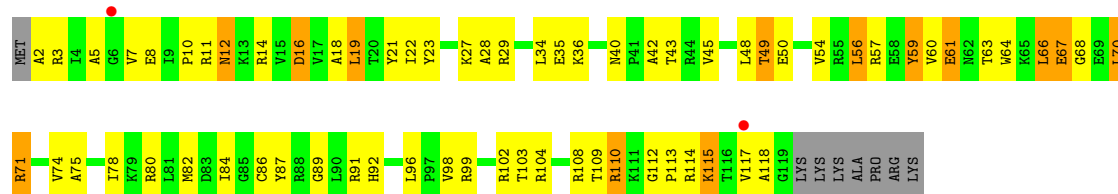
• Molecule 12: ribosomal protein S12

Chain L: 35% 38% 19% 8%



• Molecule 13: ribosomal protein S13

Chain M: 2% 40% 43% 10% 6%



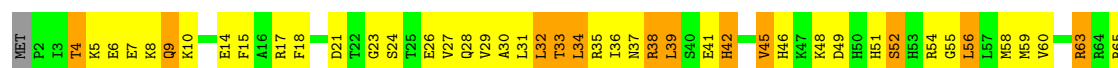
• Molecule 14: ribosomal protein S14

Chain N: 8% 41% 48% 10%



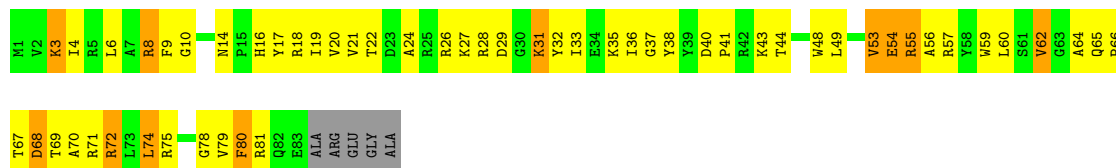
• Molecule 15: ribosomal protein S15

Chain O: 36% 46% 16%

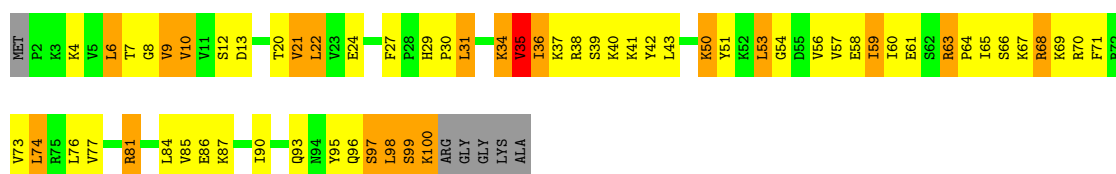
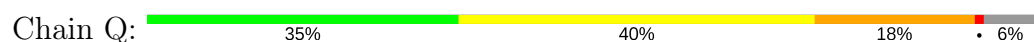




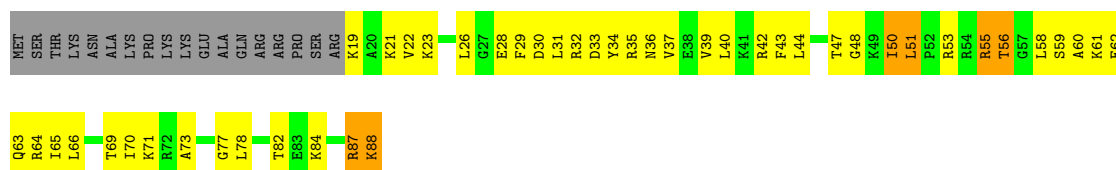
- Molecule 16: ribosomal protein S16



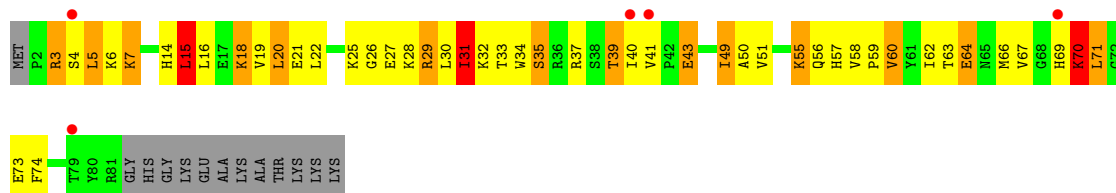
- Molecule 17: ribosomal protein S17



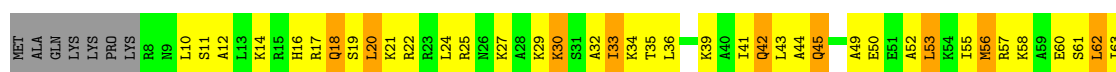
- Molecule 18: ribosomal protein S18



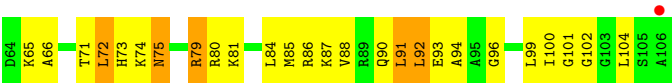
- Molecule 19: ribosomal protein S19



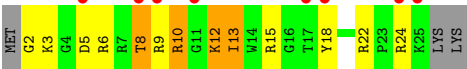
- Molecule 20: ribosomal protein S20







● Molecule 21: ribosomal protein THX



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	402.13Å 402.13Å 172.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.55 – 3.68 34.55 – 3.68	Depositor EDS
% Data completeness (in resolution range)	98.1 (34.55-3.68) 97.9 (34.55-3.68)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.92 (at 3.66Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_978)	Depositor
R, $R_{free}$	0.156 , 0.211 0.156 , 0.213	Depositor DCC
$R_{free}$ test set	7387 reflections (4.96%)	DCC
Wilson B-factor (Å <sup>2</sup> )	122.3	Xtriage
Anisotropy	0.371	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.23 , 118.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	52300	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	148.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.44% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 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	1.41	334/36041 (0.9%)	2.16	2692/56245 (4.8%)
2	B	0.91	1/1935 (0.1%)	1.06	7/2609 (0.3%)
3	C	0.70	0/1636	0.94	4/2205 (0.2%)
4	D	0.92	3/1733 (0.2%)	1.12	7/2318 (0.3%)
5	E	1.15	5/1162 (0.4%)	1.21	4/1564 (0.3%)
6	F	0.79	0/856	0.97	1/1154 (0.1%)
7	G	0.75	1/1276 (0.1%)	0.92	2/1709 (0.1%)
8	H	1.19	2/1136 (0.2%)	1.21	4/1527 (0.3%)
9	I	0.74	0/1029	0.98	1/1379 (0.1%)
10	J	0.70	0/805	0.95	0/1082
11	K	0.84	1/879 (0.1%)	1.05	1/1187 (0.1%)
12	L	0.97	1/977 (0.1%)	1.18	3/1306 (0.2%)
13	M	0.77	1/947 (0.1%)	0.95	0/1270
14	N	0.68	0/501	0.92	0/664
15	O	0.86	0/740	1.06	2/987 (0.2%)
16	P	0.95	1/716 (0.1%)	1.10	2/963 (0.2%)
17	Q	1.16	1/836 (0.1%)	1.32	9/1117 (0.8%)
18	R	0.81	0/579	0.97	0/768
19	S	0.67	0/661	0.90	1/890 (0.1%)
20	T	0.86	0/765	1.10	1/1007 (0.1%)
21	U	0.59	0/212	0.84	0/277
All	All	1.25	351/55422 (0.6%)	1.88	2741/82228 (3.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	2
4	D	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
7	G	0	1
8	H	0	1
9	I	0	1
10	J	0	2
12	L	0	1
17	Q	0	1
20	T	0	1
All	All	0	11

All (351) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	279	A	N9-C4	-14.20	1.29	1.37
1	A	1502	A	N9-C4	-12.65	1.30	1.37
1	A	917	G	N9-C4	-10.97	1.29	1.38
8	H	135	CYS	CB-SG	-10.53	1.64	1.82
1	A	1513	A	N9-C4	-10.06	1.31	1.37
1	A	279	A	N3-C4	-9.66	1.29	1.34
4	D	12	CYS	CB-SG	9.64	1.98	1.82
1	A	1508	G	N7-C5	-9.56	1.33	1.39
1	A	1227	A	N9-C4	-9.51	1.32	1.37
1	A	298	A	N9-C4	-9.37	1.32	1.37
1	A	329	A	C5-C6	-8.91	1.33	1.41
1	A	1377	A	N3-C4	-8.76	1.29	1.34
1	A	882	C	N3-C4	-8.75	1.27	1.33
1	A	1509	C	N1-C6	-8.74	1.31	1.37
1	A	266	G	N9-C4	-8.73	1.30	1.38
1	A	1502	A	C5-C6	-8.73	1.33	1.41
1	A	1394	A	N9-C4	-8.73	1.32	1.37
1	A	298	A	N3-C4	-8.63	1.29	1.34
1	A	279	A	N7-C5	-8.63	1.34	1.39
1	A	1500	A	N3-C4	-8.48	1.29	1.34
1	A	759	A	N9-C4	-8.36	1.32	1.37
1	A	1502	A	N3-C4	-8.32	1.29	1.34
1	A	1505	G	N7-C5	-8.31	1.34	1.39
1	A	1442	G	N3-C4	8.19	1.41	1.35
1	A	586	C	N1-C6	-8.16	1.32	1.37
1	A	1442	G	N9-C4	8.10	1.44	1.38
1	A	1502	A	N7-C5	-8.10	1.34	1.39
1	A	759	A	N7-C5	-8.09	1.34	1.39
1	A	901	A	N9-C4	-8.01	1.33	1.37
4	D	26	CYS	CB-SG	7.97	1.95	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	917	G	N3-C4	-7.88	1.29	1.35
1	A	876	G	C5-C4	-7.86	1.32	1.38
1	A	817	C	N1-C6	-7.80	1.32	1.37
1	A	574	A	C5-C4	-7.78	1.33	1.38
1	A	706	A	N9-C4	-7.73	1.33	1.37
1	A	88	A	N9-C4	7.71	1.42	1.37
1	A	795	C	N3-C4	7.67	1.39	1.33
1	A	1079	G	N7-C5	-7.62	1.34	1.39
1	A	905	U	C2-N3	-7.58	1.32	1.37
1	A	1401	G	N9-C8	-7.55	1.32	1.37
1	A	1499	A	N7-C5	-7.47	1.34	1.39
1	A	569	C	N3-C4	-7.44	1.28	1.33
1	A	904	C	N1-C6	-7.43	1.32	1.37
1	A	868	C	N1-C6	-7.41	1.32	1.37
1	A	860	A	N9-C4	-7.39	1.33	1.37
1	A	875	C	N1-C6	-7.39	1.32	1.37
1	A	568	G	C6-N1	-7.38	1.34	1.39
1	A	889	A	N7-C5	-7.38	1.34	1.39
2	B	12	GLU	CG-CD	7.37	1.63	1.51
1	A	1509	C	N3-C4	-7.36	1.28	1.33
1	A	1514	C	N1-C6	-7.34	1.32	1.37
1	A	795	C	C2-N3	7.29	1.41	1.35
1	A	828	A	N9-C4	-7.29	1.33	1.37
1	A	372	C	C2-O2	7.22	1.30	1.24
1	A	575	G	C6-N1	-7.21	1.34	1.39
1	A	892	A	N9-C4	-7.18	1.33	1.37
1	A	130	A	N9-C4	-7.17	1.33	1.37
1	A	130	A	N3-C4	-7.17	1.30	1.34
1	A	572	A	N3-C4	-7.16	1.30	1.34
1	A	779	C	N1-C6	-7.14	1.32	1.37
1	A	1080	A	N9-C8	-7.13	1.32	1.37
1	A	595	G	N7-C5	-7.12	1.34	1.39
1	A	580	U	C4-O4	7.12	1.29	1.23
1	A	1526	G	N7-C5	-7.11	1.34	1.39
1	A	807	A	N3-C4	-6.97	1.30	1.34
1	A	573	A	N7-C5	-6.96	1.35	1.39
1	A	730	G	N3-C4	-6.96	1.30	1.35
1	A	1543	C	N1-C2	6.94	1.47	1.40
1	A	860	A	N3-C4	-6.93	1.30	1.34
1	A	634	C	N1-C6	-6.93	1.32	1.37
1	A	1268	A	N9-C4	6.91	1.42	1.37
1	A	109	A	N7-C5	-6.87	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	758	G	N7-C5	-6.86	1.35	1.39
1	A	722	A	C5-C6	-6.77	1.34	1.41
1	A	1080	A	C5-C4	-6.77	1.34	1.38
1	A	1514	C	C2-N3	-6.76	1.30	1.35
1	A	1493	A	N9-C4	6.75	1.42	1.37
1	A	1500	A	C6-N1	-6.75	1.30	1.35
1	A	108	G	N9-C8	6.73	1.42	1.37
1	A	715	A	N9-C4	-6.72	1.33	1.37
1	A	753	A	N9-C4	-6.71	1.33	1.37
1	A	279	A	C5-C6	-6.70	1.35	1.41
1	A	791	G	N9-C4	6.70	1.43	1.38
1	A	563	A	N3-C4	-6.70	1.30	1.34
1	A	274	A	N9-C4	-6.68	1.33	1.37
1	A	16	A	N9-C4	-6.68	1.33	1.37
1	A	640	A	N3-C4	-6.67	1.30	1.34
1	A	568	G	N3-C4	-6.66	1.30	1.35
1	A	257	G	N1-C2	-6.65	1.32	1.37
1	A	144	G	N1-C2	6.65	1.43	1.37
1	A	766	A	C5-C6	-6.64	1.35	1.41
1	A	284	G	N7-C5	-6.56	1.35	1.39
1	A	1499	A	N3-C4	-6.54	1.30	1.34
1	A	1401	G	C5-C4	-6.52	1.33	1.38
1	A	1508	G	N9-C8	-6.52	1.33	1.37
1	A	482	A	N7-C5	-6.50	1.35	1.39
1	A	1524	C	N1-C6	-6.42	1.33	1.37
1	A	880	C	C4-C5	-6.41	1.37	1.43
1	A	574	A	N9-C4	-6.41	1.34	1.37
1	A	1377	A	N9-C4	-6.41	1.34	1.37
1	A	1401	G	N7-C5	-6.40	1.35	1.39
1	A	228	A	N9-C4	-6.39	1.34	1.37
1	A	899	C	C4-C5	-6.39	1.37	1.43
1	A	328	C	N1-C6	6.37	1.41	1.37
1	A	109	A	C5-C6	-6.37	1.35	1.41
1	A	822	C	N1-C6	-6.36	1.33	1.37
1	A	607	A	N3-C4	6.36	1.38	1.34
1	A	1504	G	N9-C8	-6.35	1.33	1.37
1	A	1492	A	N9-C4	6.34	1.41	1.37
1	A	726	C	N1-C6	-6.32	1.33	1.37
1	A	1499	A	N9-C4	-6.32	1.34	1.37
1	A	109	A	N9-C4	-6.31	1.34	1.37
1	A	1401	G	N9-C4	-6.31	1.32	1.38
1	A	245	C	N1-C2	-6.31	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1102	A	N7-C5	-6.30	1.35	1.39
1	A	872	A	C5-C6	-6.28	1.35	1.41
1	A	882	C	N1-C6	-6.28	1.33	1.37
1	A	811	C	N1-C6	-6.27	1.33	1.37
11	K	119	CYS	CB-SG	-6.27	1.71	1.82
1	A	880	C	P-O5'	-6.26	1.53	1.59
1	A	572	A	C6-N1	-6.26	1.31	1.35
1	A	372	C	N3-C4	6.25	1.38	1.33
1	A	938	A	N9-C4	-6.24	1.34	1.37
1	A	1241	G	N3-C4	-6.24	1.31	1.35
1	A	1482	G	N9-C4	6.23	1.43	1.38
1	A	1080	A	N9-C4	-6.22	1.34	1.37
1	A	915	A	N9-C4	-6.20	1.34	1.37
1	A	654	G	N9-C4	-6.19	1.32	1.38
1	A	151	A	N9-C4	-6.19	1.34	1.37
1	A	1514	C	N3-C4	-6.18	1.29	1.33
1	A	553	A	N9-C4	-6.18	1.34	1.37
1	A	109	A	N3-C4	-6.17	1.31	1.34
1	A	1401	G	N3-C4	-6.15	1.31	1.35
1	A	656	C	N1-C6	-6.14	1.33	1.37
1	A	822	C	N3-C4	-6.14	1.29	1.33
1	A	793	U	N1-C2	6.13	1.44	1.38
1	A	721	G	N7-C5	-6.12	1.35	1.39
1	A	862	C	N1-C6	-6.11	1.33	1.37
1	A	50	A	N9-C4	-6.10	1.34	1.37
1	A	1513	A	N3-C4	-6.08	1.31	1.34
1	A	807	A	N9-C4	-6.07	1.34	1.37
1	A	802	A	C5-C4	-6.06	1.34	1.38
1	A	790	A	N9-C4	6.06	1.41	1.37
1	A	21	G	N1-C2	-6.06	1.32	1.37
1	A	651	C	C2-O2	6.04	1.29	1.24
1	A	1501	C	N1-C6	-6.04	1.33	1.37
1	A	644	G	C5-C4	-6.03	1.34	1.38
1	A	574	A	N3-C4	-6.02	1.31	1.34
1	A	572	A	C5-C4	-5.99	1.34	1.38
1	A	250	A	C5-C4	5.98	1.43	1.38
1	A	880	C	C4-N4	-5.97	1.28	1.33
1	A	128	G	C5-C6	-5.96	1.36	1.42
1	A	1527	C	C4-C5	-5.96	1.38	1.43
1	A	298	A	C6-N1	-5.96	1.31	1.35
1	A	567	G	N3-C4	-5.96	1.31	1.35
1	A	828	A	N3-C4	-5.95	1.31	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	263	A	C5-C4	-5.95	1.34	1.38
1	A	1346	A	C3'-O3'	5.94	1.50	1.42
1	A	243	A	C3'-O3'	5.92	1.50	1.42
1	A	752	G	N3-C4	-5.92	1.31	1.35
1	A	760	G	N9-C4	-5.92	1.33	1.38
1	A	575	G	N3-C4	-5.92	1.31	1.35
1	A	632	A	N9-C4	-5.91	1.34	1.37
1	A	372	C	N1-C2	5.90	1.46	1.40
1	A	918	A	C5-C4	-5.90	1.34	1.38
1	A	802	A	N9-C4	-5.88	1.34	1.37
1	A	900	A	N7-C5	-5.88	1.35	1.39
5	E	148	VAL	CA-CB	-5.86	1.42	1.54
1	A	813	U	N1-C6	-5.85	1.32	1.38
1	A	895	G	N3-C4	-5.83	1.31	1.35
1	A	572	A	C6-N6	-5.82	1.29	1.33
1	A	53	A	C6-N1	-5.82	1.31	1.35
1	A	17	U	C4-O4	-5.81	1.19	1.23
1	A	861	G	C5-C4	-5.80	1.34	1.38
1	A	794	A	N1-C2	-5.79	1.29	1.34
1	A	1077	G	N7-C5	-5.79	1.35	1.39
1	A	1501	C	C4-C5	-5.79	1.38	1.43
1	A	788	U	N3-C4	5.78	1.43	1.38
1	A	1331	G	N9-C4	5.78	1.42	1.38
1	A	1525	G	N3-C4	-5.78	1.31	1.35
1	A	562	C	N1-C6	-5.75	1.33	1.37
1	A	666	G	N3-C4	-5.74	1.31	1.35
5	E	133	TYR	CE2-CZ	5.74	1.46	1.38
1	A	755	G	C5-C4	-5.74	1.34	1.38
1	A	778	G	N3-C4	-5.72	1.31	1.35
1	A	642	A	N3-C4	-5.71	1.31	1.34
1	A	567	G	C6-N1	-5.71	1.35	1.39
1	A	765	G	N3-C4	-5.70	1.31	1.35
1	A	862	C	C5-C6	-5.70	1.29	1.34
1	A	574	A	C6-N1	-5.69	1.31	1.35
1	A	752	G	N9-C4	-5.69	1.33	1.38
1	A	915	A	N3-C4	-5.69	1.31	1.34
1	A	363	A	N9-C4	-5.68	1.34	1.37
1	A	1236	A	C5-C4	-5.67	1.34	1.38
1	A	397	A	N3-C4	-5.65	1.31	1.34
1	A	1514	C	C2-O2	-5.65	1.19	1.24
1	A	875	C	N3-C4	-5.65	1.29	1.33
1	A	564	C	N1-C6	-5.64	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	858	G	C8-N7	-5.64	1.27	1.30
1	A	880	C	C2-O2	5.64	1.29	1.24
1	A	913	A	C3'-O3'	5.64	1.50	1.42
1	A	559	A	C6-N1	-5.64	1.31	1.35
1	A	642	A	N9-C4	-5.64	1.34	1.37
1	A	1338	G	C6-N1	-5.63	1.35	1.39
1	A	117	G	N1-C2	5.62	1.42	1.37
1	A	879	C	N1-C6	-5.61	1.33	1.37
1	A	786	G	N7-C5	-5.61	1.35	1.39
1	A	1334	G	N9-C8	-5.60	1.33	1.37
1	A	297	G	N7-C5	-5.59	1.35	1.39
1	A	675	A	N7-C5	-5.59	1.35	1.39
1	A	759	A	C5-C6	-5.59	1.36	1.41
1	A	868	C	N3-C4	-5.59	1.30	1.33
1	A	728	A	N7-C5	-5.58	1.35	1.39
1	A	825	G	N9-C8	-5.58	1.33	1.37
1	A	1080	A	C6-N1	-5.57	1.31	1.35
1	A	1094	G	C6-N1	-5.56	1.35	1.39
1	A	16	A	N9-C8	-5.55	1.33	1.37
1	A	1522	U	C4-C5	-5.55	1.38	1.43
1	A	602	A	N3-C4	-5.55	1.31	1.34
1	A	116	A	N9-C4	-5.54	1.34	1.37
1	A	1355	G	C6-N1	-5.54	1.35	1.39
1	A	1099	G	N9-C4	-5.54	1.33	1.38
1	A	128	G	N7-C5	-5.53	1.35	1.39
1	A	228	A	C5-C6	-5.53	1.36	1.41
1	A	1338	G	N3-C4	-5.53	1.31	1.35
1	A	1396	A	N9-C4	-5.53	1.34	1.37
1	A	123	C	N3-C4	-5.53	1.30	1.33
1	A	862	C	C4-C5	-5.53	1.38	1.43
1	A	935	A	N9-C4	-5.52	1.34	1.37
1	A	888	G	N3-C4	-5.52	1.31	1.35
1	A	909	A	N7-C5	-5.51	1.35	1.39
1	A	733	A	N3-C4	-5.50	1.31	1.34
4	D	5	ILE	CA-CB	5.49	1.67	1.54
17	Q	35	VAL	CA-CB	-5.49	1.43	1.54
1	A	1523	G	C2-N3	-5.48	1.28	1.32
1	A	706	A	N3-C4	-5.48	1.31	1.34
1	A	1250	A	N9-C4	-5.47	1.34	1.37
1	A	986	A	N9-C4	5.47	1.41	1.37
1	A	795	C	C2-O2	5.47	1.29	1.24
1	A	833	U	C4-O4	5.46	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1066	C	N1-C6	-5.45	1.33	1.37
1	A	1524	C	N1-C2	-5.45	1.34	1.40
1	A	918	A	N9-C8	-5.44	1.33	1.37
1	A	881	G	N9-C8	-5.43	1.34	1.37
1	A	1077	G	N9-C8	-5.43	1.34	1.37
1	A	1101	A	N3-C4	-5.43	1.31	1.34
1	A	882	C	N1-C2	-5.42	1.34	1.40
1	A	900	A	N3-C4	-5.42	1.31	1.34
1	A	577	G	N9-C4	-5.42	1.33	1.38
1	A	372	C	C2-N3	5.41	1.40	1.35
1	A	936	C	N1-C6	-5.41	1.33	1.37
1	A	902	G	C5-C4	-5.40	1.34	1.38
1	A	1101	A	C5-C4	-5.40	1.34	1.38
1	A	852	G	N3-C4	-5.39	1.31	1.35
1	A	1336	C	N1-C6	-5.39	1.33	1.37
1	A	763	G	N9-C4	-5.38	1.33	1.38
1	A	262	A	C6-N1	-5.36	1.31	1.35
1	A	715	A	N3-C4	-5.36	1.31	1.34
1	A	798	G	N3-C4	-5.34	1.31	1.35
1	A	1504	G	C5-C4	-5.33	1.34	1.38
1	A	1508	G	C5-C4	-5.33	1.34	1.38
5	E	149	GLU	CG-CD	5.33	1.59	1.51
1	A	563	A	O3'-P	-5.32	1.54	1.61
1	A	274	A	C5-C4	-5.32	1.35	1.38
1	A	803	G	N1-C2	-5.31	1.33	1.37
1	A	762	C	N1-C6	-5.31	1.33	1.37
1	A	872	A	N9-C4	-5.30	1.34	1.37
1	A	243	A	C5-C6	-5.29	1.36	1.41
1	A	1078	U	C4-C5	-5.29	1.38	1.43
1	A	15	G	C8-N7	-5.28	1.27	1.30
1	A	1103	C	N1-C6	-5.28	1.33	1.37
1	A	786	G	C5-C6	-5.28	1.37	1.42
1	A	15	G	N3-C4	-5.28	1.31	1.35
1	A	665	A	N3-C4	-5.27	1.31	1.34
1	A	765	G	C2-N3	-5.27	1.28	1.32
1	A	858	G	N9-C4	-5.27	1.33	1.38
12	L	68	ALA	CA-CB	-5.27	1.41	1.52
1	A	481	G	C8-N7	-5.27	1.27	1.30
1	A	872	A	N7-C5	-5.26	1.36	1.39
1	A	782	A	N3-C4	-5.26	1.31	1.34
1	A	269	C	N3-C4	-5.26	1.30	1.33
1	A	675	A	C5-C6	-5.26	1.36	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	350	G	N3-C4	-5.26	1.31	1.35
1	A	481	G	N3-C4	5.26	1.39	1.35
1	A	1526	G	C5-C4	-5.25	1.34	1.38
1	A	691	G	N7-C5	-5.25	1.36	1.39
1	A	918	A	N7-C5	-5.24	1.36	1.39
1	A	15	G	C6-O6	5.24	1.28	1.24
1	A	1514	C	N1-C2	-5.23	1.34	1.40
1	A	913	A	C6-N1	-5.23	1.31	1.35
1	A	867	G	C5-C6	-5.22	1.37	1.42
1	A	295	C	N1-C6	-5.22	1.34	1.37
1	A	900	A	C5-C6	-5.21	1.36	1.41
1	A	917	G	C5-C4	-5.21	1.34	1.38
1	A	67	C	N3-C4	-5.21	1.30	1.33
1	A	1515	C	N3-C4	-5.21	1.30	1.33
1	A	588	G	N9-C8	-5.20	1.34	1.37
1	A	1508	G	C6-N1	-5.20	1.35	1.39
1	A	765	G	C5-C6	-5.19	1.37	1.42
16	P	36	ILE	CA-CB	-5.19	1.43	1.54
1	A	583	A	N7-C5	-5.18	1.36	1.39
1	A	766	A	N7-C5	-5.17	1.36	1.39
1	A	1155	G	N9-C4	5.17	1.42	1.38
1	A	300	A	N7-C5	-5.17	1.36	1.39
1	A	321	A	C6-N6	-5.17	1.29	1.33
1	A	232	G	C5-C6	-5.16	1.37	1.42
1	A	602	A	N9-C4	-5.16	1.34	1.37
1	A	1339	A	C5-C4	-5.16	1.35	1.38
1	A	594	G	N7-C5	-5.16	1.36	1.39
1	A	753	A	N3-C4	-5.15	1.31	1.34
1	A	373	A	C5'-C4'	5.14	1.57	1.51
1	A	1078	U	C4-O4	-5.13	1.19	1.23
1	A	814	A	N3-C4	-5.13	1.31	1.34
1	A	659	U	N3-C4	-5.13	1.33	1.38
1	A	1513	A	C5-C4	-5.13	1.35	1.38
1	A	1515	C	C4-C5	-5.12	1.38	1.43
7	G	156	TRP	CB-CG	5.12	1.59	1.50
1	A	876	G	C6-N1	-5.12	1.35	1.39
1	A	575	G	C5-C4	-5.12	1.34	1.38
5	E	90	VAL	CA-CB	-5.11	1.44	1.54
1	A	1080	A	N7-C5	-5.11	1.36	1.39
1	A	868	C	C4-C5	-5.10	1.38	1.43
1	A	93	G	N9-C8	-5.10	1.34	1.37
1	A	566	G	N3-C4	-5.10	1.31	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	775	G	N7-C5	-5.09	1.36	1.39
1	A	895	G	N1-C2	-5.09	1.33	1.37
1	A	400	C	N3-C4	-5.08	1.30	1.33
1	A	449	C	N1-C6	-5.08	1.34	1.37
1	A	858	G	C5-C4	-5.07	1.34	1.38
1	A	903	G	N3-C4	-5.07	1.31	1.35
1	A	30	U	C2-N3	-5.07	1.34	1.37
1	A	150	C	N1-C6	-5.06	1.34	1.37
1	A	1084	G	N9-C8	-5.06	1.34	1.37
1	A	1530	G	C5-C6	-5.05	1.37	1.42
1	A	108	G	N3-C4	-5.05	1.31	1.35
13	M	64	TRP	CB-CG	-5.05	1.41	1.50
5	E	82	VAL	CA-CB	-5.05	1.44	1.54
1	A	106	C	N3-C4	-5.05	1.30	1.33
1	A	314	C	C4-N4	-5.05	1.29	1.33
1	A	634	C	C2-O2	-5.05	1.20	1.24
1	A	1236	A	N1-C2	-5.05	1.29	1.34
1	A	793	U	C1'-N1	5.04	1.56	1.48
1	A	813	U	C4-C5	-5.04	1.39	1.43
1	A	882	C	C2-O2	-5.04	1.20	1.24
8	H	124	ALA	CA-CB	-5.04	1.41	1.52
1	A	567	G	C5-C4	-5.04	1.34	1.38
1	A	917	G	N7-C5	-5.03	1.36	1.39
1	A	1529	G	N7-C5	-5.03	1.36	1.39
1	A	1261	A	N9-C4	5.03	1.40	1.37
1	A	577	G	C5-C4	-5.01	1.34	1.38
1	A	828	A	N7-C5	-5.00	1.36	1.39

All (2741) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	117	G	N1-C6-O6	20.89	132.43	119.90
1	A	279	A	C5-N7-C8	-17.64	95.08	103.90
1	A	1505	G	C8-N9-C4	-17.36	99.45	106.40
1	A	117	G	C5-C6-N1	-16.75	103.12	111.50
1	A	117	G	C2-N3-C4	-16.57	103.61	111.90
1	A	144	G	N1-C6-O6	16.04	129.53	119.90
1	A	1502	A	C5-N7-C8	-15.79	96.00	103.90
1	A	481	G	N3-C4-N9	15.15	135.09	126.00
1	A	232	G	N1-C6-O6	14.92	128.85	119.90
1	A	279	A	N7-C8-N9	14.91	121.25	113.80
1	A	1505	G	N7-C8-N9	14.57	120.39	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	251	G	N1-C6-O6	14.54	128.63	119.90
1	A	1346	A	N1-C6-N6	-14.39	109.97	118.60
1	A	1531	A	N1-C6-N6	14.34	127.21	118.60
1	A	117	G	C6-C5-N7	-14.34	121.80	130.40
1	A	128	G	N1-C6-O6	14.33	128.50	119.90
1	A	1502	A	N1-C6-N6	13.98	126.99	118.60
1	A	580	U	N3-C4-C5	-13.81	106.31	114.60
1	A	1502	A	C6-C5-N7	-13.74	122.68	132.30
1	A	795	C	C2-N3-C4	13.68	126.74	119.90
1	A	971	G	C8-N9-C4	13.61	111.84	106.40
1	A	21	G	N1-C6-O6	-13.53	111.78	119.90
1	A	1502	A	C4-C5-N7	13.44	117.42	110.70
1	A	1442	G	N3-C4-N9	13.42	134.05	126.00
1	A	1502	A	C2-N3-C4	-13.41	103.89	110.60
1	A	122	G	N1-C6-O6	13.26	127.85	119.90
1	A	232	G	C4-C5-N7	13.24	116.10	110.80
1	A	875	C	C5-C6-N1	-13.10	114.45	121.00
1	A	310	G	N1-C6-O6	13.07	127.74	119.90
1	A	284	G	N1-C6-O6	13.03	127.72	119.90
1	A	794	A	C2-N3-C4	12.92	117.06	110.60
1	A	292	G	N1-C6-O6	12.78	127.57	119.90
1	A	862	C	C6-N1-C2	12.66	125.36	120.30
1	A	1181	G	C8-N9-C4	12.65	111.46	106.40
1	A	1539	C	C6-N1-C2	12.59	125.33	120.30
1	A	1189	C	C6-N1-C2	12.36	125.24	120.30
1	A	130	A	N1-C6-N6	12.36	126.01	118.60
1	A	725	G	N1-C6-O6	12.31	127.29	119.90
1	A	232	G	N9-C4-C5	-12.25	100.50	105.40
1	A	1482	G	N3-C4-C5	-12.19	122.51	128.60
1	A	235	C	C6-N1-C2	12.07	125.13	120.30
1	A	725	G	C5-C6-O6	-12.07	121.36	128.60
1	A	822	C	C6-N1-C2	-12.03	115.49	120.30
1	A	795	C	N1-C2-N3	-11.99	110.80	119.20
1	A	559	A	C6-N1-C2	-11.98	111.41	118.60
1	A	251	G	C6-C5-N7	-11.95	123.23	130.40
1	A	232	G	C6-C5-N7	-11.92	123.25	130.40
1	A	787	A	N1-C6-N6	11.83	125.70	118.60
1	A	1126	U	C5-C6-N1	11.81	128.60	122.70
1	A	108	G	C5-N7-C8	-11.80	98.40	104.30
1	A	279	A	C8-N9-C4	-11.80	101.08	105.80
1	A	572	A	N1-C6-N6	-11.76	111.54	118.60
1	A	1543	C	N1-C2-O2	11.73	125.94	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	795	C	N3-C2-O2	11.71	130.10	121.90
1	A	1531	A	C6-C5-N7	-11.70	124.11	132.30
1	A	481	G	C8-N9-C4	11.69	111.08	106.40
1	A	15	G	C4-N9-C1'	11.64	141.63	126.50
1	A	825	G	C8-N9-C4	11.60	111.04	106.40
1	A	15	G	C8-N9-C1'	-11.58	111.95	127.00
1	A	279	A	C6-C5-N7	-11.52	124.24	132.30
1	A	88	A	C8-N9-C4	-11.49	101.20	105.80
1	A	1447	G	C4-C5-N7	11.40	115.36	110.80
1	A	279	A	C2-N3-C4	-11.38	104.91	110.60
1	A	108	G	N7-C8-N9	11.37	118.79	113.10
1	A	129(A)	G	N1-C6-O6	11.37	126.72	119.90
1	A	607	A	N9-C4-C5	-11.36	101.26	105.80
1	A	821	G	N1-C6-O6	11.36	126.72	119.90
1	A	944	G	C8-N9-C4	-11.34	101.86	106.40
1	A	336	C	C6-N1-C2	11.32	124.83	120.30
1	A	128	G	C6-C5-N7	-11.30	123.62	130.40
1	A	1442	G	C4-N9-C1'	11.28	141.17	126.50
1	A	1088	G	N1-C6-O6	11.25	126.65	119.90
1	A	567	G	C4-C5-N7	-11.21	106.32	110.80
1	A	144	G	C5-C6-N1	-11.21	105.90	111.50
1	A	782	A	N1-C2-N3	11.18	134.89	129.30
1	A	873	A	C8-N9-C4	-11.15	101.34	105.80
1	A	1505	G	C6-C5-N7	-11.13	123.72	130.40
1	A	875	C	C6-N1-C2	11.12	124.75	120.30
1	A	1377	A	N1-C6-N6	-11.06	111.96	118.60
1	A	255	G	N1-C6-O6	11.03	126.52	119.90
1	A	787	A	C2-N3-C4	-11.01	105.09	110.60
1	A	706	A	C2-N3-C4	-11.00	105.10	110.60
1	A	745	C	C6-N1-C2	11.00	124.70	120.30
1	A	481	G	N9-C4-C5	-10.98	101.01	105.40
1	A	129(A)	G	N9-C4-C5	-10.98	101.01	105.40
1	A	247	G	N1-C6-O6	10.94	126.46	119.90
1	A	817	C	C6-N1-C2	10.90	124.66	120.30
1	A	852	G	C5-C6-N1	-10.90	106.05	111.50
1	A	607	A	C4-C5-N7	10.87	116.14	110.70
1	A	627	G	N1-C6-O6	10.86	126.41	119.90
8	H	12	ARG	NE-CZ-NH1	-10.85	114.88	120.30
1	A	1502	A	N7-C8-N9	10.84	119.22	113.80
1	A	901	A	C2-N3-C4	-10.83	105.19	110.60
1	A	21	G	N3-C2-N2	10.82	127.47	119.90
1	A	1302	U	N3-C2-O2	-10.80	114.64	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	833	U	N3-C2-O2	-10.79	114.64	122.20
1	A	833	U	C4-C5-C6	10.79	126.17	119.70
1	A	228	A	C2-N3-C4	-10.78	105.21	110.60
1	A	607	A	N1-C6-N6	10.77	125.06	118.60
1	A	851	G	N1-C6-O6	10.77	126.36	119.90
1	A	266	G	N3-C4-C5	10.76	133.98	128.60
1	A	106	C	C6-N1-C2	-10.76	116.00	120.30
1	A	232	G	C5-C6-O6	-10.75	122.15	128.60
1	A	651	C	N3-C2-O2	10.70	129.39	121.90
1	A	930	C	N3-C4-C5	10.68	126.17	121.90
1	A	1455	G	N1-C6-O6	10.67	126.30	119.90
1	A	1505	G	N3-C4-C5	-10.67	123.27	128.60
1	A	1403	C	C6-N1-C2	10.65	124.56	120.30
1	A	1231	G	N1-C6-O6	10.65	126.29	119.90
1	A	266	G	C5-N7-C8	-10.62	98.99	104.30
1	A	269	C	C6-N1-C2	-10.62	116.05	120.30
1	A	1531	A	N7-C8-N9	10.59	119.09	113.80
1	A	90	U	C6-N1-C2	-10.52	114.69	121.00
1	A	1338	G	N1-C6-O6	-10.50	113.60	119.90
1	A	1088	G	C6-C5-N7	-10.48	124.11	130.40
1	A	1442	G	C8-N9-C1'	-10.48	113.38	127.00
1	A	786	G	N1-C6-O6	10.47	126.18	119.90
1	A	372	C	N1-C2-N3	-10.47	111.87	119.20
1	A	278	G	C8-N9-C4	-10.41	102.23	106.40
1	A	1236	A	C8-N9-C4	10.41	109.97	105.80
1	A	1347	G	C8-N9-C4	10.40	110.56	106.40
1	A	1334	G	C8-N9-C4	10.39	110.56	106.40
1	A	721	G	C6-C5-N7	-10.38	124.17	130.40
1	A	1442	G	C5-C6-O6	-10.37	122.38	128.60
1	A	1529	G	C8-N9-C4	-10.34	102.26	106.40
1	A	128	G	C5-C6-O6	-10.32	122.41	128.60
1	A	1530	G	C8-N9-C4	10.30	110.52	106.40
1	A	16	A	C8-N9-C4	10.30	109.92	105.80
1	A	944	G	C5-C6-O6	10.29	134.78	128.60
1	A	190(I)	G	C8-N9-C4	10.29	110.52	106.40
1	A	255	G	C6-C5-N7	-10.29	124.23	130.40
1	A	1394	A	C8-N9-C4	10.28	109.91	105.80
1	A	734	G	C5-C6-O6	-10.26	122.44	128.60
1	A	1367	C	C6-N1-C2	-10.26	116.20	120.30
1	A	820	U	N1-C2-N3	10.26	121.05	114.90
1	A	103	C	N3-C4-C5	-10.25	117.80	121.90
1	A	108	G	C8-N9-C4	-10.25	102.30	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	117	G	C4-C5-C6	10.24	124.95	118.80
1	A	310	G	C5-C6-O6	-10.22	122.47	128.60
1	A	873	A	N1-C6-N6	-10.21	112.47	118.60
1	A	309	G	C5-C6-O6	-10.16	122.50	128.60
1	A	279	A	C4-C5-N7	10.16	115.78	110.70
1	A	292	G	C5-C6-O6	-10.14	122.52	128.60
1	A	1202	G	N1-C6-O6	-10.14	113.82	119.90
1	A	309	G	C6-N1-C2	-10.12	119.03	125.10
1	A	1442	G	N1-C6-O6	10.12	125.97	119.90
1	A	1155	G	C8-N9-C4	-10.11	102.36	106.40
1	A	813	U	C5-C4-O4	-10.09	119.85	125.90
1	A	1378	C	C6-N1-C2	-10.09	116.27	120.30
1	A	1474	G	N1-C6-O6	10.08	125.95	119.90
1	A	1346	A	C5-C6-N1	10.06	122.73	117.70
1	A	284	G	C6-C5-N7	-10.05	124.37	130.40
1	A	788	U	N3-C2-O2	10.05	129.23	122.20
1	A	372	C	C6-N1-C2	10.04	124.32	120.30
1	A	788	U	N1-C2-N3	-10.03	108.88	114.90
1	A	1531	A	C4-C5-C6	10.02	122.01	117.00
1	A	1442	G	C6-C5-N7	-10.02	124.39	130.40
1	A	970	C	N1-C2-O2	10.01	124.91	118.90
1	A	769	G	N1-C6-O6	9.99	125.89	119.90
1	A	786	G	C6-C5-N7	-9.96	124.42	130.40
1	A	121	C	C6-N1-C2	9.96	124.28	120.30
1	A	1442	G	N9-C4-C5	-9.92	101.43	105.40
1	A	89	C	C5-C6-N1	9.90	125.95	121.00
1	A	1361(A)	C	N1-C2-O2	9.89	124.83	118.90
1	A	1305	G	C5-C6-N1	-9.86	106.57	111.50
1	A	873	A	C5-C6-N1	9.83	122.61	117.70
1	A	940	C	N3-C4-C5	9.82	125.83	121.90
1	A	328	C	N3-C4-C5	9.82	125.83	121.90
1	A	946	A	C6-N1-C2	-9.78	112.73	118.60
1	A	944	G	N1-C6-O6	-9.76	114.04	119.90
1	A	141	A	N1-C6-N6	9.76	124.46	118.60
1	A	230	G	C5-C6-N1	-9.74	106.63	111.50
1	A	372	C	C5-C4-N4	-9.73	113.39	120.20
1	A	1530	G	N1-C6-O6	9.72	125.73	119.90
1	A	1200	C	N1-C2-O2	9.70	124.72	118.90
1	A	880	C	N3-C4-C5	9.69	125.78	121.90
1	A	336	C	N3-C4-C5	9.67	125.77	121.90
1	A	572	A	C5-C6-N1	9.64	122.52	117.70
1	A	651	C	C6-N1-C2	9.64	124.15	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1338	G	N9-C4-C5	9.64	109.25	105.40
1	A	122	G	C5-C6-N1	-9.63	106.69	111.50
1	A	876	G	C5-C6-N1	9.63	116.31	111.50
1	A	108	G	N3-C4-C5	9.62	133.41	128.60
1	A	1365	G	C8-N9-C4	-9.62	102.55	106.40
1	A	88	A	N1-C6-N6	-9.61	112.84	118.60
1	A	880	C	C5-C4-N4	-9.60	113.48	120.20
1	A	129(A)	G	C6-C5-N7	-9.59	124.65	130.40
1	A	309	G	N3-C4-N9	9.59	131.75	126.00
1	A	279	A	N1-C6-N6	9.59	124.35	118.60
1	A	723	U	C5-C6-N1	9.58	127.49	122.70
1	A	1249	C	C2-N1-C1'	9.57	129.33	118.80
1	A	108	G	C2-N3-C4	-9.57	107.12	111.90
1	A	251	G	C5-C6-N1	-9.56	106.72	111.50
1	A	559	A	N1-C2-N3	9.55	134.07	129.30
1	A	941	G	N1-C6-O6	9.55	125.63	119.90
1	A	944	G	N3-C4-C5	-9.55	123.83	128.60
4	D	12	CYS	CA-CB-SG	9.54	131.18	114.00
1	A	640	A	C8-N9-C4	-9.53	101.99	105.80
1	A	328	C	N3-C4-N4	-9.53	111.33	118.00
1	A	793	U	C6-N1-C2	-9.50	115.30	121.00
1	A	1331	G	N1-C6-O6	-9.50	114.20	119.90
1	A	276	G	N3-C2-N2	-9.50	113.25	119.90
1	A	787	A	C4-C5-C6	9.48	121.74	117.00
1	A	791	G	C8-N9-C4	-9.48	102.61	106.40
1	A	667	G	N1-C6-O6	9.46	125.58	119.90
1	A	541	G	N1-C6-O6	9.45	125.57	119.90
1	A	946	A	N9-C4-C5	9.45	109.58	105.80
1	A	946	A	N1-C6-N6	-9.44	112.93	118.60
1	A	190(A)	C	C6-N1-C2	-9.44	116.52	120.30
1	A	787	A	C6-C5-N7	-9.44	125.69	132.30
1	A	291	C	C2-N3-C4	-9.43	115.19	119.90
1	A	24	U	N3-C2-O2	9.43	128.80	122.20
1	A	190(C)	C	C6-N1-C2	-9.42	116.53	120.30
1	A	1496	C	C5-C6-N1	9.42	125.71	121.00
1	A	384	G	N3-C4-C5	-9.40	123.90	128.60
1	A	103	C	C6-N1-C2	-9.40	116.54	120.30
1	A	481	G	N3-C4-C5	-9.39	123.91	128.60
1	A	372	C	N1-C2-O2	9.37	124.52	118.90
1	A	1531	A	C5-C6-N1	-9.37	113.02	117.70
1	A	567	G	N9-C4-C5	9.36	109.14	105.40
1	A	904	C	C6-N1-C2	-9.36	116.56	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1377	A	N9-C4-C5	9.36	109.54	105.80
1	A	572	A	C6-N1-C2	-9.35	112.99	118.60
1	A	21	G	N3-C4-N9	9.32	131.59	126.00
1	A	573	A	C8-N9-C4	-9.32	102.07	105.80
1	A	117	G	N3-C2-N2	-9.32	113.38	119.90
1	A	890	G	C4-C5-N7	-9.31	107.07	110.80
1	A	1442	G	C4-C5-N7	9.30	114.52	110.80
1	A	260	G	N1-C6-O6	9.28	125.47	119.90
1	A	722	A	C2-N3-C4	-9.25	105.97	110.60
1	A	129(A)	G	C8-N9-C1'	-9.25	114.98	127.00
1	A	266	G	C2-N3-C4	-9.24	107.28	111.90
1	A	755	G	C5-C6-N1	9.24	116.12	111.50
1	A	878	G	N1-C2-N3	9.23	129.44	123.90
1	A	1339	A	N1-C6-N6	-9.22	113.06	118.60
1	A	324	G	C8-N9-C4	-9.22	102.71	106.40
1	A	1367	C	C5-C6-N1	9.22	125.61	121.00
1	A	779	C	C4-C5-C6	9.22	122.01	117.40
1	A	474	G	N1-C6-O6	9.21	125.42	119.90
1	A	788	U	C5-C6-N1	9.20	127.30	122.70
1	A	734	G	C4-C5-N7	9.20	114.48	110.80
1	A	284	G	C5-C6-O6	-9.19	123.09	128.60
1	A	1505	G	C4-C5-C6	9.18	124.31	118.80
1	A	795	C	C5-C6-N1	9.18	125.59	121.00
1	A	285	G	C2-N3-C4	-9.17	107.31	111.90
1	A	822	C	N1-C2-N3	9.17	125.62	119.20
1	A	1389	C	C6-N1-C2	9.17	123.97	120.30
1	A	1249	C	N1-C2-O2	9.16	124.40	118.90
1	A	1296	C	N3-C4-C5	-9.16	118.23	121.90
1	A	89	C	C6-N1-C2	-9.16	116.64	120.30
1	A	735	C	C6-N1-C2	9.16	123.96	120.30
1	A	946	A	N1-C2-N3	9.15	133.88	129.30
1	A	326	G	N3-C4-C5	-9.15	124.02	128.60
1	A	1526	G	N1-C6-O6	9.15	125.39	119.90
1	A	890	G	C5-N7-C8	9.15	108.88	104.30
1	A	1524	C	C6-N1-C2	-9.14	116.64	120.30
1	A	1084	G	N3-C4-C5	-9.14	124.03	128.60
1	A	108	G	N3-C4-N9	-9.14	120.52	126.00
1	A	269	C	N3-C2-O2	-9.13	115.51	121.90
1	A	250	A	C2-N3-C4	-9.13	106.04	110.60
1	A	971	G	N7-C8-N9	-9.12	108.54	113.10
1	A	247	G	C5-C6-N1	-9.11	106.94	111.50
1	A	108	G	C4-C5-N7	9.11	114.44	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	21	G	C5-C6-N1	9.10	116.05	111.50
1	A	1530	G	N3-C4-C5	9.10	133.15	128.60
1	A	21	G	N3-C4-C5	-9.09	124.05	128.60
1	A	901	A	N1-C2-N3	9.09	133.84	129.30
1	A	872	A	N9-C4-C5	-9.08	102.17	105.80
1	A	1296	C	N1-C2-O2	-9.07	113.46	118.90
1	A	1443	G	C8-N9-C4	9.07	110.03	106.40
1	A	144	G	N3-C2-N2	-9.06	113.56	119.90
1	A	731	G	N1-C6-O6	9.06	125.33	119.90
1	A	1502	A	C5-C6-N1	-9.04	113.18	117.70
1	A	1543	C	C5-C6-N1	9.04	125.52	121.00
1	A	599	C	C6-N1-C2	9.03	123.91	120.30
1	A	813	U	N3-C4-O4	9.03	125.72	119.40
1	A	15	G	C5-C6-N1	-9.02	106.99	111.50
1	A	586	C	C5-C6-N1	-9.01	116.49	121.00
1	A	234	C	C6-N1-C2	8.99	123.90	120.30
1	A	963	G	C8-N9-C4	-8.99	102.80	106.40
1	A	1524	C	N3-C4-C5	-8.98	118.31	121.90
1	A	259	G	C8-N9-C4	-8.97	102.81	106.40
1	A	569	C	N1-C2-O2	-8.97	113.52	118.90
1	A	308	C	C5-C4-N4	-8.96	113.93	120.20
1	A	882	C	N1-C2-N3	8.95	125.47	119.20
1	A	734	G	N1-C6-O6	8.95	125.27	119.90
1	A	916	G	C6-N1-C2	-8.94	119.73	125.10
1	A	1200	C	C2-N1-C1'	8.92	128.62	118.80
1	A	685	G	N3-C4-C5	8.91	133.06	128.60
1	A	580	U	C4-C5-C6	8.91	125.05	119.70
1	A	15	G	C6-C5-N7	-8.91	125.05	130.40
1	A	825	G	N7-C8-N9	-8.91	108.65	113.10
1	A	631	G	C8-N9-C4	-8.90	102.84	106.40
1	A	941	G	C5-C6-O6	-8.90	123.26	128.60
1	A	945	G	C5-C6-N1	8.90	115.95	111.50
1	A	308	C	N3-C4-N4	8.89	124.22	118.00
1	A	589	C	C2-N1-C1'	-8.89	109.02	118.80
1	A	797	C	C6-N1-C2	8.88	123.85	120.30
1	A	322	C	N1-C2-O2	-8.87	113.58	118.90
1	A	1331	G	N3-C4-C5	-8.87	124.17	128.60
1	A	747	C	C6-N1-C2	8.87	123.85	120.30
1	A	794	A	N1-C6-N6	-8.86	113.28	118.60
1	A	586	C	C6-N1-C2	8.86	123.84	120.30
1	A	1084	G	C4-C5-N7	-8.85	107.26	110.80
1	A	88	A	N9-C4-C5	8.84	109.33	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	821	G	C5-C6-O6	-8.83	123.30	128.60
1	A	761	G	C6-C5-N7	-8.83	125.10	130.40
1	A	1099	G	N3-C4-C5	8.82	133.01	128.60
1	A	591	U	N3-C4-O4	8.82	125.57	119.40
1	A	1080	A	N1-C6-N6	-8.82	113.31	118.60
1	A	723	U	C2-N1-C1'	8.81	128.27	117.70
1	A	946	A	C8-N9-C4	-8.81	102.28	105.80
1	A	1181	G	N7-C8-N9	-8.81	108.69	113.10
1	A	1524	C	N1-C2-O2	-8.80	113.62	118.90
1	A	297	G	C6-C5-N7	-8.79	125.12	130.40
1	A	1331	G	C4-C5-N7	-8.79	107.28	110.80
1	A	872	A	N1-C6-N6	8.79	123.87	118.60
1	A	638	G	N1-C2-N2	-8.78	108.30	116.20
1	A	881	G	N1-C6-O6	8.78	125.17	119.90
1	A	823	G	C2-N3-C4	-8.77	107.51	111.90
1	A	1394	A	C2-N3-C4	-8.77	106.22	110.60
1	A	1447	G	C5-N7-C8	-8.77	99.92	104.30
1	A	1531	A	C8-N9-C4	-8.76	102.30	105.80
1	A	260	G	C8-N9-C4	-8.76	102.90	106.40
1	A	793	U	C2-N1-C1'	8.75	128.20	117.70
1	A	1338	G	C5-C6-O6	8.75	133.85	128.60
1	A	1543	C	C2-N1-C1'	8.75	128.42	118.80
1	A	130	A	C4-C5-C6	8.74	121.37	117.00
1	A	328	C	C4-C5-C6	-8.74	113.03	117.40
1	A	235	C	N3-C4-C5	8.74	125.39	121.90
1	A	474	G	C6-C5-N7	-8.73	125.16	130.40
1	A	722	A	N1-C6-N6	8.73	123.84	118.60
1	A	277	C	C6-N1-C2	8.72	123.79	120.30
1	A	1189	C	C5-C6-N1	-8.72	116.64	121.00
1	A	1055	A	N1-C6-N6	-8.71	113.38	118.60
1	A	1079	G	N3-C4-C5	-8.71	124.25	128.60
1	A	1241	G	N3-C4-N9	-8.70	120.78	126.00
1	A	1060	C	N1-C2-O2	8.70	124.12	118.90
1	A	595	G	C6-C5-N7	-8.69	125.19	130.40
1	A	130	A	C6-C5-N7	-8.69	126.22	132.30
1	A	1340	A	N1-C2-N3	8.69	133.64	129.30
1	A	38	G	N3-C4-C5	8.68	132.94	128.60
1	A	824	C	N3-C4-C5	8.66	125.36	121.90
1	A	400	C	N3-C4-N4	-8.66	111.94	118.00
1	A	1236	A	N7-C8-N9	-8.66	109.47	113.80
1	A	788	U	C4-C5-C6	-8.65	114.51	119.70
1	A	930	C	N3-C4-N4	-8.65	111.94	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	389	A	C8-N9-C4	-8.65	102.34	105.80
1	A	989	C	C6-N1-C2	-8.64	116.84	120.30
1	A	591	U	C5-C4-O4	-8.63	120.72	125.90
1	A	875	C	C2-N3-C4	-8.64	115.58	119.90
1	A	266	G	C4-C5-N7	8.63	114.25	110.80
1	A	309	G	C5-C6-N1	8.63	115.81	111.50
1	A	412	A	C8-N9-C4	8.63	109.25	105.80
1	A	556	C	C2-N3-C4	-8.63	115.59	119.90
1	A	252	U	C5-C6-N1	-8.62	118.39	122.70
1	A	787	A	N1-C2-N3	8.62	133.61	129.30
1	A	176	C	C6-N1-C2	8.61	123.74	120.30
1	A	1074	G	C5-C6-N1	-8.60	107.20	111.50
1	A	309	G	N9-C4-C5	-8.59	101.96	105.40
1	A	129(A)	G	C5-C6-O6	-8.59	123.44	128.60
1	A	481	G	C8-N9-C1'	-8.59	115.83	127.00
1	A	710	G	N1-C6-O6	8.59	125.06	119.90
1	A	113	G	N1-C6-O6	8.59	125.05	119.90
1	A	916	G	N3-C4-C5	-8.59	124.31	128.60
1	A	833	U	N3-C4-C5	-8.58	109.45	114.60
1	A	1482	G	C8-N9-C4	-8.58	102.97	106.40
1	A	820	U	N1-C2-O2	-8.58	116.80	122.80
1	A	511	C	C2-N1-C1'	-8.57	109.38	118.80
1	A	372	C	N3-C4-N4	8.56	124.00	118.00
1	A	482	A	N1-C6-N6	8.56	123.74	118.60
1	A	113	G	C6-C5-N7	-8.56	125.27	130.40
1	A	569	C	C5-C6-N1	-8.55	116.72	121.00
1	A	190(D)	U	C5-C6-N1	-8.53	118.44	122.70
1	A	279	A	N1-C2-N3	8.53	133.56	129.30
1	A	721	G	N1-C6-O6	8.52	125.01	119.90
1	A	589	C	C6-N1-C2	8.52	123.71	120.30
1	A	1303	C	C6-N1-C2	8.52	123.71	120.30
1	A	447	G	C5-C6-O6	8.51	133.70	128.60
1	A	1436	U	N3-C2-O2	-8.51	116.25	122.20
1	A	190	C	C6-N1-C2	-8.49	116.91	120.30
1	A	1491	G	N3-C4-C5	-8.48	124.36	128.60
1	A	1490	C	C5-C6-N1	8.48	125.24	121.00
1	A	276	G	N3-C4-C5	8.47	132.84	128.60
1	A	360	A	C5-N7-C8	-8.47	99.66	103.90
1	A	130	A	C5-C6-N1	-8.47	113.47	117.70
1	A	1355	G	C8-N9-C4	-8.47	103.01	106.40
1	A	1526	G	C6-C5-N7	-8.47	125.32	130.40
1	A	882	C	C6-N1-C2	-8.46	116.92	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	129(A)	G	C4-C5-N7	8.45	114.18	110.80
1	A	350	G	C8-N9-C4	-8.44	103.02	106.40
1	A	500	G	N1-C6-O6	8.44	124.96	119.90
2	B	158	LEU	CA-CB-CG	-8.43	95.92	115.30
1	A	570	G	C4-N9-C1'	8.42	137.45	126.50
1	A	740	U	N3-C2-O2	-8.42	116.30	122.20
1	A	326	G	N1-C6-O6	-8.42	114.85	119.90
1	A	708	C	C6-N1-C2	8.42	123.67	120.30
1	A	1490	C	C6-N1-C2	-8.41	116.94	120.30
1	A	511	C	N3-C4-N4	-8.41	112.11	118.00
1	A	794	A	C8-N9-C4	-8.40	102.44	105.80
1	A	21	G	C2-N3-C4	8.40	116.10	111.90
1	A	251	G	C4-C5-C6	8.40	123.84	118.80
1	A	570	G	C8-N9-C1'	-8.40	116.08	127.00
1	A	1508	G	C8-N9-C4	-8.38	103.05	106.40
1	A	874	G	C8-N9-C4	8.38	109.75	106.40
1	A	29	G	N1-C2-N3	8.36	128.92	123.90
1	A	794	A	N9-C4-C5	8.36	109.14	105.80
1	A	562	C	C5-C6-N1	-8.36	116.82	121.00
1	A	812	C	N1-C2-O2	-8.35	113.89	118.90
1	A	556	C	C5-C6-N1	-8.34	116.83	121.00
1	A	568	G	C8-N9-C4	-8.34	103.06	106.40
1	A	765	G	C4-C5-N7	8.34	114.14	110.80
1	A	1231	G	C4-C5-N7	8.34	114.14	110.80
1	A	1333	A	C8-N9-C4	-8.34	102.47	105.80
1	A	316	G	N1-C6-O6	8.33	124.90	119.90
1	A	746	A	C8-N9-C4	8.33	109.13	105.80
1	A	1370	G	N1-C6-O6	8.33	124.90	119.90
1	A	316	G	C6-C5-N7	-8.33	125.40	130.40
1	A	707	C	C6-N1-C2	8.33	123.63	120.30
1	A	113	G	C5-C6-O6	-8.31	123.61	128.60
1	A	776	G	N3-C4-C5	8.31	132.76	128.60
1	A	15	G	N1-C6-O6	8.30	124.88	119.90
1	A	79	G	C5-C6-N1	-8.30	107.35	111.50
1	A	79	G	N1-C6-O6	8.30	124.88	119.90
1	A	266	G	N3-C4-N9	-8.29	121.02	126.00
1	A	1389	C	N3-C4-C5	8.29	125.22	121.90
1	A	1490	C	N1-C2-O2	-8.29	113.92	118.90
1	A	1246	C	N3-C2-O2	8.28	127.69	121.90
1	A	1238	A	C5-C6-N6	8.28	130.32	123.70
1	A	1165	C	C6-N1-C2	-8.27	116.99	120.30
1	A	698	G	C8-N9-C4	-8.26	103.09	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	793	U	C5-C6-N1	8.26	126.83	122.70
1	A	128	G	C4-C5-N7	8.26	114.10	110.80
1	A	295	C	C6-N1-C2	8.25	123.60	120.30
1	A	642	A	C8-N9-C4	-8.25	102.50	105.80
1	A	881	G	C5-C6-O6	-8.25	123.65	128.60
1	A	108	G	N1-C6-O6	8.24	124.84	119.90
1	A	862	C	N3-C4-C5	8.24	125.19	121.90
1	A	27	G	N3-C4-N9	8.23	130.94	126.00
1	A	788	U	C5-C4-O4	-8.23	120.96	125.90
1	A	576	G	C5-C6-O6	-8.23	123.66	128.60
1	A	93	G	N3-C4-N9	8.23	130.94	126.00
1	A	1200	C	C6-N1-C1'	-8.23	110.93	120.80
1	A	1461	G	C8-N9-C4	8.22	109.69	106.40
1	A	607	A	C6-N1-C2	8.22	123.53	118.60
1	A	627	G	C6-C5-N7	-8.21	125.47	130.40
1	A	926	G	N3-C4-N9	8.21	130.93	126.00
1	A	1346	A	C2-N3-C4	8.21	114.71	110.60
1	A	1527	C	C6-N1-C2	-8.21	117.02	120.30
1	A	190(F)	G	N3-C4-N9	-8.21	121.08	126.00
1	A	580	U	N1-C2-O2	-8.21	117.05	122.80
1	A	948	C	C6-N1-C2	8.21	123.58	120.30
1	A	1530	G	C5-C6-O6	-8.20	123.68	128.60
1	A	481	G	N3-C2-N2	8.20	125.64	119.90
1	A	694	A	C5-C6-N1	-8.20	113.60	117.70
1	A	79	G	C8-N9-C4	-8.19	103.13	106.40
1	A	78	G	C4-C5-N7	8.18	114.07	110.80
1	A	197	A	N1-C6-N6	-8.18	113.69	118.60
1	A	859	A	N3-C4-C5	-8.18	121.08	126.80
1	A	1079	G	C6-C5-N7	-8.18	125.49	130.40
1	A	872	A	C4-C5-N7	8.17	114.79	110.70
1	A	1442	G	N3-C4-C5	-8.17	124.51	128.60
1	A	1254	C	C6-N1-C2	-8.17	117.03	120.30
1	A	144	G	C6-C5-N7	-8.17	125.50	130.40
1	A	545	C	C6-N1-C2	-8.16	117.03	120.30
1	A	297	G	N1-C6-O6	8.16	124.80	119.90
1	A	907	A	N1-C6-N6	-8.16	113.70	118.60
1	A	650	G	N1-C6-O6	8.15	124.79	119.90
1	A	29	G	C5-N7-C8	8.15	108.37	104.30
1	A	913	A	N1-C6-N6	-8.15	113.71	118.60
1	A	822	C	N1-C2-O2	-8.14	114.01	118.90
1	A	117	G	N1-C2-N3	8.14	128.78	123.90
1	A	456	C	N1-C2-O2	8.14	123.78	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	450	G	C8-N9-C4	8.14	109.66	106.40
1	A	730	G	C5-C6-O6	8.14	133.48	128.60
1	A	899	C	C5-C6-N1	8.14	125.07	121.00
1	A	1064	G	C6-C5-N7	-8.13	125.52	130.40
1	A	176	C	N3-C4-C5	8.12	125.15	121.90
1	A	607	A	C5-N7-C8	-8.12	99.84	103.90
1	A	328	C	N1-C2-O2	8.12	123.77	118.90
1	A	329	A	C4-C5-N7	8.12	114.76	110.70
1	A	1367	C	N1-C2-O2	8.12	123.77	118.90
1	A	141	A	C2-N3-C4	-8.12	106.54	110.60
1	A	323	U	N3-C2-O2	8.11	127.88	122.20
1	A	314	C	N3-C4-C5	8.11	125.14	121.90
1	A	872	A	C2-N3-C4	-8.11	106.55	110.60
1	A	1375	A	N7-C8-N9	-8.09	109.75	113.80
1	A	859	A	C2-N3-C4	8.09	114.64	110.60
1	A	729	A	C5-N7-C8	-8.08	99.86	103.90
1	A	919	A	C8-N9-C4	8.08	109.03	105.80
1	A	916	G	N3-C4-N9	8.08	130.85	126.00
1	A	80	G	C6-C5-N7	-8.08	125.55	130.40
1	A	401	C	C6-N1-C2	-8.08	117.07	120.30
1	A	930	C	C2-N3-C4	-8.07	115.86	119.90
1	A	1152	A	N1-C6-N6	-8.07	113.76	118.60
1	A	117	G	N3-C4-C5	8.07	132.63	128.60
1	A	995	C	C2-N1-C1'	8.07	127.67	118.80
1	A	322	C	N3-C4-C5	-8.06	118.68	121.90
1	A	632	A	N1-C6-N6	8.06	123.44	118.60
1	A	873	A	C2-N3-C4	8.06	114.63	110.60
1	A	35	G	N1-C6-O6	8.05	124.73	119.90
1	A	255	G	C8-N9-C1'	-8.05	116.53	127.00
1	A	703	G	C4-C5-N7	-8.05	107.58	110.80
1	A	916	G	N1-C2-N3	8.05	128.73	123.90
1	A	647	C	C6-N1-C2	8.05	123.52	120.30
1	A	1249	C	C5-C6-N1	8.05	125.02	121.00
1	A	950	U	N3-C4-C5	-8.04	109.78	114.60
1	A	230	G	C2-N3-C4	-8.04	107.88	111.90
1	A	832	C	N3-C2-O2	8.03	127.52	121.90
1	A	567	G	C5-N7-C8	8.02	108.31	104.30
1	A	481	G	C2-N3-C4	8.01	115.91	111.90
1	A	885	G	N7-C8-N9	8.00	117.10	113.10
1	A	1063	C	C6-N1-C2	-8.00	117.10	120.30
1	A	708	C	N3-C4-C5	7.99	125.10	121.90
1	A	859	A	C5-C6-N6	-7.99	117.31	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	725	G	C4-C5-N7	7.99	114.00	110.80
1	A	1408	A	N1-C6-N6	7.99	123.39	118.60
1	A	108	G	C5-C6-N1	-7.98	107.51	111.50
1	A	29	G	C5-C6-N1	-7.97	107.51	111.50
1	A	1455	G	C8-N9-C4	-7.97	103.21	106.40
1	A	285	G	C5-C6-N1	-7.97	107.52	111.50
1	A	1069	C	C6-N1-C2	7.97	123.49	120.30
1	A	776	G	N3-C4-N9	-7.96	121.22	126.00
1	A	400	C	N1-C2-O2	7.96	123.67	118.90
1	A	942	G	N1-C6-O6	7.95	124.67	119.90
1	A	791	G	N3-C4-C5	-7.95	124.62	128.60
1	A	1249	C	C6-N1-C1'	-7.95	111.26	120.80
1	A	774	G	N3-C4-N9	7.94	130.76	126.00
1	A	795	C	N3-C4-N4	7.94	123.56	118.00
1	A	627	G	C2-N3-C4	-7.94	107.93	111.90
1	A	823	G	N1-C2-N3	7.94	128.66	123.90
1	A	780	A	C6-N1-C2	-7.94	113.84	118.60
1	A	793	U	N3-C2-O2	-7.93	116.65	122.20
1	A	607	A	N1-C2-N3	-7.93	125.33	129.30
1	A	889	A	C8-N9-C4	-7.92	102.63	105.80
8	H	12	ARG	NE-CZ-NH2	7.92	124.26	120.30
1	A	1342	C	N1-C2-O2	-7.92	114.15	118.90
1	A	1279	A	N7-C8-N9	7.91	117.75	113.80
1	A	1084	G	N1-C6-O6	-7.90	115.16	119.90
1	A	299	G	N1-C6-O6	7.90	124.64	119.90
1	A	384	G	N3-C4-N9	7.89	130.73	126.00
1	A	1060	C	N3-C2-O2	-7.89	116.38	121.90
1	A	292	G	C8-N9-C4	7.88	109.55	106.40
1	A	595	G	C4-C5-C6	7.88	123.53	118.80
1	A	875	C	N1-C2-O2	-7.88	114.17	118.90
1	A	623	C	N3-C4-C5	7.87	125.05	121.90
1	A	787	A	C5-C6-N1	-7.87	113.77	117.70
1	A	1064	G	N1-C6-O6	7.87	124.62	119.90
1	A	190(F)	G	N3-C4-C5	7.86	132.53	128.60
1	A	1370	G	C4-N9-C1'	7.86	136.72	126.50
1	A	98	U	C6-N1-C2	-7.86	116.28	121.00
1	A	569	C	C2-N3-C4	-7.86	115.97	119.90
1	A	570	G	C6-C5-N7	-7.86	125.69	130.40
1	A	778	G	C2-N3-C4	-7.86	107.97	111.90
1	A	1514	C	C2-N3-C4	-7.86	115.97	119.90
1	A	659	U	C5-C6-N1	-7.85	118.78	122.70
1	A	919	A	N1-C2-N3	-7.85	125.38	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1542	U	N3-C4-C5	-7.85	109.89	114.60
1	A	43	C	C6-N1-C2	7.84	123.44	120.30
1	A	852	G	C2-N3-C4	-7.84	107.98	111.90
1	A	867	G	C6-C5-N7	-7.84	125.69	130.40
1	A	20	U	C3'-C2'-C1'	-7.84	95.23	101.50
1	A	400	C	N3-C4-C5	7.83	125.03	121.90
1	A	1179	A	N1-C6-N6	-7.83	113.90	118.60
1	A	199	G	N1-C6-O6	7.83	124.60	119.90
1	A	567	G	C5-C6-O6	7.83	133.30	128.60
1	A	62	U	N3-C2-O2	-7.83	116.72	122.20
1	A	21	G	N1-C2-N2	-7.82	109.16	116.20
1	A	255	G	C4-N9-C1'	7.82	136.66	126.50
1	A	481	G	N7-C8-N9	-7.82	109.19	113.10
1	A	580	U	C6-N1-C2	-7.81	116.31	121.00
1	A	1182	G	N1-C6-O6	7.81	124.59	119.90
1	A	218	C	C5-C6-N1	7.81	124.90	121.00
1	A	875	C	C4-C5-C6	7.80	121.30	117.40
1	A	610	G	C8-N9-C4	-7.80	103.28	106.40
1	A	285	G	N1-C6-O6	7.79	124.58	119.90
1	A	606	G	N3-C4-C5	-7.79	124.70	128.60
1	A	1482	G	N3-C4-N9	7.79	130.67	126.00
1	A	43	C	C5-C6-N1	-7.78	117.11	121.00
1	A	703	G	C5-C6-O6	7.78	133.27	128.60
1	A	719	C	N3-C2-O2	-7.76	116.47	121.90
1	A	1069	C	N3-C2-O2	7.76	127.33	121.90
1	A	331	G	C5-C6-N1	-7.76	107.62	111.50
1	A	765	G	C5-N7-C8	-7.76	100.42	104.30
1	A	638	G	N1-C2-N3	7.76	128.56	123.90
1	A	717	C	C6-N1-C2	7.76	123.40	120.30
1	A	559	A	C5-C6-N1	7.75	121.58	117.70
1	A	15	G	C4-C5-C6	7.75	123.45	118.80
1	A	728	A	C8-N9-C4	-7.75	102.70	105.80
1	A	1334	G	N7-C8-N9	-7.74	109.23	113.10
1	A	786	G	C5-C6-O6	-7.74	123.95	128.60
1	A	1265	G	N1-C6-O6	7.74	124.55	119.90
1	A	132	C	C4-C5-C6	7.74	121.27	117.40
1	A	1088	G	C8-N9-C4	-7.74	103.31	106.40
1	A	1484	C	C6-N1-C2	-7.73	117.21	120.30
1	A	1346	A	C6-C5-N7	7.73	137.71	132.30
1	A	323	U	C5-C4-O4	-7.72	121.27	125.90
1	A	88	A	N3-C4-C5	-7.72	121.40	126.80
1	A	1521	G	C5-C6-N1	7.71	115.36	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	780	A	C5-C6-N1	7.71	121.56	117.70
1	A	599	C	C5-C6-N1	-7.71	117.14	121.00
1	A	927	G	C5-C6-N1	-7.71	107.65	111.50
1	A	703	G	N1-C6-O6	-7.70	115.28	119.90
1	A	881	G	C4-C5-C6	7.70	123.42	118.80
1	A	881	G	C6-C5-N7	-7.70	125.78	130.40
1	A	251	G	C4-N9-C1'	7.69	136.50	126.50
1	A	1181	G	N3-C4-C5	7.69	132.45	128.60
1	A	309	G	C8-N9-C4	7.69	109.48	106.40
1	A	867	G	C5-C6-O6	-7.68	123.99	128.60
1	A	1088	G	N7-C8-N9	7.68	116.94	113.10
1	A	1375	A	C8-N9-C4	7.68	108.87	105.80
1	A	1355	G	N1-C6-O6	-7.67	115.30	119.90
1	A	7	G	C2-N3-C4	7.67	115.74	111.90
1	A	1152	A	N9-C4-C5	7.67	108.87	105.80
1	A	650	G	C5-C6-O6	-7.67	124.00	128.60
1	A	919	A	C4-C5-C6	-7.66	113.17	117.00
1	A	1084	G	C5-N7-C8	7.66	108.13	104.30
1	A	230	G	N1-C2-N3	7.66	128.50	123.90
1	A	890	G	N7-C8-N9	-7.66	109.27	113.10
1	A	1348	U	C2-N1-C1'	7.66	126.89	117.70
1	A	812	C	N3-C4-C5	-7.65	118.84	121.90
1	A	1512	U	N1-C2-O2	-7.65	117.44	122.80
12	L	66	VAL	CB-CA-C	-7.65	96.86	111.40
1	A	782	A	C4-C5-C6	7.64	120.82	117.00
1	A	860	A	C2-N3-C4	-7.64	106.78	110.60
1	A	236	G	C4-N9-C1'	7.64	136.43	126.50
1	A	685	G	C2-N3-C4	-7.64	108.08	111.90
1	A	144	G	C2-N3-C4	-7.63	108.08	111.90
1	A	1526	G	C4-N9-C1'	7.63	136.42	126.50
1	A	97	G	C8-N9-C4	-7.63	103.35	106.40
1	A	190	C	N3-C2-O2	-7.63	116.56	121.90
1	A	1380	U	N3-C2-O2	-7.63	116.86	122.20
1	A	39	G	C5-C6-N1	7.62	115.31	111.50
1	A	1279	A	C6-C5-N7	-7.62	126.97	132.30
1	A	745	C	N3-C4-C5	7.61	124.94	121.90
1	A	139	G	N1-C6-O6	7.60	124.46	119.90
1	A	368	U	C5-C6-N1	-7.60	118.90	122.70
1	A	75	G	N3-C4-N9	7.60	130.56	126.00
1	A	755	G	N1-C2-N3	-7.60	119.34	123.90
1	A	673	G	N3-C4-N9	7.60	130.56	126.00
1	A	824	C	C2-N3-C4	-7.59	116.10	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1346	A	N9-C4-C5	7.59	108.84	105.80
1	A	859	A	N7-C8-N9	7.59	117.59	113.80
1	A	557	G	C6-C5-N7	-7.59	125.85	130.40
1	A	113	G	C8-N9-C1'	-7.58	117.15	127.00
1	A	132	C	N1-C2-N3	7.57	124.50	119.20
1	A	357	G	C5-C6-N1	-7.57	107.71	111.50
1	A	941	G	N3-C2-N2	-7.57	114.60	119.90
1	A	851	G	N3-C2-N2	-7.57	114.60	119.90
1	A	1416	G	C5-C6-N1	-7.57	107.72	111.50
1	A	24	U	C5-C4-O4	-7.56	121.36	125.90
1	A	238	G	C2-N3-C4	-7.56	108.12	111.90
1	A	1369	C	C6-N1-C2	-7.56	117.28	120.30
1	A	106	C	N1-C2-N3	7.56	124.49	119.20
1	A	570	G	N1-C2-N3	7.56	128.44	123.90
3	C	179	ARG	N-CA-C	-7.55	90.60	111.00
1	A	1455	G	C4-C5-N7	7.55	113.82	110.80
1	A	1497	G	C4-C5-N7	7.55	113.82	110.80
1	A	1455	G	C5-N7-C8	-7.55	100.53	104.30
1	A	483	C	C2-N1-C1'	-7.54	110.50	118.80
1	A	1409	C	C6-N1-C2	-7.54	117.28	120.30
20	T	94	ALA	N-CA-C	-7.54	90.65	111.00
1	A	1148	U	C5-C6-N1	7.53	126.47	122.70
1	A	317	G	C5-C6-O6	-7.53	124.08	128.60
1	A	1529	G	N7-C8-N9	7.53	116.86	113.10
1	A	586	C	C2-N3-C4	-7.53	116.14	119.90
1	A	29	G	C2-N3-C4	-7.52	108.14	111.90
1	A	257	G	N3-C2-N2	7.52	125.16	119.90
1	A	798	G	C2-N3-C4	-7.51	108.14	111.90
1	A	859	A	N1-C6-N6	7.51	123.11	118.60
1	A	654	G	C2-N3-C4	-7.51	108.15	111.90
1	A	873	A	N9-C4-C5	7.50	108.80	105.80
1	A	326	G	C2-N3-C4	7.50	115.65	111.90
1	A	809	G	C8-N9-C4	-7.50	103.40	106.40
1	A	280	C	C6-N1-C2	7.49	123.30	120.30
1	A	1241	G	C5-C6-N1	-7.49	107.75	111.50
1	A	66	G	C5-N7-C8	-7.49	100.56	104.30
1	A	30	U	N3-C4-C5	7.48	119.09	114.60
1	A	755	G	C2-N3-C4	7.48	115.64	111.90
1	A	1513	A	C2-N3-C4	-7.48	106.86	110.60
1	A	730	G	N1-C2-N3	7.48	128.39	123.90
1	A	190(G)	G	C8-N9-C4	-7.48	103.41	106.40
1	A	16	A	N7-C8-N9	-7.47	110.06	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1521	G	N1-C6-O6	-7.47	115.42	119.90
1	A	859	A	N3-C4-N9	7.46	133.37	127.40
1	A	1279	A	C5-N7-C8	-7.45	100.17	103.90
1	A	518	C	C6-N1-C2	7.45	123.28	120.30
1	A	113	G	N3-C4-N9	7.44	130.46	126.00
1	A	580	U	N3-C4-O4	7.44	124.61	119.40
1	A	708	C	C5-C6-N1	-7.44	117.28	121.00
1	A	257	G	N1-C2-N2	-7.44	109.51	116.20
1	A	295	C	N3-C4-C5	7.43	124.87	121.90
1	A	721	G	C4-C5-N7	7.43	113.77	110.80
1	A	1347	G	N7-C8-N9	-7.42	109.39	113.10
1	A	325	A	N9-C4-C5	7.42	108.77	105.80
1	A	524	G	C5-C6-O6	-7.42	124.15	128.60
1	A	811	C	N3-C4-C5	-7.42	118.93	121.90
1	A	559	A	N3-C4-C5	-7.41	121.61	126.80
1	A	1074	G	C6-C5-N7	-7.41	125.95	130.40
1	A	1155	G	N7-C8-N9	7.41	116.80	113.10
1	A	899	C	N3-C4-N4	7.40	123.18	118.00
1	A	141	A	C4-C5-N7	7.40	114.40	110.70
1	A	1241	G	C2-N3-C4	-7.39	108.20	111.90
1	A	928	G	C4-C5-N7	7.39	113.76	110.80
1	A	1529	G	C4-N9-C1'	7.39	136.10	126.50
1	A	1338	G	N3-C4-N9	-7.39	121.57	126.00
1	A	1192	C	C2-N3-C4	-7.38	116.21	119.90
1	A	1382	C	C6-N1-C2	-7.38	117.35	120.30
1	A	1494	G	N1-C6-O6	7.38	124.33	119.90
1	A	122	G	C2-N3-C4	-7.37	108.21	111.90
1	A	128	G	N9-C4-C5	-7.37	102.45	105.40
1	A	722	A	C6-C5-N7	-7.37	127.14	132.30
1	A	329	A	C5-C6-N6	-7.36	117.81	123.70
1	A	721	G	N9-C4-C5	-7.36	102.46	105.40
1	A	1328	C	C6-N1-C2	-7.35	117.36	120.30
1	A	1435	G	N1-C6-O6	7.35	124.31	119.90
1	A	393	A	N1-C6-N6	7.35	123.01	118.60
1	A	944	G	N7-C8-N9	7.35	116.78	113.10
1	A	1279	A	N1-C6-N6	7.35	123.01	118.60
1	A	238	G	C5-C6-N1	-7.35	107.83	111.50
1	A	128	G	C2-N3-C4	-7.34	108.23	111.90
1	A	707	C	C2-N1-C1'	-7.34	110.72	118.80
1	A	416	G	N1-C6-O6	7.34	124.30	119.90
1	A	1455	G	N7-C8-N9	7.34	116.77	113.10
1	A	773	G	N1-C6-O6	7.33	124.30	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1080	A	N7-C8-N9	-7.33	110.14	113.80
1	A	372	C	C6-N1-C1'	-7.33	112.01	120.80
1	A	741	G	C4-C5-N7	-7.33	107.87	110.80
1	A	865	A	C5-C6-N1	7.32	121.36	117.70
1	A	971	G	N1-C6-O6	7.32	124.29	119.90
1	A	669	U	C6-N1-C2	7.32	125.39	121.00
1	A	451	A	C4-C5-C6	-7.32	113.34	117.00
1	A	499	A	N9-C4-C5	7.32	108.73	105.80
1	A	1181	G	C4-N9-C1'	-7.32	116.99	126.50
1	A	93	G	N3-C4-C5	-7.32	124.94	128.60
1	A	80	G	C8-N9-C4	-7.31	103.47	106.40
1	A	557	G	N1-C6-O6	7.31	124.29	119.90
1	A	146	G	N1-C6-O6	7.30	124.28	119.90
1	A	627	G	N9-C4-C5	-7.30	102.48	105.40
1	A	98	U	C5-C6-N1	7.30	126.35	122.70
1	A	7	G	C4-C5-N7	-7.30	107.88	110.80
1	A	122	G	C6-C5-N7	-7.30	126.02	130.40
1	A	926	G	N3-C4-C5	-7.30	124.95	128.60
1	A	507	C	N3-C4-C5	7.30	124.82	121.90
1	A	1200	C	C5-C6-N1	7.30	124.65	121.00
1	A	1348	U	N3-C4-O4	7.29	124.51	119.40
1	A	27	G	C6-C5-N7	-7.29	126.02	130.40
1	A	481	G	C5-C6-O6	-7.29	124.22	128.60
1	A	417	C	C5-C6-N1	7.29	124.64	121.00
1	A	119	A	N1-C6-N6	-7.28	114.23	118.60
1	A	827	U	N1-C2-N3	7.28	119.27	114.90
1	A	882	C	N1-C2-O2	-7.28	114.53	118.90
1	A	731	G	C4-C5-N7	7.28	113.71	110.80
1	A	1469	G	N1-C6-O6	7.28	124.27	119.90
1	A	251	G	N7-C8-N9	7.27	116.74	113.10
1	A	782	A	C6-N1-C2	-7.27	114.24	118.60
1	A	927	G	N3-C4-C5	7.27	132.23	128.60
1	A	971	G	C5-C6-N1	-7.27	107.87	111.50
1	A	228	A	N1-C6-N6	7.26	122.96	118.60
1	A	927	G	N1-C6-O6	7.26	124.26	119.90
1	A	755	G	N1-C2-N2	7.26	122.73	116.20
1	A	628	G	N3-C4-N9	7.25	130.35	126.00
1	A	1238	A	N1-C6-N6	-7.25	114.25	118.60
1	A	1202	G	C5-C6-O6	7.25	132.95	128.60
1	A	852	G	N1-C6-O6	7.24	124.25	119.90
1	A	1465	C	C5-C4-N4	-7.24	115.13	120.20
1	A	1447	G	N7-C8-N9	7.24	116.72	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1370	G	C5-C6-O6	-7.24	124.26	128.60
1	A	499	A	C8-N9-C4	-7.24	102.91	105.80
1	A	106	C	C4-C5-C6	7.23	121.01	117.40
1	A	483	C	C5-C6-N1	-7.23	117.39	121.00
1	A	129(A)	G	C4-N9-C1'	7.23	135.90	126.50
1	A	919	A	C5-C6-N1	7.23	121.31	117.70
1	A	244	U	C5-C6-N1	-7.22	119.09	122.70
1	A	640	A	N9-C4-C5	7.22	108.69	105.80
1	A	1061	G	N1-C6-O6	7.22	124.23	119.90
1	A	519	C	N3-C4-C5	-7.22	119.01	121.90
1	A	1208	C	C6-N1-C2	-7.22	117.41	120.30
1	A	190(G)	G	N7-C8-N9	7.22	116.71	113.10
1	A	44	G	C6-C5-N7	-7.22	126.07	130.40
1	A	238	G	N1-C6-O6	7.21	124.23	119.90
1	A	651	C	N1-C2-N3	-7.21	114.15	119.20
1	A	1409	C	C5-C6-N1	7.21	124.61	121.00
1	A	310	G	C4-C5-N7	7.21	113.68	110.80
1	A	881	G	N3-C4-N9	7.21	130.33	126.00
1	A	927	G	C2-N3-C4	-7.21	108.30	111.90
1	A	1496	C	C4-C5-C6	-7.20	113.80	117.40
1	A	1219	U	C6-N1-C2	-7.20	116.68	121.00
1	A	589	C	C5-C6-N1	-7.19	117.40	121.00
1	A	1469	G	C5-C6-O6	-7.19	124.28	128.60
1	A	1152	A	C8-N9-C4	-7.19	102.92	105.80
1	A	1373	G	N3-C4-C5	-7.19	125.01	128.60
17	Q	35	VAL	CB-CA-C	-7.19	97.74	111.40
1	A	276	G	N3-C4-N9	-7.18	121.69	126.00
1	A	857	C	C6-N1-C2	-7.18	117.43	120.30
1	A	821	G	C8-N9-C4	7.18	109.27	106.40
1	A	766	A	C2-N3-C4	-7.17	107.02	110.60
1	A	1344	C	C2-N3-C4	-7.17	116.32	119.90
1	A	1241	G	N3-C4-C5	7.16	132.18	128.60
1	A	288	A	C2-N3-C4	-7.16	107.02	110.60
1	A	1528	U	C6-N1-C2	7.16	125.30	121.00
1	A	108	G	C6-C5-N7	-7.16	126.11	130.40
1	A	1240	U	C5-C4-O4	7.15	130.19	125.90
1	A	1377	A	C5-C6-N6	7.15	129.42	123.70
1	A	920	U	C5-C4-O4	7.15	130.19	125.90
1	A	329	A	N1-C6-N6	7.15	122.89	118.60
1	A	157	G	N1-C6-O6	7.14	124.19	119.90
1	A	197	A	C5-C6-N1	7.14	121.27	117.70
1	A	265	G	C8-N9-C4	7.14	109.26	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1231	G	C2-N3-C4	-7.14	108.33	111.90
1	A	266	G	N7-C8-N9	7.13	116.67	113.10
1	A	247	G	C2-N3-C4	-7.13	108.33	111.90
1	A	673	G	C6-C5-N7	-7.13	126.12	130.40
1	A	731	G	C5-C6-O6	-7.13	124.32	128.60
1	A	870	U	N1-C2-O2	7.13	127.79	122.80
1	A	900	A	C2-N3-C4	-7.13	107.04	110.60
1	A	933	G	N3-C4-C5	7.13	132.16	128.60
1	A	1436	U	N1-C2-O2	7.13	127.79	122.80
1	A	240	C	C5-C4-N4	-7.12	115.21	120.20
1	A	373	A	C2-N3-C4	-7.12	107.04	110.60
1	A	1517	G	C8-N9-C4	-7.12	103.55	106.40
1	A	616	G	C5-C6-N1	-7.12	107.94	111.50
1	A	779	C	N1-C2-N3	7.11	124.18	119.20
1	A	190(D)	U	C2-N1-C1'	-7.11	109.17	117.70
1	A	383	A	N1-C6-N6	7.11	122.87	118.60
1	A	572	A	N7-C8-N9	-7.11	110.25	113.80
1	A	109	A	N1-C6-N6	7.10	122.86	118.60
1	A	750	G	N1-C2-N3	7.10	128.16	123.90
1	A	319	G	C6-C5-N7	-7.09	126.14	130.40
1	A	755	G	C5-C6-O6	-7.09	124.34	128.60
1	A	1182	G	C5-C6-O6	-7.09	124.34	128.60
1	A	309	G	N1-C2-N3	7.09	128.15	123.90
1	A	1238	A	C4-C5-N7	-7.09	107.16	110.70
1	A	1367	C	C2-N1-C1'	7.09	126.60	118.80
1	A	656	C	C2-N3-C4	-7.09	116.36	119.90
1	A	1441	G	C5-C6-O6	7.08	132.85	128.60
1	A	121	C	C2-N1-C1'	-7.08	111.01	118.80
1	A	858	G	N3-C4-C5	7.08	132.14	128.60
1	A	291	C	N1-C2-N3	7.08	124.16	119.20
1	A	1494	G	N9-C4-C5	-7.07	102.57	105.40
1	A	234	C	N3-C4-C5	7.07	124.73	121.90
1	A	80	G	N7-C8-N9	7.07	116.63	113.10
1	A	144	G	N7-C8-N9	7.07	116.63	113.10
1	A	779	C	N1-C2-O2	-7.07	114.66	118.90
1	A	234	C	C5-C6-N1	-7.07	117.47	121.00
1	A	1071	C	C5-C4-N4	-7.07	115.25	120.20
1	A	255	G	C4-C5-C6	7.06	123.04	118.80
1	A	1474	G	C5-C6-O6	-7.06	124.36	128.60
1	A	59	A	C5-C6-N1	7.06	121.23	117.70
1	A	29	G	N7-C8-N9	-7.06	109.57	113.10
1	A	1455	G	C6-C5-N7	-7.05	126.17	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1452	C	N1-C2-O2	7.05	123.13	118.90
1	A	1100	C	C6-N1-C2	-7.04	117.48	120.30
1	A	167	G	C8-N9-C4	-7.04	103.59	106.40
1	A	310	G	C6-C5-N7	-7.04	126.18	130.40
1	A	606	G	C8-N9-C4	-7.04	103.59	106.40
1	A	653	A	C8-N9-C4	-7.04	102.99	105.80
1	A	779	C	N3-C4-C5	-7.03	119.09	121.90
1	A	782	A	C2-N3-C4	-7.03	107.09	110.60
1	A	888	G	N9-C4-C5	7.02	108.21	105.40
1	A	1499	A	N1-C6-N6	7.02	122.81	118.60
1	A	928	G	C5-C6-O6	-7.02	124.39	128.60
1	A	645	C	C5-C6-N1	7.02	124.51	121.00
2	B	23	ARG	N-CA-C	-7.02	92.06	111.00
1	A	1497	G	C5-N7-C8	-7.01	100.79	104.30
1	A	1043	C	C6-N1-C2	-7.01	117.50	120.30
1	A	706	A	N1-C2-N3	7.01	132.81	129.30
1	A	711	G	N1-C6-O6	7.01	124.11	119.90
1	A	908	A	C8-N9-C4	-7.01	103.00	105.80
1	A	764	C	N3-C4-C5	7.01	124.70	121.90
1	A	701	C	N3-C4-N4	-7.01	113.09	118.00
1	A	18	C	C6-N1-C2	7.00	123.10	120.30
1	A	481	G	C5-N7-C8	7.00	107.80	104.30
1	A	142	G	N3-C4-C5	-6.99	125.10	128.60
1	A	1338	G	N1-C2-N3	6.99	128.10	123.90
1	A	1231	G	C6-C5-N7	-6.99	126.20	130.40
1	A	168	G	C6-C5-N7	-6.98	126.21	130.40
1	A	407	G	C2-N3-C4	-6.98	108.41	111.90
1	A	563	A	C8-N9-C1'	-6.98	115.13	127.70
1	A	399	G	C2-N3-C4	-6.98	108.41	111.90
1	A	1425	U	C5-C4-O4	6.98	130.09	125.90
1	A	719	C	C5-C6-N1	-6.98	117.51	121.00
1	A	862	C	C5-C6-N1	-6.98	117.51	121.00
1	A	1522	U	C5-C6-N1	6.97	126.19	122.70
1	A	565	U	N1-C2-N3	-6.97	110.72	114.90
1	A	1310	G	C8-N9-C1'	-6.97	117.94	127.00
1	A	598	U	C5-C6-N1	-6.96	119.22	122.70
1	A	563	A	C4-C5-C6	6.96	120.48	117.00
1	A	707	C	N3-C4-N4	-6.95	113.13	118.00
5	E	41	VAL	CB-CA-C	-6.95	98.19	111.40
1	A	322	C	N3-C4-N4	6.95	122.86	118.00
1	A	898	G	C2-N3-C4	-6.95	108.43	111.90
1	A	145	G	N1-C6-O6	6.95	124.07	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	759	A	C5-N7-C8	-6.94	100.43	103.90
1	A	319	G	C5-C6-O6	-6.94	124.44	128.60
1	A	1302	U	N1-C2-O2	6.94	127.66	122.80
1	A	1079	G	C6-N1-C2	-6.94	120.94	125.10
1	A	274	A	C8-N9-C4	6.94	108.58	105.80
1	A	658	G	C8-N9-C4	6.94	109.17	106.40
1	A	785	G	C6-C5-N7	-6.94	126.24	130.40
1	A	30	U	C5-C6-N1	-6.93	119.23	122.70
1	A	769	G	C6-C5-N7	-6.93	126.24	130.40
1	A	117	G	C5-C6-O6	-6.93	124.44	128.60
1	A	705	U	N1-C2-O2	-6.93	117.95	122.80
1	A	1084	G	C5-C6-O6	6.93	132.76	128.60
1	A	874	G	N1-C2-N3	6.92	128.05	123.90
1	A	627	G	C5-C6-O6	-6.92	124.45	128.60
1	A	867	G	N1-C6-O6	6.92	124.05	119.90
1	A	262	A	C8-N9-C4	-6.92	103.03	105.80
1	A	754	C	N3-C4-C5	6.92	124.67	121.90
1	A	948	C	N3-C4-C5	6.92	124.67	121.90
1	A	1082	G	N9-C4-C5	-6.92	102.63	105.40
1	A	511	C	N3-C4-C5	6.91	124.67	121.90
1	A	1189	C	C2-N1-C1'	-6.91	111.20	118.80
1	A	296	U	C5-C6-N1	-6.91	119.25	122.70
1	A	704	A	C2-N3-C4	-6.91	107.15	110.60
1	A	777	A	C5-C6-N6	-6.91	118.17	123.70
1	A	627	G	C4-C5-N7	6.91	113.56	110.80
1	A	656	C	C4-C5-C6	6.91	120.85	117.40
1	A	1236	A	C4-C5-C6	-6.91	113.55	117.00
1	A	885	G	C5-N7-C8	-6.90	100.85	104.30
1	A	1331	G	C5-N7-C8	6.90	107.75	104.30
1	A	190(D)	U	C5-C4-O4	6.90	130.04	125.90
1	A	251	G	C8-N9-C1'	-6.90	118.03	127.00
1	A	1339	A	C5-C6-N1	6.89	121.15	117.70
1	A	1088	G	C5-C6-O6	-6.89	124.47	128.60
1	A	1531	A	C5-N7-C8	-6.89	100.45	103.90
1	A	1064	G	C5-C6-O6	-6.89	124.47	128.60
1	A	1064	G	C8-N9-C1'	-6.89	118.05	127.00
1	A	766	A	C5-N7-C8	-6.88	100.46	103.90
1	A	1447	G	C5-C6-O6	-6.88	124.47	128.60
1	A	1532	U	C5-C6-N1	6.88	126.14	122.70
1	A	945	G	C5-C6-O6	-6.88	124.47	128.60
1	A	565	U	C5-C4-O4	-6.87	121.78	125.90
1	A	898	G	C8-N9-C4	6.87	109.15	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	517	G	C4-C5-N7	-6.87	108.05	110.80
1	A	1344	C	C5-C6-N1	-6.87	117.57	121.00
1	A	1486	G	N1-C6-O6	6.86	124.02	119.90
1	A	260	G	N3-C2-N2	-6.86	115.10	119.90
1	A	760	G	C2-N3-C4	-6.86	108.47	111.90
1	A	1233	G	C8-N9-C4	6.86	109.14	106.40
1	A	373	A	N7-C8-N9	6.86	117.23	113.80
1	A	66	G	C4-C5-N7	6.85	113.54	110.80
1	A	109	A	C5-N7-C8	-6.85	100.47	103.90
1	A	240	C	N3-C4-N4	6.85	122.80	118.00
1	A	759	A	C2-N3-C4	-6.85	107.17	110.60
1	A	1240	U	N1-C2-N3	6.85	119.01	114.90
1	A	1077	G	C5-C6-N1	-6.85	108.07	111.50
1	A	1512	U	N1-C2-N3	6.85	119.01	114.90
1	A	190(G)	G	C6-C5-N7	-6.85	126.29	130.40
1	A	1281	U	C5-C6-N1	6.85	126.12	122.70
1	A	357	G	C8-N9-C4	6.84	109.14	106.40
1	A	879	C	C5-C4-N4	-6.84	115.41	120.20
1	A	167	G	N9-C4-C5	6.84	108.14	105.40
17	Q	21	VAL	CB-CA-C	-6.84	98.41	111.40
1	A	705	U	C6-N1-C1'	6.83	130.77	121.20
1	A	574	A	N7-C8-N9	-6.83	110.38	113.80
1	A	771	G	C2-N3-C4	-6.83	108.48	111.90
1	A	376	G	N1-C6-O6	6.83	124.00	119.90
1	A	1338	G	C8-N9-C4	-6.83	103.67	106.40
1	A	1416	G	C2-N3-C4	-6.83	108.48	111.90
1	A	1505	G	N1-C6-O6	6.83	124.00	119.90
1	A	277	C	C5-C6-N1	-6.83	117.59	121.00
1	A	1099	G	N3-C4-N9	-6.83	121.91	126.00
1	A	129(A)	G	N3-C4-N9	6.82	130.09	126.00
1	A	1064	G	N9-C4-C5	-6.82	102.67	105.40
1	A	90	U	N3-C4-C5	-6.82	110.51	114.60
1	A	357	G	N1-C6-O6	6.82	123.99	119.90
1	A	377	G	C2-N3-C4	-6.82	108.49	111.90
1	A	521	G	C6-C5-N7	6.82	134.49	130.40
1	A	1494	G	C6-C5-N7	-6.82	126.31	130.40
1	A	839	U	N1-C2-O2	6.82	127.57	122.80
1	A	707	C	C5-C6-N1	-6.82	117.59	121.00
1	A	790	A	C8-N9-C4	-6.82	103.07	105.80
1	A	319	G	N3-C4-N9	6.81	130.09	126.00
1	A	637	G	C8-N9-C1'	-6.81	118.14	127.00
1	A	27	G	C8-N9-C1'	-6.81	118.14	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1530	G	N9-C4-C5	-6.81	102.67	105.40
17	Q	98	LEU	CA-CB-CG	6.81	130.97	115.30
1	A	833	U	N1-C2-N3	6.81	118.99	114.90
1	A	373	A	N1-C2-N3	6.81	132.70	129.30
1	A	634	C	C6-N1-C2	-6.80	117.58	120.30
1	A	46	G	N3-C4-C5	-6.80	125.20	128.60
1	A	628	G	N3-C4-C5	-6.80	125.20	128.60
1	A	746	A	N9-C4-C5	-6.80	103.08	105.80
1	A	1340	A	C2-N3-C4	-6.80	107.20	110.60
1	A	568	G	C6-N1-C2	-6.79	121.03	125.10
1	A	366	C	N1-C2-O2	6.79	122.97	118.90
1	A	862	C	C5-C4-N4	-6.79	115.45	120.20
1	A	123	C	N1-C2-N3	6.78	123.95	119.20
1	A	229	U	C6-N1-C2	-6.78	116.93	121.00
1	A	944	G	N1-C2-N2	-6.78	110.10	116.20
1	A	336	C	N3-C2-O2	6.78	126.64	121.90
1	A	1335	C	C6-N1-C1'	6.78	128.94	120.80
1	A	404	U	N1-C2-O2	-6.78	118.06	122.80
1	A	259	G	N7-C8-N9	6.77	116.49	113.10
1	A	760	G	N3-C4-C5	6.77	131.99	128.60
1	A	230	G	N1-C6-O6	6.77	123.96	119.90
1	A	780	A	N1-C6-N6	-6.77	114.54	118.60
1	A	262	A	N1-C6-N6	-6.77	114.54	118.60
1	A	1099	G	N1-C6-O6	6.77	123.96	119.90
1	A	606	G	C4-C5-N7	-6.76	108.10	110.80
1	A	1264	C	C6-N1-C2	-6.75	117.60	120.30
1	A	1182	G	C4-C5-N7	6.75	113.50	110.80
1	A	1087	G	C4-C5-N7	6.75	113.50	110.80
1	A	255	G	C5-C6-O6	-6.75	124.55	128.60
1	A	541	G	N3-C2-N2	-6.75	115.18	119.90
1	A	553	A	C5-C6-N1	6.75	121.07	117.70
1	A	794	A	N3-C4-C5	-6.75	122.08	126.80
1	A	761	G	N1-C6-O6	6.75	123.95	119.90
1	A	814	A	N1-C2-N3	6.75	132.67	129.30
1	A	265	G	C2-N3-C4	-6.75	108.53	111.90
1	A	832	C	C5-C4-N4	-6.75	115.48	120.20
1	A	1403	C	C4-C5-C6	-6.75	114.03	117.40
1	A	1443	G	N9-C4-C5	-6.74	102.70	105.40
1	A	930	C	N3-C2-O2	-6.74	117.19	121.90
1	A	1060	C	C2-N1-C1'	6.73	126.21	118.80
1	A	129(A)	G	C8-N9-C4	6.73	109.09	106.40
1	A	1539	C	N3-C4-C5	6.73	124.59	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	Q	22	LEU	CA-CB-CG	-6.73	99.82	115.30
1	A	260	G	C5-C6-N1	-6.73	108.14	111.50
1	A	753	A	C2-N3-C4	-6.72	107.24	110.60
1	A	1084	G	C2-N3-C4	6.72	115.26	111.90
1	A	1233	G	N7-C8-N9	-6.72	109.74	113.10
1	A	559	A	C4-C5-C6	6.72	120.36	117.00
1	A	878	G	N1-C2-N2	-6.72	110.15	116.20
1	A	1157	A	C5-C6-N6	6.72	129.08	123.70
1	A	277	C	N3-C4-C5	6.72	124.59	121.90
1	A	906	G	C4-C5-N7	6.72	113.49	110.80
1	A	144	G	C5-N7-C8	-6.72	100.94	104.30
1	A	27	G	N1-C2-N3	6.71	127.93	123.90
1	A	484	G	N3-C4-N9	6.71	130.03	126.00
1	A	236	G	C8-N9-C1'	-6.71	118.28	127.00
1	A	144	G	C5-C6-O6	-6.71	124.58	128.60
1	A	1370	G	C8-N9-C1'	-6.71	118.28	127.00
1	A	243	A	P-O3'-C3'	6.70	127.75	119.70
1	A	1108	G	N3-C4-C5	-6.70	125.25	128.60
1	A	1482	G	N1-C2-N2	-6.70	110.17	116.20
1	A	1544	U	N3-C2-O2	6.70	126.89	122.20
1	A	833	U	C5-C6-N1	-6.70	119.35	122.70
1	A	649	G	C5-C6-O6	-6.70	124.58	128.60
1	A	725	G	C5-N7-C8	-6.70	100.95	104.30
1	A	244	U	C6-N1-C2	6.70	125.02	121.00
1	A	634	C	N3-C4-C5	-6.69	119.22	121.90
1	A	113	G	C4-N9-C1'	6.69	135.20	126.50
1	A	786	G	C4-C5-N7	6.69	113.48	110.80
1	A	1051	C	N3-C4-C5	-6.69	119.22	121.90
1	A	577	G	C2-N3-C4	-6.69	108.56	111.90
1	A	269	C	N1-C2-N3	6.68	123.88	119.20
1	A	575	G	C5-C6-N1	6.68	114.84	111.50
1	A	705	U	N3-C4-C5	-6.68	110.59	114.60
1	A	876	G	C6-N1-C2	-6.68	121.09	125.10
1	A	928	G	N9-C4-C5	-6.68	102.73	105.40
1	A	309	G	N1-C2-N2	-6.68	110.19	116.20
1	A	631	G	N7-C8-N9	6.68	116.44	113.10
1	A	703	G	N3-C4-C5	-6.68	125.26	128.60
1	A	1047	G	N3-C4-C5	-6.68	125.26	128.60
1	A	1419	G	C5-C6-N1	-6.68	108.16	111.50
1	A	278	G	N7-C8-N9	6.68	116.44	113.10
1	A	62	U	N1-C2-O2	6.67	127.47	122.80
1	A	380	G	C5-C6-N1	-6.67	108.16	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	612	C	N1-C2-O2	6.67	122.91	118.90
1	A	634	C	N1-C2-N3	6.67	123.87	119.20
1	A	384	G	C6-N1-C2	-6.67	121.10	125.10
1	A	1505	G	C5-N7-C8	-6.67	100.96	104.30
1	A	47	C	C2-N1-C1'	6.67	126.13	118.80
1	A	1370	G	C6-C5-N7	-6.67	126.40	130.40
1	A	78	G	N9-C4-C5	-6.67	102.73	105.40
1	A	256	U	C5-C4-O4	-6.67	121.90	125.90
1	A	307	C	N1-C2-O2	6.67	122.90	118.90
1	A	75	G	N3-C4-C5	-6.66	125.27	128.60
1	A	572	A	N9-C4-C5	6.66	108.47	105.80
1	A	1079	G	C4-C5-C6	6.66	122.80	118.80
1	A	521	G	N1-C6-O6	-6.66	115.90	119.90
1	A	27	G	C4-N9-C1'	6.66	135.16	126.50
1	A	1126	U	C6-N1-C2	-6.66	117.01	121.00
1	A	1200	C	C4-C5-C6	-6.65	114.07	117.40
1	A	358	U	N1-C2-N3	6.65	118.89	114.90
1	A	867	G	C4-C5-N7	6.65	113.46	110.80
1	A	1329	A	N1-C6-N6	6.65	122.59	118.60
1	A	1482	G	C4-N9-C1'	6.65	135.14	126.50
1	A	93	G	N3-C2-N2	6.64	124.55	119.90
1	A	1394	A	N7-C8-N9	-6.64	110.48	113.80
1	A	260	G	N7-C8-N9	6.63	116.42	113.10
1	A	562	C	C4-C5-C6	6.63	120.72	117.40
1	A	30	U	C2-N3-C4	-6.62	123.03	127.00
1	A	93	G	N1-C2-N2	-6.62	110.24	116.20
1	A	563	A	C4-N9-C1'	6.62	138.22	126.30
1	A	722	A	C4-C5-N7	6.62	114.01	110.70
1	A	588	G	C8-N9-C1'	-6.62	118.40	127.00
1	A	700	G	N3-C4-C5	-6.62	125.29	128.60
1	A	263	A	C5-C6-N1	6.62	121.01	117.70
1	A	673	G	C8-N9-C1'	-6.62	118.40	127.00
1	A	1532	U	C4-C5-C6	-6.61	115.73	119.70
1	A	257	G	N3-C4-N9	6.61	129.97	126.00
1	A	416	G	C4-C5-N7	6.61	113.44	110.80
1	A	474	G	C4-C5-N7	6.61	113.44	110.80
1	A	1291	G	C8-N9-C1'	-6.61	118.41	127.00
1	A	1285	A	C5-N7-C8	-6.61	100.60	103.90
1	A	725	G	C6-C5-N7	-6.60	126.44	130.40
1	A	1323	G	N1-C6-O6	6.60	123.86	119.90
1	A	1116	C	C6-N1-C2	6.60	122.94	120.30
1	A	416	G	N3-C4-C5	6.60	131.90	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	770	C	C2-N3-C4	-6.60	116.60	119.90
1	A	27	G	N3-C4-C5	-6.59	125.30	128.60
1	A	765	G	N3-C4-C5	6.59	131.90	128.60
1	A	922	G	C8-N9-C4	-6.59	103.76	106.40
1	A	235	C	C5-C6-N1	-6.59	117.70	121.00
1	A	731	G	N9-C4-C5	-6.59	102.76	105.40
1	A	250	A	C5-C6-N1	-6.59	114.41	117.70
1	A	1529	G	N3-C2-N2	-6.59	115.29	119.90
1	A	1526	G	C4-C5-C6	6.59	122.75	118.80
1	A	723	U	C6-N1-C2	-6.58	117.05	121.00
1	A	771	G	C8-N9-C4	6.58	109.03	106.40
1	A	944	G	N9-C4-C5	6.58	108.03	105.40
1	A	971	G	N9-C4-C5	-6.58	102.77	105.40
1	A	1331	G	N9-C4-C5	6.58	108.03	105.40
1	A	232	G	N3-C4-N9	6.57	129.94	126.00
1	A	251	G	C5-C6-O6	-6.57	124.66	128.60
1	A	837	G	C8-N9-C4	6.57	109.03	106.40
1	A	1387	G	N1-C2-N2	-6.57	110.28	116.20
1	A	234	C	C2-N3-C4	-6.57	116.61	119.90
1	A	500	G	C5-C6-O6	-6.57	124.66	128.60
1	A	201	C	C2-N1-C1'	6.57	126.02	118.80
1	A	314	C	N3-C4-N4	-6.57	113.40	118.00
1	A	1403	C	N1-C2-N3	-6.57	114.60	119.20
1	A	1489	G	C8-N9-C4	-6.56	103.78	106.40
1	A	119	A	C5-C6-N6	6.55	128.94	123.70
1	A	928	G	N3-C4-C5	6.55	131.88	128.60
1	A	1394	A	N3-C4-C5	6.55	131.39	126.80
1	A	730	G	C5-C6-N1	-6.55	108.22	111.50
1	A	906	G	C5-C6-O6	-6.55	124.67	128.60
1	A	740	U	N1-C2-N3	6.55	118.83	114.90
1	A	119	A	C4-C5-N7	-6.55	107.43	110.70
1	A	456	C	N3-C2-O2	-6.54	117.32	121.90
1	A	1231	G	N9-C4-C5	-6.54	102.78	105.40
1	A	38	G	C4-N9-C1'	-6.54	118.00	126.50
1	A	785	G	N1-C6-O6	6.54	123.82	119.90
1	A	1194	U	C6-N1-C2	-6.54	117.08	121.00
1	A	906	G	N1-C6-O6	6.54	123.82	119.90
1	A	190(F)	G	C4-N9-C1'	-6.54	118.00	126.50
1	A	1502	A	N9-C4-C5	-6.54	103.19	105.80
1	A	281	G	N1-C6-O6	6.53	123.82	119.90
1	A	995	C	C5-C6-N1	6.53	124.27	121.00
1	A	1333	A	N7-C8-N9	6.53	117.07	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	900	A	C5-N7-C8	-6.53	100.63	103.90
1	A	1086	U	C5-C6-N1	6.53	125.97	122.70
1	A	518	C	N1-C2-O2	6.53	122.82	118.90
1	A	121	C	C5-C6-N1	-6.53	117.73	121.00
1	A	602	A	N1-C2-N3	6.53	132.56	129.30
1	A	778	G	N1-C2-N3	6.53	127.81	123.90
1	A	1187	G	N1-C6-O6	6.53	123.81	119.90
4	D	30	LYS	N-CA-C	6.53	128.62	111.00
1	A	765	G	N1-C6-O6	6.52	123.81	119.90
1	A	509	A	C3'-C2'-C1'	-6.52	96.28	101.50
1	A	1491	G	N3-C4-N9	6.52	129.91	126.00
1	A	382	A	C8-N9-C4	-6.51	103.20	105.80
1	A	117	G	N9-C4-C5	-6.51	102.80	105.40
1	A	628	G	C4-N9-C1'	6.51	134.96	126.50
1	A	919	A	C2-N3-C4	6.51	113.85	110.60
1	A	324	G	N9-C4-C5	6.50	108.00	105.40
1	A	584	G	C5-C6-O6	-6.50	124.70	128.60
1	A	1155	G	C6-C5-N7	-6.50	126.50	130.40
1	A	1512	U	N3-C4-C5	-6.50	110.70	114.60
1	A	666	G	C5-C6-N1	-6.50	108.25	111.50
1	A	1192	C	N1-C2-N3	6.50	123.75	119.20
1	A	815	A	N7-C8-N9	-6.49	110.55	113.80
1	A	1502	A	N3-C4-C5	6.49	131.35	126.80
1	A	130	A	C8-N9-C1'	-6.49	116.02	127.70
1	A	1078	U	C5-C6-N1	6.49	125.95	122.70
1	A	1482	G	N1-C6-O6	-6.49	116.01	119.90
1	A	557	G	C4-C5-C6	6.49	122.69	118.80
1	A	705	U	N1-C2-N3	6.49	118.79	114.90
1	A	1492	A	C8-N9-C4	-6.49	103.20	105.80
1	A	236	G	N1-C6-O6	-6.49	116.01	119.90
1	A	309	G	C8-N9-C1'	-6.48	118.57	127.00
1	A	877	C	C4-C5-C6	6.48	120.64	117.40
1	A	460	A	C8-N9-C4	-6.48	103.21	105.80
1	A	360	A	N7-C8-N9	6.47	117.04	113.80
1	A	1157	A	N1-C6-N6	-6.47	114.72	118.60
1	A	572	A	C4-C5-N7	-6.47	107.46	110.70
8	H	112	LEU	CA-CB-CG	-6.47	100.41	115.30
1	A	579	G	C4-C5-N7	6.47	113.39	110.80
1	A	53	A	N1-C2-N3	6.47	132.53	129.30
1	A	560	U	N3-C4-C5	-6.47	110.72	114.60
1	A	666	G	N1-C2-N3	6.47	127.78	123.90
1	A	805	C	N3-C4-C5	6.47	124.49	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	798	G	N1-C2-N3	6.46	127.78	123.90
1	A	1300	G	P-O3'-C3'	6.46	127.46	119.70
1	A	292	G	N9-C4-C5	-6.46	102.81	105.40
1	A	1377	A	C6-C5-N7	6.46	136.82	132.30
1	A	796	C	C2-N3-C4	-6.46	116.67	119.90
1	A	1398	A	C6-N1-C2	-6.46	114.72	118.60
1	A	17	U	N3-C4-C5	6.46	118.47	114.60
1	A	59	A	C4-C5-N7	6.46	113.93	110.70
1	A	766	A	N1-C6-N6	6.46	122.48	118.60
1	A	1310	G	C4-N9-C1'	6.46	134.90	126.50
1	A	1223	C	C6-N1-C2	-6.46	117.72	120.30
1	A	99	C	C5-C6-N1	6.45	124.23	121.00
1	A	589	C	N3-C4-N4	-6.45	113.48	118.00
1	A	1416	G	N1-C6-O6	6.45	123.77	119.90
1	A	569	C	C2-N1-C1'	-6.45	111.71	118.80
1	A	1266	G	N3-C4-C5	6.45	131.82	128.60
1	A	1080	A	C5-N7-C8	6.44	107.12	103.90
1	A	1285	A	N7-C8-N9	6.44	117.02	113.80
1	A	1192	C	N1-C2-O2	-6.44	115.04	118.90
1	A	1077	G	C6-C5-N7	-6.44	126.54	130.40
1	A	632	A	C5-N7-C8	-6.44	100.68	103.90
1	A	638	G	N3-C4-N9	6.44	129.86	126.00
1	A	1310	G	C5-C6-N1	-6.44	108.28	111.50
1	A	1341	U	C2-N1-C1'	-6.44	109.98	117.70
1	A	1383	C	N3-C4-N4	6.44	122.51	118.00
1	A	190(I)	G	N7-C8-N9	-6.43	109.88	113.10
1	A	774	G	C6-C5-N7	-6.43	126.54	130.40
1	A	822	C	C4-C5-C6	6.43	120.61	117.40
1	A	1078	U	C6-N1-C2	-6.43	117.14	121.00
1	A	916	G	C8-N9-C1'	-6.43	118.64	127.00
1	A	482	A	C6-C5-N7	-6.42	127.80	132.30
1	A	721	G	C8-N9-C1'	-6.42	118.65	127.00
1	A	1469	G	C6-C5-N7	-6.42	126.55	130.40
1	A	707	C	N3-C4-C5	6.42	124.47	121.90
1	A	1135	U	C2-N1-C1'	6.42	125.41	117.70
1	A	1312	G	C4-C5-N7	6.41	113.36	110.80
1	A	1203	C	C2-N1-C1'	6.41	125.85	118.80
1	A	1346	A	P-O3'-C3'	6.41	127.39	119.70
1	A	1212	U	C2-N1-C1'	6.40	125.38	117.70
1	A	1335	C	C2-N1-C1'	-6.40	111.76	118.80
1	A	833	U	C5-C4-O4	6.40	129.74	125.90
1	A	249	U	C5-C4-O4	6.40	129.74	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	876	G	C5-C6-O6	-6.40	124.76	128.60
1	A	860	A	C5-N7-C8	-6.39	100.70	103.90
1	A	156	G	N1-C6-O6	6.39	123.73	119.90
1	A	995	C	N1-C2-O2	6.39	122.73	118.90
1	A	348	G	N1-C6-O6	6.39	123.73	119.90
1	A	1512	U	C6-N1-C2	-6.39	117.17	121.00
1	A	7	G	C5-C6-N1	6.38	114.69	111.50
1	A	1514	C	N3-C4-C5	6.38	124.45	121.90
1	A	123	C	C6-N1-C2	-6.38	117.75	120.30
1	A	879	C	N3-C4-C5	6.38	124.45	121.90
1	A	190(F)	G	C8-N9-C1'	6.38	135.29	127.00
1	A	734	G	N9-C4-C5	-6.37	102.85	105.40
1	A	276	G	N1-C6-O6	6.37	123.72	119.90
1	A	795	C	C4-C5-C6	-6.37	114.22	117.40
1	A	878	G	C6-N1-C2	-6.37	121.28	125.10
1	A	1354	C	N3-C4-C5	6.37	124.45	121.90
1	A	888	G	C4-C5-N7	-6.37	108.25	110.80
1	A	32	A	N1-C2-N3	6.37	132.48	129.30
1	A	275	G	N1-C6-O6	6.37	123.72	119.90
1	A	1282	C	N3-C4-C5	-6.36	119.35	121.90
1	A	1079	G	N3-C4-N9	6.36	129.81	126.00
1	A	812	C	C5-C4-N4	6.36	124.65	120.20
1	A	130	A	C2-N3-C4	-6.36	107.42	110.60
1	A	551	U	C2-N1-C1'	6.36	125.33	117.70
1	A	595	G	N3-C4-C5	-6.36	125.42	128.60
1	A	1238	A	N9-C4-C5	6.36	108.34	105.80
1	A	1099	G	C2-N3-C4	-6.35	108.72	111.90
1	A	53	A	N1-C6-N6	-6.35	114.79	118.60
1	A	1531	A	C4-C5-N7	6.35	113.88	110.70
1	A	199	G	C6-C5-N7	-6.35	126.59	130.40
1	A	373	A	C8-N9-C4	-6.35	103.26	105.80
1	A	706	A	C8-N9-C4	6.35	108.34	105.80
1	A	558	G	N1-C6-O6	6.35	123.71	119.90
1	A	973	G	C8-N9-C1'	-6.35	118.75	127.00
1	A	1502	A	C4-N9-C1'	6.35	137.72	126.30
1	A	821	G	C6-C5-N7	-6.34	126.59	130.40
1	A	832	C	N1-C2-O2	-6.34	115.09	118.90
1	A	328	C	P-O3'-C3'	6.34	127.31	119.70
1	A	329	A	C5-N7-C8	-6.34	100.73	103.90
1	A	556	C	N3-C4-N4	-6.34	113.56	118.00
1	A	676	A	C8-N9-C4	6.34	108.34	105.80
1	A	1112	C	C6-N1-C2	6.34	122.84	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	404	U	N3-C2-O2	6.34	126.64	122.20
1	A	818	G	N1-C6-O6	6.34	123.70	119.90
1	A	1398	A	N1-C6-N6	-6.34	114.80	118.60
1	A	300	A	N7-C8-N9	6.34	116.97	113.80
1	A	1079	G	C8-N9-C4	-6.33	103.87	106.40
1	A	815	A	C5-N7-C8	6.33	107.07	103.90
1	A	30	U	N3-C4-O4	-6.33	114.97	119.40
1	A	1543	C	C5-C4-N4	-6.33	115.77	120.20
1	A	350	G	N7-C8-N9	6.33	116.27	113.10
1	A	1088	G	C4-C5-C6	6.32	122.59	118.80
1	A	319	G	C4-C5-N7	6.32	113.33	110.80
1	A	1481	U	C5-C4-O4	6.32	129.69	125.90
1	A	103	C	C4-C5-C6	6.32	120.56	117.40
1	A	872	A	C6-C5-N7	-6.32	127.88	132.30
1	A	926	G	C6-C5-N7	-6.32	126.61	130.40
1	A	1087	G	C5-C6-O6	-6.32	124.81	128.60
1	A	1106	G	C2-N3-C4	-6.32	108.74	111.90
1	A	877	C	C2-N3-C4	-6.31	116.75	119.90
1	A	51	A	C5-N7-C8	-6.31	100.75	103.90
1	A	93	G	C8-N9-C1'	-6.31	118.80	127.00
1	A	1411	C	C6-N1-C2	-6.31	117.78	120.30
1	A	345	C	C6-N1-C2	-6.31	117.78	120.30
1	A	1219	U	N3-C2-O2	-6.31	117.79	122.20
1	A	1505	G	C4-N9-C1'	6.31	134.70	126.50
1	A	130	A	N1-C2-N3	6.30	132.45	129.30
1	A	795	C	C6-N1-C2	6.30	122.82	120.30
1	A	918	A	N7-C8-N9	-6.30	110.65	113.80
1	A	700	G	N3-C4-N9	6.30	129.78	126.00
1	A	1030	C	C6-N1-C2	-6.30	117.78	120.30
1	A	141	A	C5-N7-C8	-6.30	100.75	103.90
1	A	511	C	C6-N1-C1'	6.30	128.36	120.80
1	A	1346	A	C6-N1-C2	-6.30	114.82	118.60
1	A	88	A	C2-N3-C4	6.29	113.75	110.60
1	A	1403	C	N3-C4-C5	6.29	124.42	121.90
1	A	245	C	C6-N1-C1'	6.29	128.35	120.80
1	A	766	A	C4-C5-N7	6.29	113.84	110.70
1	A	1166	G	C8-N9-C4	-6.29	103.88	106.40
1	A	1408	A	C4-C5-N7	6.29	113.84	110.70
1	A	322	C	N3-C2-O2	6.29	126.30	121.90
1	A	385	C	N3-C2-O2	-6.29	117.50	121.90
1	A	384	G	C8-N9-C1'	-6.29	118.83	127.00
1	A	1436	U	C2-N1-C1'	6.29	125.24	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	178	C	N1-C2-O2	6.28	122.67	118.90
1	A	625	G	C8-N9-C4	-6.28	103.89	106.40
1	A	22	G	N3-C2-N2	6.28	124.30	119.90
1	A	284	G	C4-C5-C6	6.28	122.57	118.80
1	A	838	G	C8-N9-C4	6.28	108.91	106.40
1	A	1508	G	N3-C4-C5	-6.28	125.46	128.60
1	A	708	C	N3-C4-N4	-6.28	113.61	118.00
1	A	865	A	N1-C6-N6	-6.28	114.83	118.60
1	A	1231	G	N3-C4-C5	6.28	131.74	128.60
1	A	122	G	N3-C4-C5	6.27	131.74	128.60
1	A	790	A	N7-C8-N9	6.27	116.94	113.80
1	A	258	G	N1-C6-O6	6.27	123.66	119.90
1	A	1080	A	C4-C5-N7	-6.27	107.57	110.70
1	A	1331	G	C5-C6-O6	6.27	132.36	128.60
1	A	113	G	N9-C4-C5	-6.27	102.89	105.40
1	A	232	G	C5-N7-C8	-6.27	101.17	104.30
1	A	29	G	C4-C5-N7	-6.27	108.29	110.80
1	A	367	U	C5-C4-O4	-6.27	122.14	125.90
1	A	451	A	C8-N9-C4	6.26	108.31	105.80
1	A	1358	U	C6-N1-C2	-6.26	117.24	121.00
1	A	1520	G	C5-C6-O6	-6.26	124.84	128.60
1	A	703	G	C5-N7-C8	6.26	107.43	104.30
1	A	789	U	C5-C6-N1	6.26	125.83	122.70
1	A	1513	A	N3-C4-C5	6.26	131.18	126.80
1	A	247	G	N3-C2-N2	-6.26	115.52	119.90
1	A	759	A	N1-C6-N6	6.26	122.35	118.60
1	A	1499	A	C6-C5-N7	-6.25	127.92	132.30
1	A	96	G	N1-C6-O6	6.25	123.65	119.90
1	A	363	A	C2-N3-C4	-6.25	107.47	110.60
1	A	1023	G	N3-C4-N9	6.25	129.75	126.00
1	A	301	G	C4-C5-C6	6.25	122.55	118.80
1	A	394	G	C5-C6-N1	-6.25	108.38	111.50
1	A	179	A	N1-C2-N3	6.25	132.42	129.30
1	A	384	G	C5-N7-C8	6.25	107.42	104.30
1	A	125	U	C5-C6-N1	-6.24	119.58	122.70
1	A	1023	G	N3-C4-C5	-6.24	125.48	128.60
1	A	1088	G	C4-C5-N7	6.24	113.30	110.80
1	A	1089	G	N3-C4-C5	-6.24	125.48	128.60
1	A	673	G	N1-C2-N3	6.24	127.64	123.90
1	A	743	U	C5-C4-O4	6.24	129.64	125.90
1	A	1530	G	C4-N9-C1'	-6.24	118.39	126.50
1	A	859	A	C6-N1-C2	-6.24	114.86	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1516	G	N3-C4-C5	6.24	131.72	128.60
1	A	146	G	C5-C6-N1	-6.23	108.38	111.50
1	A	301	G	C6-C5-N7	-6.23	126.66	130.40
1	A	886	G	C2-N3-C4	-6.23	108.78	111.90
1	A	1348	U	C6-N1-C1'	-6.23	112.48	121.20
1	A	1524	C	N1-C2-N3	6.23	123.56	119.20
1	A	78	G	C5-C6-O6	-6.23	124.86	128.60
1	A	300	A	C8-N9-C4	-6.23	103.31	105.80
1	A	818	G	C8-N9-C4	-6.23	103.91	106.40
1	A	928	G	C8-N9-C4	6.23	108.89	106.40
1	A	852	G	C4-C5-C6	6.22	122.53	118.80
1	A	941	G	N3-C4-C5	6.22	131.71	128.60
1	A	1082	G	C6-C5-N7	-6.22	126.67	130.40
1	A	1193	G	N1-C6-O6	6.22	123.64	119.90
1	A	144	G	N3-C4-C5	6.22	131.71	128.60
1	A	46	G	C4-C5-C6	6.21	122.53	118.80
1	A	336	C	C5-C4-N4	-6.21	115.85	120.20
1	A	900	A	C8-N9-C4	-6.21	103.31	105.80
1	A	926	G	N3-C2-N2	6.21	124.25	119.90
1	A	852	G	C6-C5-N7	-6.21	126.67	130.40
1	A	568	G	N1-C2-N3	6.21	127.63	123.90
1	A	1132	C	C6-N1-C2	-6.21	117.82	120.30
1	A	1393	U	C4-C5-C6	6.21	123.42	119.70
1	A	735	C	C5-C6-N1	-6.20	117.90	121.00
1	A	265	G	N1-C2-N2	-6.20	110.62	116.20
1	A	719	C	N1-C2-O2	6.20	122.62	118.90
1	A	909	A	C6-N1-C2	-6.20	114.88	118.60
1	A	989	C	N3-C4-C5	-6.20	119.42	121.90
1	A	80	G	C4-N9-C1'	6.20	134.55	126.50
1	A	360	A	C8-N9-C4	-6.20	103.32	105.80
1	A	59	A	C4-C5-C6	-6.19	113.90	117.00
1	A	813	U	N1-C2-N3	6.19	118.62	114.90
1	A	393	A	C2-N3-C4	-6.19	107.50	110.60
1	A	511	C	C5-C6-N1	-6.19	117.91	121.00
1	A	1539	C	N1-C2-O2	6.19	122.61	118.90
1	A	786	G	C2-N3-C4	-6.19	108.81	111.90
1	A	1375	A	C5-N7-C8	6.19	106.99	103.90
1	A	632	A	C2-N3-C4	-6.19	107.51	110.60
1	A	1186	G	C5-C6-N1	-6.19	108.41	111.50
1	A	1386	G	N7-C8-N9	-6.19	110.01	113.10
1	A	821	G	N9-C4-C5	-6.19	102.93	105.40
1	A	567	G	N3-C4-C5	-6.18	125.51	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1401	G	C6-C5-N7	-6.18	126.69	130.40
1	A	669	U	C5-C6-N1	-6.18	119.61	122.70
1	A	1293	G	C8-N9-C4	-6.18	103.93	106.40
1	A	774	G	N9-C4-C5	-6.18	102.93	105.40
1	A	595	G	C4-N9-C1'	6.18	134.53	126.50
1	A	381	C	N1-C2-O2	6.18	122.61	118.90
1	A	240	C	N1-C2-O2	-6.17	115.20	118.90
1	A	643	C	N3-C4-N4	6.17	122.32	118.00
17	Q	31	LEU	CA-CB-CG	-6.17	101.11	115.30
1	A	878	G	C2-N3-C4	-6.17	108.82	111.90
1	A	66	G	N3-C4-C5	6.17	131.68	128.60
1	A	874	G	N7-C8-N9	-6.17	110.02	113.10
1	A	241	C	C2-N3-C4	-6.17	116.82	119.90
1	A	856	C	N3-C4-C5	-6.17	119.43	121.90
1	A	1499	A	C4-C5-C6	6.17	120.08	117.00
1	A	144	G	N1-C2-N2	6.16	121.75	116.20
1	A	245	C	C2-N1-C1'	-6.16	112.02	118.80
1	A	605	U	N1-C2-N3	6.16	118.60	114.90
1	A	932	C	C6-N1-C2	-6.16	117.83	120.30
1	A	88	A	C4-C5-N7	-6.16	107.62	110.70
1	A	797	C	C5-C6-N1	-6.16	117.92	121.00
1	A	1132	C	C5-C6-N1	6.16	124.08	121.00
1	A	945	G	C4-C5-N7	6.15	113.26	110.80
1	A	1228	C	C6-N1-C2	-6.15	117.84	120.30
1	A	638	G	C8-N9-C1'	-6.15	119.00	127.00
1	A	1107	C	C6-N1-C2	-6.15	117.84	120.30
1	A	1526	G	C8-N9-C1'	-6.15	119.01	127.00
1	A	1246	C	C6-N1-C2	6.15	122.76	120.30
1	A	1279	A	C4-C5-N7	6.15	113.77	110.70
1	A	41	G	C8-N9-C4	-6.15	103.94	106.40
1	A	117	G	C4-C5-N7	6.14	113.26	110.80
1	A	107	G	C6-C5-N7	-6.14	126.72	130.40
1	A	595	G	N3-C4-N9	6.14	129.68	126.00
1	A	661	G	C2-N3-C4	-6.14	108.83	111.90
1	A	685	G	C4-C5-N7	6.13	113.25	110.80
1	A	1187	G	C8-N9-C4	-6.13	103.95	106.40
1	A	1543	C	C6-N1-C1'	-6.13	113.44	120.80
1	A	908	A	C5-C6-N6	6.13	128.61	123.70
1	A	718	G	N1-C6-O6	6.13	123.58	119.90
1	A	164	U	C5-C4-O4	6.13	129.58	125.90
1	A	693	G	N9-C4-C5	-6.13	102.95	105.40
1	A	1227	A	N3-C4-C5	6.13	131.09	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	275	G	C8-N9-C4	6.12	108.85	106.40
1	A	904	C	N1-C2-N3	6.12	123.49	119.20
4	D	135	LEU	CB-CG-CD1	-6.12	100.59	111.00
1	A	633	G	N3-C4-C5	6.12	131.66	128.60
1	A	109	A	C6-C5-N7	-6.12	128.02	132.30
1	A	278	G	N9-C4-C5	6.12	107.85	105.40
1	A	1517	G	N7-C8-N9	6.12	116.16	113.10
1	A	676	A	N1-C6-N6	6.12	122.27	118.60
1	A	763	G	C8-N9-C4	6.12	108.85	106.40
1	A	1177	G	C8-N9-C4	-6.12	103.95	106.40
1	A	975	A	N1-C6-N6	6.11	122.27	118.60
1	A	108	G	N3-C2-N2	-6.11	115.62	119.90
1	A	793	U	N1-C2-O2	6.11	127.08	122.80
1	A	1378	C	C5-C6-N1	6.11	124.06	121.00
1	A	79	G	N7-C8-N9	6.11	116.15	113.10
1	A	90	U	C5-C6-N1	6.11	125.75	122.70
1	A	8	A	N1-C6-N6	-6.10	114.94	118.60
1	A	1527	C	N1-C2-O2	-6.10	115.24	118.90
1	A	573	A	N7-C8-N9	6.10	116.85	113.80
1	A	1250	A	N1-C6-N6	-6.10	114.94	118.60
1	A	147	G	C5-C6-N1	-6.10	108.45	111.50
1	A	368	U	N3-C4-O4	-6.10	115.13	119.40
1	A	693	G	C8-N9-C4	6.10	108.84	106.40
1	A	120	A	C2-N3-C4	-6.10	107.55	110.60
1	A	637	G	N3-C4-N9	6.10	129.66	126.00
1	A	1318	A	C8-N9-C4	6.10	108.24	105.80
1	A	608	A	C2-N3-C4	-6.09	107.55	110.60
1	A	1493	A	C2-N3-C4	6.09	113.65	110.60
1	A	671	G	N1-C6-O6	6.09	123.56	119.90
1	A	1069	C	N1-C2-N3	-6.09	114.94	119.20
1	A	1234	C	C5-C6-N1	6.09	124.05	121.00
1	A	416	G	C5-N7-C8	-6.09	101.25	104.30
1	A	1246	C	C2-N1-C1'	-6.09	112.10	118.80
1	A	1370	G	N3-C4-N9	6.09	129.66	126.00
1	A	1393	U	C5-C6-N1	-6.09	119.65	122.70
1	A	78	G	C5-C6-N1	6.09	114.54	111.50
1	A	200	G	C5-C6-N1	-6.09	108.46	111.50
1	A	401	C	N1-C2-N3	6.09	123.46	119.20
1	A	610	G	N7-C8-N9	6.09	116.14	113.10
1	A	1455	G	C2-N3-C4	-6.09	108.86	111.90
1	A	271	C	N1-C2-O2	-6.08	115.25	118.90
1	A	305	G	C8-N9-C4	-6.08	103.97	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1451	A	N1-C6-N6	6.08	122.25	118.60
1	A	1346	A	C4-C5-N7	-6.08	107.66	110.70
1	A	6	G	N1-C6-O6	6.08	123.55	119.90
1	A	851	G	C5-C6-O6	-6.08	124.95	128.60
1	A	903	G	N1-C2-N3	6.08	127.55	123.90
1	A	909	A	C5-C6-N6	-6.08	118.84	123.70
1	A	324	G	C5-C6-N1	-6.08	108.46	111.50
1	A	325	A	N1-C6-N6	-6.08	114.95	118.60
1	A	809	G	N9-C4-C5	6.08	107.83	105.40
1	A	628	G	C6-C5-N7	-6.07	126.76	130.40
1	A	1366	C	N3-C4-C5	6.07	124.33	121.90
1	A	885	G	C4-C5-N7	6.07	113.23	110.80
1	A	708	C	C2-N3-C4	-6.07	116.86	119.90
1	A	805	C	C6-N1-C2	6.07	122.73	120.30
1	A	673	G	C4-N9-C1'	6.07	134.39	126.50
1	A	722	A	C5-C6-N1	-6.07	114.67	117.70
1	A	1048	G	N3-C4-N9	-6.07	122.36	126.00
1	A	1264	C	C5-C6-N1	6.06	124.03	121.00
1	A	265	G	N9-C4-C5	-6.06	102.97	105.40
1	A	945	G	C4-C5-C6	-6.06	115.16	118.80
1	A	1305	G	C8-N9-C4	-6.06	103.97	106.40
1	A	1236	A	N1-C2-N3	-6.06	126.27	129.30
1	A	1442	G	N3-C2-N2	6.06	124.14	119.90
1	A	450	G	N7-C8-N9	-6.06	110.07	113.10
1	A	696	A	C8-N9-C4	6.06	108.22	105.80
1	A	1495	U	C5-C4-O4	-6.06	122.26	125.90
1	A	331	G	N1-C6-O6	6.06	123.53	119.90
1	A	1495	U	N3-C4-C5	6.06	118.23	114.60
1	A	276	G	C2-N3-C4	-6.06	108.87	111.90
1	A	532	A	C4-C5-C6	-6.05	113.97	117.00
1	A	647	C	C5-C6-N1	-6.05	117.97	121.00
1	A	228	A	C5-C6-N1	-6.05	114.67	117.70
1	A	1192	C	N3-C4-N4	6.05	122.24	118.00
1	A	1367	C	N3-C2-O2	-6.05	117.67	121.90
1	A	363	A	C5-N7-C8	-6.05	100.88	103.90
1	A	373	A	C5-C6-N1	-6.05	114.68	117.70
1	A	487	A	C8-N9-C4	6.05	108.22	105.80
1	A	909	A	C5-C6-N1	6.05	120.72	117.70
1	A	628	G	C4-C5-C6	6.04	122.43	118.80
1	A	628	G	C8-N9-C1'	-6.04	119.14	127.00
1	A	761	G	C5-C6-N1	-6.04	108.48	111.50
1	A	1083	U	N3-C4-C5	-6.04	110.97	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	230	G	C4-C5-C6	6.04	122.42	118.80
1	A	832	C	C6-N1-C2	6.04	122.72	120.30
1	A	328	C	C5-C6-N1	6.03	124.02	121.00
1	A	723	U	N1-C2-O2	6.03	127.02	122.80
1	A	799	G	C4-C5-N7	6.03	113.21	110.80
1	A	665	A	C6-N1-C2	-6.03	114.98	118.60
1	A	933	G	C2-N3-C4	-6.03	108.89	111.90
1	A	640	A	N7-C8-N9	6.03	116.81	113.80
1	A	940	C	N3-C2-O2	-6.03	117.68	121.90
1	A	1353	G	N3-C4-C5	-6.03	125.59	128.60
1	A	698	G	C4-N9-C1'	6.03	134.33	126.50
1	A	1328	C	N3-C2-O2	-6.03	117.68	121.90
1	A	593	G	C5-C6-N1	-6.02	108.49	111.50
1	A	111	G	N3-C4-N9	-6.02	122.39	126.00
15	O	63	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	A	114	U	C6-N1-C2	6.02	124.61	121.00
1	A	1342	C	N3-C2-O2	6.02	126.11	121.90
1	A	228	A	N3-C4-C5	6.02	131.01	126.80
1	A	773	G	C4-C5-N7	6.02	113.21	110.80
1	A	951	G	N7-C8-N9	-6.02	110.09	113.10
1	A	899	C	C5-C4-N4	-6.01	115.99	120.20
1	A	803	G	N1-C2-N3	6.01	127.51	123.90
1	A	706	A	N3-C4-C5	6.01	131.00	126.80
1	A	1455	G	C5-C6-O6	-6.01	125.00	128.60
1	A	1442	G	N7-C8-N9	6.00	116.10	113.10
1	A	638	G	C6-C5-N7	-6.00	126.80	130.40
1	A	1455	G	N3-C2-N2	-6.00	115.70	119.90
1	A	1527	C	C5-C4-N4	-6.00	116.00	120.20
1	A	710	G	C2-N3-C4	-6.00	108.90	111.90
1	A	1231	G	C5-C6-N1	-6.00	108.50	111.50
1	A	1355	G	N9-C4-C5	6.00	107.80	105.40
1	A	1408	A	C5-N7-C8	-6.00	100.90	103.90
1	A	116	A	C2-N3-C4	-6.00	107.60	110.60
1	A	1009	G	C8-N9-C4	-5.99	104.00	106.40
1	A	1377	A	C4-C5-N7	-5.99	107.70	110.70
1	A	971	G	C2-N3-C4	-5.99	108.90	111.90
1	A	1268	A	C8-N9-C4	-5.99	103.40	105.80
1	A	1063	C	C4-C5-C6	5.99	120.40	117.40
1	A	830	G	C4-C5-C6	5.99	122.39	118.80
1	A	1435	G	C5-C6-N1	-5.99	108.50	111.50
1	A	773	G	C5-C6-O6	-5.99	125.01	128.60
1	A	92	C	N1-C2-O2	5.99	122.49	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1075	C	N3-C4-C5	5.99	124.29	121.90
1	A	1522	U	C6-N1-C2	-5.99	117.41	121.00
1	A	119	A	N9-C4-C5	5.98	108.19	105.80
1	A	298	A	C2-N3-C4	-5.98	107.61	110.60
1	A	334	C	C6-N1-C2	5.98	122.69	120.30
1	A	7	G	N1-C6-O6	-5.98	116.31	119.90
1	A	291	C	C4-C5-C6	5.98	120.39	117.40
1	A	109	A	C2-N3-C4	-5.98	107.61	110.60
1	A	97	G	N7-C8-N9	5.97	116.09	113.10
1	A	38	G	C8-N9-C4	5.97	108.79	106.40
1	A	61	G	N1-C6-O6	5.97	123.48	119.90
1	A	752	G	C5-C6-N1	-5.97	108.51	111.50
1	A	350	G	N9-C4-C5	5.97	107.79	105.40
1	A	942	G	C5-C6-N1	-5.97	108.52	111.50
1	A	451	A	C4-C5-N7	5.97	113.68	110.70
1	A	659	U	N3-C4-O4	-5.97	115.22	119.40
1	A	301	G	N1-C2-N3	5.97	127.48	123.90
1	A	1194	U	C5-C6-N1	5.97	125.68	122.70
1	A	1396	A	C2-N3-C4	-5.97	107.62	110.60
1	A	1491	G	C2-N3-C4	5.96	114.88	111.90
1	A	607	A	C5-C6-N6	-5.96	118.93	123.70
1	A	642	A	N9-C4-C5	5.96	108.19	105.80
1	A	279	A	C4-C5-C6	5.96	119.98	117.00
1	A	360	A	C4-C5-N7	5.96	113.68	110.70
1	A	799	G	C2-N3-C4	-5.96	108.92	111.90
1	A	1544	U	N3-C4-O4	5.96	123.57	119.40
1	A	477	G	N1-C6-O6	5.96	123.48	119.90
1	A	1481	U	N3-C4-C5	-5.96	111.02	114.60
1	A	79	G	C6-C5-N7	-5.96	126.83	130.40
1	A	301	G	C4-N9-C1'	5.96	134.24	126.50
3	C	138	VAL	CB-CA-C	-5.96	100.08	111.40
1	A	285	G	N3-C4-C5	5.95	131.57	128.60
1	A	933	G	N1-C6-O6	5.95	123.47	119.90
1	A	1377	A	N1-C2-N3	5.95	132.27	129.30
1	A	375	U	C6-N1-C2	-5.95	117.43	121.00
1	A	975	A	C5-N7-C8	-5.95	100.93	103.90
1	A	1223	C	C5-C6-N1	5.95	123.97	121.00
1	A	816	A	N1-C2-N3	5.94	132.27	129.30
1	A	389	A	N7-C8-N9	5.94	116.77	113.80
1	A	571	U	N3-C4-O4	-5.94	115.24	119.40
1	A	190(G)	G	N1-C6-O6	5.94	123.47	119.90
1	A	752	G	N3-C4-C5	5.94	131.57	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	860	A	N1-C2-N3	5.94	132.27	129.30
1	A	1250	A	C5-C6-N6	5.94	128.45	123.70
1	A	21	G	C5-C6-O6	5.94	132.16	128.60
1	A	1361(A)	C	N3-C2-O2	-5.94	117.74	121.90
1	A	1398	A	N9-C4-C5	5.94	108.17	105.80
1	A	37	U	N3-C2-O2	-5.94	118.04	122.20
1	A	556	C	N1-C2-N3	5.94	123.36	119.20
1	A	240	C	N3-C2-O2	5.93	126.05	121.90
1	A	642	A	N7-C8-N9	5.93	116.77	113.80
1	A	1291	G	N9-C4-C5	-5.93	103.03	105.40
1	A	764	C	C2-N3-C4	-5.93	116.94	119.90
1	A	831	U	C6-N1-C2	-5.93	117.44	121.00
1	A	918	A	C8-N9-C4	5.93	108.17	105.80
1	A	150	C	C2-N1-C1'	5.93	125.32	118.80
1	A	377	G	N1-C2-N3	5.93	127.46	123.90
1	A	935	A	C8-N9-C4	5.93	108.17	105.80
1	A	1008	C	C5-C6-N1	5.93	123.96	121.00
1	A	1398	A	N1-C2-N3	5.93	132.26	129.30
1	A	672	U	C6-N1-C2	5.93	124.56	121.00
1	A	19	C	C2-N3-C4	-5.92	116.94	119.90
1	A	877	C	N1-C2-O2	-5.92	115.35	118.90
1	A	484	G	C8-N9-C1'	-5.92	119.30	127.00
1	A	565	U	C4-C5-C6	-5.92	116.15	119.70
1	A	776	G	C2-N3-C4	-5.92	108.94	111.90
1	A	668	G	C8-N9-C4	5.92	108.77	106.40
1	A	733	A	N1-C2-N3	5.92	132.26	129.30
1	A	99	C	C6-N1-C2	-5.92	117.93	120.30
1	A	297	G	C4-C5-N7	5.91	113.17	110.80
1	A	699	C	N1-C2-O2	-5.91	115.35	118.90
1	A	717	C	N3-C2-O2	5.91	126.04	121.90
1	A	769	G	C5-C6-O6	-5.91	125.05	128.60
1	A	796	C	N3-C4-C5	5.91	124.26	121.90
1	A	1099	G	N3-C2-N2	-5.91	115.76	119.90
1	A	1323	G	C2-N3-C4	-5.91	108.94	111.90
1	A	917	G	C8-N9-C1'	-5.91	119.32	127.00
1	A	989	C	C2-N1-C1'	5.91	125.30	118.80
1	A	1376	U	N1-C2-N3	5.91	118.44	114.90
1	A	316	G	C4-C5-C6	5.91	122.34	118.80
1	A	1476	G	C8-N9-C4	-5.91	104.04	106.40
1	A	723	U	C2-N3-C4	5.90	130.54	127.00
1	A	171	A	C6-N1-C2	-5.90	115.06	118.60
1	A	258	G	C4-C5-N7	5.90	113.16	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1180	A	C8-N9-C4	-5.90	103.44	105.80
1	A	1265	G	C5-C6-N1	-5.90	108.55	111.50
1	A	1387	G	N1-C2-N3	5.90	127.44	123.90
1	A	1393	U	N1-C2-N3	5.89	118.44	114.90
1	A	29	G	C8-N9-C4	5.89	108.76	106.40
1	A	1107	C	N3-C4-C5	-5.89	119.54	121.90
1	A	168	G	C8-N9-C4	-5.89	104.04	106.40
1	A	120	A	N1-C2-N3	5.89	132.25	129.30
1	A	298	A	N3-C4-N9	-5.89	122.69	127.40
1	A	190(G)	G	C5-C6-N1	-5.89	108.56	111.50
1	A	299	G	C6-C5-N7	-5.89	126.87	130.40
1	A	482	A	C5-C6-N6	-5.89	118.99	123.70
1	A	1305	G	C4-C5-C6	5.89	122.33	118.80
1	A	1335	C	N3-C2-O2	-5.88	117.78	121.90
1	A	1530	G	N7-C8-N9	-5.88	110.16	113.10
1	A	242	C	C4-C5-C6	5.88	120.34	117.40
1	A	1530	G	C4-C5-N7	5.88	113.15	110.80
1	A	110	C	C4-C5-C6	5.88	120.34	117.40
1	A	541	G	N3-C4-C5	5.88	131.54	128.60
1	A	1064	G	N3-C4-N9	5.88	129.53	126.00
1	A	145	G	C5-C6-N1	-5.88	108.56	111.50
1	A	615	C	C5-C4-N4	-5.87	116.09	120.20
1	A	885	G	C2-N3-C4	-5.87	108.96	111.90
1	A	1145	C	C2-N1-C1'	-5.87	112.34	118.80
1	A	27	G	C4-C5-C6	5.87	122.32	118.80
1	A	225	C	C2-N3-C4	-5.87	116.97	119.90
1	A	607	A	N3-C4-C5	5.87	130.91	126.80
1	A	285	G	N1-C2-N3	5.86	127.42	123.90
1	A	592	G	N1-C6-O6	-5.86	116.38	119.90
1	A	577	G	C5-C6-O6	-5.86	125.08	128.60
1	A	1048	G	N3-C4-C5	5.86	131.53	128.60
1	A	429	U	C5-C6-N1	-5.86	119.77	122.70
4	D	94	LEU	CA-CB-CG	-5.86	101.83	115.30
1	A	719	C	C2-N3-C4	-5.86	116.97	119.90
1	A	632	A	C4-C5-N7	5.86	113.63	110.70
1	A	1542	U	C6-N1-C2	-5.86	117.49	121.00
1	A	799	G	C5-C6-O6	-5.85	125.09	128.60
1	A	317	G	C4-C5-N7	5.85	113.14	110.80
1	A	551	U	N3-C4-C5	-5.85	111.09	114.60
1	A	705	U	C2-N1-C1'	-5.85	110.68	117.70
1	A	1250	A	N3-C4-N9	-5.85	122.72	127.40
1	A	423	G	C4-C5-N7	5.85	113.14	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	274	A	N7-C8-N9	-5.85	110.88	113.80
1	A	819	A	C2-N3-C4	-5.85	107.68	110.60
1	A	1156	G	C8-N9-C4	-5.85	104.06	106.40
1	A	38	G	N3-C4-N9	-5.84	122.49	126.00
1	A	899	C	C2-N3-C4	5.84	122.82	119.90
1	A	1416	G	N3-C2-N2	-5.84	115.81	119.90
1	A	1505	G	N3-C4-N9	5.84	129.50	126.00
1	A	1529	G	N9-C4-C5	5.84	107.74	105.40
1	A	900	A	N7-C8-N9	5.84	116.72	113.80
1	A	396	G	N3-C4-C5	-5.84	125.68	128.60
1	A	541	G	C2-N3-C4	-5.84	108.98	111.90
1	A	1074	G	C4-C5-C6	5.84	122.30	118.80
16	P	80	PHE	N-CA-C	5.84	126.76	111.00
1	A	417	C	C6-N1-C2	-5.83	117.97	120.30
1	A	483	C	C5-C4-N4	5.83	124.28	120.20
1	A	721	G	C4-N9-C1'	5.83	134.08	126.50
1	A	1196	U	N3-C4-O4	-5.83	115.32	119.40
1	A	292	G	C6-C5-N7	-5.83	126.90	130.40
1	A	877	C	C5-C6-N1	-5.83	118.08	121.00
1	A	1325	C	C6-N1-C2	5.83	122.63	120.30
1	A	635	G	N1-C2-N3	5.83	127.40	123.90
1	A	897	C	C6-N1-C2	5.83	122.63	120.30
1	A	218	C	C6-N1-C2	-5.83	117.97	120.30
1	A	762	C	C5-C4-N4	-5.83	116.12	120.20
1	A	957	U	C4-C5-C6	5.83	123.20	119.70
1	A	1251	A	N9-C4-C5	5.83	108.13	105.80
1	A	1373	G	N3-C4-N9	5.83	129.50	126.00
1	A	787	A	N9-C4-C5	-5.83	103.47	105.80
1	A	1499	A	C2-N3-C4	-5.83	107.69	110.60
12	L	119	LYS	N-CA-C	-5.83	95.27	111.00
1	A	90	U	N1-C2-N3	5.82	118.39	114.90
1	A	635	G	C4-C5-C6	5.82	122.29	118.80
1	A	1125	U	C5-C6-N1	5.82	125.61	122.70
1	A	21	G	C5-N7-C8	5.82	107.21	104.30
1	A	326	G	C4-C5-N7	-5.82	108.47	110.80
1	A	761	G	C2-N3-C4	-5.82	108.99	111.90
1	A	141	A	C5-C6-N6	-5.82	119.05	123.70
1	A	825	G	C5-C6-O6	-5.82	125.11	128.60
1	A	881	G	N3-C4-C5	-5.82	125.69	128.60
1	A	881	G	C6-N1-C2	-5.82	121.61	125.10
1	A	1335	C	N3-C4-N4	-5.82	113.93	118.00
1	A	203	U	C5-C4-O4	-5.82	122.41	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	557	G	C5-C6-N1	-5.82	108.59	111.50
1	A	799	G	N1-C6-O6	5.82	123.39	119.90
1	A	908	A	N9-C4-C5	5.82	108.13	105.80
3	C	25	GLY	N-CA-C	5.82	127.64	113.10
1	A	44	G	N1-C6-O6	5.81	123.39	119.90
1	A	565	U	N3-C4-C5	5.81	118.09	114.60
1	A	859	A	C4-C5-C6	5.81	119.91	117.00
1	A	1281	U	C6-N1-C2	-5.81	117.51	121.00
1	A	481	G	C5-C6-N1	5.81	114.40	111.50
1	A	730	G	N9-C4-C5	5.81	107.72	105.40
1	A	1093	A	N1-C6-N6	5.81	122.08	118.60
1	A	1512	U	C4-C5-C6	5.81	123.19	119.70
1	A	570	G	C4-C5-C6	5.81	122.28	118.80
1	A	514	C	C6-N1-C2	-5.80	117.98	120.30
1	A	147	G	N1-C6-O6	5.80	123.38	119.90
1	A	328	C	N3-C2-O2	-5.80	117.84	121.90
1	A	885	G	C8-N9-C4	-5.80	104.08	106.40
1	A	494	G	C5-C6-N1	-5.80	108.60	111.50
1	A	743	U	C5-C6-N1	-5.80	119.80	122.70
6	F	9	VAL	CB-CA-C	-5.80	100.38	111.40
1	A	825	G	C8-N9-C1'	-5.80	119.47	127.00
1	A	1454	G	C4-C5-N7	5.80	113.12	110.80
1	A	112	G	N3-C2-N2	-5.79	115.84	119.90
1	A	128	G	C4-C5-C6	5.79	122.28	118.80
1	A	551	U	C6-N1-C2	-5.79	117.52	121.00
1	A	659	U	C2-N3-C4	-5.79	123.52	127.00
1	A	859	A	C6-C5-N7	-5.79	128.25	132.30
1	A	1067	A	C2-N3-C4	5.79	113.50	110.60
1	A	108	G	C4-N9-C1'	5.79	134.03	126.50
1	A	175	C	N3-C4-C5	5.79	124.22	121.90
1	A	774	G	C4-C5-N7	5.79	113.12	110.80
1	A	856	C	C4-C5-C6	5.79	120.29	117.40
1	A	81	U	N3-C2-O2	-5.79	118.15	122.20
1	A	566	G	N9-C4-C5	5.79	107.71	105.40
1	A	617	G	C8-N9-C1'	-5.78	119.48	127.00
1	A	1358	U	C5-C6-N1	5.78	125.59	122.70
2	B	51	LEU	CA-CB-CG	-5.78	102.00	115.30
1	A	1493	A	C8-N9-C4	-5.78	103.49	105.80
1	A	610	G	C4-N9-C1'	5.78	134.01	126.50
1	A	886	G	C5-C6-N1	-5.78	108.61	111.50
1	A	936	C	C6-N1-C2	5.78	122.61	120.30
1	A	1061	G	C6-C5-N7	-5.78	126.93	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1063	C	N1-C2-N3	5.78	123.24	119.20
1	A	1067	A	N3-C4-C5	-5.78	122.75	126.80
1	A	1335	C	C5-C4-N4	5.78	124.24	120.20
1	A	182	U	C5-C6-N1	5.78	125.59	122.70
1	A	399	G	N1-C2-N3	5.78	127.36	123.90
1	A	820	U	C2-N3-C4	-5.78	123.53	127.00
1	A	335	C	C2-N3-C4	-5.77	117.01	119.90
1	A	730	G	C4-C5-C6	5.77	122.26	118.80
1	A	1523	G	N1-C2-N2	5.77	121.40	116.20
1	A	691	G	C6-C5-N7	-5.77	126.94	130.40
1	A	877	C	N1-C2-N3	5.77	123.24	119.20
1	A	555	C	C5-C4-N4	-5.77	116.16	120.20
1	A	568	G	N3-C2-N2	-5.77	115.86	119.90
1	A	1338	G	C8-N9-C1'	5.77	134.50	127.00
1	A	859	A	C8-N9-C4	-5.77	103.49	105.80
1	A	79	G	C4-C5-C6	5.77	122.26	118.80
2	B	16	HIS	CB-CA-C	-5.77	98.87	110.40
1	A	285	G	C8-N9-C4	5.76	108.71	106.40
1	A	319	G	N9-C4-C5	-5.76	103.09	105.40
1	A	551	U	N3-C2-O2	-5.76	118.17	122.20
1	A	791	G	N7-C8-N9	5.76	115.98	113.10
1	A	1268	A	N3-C4-C5	-5.76	122.77	126.80
1	A	487	A	N7-C8-N9	-5.76	110.92	113.80
1	A	861	G	C5-C6-N1	5.76	114.38	111.50
1	A	816	A	C6-N1-C2	-5.76	115.15	118.60
1	A	1522	U	C2-N1-C1'	5.76	124.61	117.70
1	A	75	G	C4-N9-C1'	5.75	133.98	126.50
1	A	568	G	N9-C4-C5	5.75	107.70	105.40
1	A	580	U	N1-C2-N3	5.75	118.35	114.90
1	A	717	C	N3-C4-C5	5.75	124.20	121.90
1	A	852	G	N1-C2-N3	5.75	127.35	123.90
1	A	984	C	N3-C4-C5	-5.75	119.60	121.90
1	A	572	A	C6-C5-N7	5.75	136.33	132.30
1	A	588	G	N1-C2-N3	5.75	127.35	123.90
1	A	1254	C	N3-C4-C5	-5.75	119.60	121.90
1	A	1502	A	C4-C5-C6	5.75	119.88	117.00
1	A	661	G	C5-C6-N1	-5.75	108.62	111.50
1	A	824	C	C6-N1-C2	5.75	122.60	120.30
1	A	696	A	N7-C8-N9	-5.75	110.93	113.80
1	A	261	U	N3-C4-C5	-5.75	111.15	114.60
1	A	888	G	N3-C2-N2	-5.75	115.88	119.90
1	A	975	A	N7-C8-N9	5.75	116.67	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1522	U	N3-C4-O4	5.75	123.42	119.40
1	A	916	G	C4-N9-C1'	5.75	133.97	126.50
1	A	243	A	N1-C6-N6	5.74	122.05	118.60
1	A	881	G	C8-N9-C1'	-5.74	119.54	127.00
1	A	730	G	C4-C5-N7	-5.74	108.50	110.80
1	A	768	A	N1-C2-N3	5.74	132.17	129.30
1	A	1361(A)	C	N3-C4-C5	5.74	124.19	121.90
1	A	1469	G	C4-C5-N7	5.74	113.09	110.80
1	A	250	A	N3-C4-C5	5.74	130.81	126.80
1	A	1490	C	N3-C2-O2	5.74	125.91	121.90
1	A	777	A	N1-C6-N6	5.73	122.04	118.60
1	A	895	G	C8-N9-C4	-5.73	104.11	106.40
1	A	49	U	N1-C2-O2	-5.73	118.79	122.80
1	A	258	G	C6-C5-N7	-5.73	126.96	130.40
1	A	310	G	C5-N7-C8	-5.73	101.43	104.30
1	A	491	G	N1-C6-O6	5.73	123.34	119.90
1	A	20	U	P-O3'-C3'	5.73	126.57	119.70
1	A	263	A	C2-N3-C4	5.73	113.46	110.60
1	A	451	A	N9-C4-C5	-5.73	103.51	105.80
1	A	1366	C	C4-C5-C6	-5.73	114.54	117.40
1	A	98	U	N3-C4-O4	5.72	123.41	119.40
1	A	600	C	C5-C6-N1	-5.72	118.14	121.00
1	A	760	G	N3-C4-N9	-5.72	122.56	126.00
1	A	784	C	C5-C4-N4	-5.72	116.19	120.20
1	A	1416	G	C8-N9-C4	-5.72	104.11	106.40
1	A	812	C	C4-C5-C6	5.72	120.26	117.40
1	A	606	G	N9-C4-C5	5.72	107.69	105.40
1	A	1374	A	C8-N9-C4	-5.72	103.51	105.80
1	A	137	C	N3-C4-N4	-5.72	114.00	118.00
1	A	951	G	C8-N9-C4	5.72	108.69	106.40
1	A	771	G	N9-C4-C5	-5.71	103.11	105.40
1	A	300	A	C5-N7-C8	-5.71	101.05	103.90
1	A	778	G	C5-C6-N1	-5.71	108.65	111.50
1	A	1299	A	C5-N7-C8	-5.71	101.05	103.90
1	A	1354	C	N3-C2-O2	-5.71	117.91	121.90
1	A	944	G	N3-C2-N2	5.71	123.89	119.90
1	A	973	G	N3-C4-N9	5.70	129.42	126.00
1	A	1243	C	N3-C4-N4	-5.70	114.01	118.00
1	A	132	C	C5-C6-N1	-5.70	118.15	121.00
1	A	1513	A	N3-C4-N9	-5.70	122.84	127.40
1	A	164	U	C2-N1-C1'	-5.69	110.87	117.70
1	A	166	G	C8-N9-C4	5.69	108.68	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	461	C	N1-C2-O2	5.69	122.31	118.90
2	B	44	LEU	CA-CB-CG	-5.69	102.21	115.30
1	A	588	G	C8-N9-C4	5.69	108.68	106.40
1	A	608	A	N1-C2-N3	5.69	132.15	129.30
1	A	694	A	C2-N3-C4	-5.69	107.75	110.60
1	A	482	A	C4-C5-C6	5.69	119.84	117.00
1	A	1231	G	C5-N7-C8	-5.69	101.46	104.30
1	A	375	U	N3-C4-C5	-5.68	111.19	114.60
1	A	1337	G	N1-C2-N3	5.68	127.31	123.90
1	A	276	G	N1-C2-N2	5.68	121.31	116.20
1	A	315	A	C8-N9-C4	-5.68	103.53	105.80
1	A	141	A	C6-C5-N7	-5.68	128.32	132.30
1	A	711	G	C6-C5-N7	-5.68	126.99	130.40
1	A	157	G	C5-C6-N1	-5.68	108.66	111.50
1	A	342	C	C5-C6-N1	5.68	123.84	121.00
1	A	694	A	N1-C6-N6	5.68	122.01	118.60
1	A	905	U	N3-C2-O2	-5.68	118.22	122.20
1	A	1526	G	N3-C4-C5	-5.68	125.76	128.60
1	A	323	U	N3-C4-O4	5.68	123.37	119.40
1	A	827	U	C4-C5-C6	5.68	123.11	119.70
1	A	474	G	C5-N7-C8	-5.68	101.46	104.30
1	A	913	A	P-O3'-C3'	5.68	126.51	119.70
1	A	1248	A	N1-C6-N6	5.68	122.01	118.60
1	A	1521	G	C2-N3-C4	5.68	114.74	111.90
1	A	260	G	C6-C5-N7	-5.67	127.00	130.40
1	A	331	G	C6-C5-N7	-5.67	127.00	130.40
1	A	885	G	C6-C5-N7	-5.67	127.00	130.40
1	A	1088	G	C5-N7-C8	-5.67	101.46	104.30
1	A	1286	A	C2-N3-C4	-5.67	107.76	110.60
1	A	904	C	N3-C4-N4	5.67	121.97	118.00
1	A	14	U	C6-N1-C2	-5.67	117.60	121.00
1	A	1499	A	N1-C2-N3	5.67	132.13	129.30
1	A	253	U	C5-C6-N1	-5.67	119.87	122.70
1	A	794	A	C4-C5-N7	-5.67	107.87	110.70
1	A	583	A	N1-C6-N6	5.66	122.00	118.60
1	A	732	C	N1-C2-O2	5.66	122.30	118.90
1	A	1374	A	N1-C6-N6	-5.66	115.20	118.60
1	A	1294	G	N3-C4-C5	5.66	131.43	128.60
1	A	447	G	N1-C6-O6	-5.66	116.50	119.90
1	A	474	G	C5-C6-N1	-5.66	108.67	111.50
1	A	725	G	N3-C2-N2	-5.66	115.94	119.90
1	A	874	G	C2-N3-C4	-5.66	109.07	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	741	G	N9-C4-C5	5.65	107.66	105.40
1	A	940	C	N1-C2-O2	5.65	122.29	118.90
1	A	1153	C	N1-C2-O2	5.65	122.29	118.90
1	A	1461	G	N1-C6-O6	5.65	123.29	119.90
1	A	1542	U	C4-C5-C6	5.65	123.09	119.70
1	A	66	G	N3-C2-N2	-5.65	115.94	119.90
1	A	329	A	C2-N3-C4	-5.65	107.78	110.60
1	A	546	G	N3-C4-N9	5.65	129.39	126.00
1	A	729	A	N7-C8-N9	5.65	116.62	113.80
1	A	1231	G	C5-C6-O6	-5.65	125.21	128.60
1	A	1129	C	C6-N1-C2	-5.65	118.04	120.30
1	A	1187	G	N7-C8-N9	5.65	115.92	113.10
1	A	262	A	N9-C4-C5	5.64	108.06	105.80
1	A	667	G	C2-N3-C4	-5.64	109.08	111.90
1	A	1227	A	N3-C4-N9	-5.64	122.89	127.40
1	A	649	G	C4-C5-N7	5.64	113.06	110.80
1	A	734	G	C6-C5-N7	-5.64	127.02	130.40
1	A	856	C	C6-N1-C2	-5.64	118.05	120.30
1	A	748	C	C5-C6-N1	-5.64	118.18	121.00
1	A	281	G	C5-N7-C8	-5.63	101.48	104.30
1	A	284	G	C4-C5-N7	5.63	113.05	110.80
1	A	933	G	C5-C6-O6	-5.63	125.22	128.60
1	A	1203	C	N3-C4-C5	-5.63	119.65	121.90
17	Q	99	SER	N-CA-C	5.63	126.21	111.00
1	A	218	C	N1-C2-O2	5.63	122.28	118.90
1	A	1528	U	N3-C4-C5	5.63	117.98	114.60
1	A	375	U	N1-C2-N3	5.63	118.28	114.90
1	A	637	G	C4-N9-C1'	5.63	133.82	126.50
1	A	1398	A	C4-C5-N7	-5.63	107.88	110.70
1	A	729	A	C5-C6-N6	-5.63	119.20	123.70
1	A	851	G	C5-C6-N1	-5.63	108.69	111.50
1	A	230	G	C6-C5-N7	-5.63	127.02	130.40
1	A	372	C	C2-N3-C4	5.63	122.71	119.90
1	A	914	G	N1-C2-N3	5.63	127.28	123.90
1	A	79	G	N3-C2-N2	-5.62	115.96	119.90
1	A	1406	U	N3-C2-O2	5.62	126.14	122.20
1	A	913	A	N9-C4-C5	5.62	108.05	105.80
1	A	1377	A	N3-C4-N9	-5.62	122.90	127.40
1	A	1432	G	N3-C4-N9	-5.62	122.63	126.00
1	A	190(A)	C	C5-C6-N1	5.62	123.81	121.00
1	A	1173	G	C8-N9-C4	5.62	108.65	106.40
1	A	1373	G	C4-N9-C1'	5.62	133.81	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	123	C	C5-C4-N4	5.62	124.13	120.20
1	A	325	A	C5-C6-N6	5.62	128.19	123.70
1	A	1212	U	C6-N1-C1'	-5.62	113.34	121.20
1	A	81	U	N1-C2-O2	5.62	126.73	122.80
1	A	1108	G	C8-N9-C4	-5.62	104.15	106.40
1	A	297	G	N7-C8-N9	5.61	115.91	113.10
1	A	643	C	C6-N1-C2	-5.61	118.06	120.30
1	A	1098	C	C6-N1-C2	5.61	122.55	120.30
1	A	1268	A	C2-N3-C4	5.61	113.41	110.60
1	A	18	C	C5-C6-N1	-5.61	118.19	121.00
1	A	92	C	C5-C6-N1	-5.61	118.19	121.00
1	A	326	G	C5-C6-O6	5.61	131.97	128.60
1	A	24	U	N1-C2-N3	-5.61	111.53	114.90
1	A	248	C	C5-C4-N4	-5.61	116.28	120.20
1	A	376	G	N3-C2-N2	-5.61	115.98	119.90
1	A	1009	G	C4-N9-C1'	5.61	133.79	126.50
1	A	1294	G	N1-C6-O6	5.61	123.26	119.90
7	G	22	LEU	CA-CB-CG	-5.61	102.41	115.30
1	A	1155	G	N1-C6-O6	5.60	123.26	119.90
1	A	1203	C	N3-C4-N4	5.60	121.92	118.00
1	A	1227	A	C2-N3-C4	-5.60	107.80	110.60
1	A	1442	G	C2-N3-C4	5.60	114.70	111.90
1	A	299	G	C2-N3-C4	-5.60	109.10	111.90
1	A	671	G	C5-C6-N1	-5.60	108.70	111.50
1	A	1455	G	C5-C6-N1	-5.60	108.70	111.50
1	A	1494	G	C8-N9-C1'	-5.60	119.72	127.00
1	A	541	G	C5-C6-N1	-5.60	108.70	111.50
1	A	662	G	C4-N9-C1'	5.60	133.78	126.50
1	A	1179	A	N9-C4-C5	5.59	108.04	105.80
1	A	1474	G	C6-C5-N7	-5.59	127.04	130.40
1	A	292	G	N3-C2-N2	-5.59	115.98	119.90
1	A	581	G	N3-C4-N9	-5.59	122.64	126.00
1	A	1365	G	N7-C8-N9	5.59	115.90	113.10
1	A	44	G	C4-C5-N7	5.59	113.04	110.80
1	A	624	C	C6-N1-C2	5.59	122.54	120.30
1	A	654	G	N1-C2-N3	5.59	127.25	123.90
1	A	1253	G	C4-C5-N7	5.59	113.03	110.80
1	A	1339	A	N9-C4-C5	5.59	108.03	105.80
1	A	1526	G	C5-C6-O6	-5.59	125.25	128.60
1	A	245	C	N1-C2-O2	-5.58	115.55	118.90
1	A	540	G	C5-C6-O6	-5.58	125.25	128.60
1	A	777	A	C2-N3-C4	5.58	113.39	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1241	G	N3-C2-N2	-5.58	115.99	119.90
12	L	85	ILE	CB-CA-C	-5.58	100.43	111.60
1	A	774	G	C5-C6-O6	-5.58	125.25	128.60
1	A	383	A	C4-C5-N7	5.58	113.49	110.70
17	Q	100	LYS	CD-CE-NZ	5.58	124.54	111.70
1	A	113	G	C4-C5-N7	5.58	113.03	110.80
1	A	551	U	C4-C5-C6	5.58	123.05	119.70
1	A	591	U	N1-C2-N3	5.58	118.25	114.90
1	A	264	U	N1-C2-N3	5.58	118.25	114.90
1	A	123	C	C4-C5-C6	5.58	120.19	117.40
1	A	732	C	C6-N1-C1'	-5.58	114.11	120.80
1	A	759	A	C6-C5-N7	-5.58	128.40	132.30
1	A	27	G	N1-C6-O6	5.57	123.24	119.90
1	A	673	G	N3-C4-C5	-5.57	125.81	128.60
1	A	1159	U	N3-C4-O4	5.57	123.30	119.40
1	A	403	C	N3-C4-N4	5.57	121.90	118.00
1	A	944	G	C4-N9-C1'	5.57	133.74	126.50
1	A	325	A	C4-C5-N7	-5.57	107.92	110.70
1	A	1095	U	C5-C4-O4	-5.57	122.56	125.90
1	A	609	A	C8-N9-C4	-5.57	103.57	105.80
1	A	1192	C	C5-C4-N4	-5.57	116.30	120.20
7	G	59	LEU	CA-CB-CG	5.57	128.10	115.30
1	A	654	G	N3-C4-C5	5.56	131.38	128.60
1	A	1417	G	N3-C4-C5	-5.56	125.82	128.60
1	A	858	G	C8-N9-C4	5.56	108.62	106.40
1	A	562	C	N3-C2-O2	-5.56	118.01	121.90
1	A	593	G	C2-N3-C4	-5.56	109.12	111.90
1	A	614	A	C8-N9-C4	-5.56	103.58	105.80
1	A	1233	G	C5-C6-N1	5.56	114.28	111.50
1	A	327	A	C6-N1-C2	-5.56	115.27	118.60
1	A	579	G	C5-C6-O6	-5.56	125.27	128.60
1	A	630	G	N1-C6-O6	5.56	123.23	119.90
1	A	1172	C	C2-N1-C1'	-5.56	112.69	118.80
1	A	1229	A	N3-C4-C5	5.56	130.69	126.80
1	A	1516	G	N3-C4-N9	-5.56	122.67	126.00
1	A	1543	C	N3-C2-O2	-5.56	118.01	121.90
1	A	203	U	N1-C2-N3	-5.56	111.57	114.90
1	A	864	A	N1-C6-N6	-5.55	115.27	118.60
1	A	186	C	C2-N3-C4	-5.55	117.12	119.90
1	A	186	C	N3-C2-O2	-5.55	118.01	121.90
4	D	31	CYS	N-CA-CB	5.55	120.60	110.60
1	A	190(J)	U	C4-C5-C6	5.55	123.03	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	115	G	C8-N9-C4	5.55	108.62	106.40
1	A	190(G)	G	C4-C5-C6	5.55	122.13	118.80
1	A	1047	G	N3-C4-N9	5.55	129.33	126.00
1	A	373	A	C4-C5-C6	5.54	119.77	117.00
1	A	499	A	C2-N3-C4	5.54	113.37	110.60
16	P	6	LEU	CA-CB-CG	-5.54	102.55	115.30
1	A	102	G	C8-N9-C4	-5.54	104.18	106.40
1	A	546	G	C8-N9-C1'	-5.54	119.80	127.00
1	A	553	A	C6-N1-C2	-5.54	115.28	118.60
1	A	553	A	C5-C6-N6	-5.54	119.27	123.70
1	A	1082	G	C8-N9-C1'	-5.54	119.80	127.00
1	A	1116	C	N3-C4-C5	5.54	124.12	121.90
1	A	1229	A	C4-C5-C6	-5.54	114.23	117.00
1	A	256	U	N1-C2-N3	-5.54	111.58	114.90
1	A	765	G	N3-C4-N9	-5.54	122.68	126.00
1	A	104	G	C2-N3-C4	-5.54	109.13	111.90
1	A	1077	G	C4-C5-C6	5.54	122.12	118.80
1	A	522	C	C5-C4-N4	5.53	124.07	120.20
1	A	963	G	N9-C4-C5	5.53	107.61	105.40
1	A	1295	G	C8-N9-C4	-5.53	104.19	106.40
1	A	171	A	N1-C6-N6	-5.53	115.28	118.60
1	A	1199	U	N3-C4-C5	-5.53	111.28	114.60
1	A	1523	G	N3-C2-N2	-5.53	116.03	119.90
1	A	461	C	C6-N1-C2	-5.53	118.09	120.30
1	A	563	A	C5-C6-N1	-5.53	114.94	117.70
1	A	950	U	C5-C4-O4	5.53	129.22	125.90
1	A	578	C	C4-C5-C6	5.53	120.16	117.40
1	A	366	C	N3-C2-O2	-5.52	118.03	121.90
1	A	366	C	C2-N1-C1'	5.52	124.88	118.80
1	A	801	U	N3-C4-O4	-5.52	115.53	119.40
1	A	1064	G	C4-C5-N7	5.52	113.01	110.80
1	A	483	C	C4-C5-C6	5.52	120.16	117.40
1	A	666	G	C8-N9-C1'	-5.52	119.83	127.00
1	A	483	C	C6-N1-C1'	5.52	127.42	120.80
1	A	1340	A	C6-N1-C2	-5.52	115.29	118.60
1	A	995	C	C6-N1-C1'	-5.51	114.18	120.80
1	A	92	C	C6-N1-C2	5.51	122.50	120.30
1	A	1324	A	N1-C6-N6	5.51	121.91	118.60
1	A	101	A	C5-C6-N1	5.51	120.45	117.70
1	A	417	C	C2-N1-C1'	5.51	124.86	118.80
1	A	735	C	C2-N1-C1'	-5.51	112.74	118.80
1	A	1067	A	P-O3'-C3'	5.51	126.31	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	457	C	C5-C6-N1	5.50	123.75	121.00
1	A	799	G	C6-C5-N7	-5.50	127.10	130.40
1	A	78	G	N3-C2-N2	5.50	123.75	119.90
1	A	774	G	C8-N9-C1'	-5.50	119.85	127.00
1	A	786	G	C4-C5-C6	5.50	122.10	118.80
1	A	1189	C	N3-C4-N4	-5.50	114.15	118.00
1	A	848	C	C6-N1-C2	5.50	122.50	120.30
2	B	48	MET	CG-SD-CE	5.50	109.00	100.20
1	A	707	C	C2-N3-C4	-5.50	117.15	119.90
1	A	1331	G	C2-N3-C4	5.50	114.65	111.90
1	A	116	A	N1-C2-N3	5.50	132.05	129.30
1	A	255	G	N9-C4-C5	-5.50	103.20	105.40
1	A	1277	C	C6-N1-C2	-5.49	118.10	120.30
1	A	154	C	C5-C6-N1	5.49	123.75	121.00
1	A	167	G	C4-C5-N7	-5.49	108.60	110.80
1	A	834	C	C2-N3-C4	5.49	122.65	119.90
1	A	190(D)	U	N3-C4-O4	-5.49	115.56	119.40
1	A	319	G	C8-N9-C1'	-5.49	119.86	127.00
1	A	348	G	C4-C5-N7	5.49	113.00	110.80
1	A	700	G	C4-C5-C6	5.49	122.09	118.80
1	A	946	A	C5-C6-N1	5.49	120.44	117.70
1	A	1299	A	N7-C8-N9	5.49	116.55	113.80
1	A	315	A	C2-N3-C4	-5.49	107.86	110.60
1	A	494	G	C8-N9-C4	-5.49	104.20	106.40
1	A	1092	A	C4-C5-C6	-5.49	114.26	117.00
9	I	107	ARG	NE-CZ-NH1	5.49	123.04	120.30
1	A	66	G	N3-C4-N9	-5.48	122.71	126.00
1	A	667	G	C5-C6-O6	-5.48	125.31	128.60
1	A	908	A	N3-C4-N9	-5.48	123.01	127.40
1	A	241	C	C5-C6-N1	-5.48	118.26	121.00
1	A	901	A	C4-C5-C6	5.48	119.74	117.00
1	A	546	G	C4-N9-C1'	5.48	133.62	126.50
1	A	734	G	C5-N7-C8	-5.48	101.56	104.30
1	A	1126	U	C5-C4-O4	-5.48	122.61	125.90
1	A	578	C	N3-C4-C5	-5.48	119.71	121.90
1	A	770	C	N3-C4-N4	-5.48	114.17	118.00
1	A	1331	G	C8-N9-C4	-5.48	104.21	106.40
1	A	869	G	C5-C6-O6	5.48	131.89	128.60
1	A	508	C	C2-N1-C1'	5.47	124.82	118.80
1	A	583	A	C4-C5-C6	5.47	119.74	117.00
1	A	924	C	N3-C4-N4	5.47	121.83	118.00
1	A	247	G	C6-C5-N7	-5.47	127.12	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	559	A	C8-N9-C4	-5.47	103.61	105.80
1	A	643	C	C5-C6-N1	5.47	123.74	121.00
1	A	705	U	C4-C5-C6	5.47	122.98	119.70
1	A	730	G	N1-C2-N2	-5.47	111.28	116.20
1	A	748	C	C4-C5-C6	5.47	120.14	117.40
1	A	752	G	C2-N3-C4	-5.47	109.16	111.90
1	A	895	G	N1-C2-N3	5.47	127.18	123.90
1	A	673	G	N1-C2-N2	-5.47	111.28	116.20
1	A	746	A	C2-N3-C4	-5.47	107.86	110.60
1	A	1187	G	C6-C5-N7	-5.47	127.12	130.40
19	S	15	LEU	CA-CB-CG	5.47	127.88	115.30
1	A	8	A	N9-C4-C5	5.47	107.99	105.80
1	A	198	G	C8-N9-C1'	-5.47	119.89	127.00
1	A	910	C	N3-C4-C5	5.47	124.09	121.90
1	A	230	G	C8-N9-C1'	-5.46	119.90	127.00
1	A	75	G	C8-N9-C1'	-5.46	119.90	127.00
1	A	1087	G	C5-N7-C8	-5.46	101.57	104.30
1	A	384	G	C4-C5-N7	-5.45	108.62	110.80
1	A	874	G	C8-N9-C1'	-5.45	119.91	127.00
1	A	167	G	C2-N3-C4	5.45	114.63	111.90
1	A	582	U	C2-N3-C4	-5.45	123.73	127.00
1	A	926	G	N1-C2-N2	-5.45	111.29	116.20
1	A	546	G	N3-C4-C5	-5.45	125.88	128.60
1	A	554	C	C6-N1-C1'	5.45	127.34	120.80
1	A	873	A	N7-C8-N9	5.45	116.52	113.80
1	A	1301	U	N3-C4-O4	5.45	123.22	119.40
1	A	7	G	C5-N7-C8	5.45	107.02	104.30
1	A	274	A	C5-C6-N1	5.45	120.42	117.70
1	A	795	C	N3-C4-C5	-5.45	119.72	121.90
1	A	718	G	C5-C6-N1	-5.44	108.78	111.50
1	A	1082	G	N3-C4-N9	5.44	129.27	126.00
1	A	115	G	N1-C6-O6	5.44	123.17	119.90
1	A	226	G	N1-C2-N3	5.44	127.17	123.90
1	A	1353	G	N3-C4-N9	5.44	129.27	126.00
1	A	1461	G	N9-C4-C5	-5.44	103.22	105.40
1	A	245	C	C5-C6-N1	5.44	123.72	121.00
1	A	888	G	N3-C4-N9	-5.44	122.74	126.00
1	A	1026	G	N3-C4-C5	5.44	131.32	128.60
1	A	1192	C	C4-C5-C6	5.44	120.12	117.40
1	A	24	U	C6-N1-C2	5.44	124.26	121.00
1	A	141	A	N9-C4-C5	-5.43	103.63	105.80
1	A	865	A	C2-N3-C4	5.43	113.32	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1543	C	C6-N1-C2	-5.43	118.13	120.30
1	A	721	G	C4-C5-C6	5.43	122.06	118.80
1	A	574	A	N1-C6-N6	-5.43	115.34	118.60
1	A	654	G	N3-C4-N9	-5.43	122.74	126.00
1	A	687	A	P-O3'-C3'	5.43	126.22	119.70
1	A	879	C	C2-N3-C4	-5.43	117.19	119.90
1	A	306	G	C8-N9-C4	5.43	108.57	106.40
1	A	1296	C	C6-N1-C2	-5.43	118.13	120.30
1	A	1416	G	C6-C5-N7	-5.43	127.14	130.40
1	A	615	C	C5-C6-N1	5.43	123.71	121.00
1	A	823	G	C8-N9-C4	5.43	108.57	106.40
1	A	995	C	C6-N1-C2	-5.43	118.13	120.30
1	A	834	C	N3-C2-O2	5.42	125.70	121.90
1	A	511	C	C2-N3-C4	-5.42	117.19	119.90
1	A	682	G	N1-C6-O6	5.42	123.15	119.90
1	A	928	G	C4-N9-C1'	-5.42	119.45	126.50
1	A	667	G	N3-C2-N2	-5.42	116.11	119.90
1	A	785	G	C5-C6-O6	-5.42	125.35	128.60
1	A	1047	G	C4-N9-C1'	5.42	133.55	126.50
1	A	1116	C	N3-C4-N4	-5.42	114.20	118.00
1	A	364	A	C2-N3-C4	-5.42	107.89	110.60
1	A	561	U	N3-C4-O4	5.42	123.19	119.40
1	A	265	G	C5-C6-N1	-5.42	108.79	111.50
1	A	287	U	C6-N1-C2	-5.42	117.75	121.00
1	A	309	G	C6-C5-N7	-5.41	127.15	130.40
1	A	1234	C	C5-C4-N4	-5.41	116.41	120.20
1	A	257	G	N1-C6-O6	-5.41	116.65	119.90
1	A	316	G	C5-C6-N1	-5.41	108.79	111.50
1	A	262	A	C5-C6-N6	5.41	128.03	123.70
1	A	131	C	N3-C2-O2	-5.41	118.11	121.90
1	A	661	G	C8-N9-C4	-5.41	104.24	106.40
1	A	1186	G	N3-C4-C5	5.41	131.31	128.60
1	A	1387	G	C8-N9-C4	5.41	108.56	106.40
1	A	324	G	C5-C6-O6	5.41	131.84	128.60
1	A	946	A	N3-C4-C5	-5.41	123.02	126.80
1	A	1212	U	C5-C6-N1	5.41	125.40	122.70
1	A	712	A	N1-C2-N3	5.40	132.00	129.30
1	A	242	C	C5-C6-N1	-5.40	118.30	121.00
1	A	577	G	N3-C4-C5	5.40	131.30	128.60
1	A	364	A	N1-C2-N3	5.40	132.00	129.30
1	A	581	G	C8-N9-C1'	5.40	134.02	127.00
1	A	1066	C	C6-N1-C2	5.40	122.46	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1289	A	C2-N3-C4	5.40	113.30	110.60
1	A	1291	G	N3-C4-N9	5.40	129.24	126.00
1	A	591	U	C4-C5-C6	5.40	122.94	119.70
1	A	913	A	C8-N9-C4	-5.40	103.64	105.80
1	A	406	G	C6-C5-N7	-5.40	127.16	130.40
1	A	569	C	N3-C4-N4	-5.40	114.22	118.00
1	A	1062	U	C5-C4-O4	5.40	129.14	125.90
1	A	386	C	N1-C2-O2	-5.39	115.66	118.90
1	A	825	G	N1-C6-O6	5.39	123.14	119.90
1	A	255	G	N3-C4-N9	5.39	129.24	126.00
1	A	290	C	N3-C4-C5	5.39	124.06	121.90
1	A	786	G	N1-C2-N3	5.39	127.14	123.90
1	A	575	G	N1-C6-O6	-5.39	116.67	119.90
1	A	971	G	N3-C4-C5	5.39	131.29	128.60
1	A	1141	C	N1-C2-O2	5.39	122.13	118.90
1	A	709	G	C5-C6-O6	-5.39	125.37	128.60
1	A	229	U	N3-C4-O4	5.38	123.17	119.40
1	A	589	C	C6-N1-C1'	5.38	127.26	120.80
1	A	200	G	C4-C5-C6	5.38	122.03	118.80
1	A	660	G	N3-C4-C5	5.38	131.29	128.60
1	A	644	G	C5-C6-O6	-5.38	125.37	128.60
1	A	46	G	N3-C4-N9	5.38	129.23	126.00
1	A	569	C	N3-C4-C5	5.38	124.05	121.90
1	A	872	A	C5-C6-N6	-5.38	119.40	123.70
1	A	1361	G	N1-C6-O6	-5.38	116.67	119.90
1	A	364	A	C4-C5-C6	5.37	119.69	117.00
1	A	550	G	N3-C2-N2	-5.37	116.14	119.90
1	A	1387	G	N9-C4-C5	-5.37	103.25	105.40
1	A	326	G	C5-N7-C8	5.37	106.98	104.30
1	A	439	A	C8-N9-C4	-5.37	103.65	105.80
1	A	623	C	N1-C2-O2	-5.37	115.68	118.90
1	A	752	G	N3-C4-N9	-5.37	122.78	126.00
1	A	919	A	N7-C8-N9	-5.37	111.11	113.80
1	A	1520	G	C6-N1-C2	-5.37	121.88	125.10
1	A	168	G	N7-C8-N9	5.37	115.78	113.10
1	A	447	G	C4-N9-C1'	5.37	133.48	126.50
1	A	807	A	N1-C2-N3	5.37	131.98	129.30
1	A	834	C	N3-C4-C5	-5.37	119.75	121.90
1	A	1059	C	C4-C5-C6	5.37	120.08	117.40
1	A	484	G	N3-C4-C5	-5.36	125.92	128.60
1	A	938	A	N1-C6-N6	-5.36	115.38	118.60
1	A	1059	C	N3-C4-C5	-5.36	119.75	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1082	G	C8-N9-C4	5.36	108.55	106.40
1	A	1414	U	C5-C6-N1	-5.36	120.02	122.70
1	A	353	A	N1-C6-N6	-5.36	115.38	118.60
1	A	914	G	N1-C2-N2	-5.36	111.38	116.20
1	A	1149	C	C6-N1-C2	-5.36	118.16	120.30
1	A	279	A	C5-C6-N6	-5.36	119.41	123.70
1	A	1064	G	N1-C2-N3	5.36	127.12	123.90
1	A	89	C	C5-C4-N4	-5.36	116.45	120.20
1	A	236	G	C5-C6-O6	5.36	131.81	128.60
1	A	310	G	N3-C2-N2	-5.36	116.15	119.90
1	A	555	C	N3-C4-N4	5.36	121.75	118.00
1	A	1279	A	C4-N9-C1'	5.36	135.94	126.30
1	A	673	G	C4-C5-C6	5.36	122.01	118.80
1	A	236	G	N3-C4-C5	-5.35	125.92	128.60
5	E	126	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	A	403	C	N3-C2-O2	-5.35	118.15	121.90
1	A	1419	G	N1-C6-O6	5.35	123.11	119.90
1	A	653	A	N1-C2-N3	5.35	131.97	129.30
1	A	1093	A	C5-C6-N6	-5.35	119.42	123.70
1	A	190(J)	U	N3-C4-C5	-5.34	111.39	114.60
1	A	904	C	C4-C5-C6	5.34	120.07	117.40
1	A	1251	A	N1-C6-N6	-5.34	115.39	118.60
4	D	12	CYS	N-CA-C	-5.34	96.57	111.00
1	A	257	G	C5-C6-N1	5.34	114.17	111.50
1	A	1019	C	N1-C2-O2	5.34	122.10	118.90
1	A	818	G	N7-C8-N9	5.34	115.77	113.10
1	A	1227	A	C5-N7-C8	-5.34	101.23	103.90
1	A	74	C	C5-C6-N1	5.34	123.67	121.00
1	A	245	C	N3-C2-O2	5.34	125.64	121.90
1	A	1063	C	N3-C2-O2	-5.34	118.17	121.90
1	A	109	A	C4-C5-N7	5.33	113.37	110.70
1	A	685	G	C8-N9-C4	5.33	108.53	106.40
1	A	854	G	C4-C5-N7	5.33	112.93	110.80
1	A	1165	C	C5-C6-N1	5.33	123.67	121.00
1	A	922	G	N7-C8-N9	5.33	115.77	113.10
1	A	1484	C	C5-C6-N1	5.33	123.67	121.00
1	A	644	G	C5-C6-N1	5.33	114.16	111.50
1	A	911	U	C5-C4-O4	-5.33	122.70	125.90
1	A	1301	U	P-O3'-C3'	5.33	126.09	119.70
1	A	588	G	N1-C2-N2	-5.33	111.41	116.20
1	A	666	G	C4-N9-C1'	5.33	133.42	126.50
1	A	251	G	C4-C5-N7	5.32	112.93	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	336	C	C2-N1-C1'	-5.32	112.94	118.80
1	A	384	G	C4-N9-C1'	5.32	133.42	126.50
1	A	515	G	C2-N3-C4	-5.32	109.24	111.90
1	A	703	G	N1-C2-N2	-5.32	111.41	116.20
1	A	814	A	C2-N3-C4	-5.32	107.94	110.60
1	A	819	A	C5-N7-C8	-5.32	101.24	103.90
1	A	854	G	C5-C6-N1	5.32	114.16	111.50
1	A	17	U	C2-N3-C4	-5.32	123.81	127.00
1	A	457	C	N3-C4-N4	5.32	121.72	118.00
1	A	309	G	C4-C5-N7	5.32	112.93	110.80
1	A	1234	C	N3-C4-N4	5.32	121.72	118.00
1	A	1368	G	C5-C6-N1	5.32	114.16	111.50
1	A	638	G	C4-N9-C1'	5.32	133.41	126.50
1	A	856	C	N1-C2-N3	5.32	122.92	119.20
1	A	858	G	N7-C8-N9	-5.32	110.44	113.10
1	A	916	G	C4-C5-C6	5.32	121.99	118.80
1	A	1080	A	C6-N1-C2	-5.32	115.41	118.60
1	A	1502	A	C8-N9-C1'	-5.32	118.13	127.70
1	A	297	G	C5-N7-C8	-5.32	101.64	104.30
1	A	761	G	C4-C5-C6	5.32	121.99	118.80
1	A	29	G	C4-C5-C6	5.31	121.99	118.80
1	A	92	C	N3-C2-O2	-5.31	118.18	121.90
1	A	574	A	C8-N9-C4	5.31	107.92	105.80
1	A	716	A	N1-C6-N6	-5.31	115.41	118.60
1	A	567	G	C4-C5-C6	5.31	121.99	118.80
1	A	781	A	C5-N7-C8	-5.31	101.24	103.90
1	A	688	G	C8-N9-C4	-5.31	104.28	106.40
1	A	1152	A	C5-C6-N6	5.31	127.95	123.70
1	A	1186	G	N3-C4-N9	-5.31	122.81	126.00
1	A	762	C	C6-N1-C2	5.31	122.42	120.30
1	A	1356	G	C8-N9-C4	-5.31	104.28	106.40
1	A	1511	G	N1-C6-O6	-5.31	116.72	119.90
1	A	252	U	C4-C5-C6	5.31	122.88	119.70
1	A	1112	C	C5-C6-N1	-5.30	118.35	121.00
1	A	407	G	N1-C6-O6	5.30	123.08	119.90
1	A	573	A	C4-C5-C6	5.30	119.65	117.00
1	A	1432	G	C5-C6-N1	-5.30	108.85	111.50
1	A	420	U	N3-C4-C5	-5.30	111.42	114.60
1	A	1268	A	N9-C4-C5	5.30	107.92	105.80
1	A	89	C	N3-C4-N4	5.30	121.71	118.00
1	A	362	G	C5-C6-N1	-5.30	108.85	111.50
1	A	394	G	C4-C5-N7	-5.30	108.68	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	580	U	C5-C4-O4	5.30	129.08	125.90
17	Q	63	ARG	NE-CZ-NH1	-5.30	117.65	120.30
1	A	1383	C	C5-C4-N4	-5.29	116.49	120.20
1	A	307	C	C4-C5-C6	-5.29	114.75	117.40
1	A	459	G	C8-N9-C4	-5.29	104.28	106.40
1	A	1074	G	N1-C6-O6	5.29	123.08	119.90
1	A	1246	C	N1-C2-O2	-5.29	115.72	118.90
1	A	1332	A	N1-C6-N6	-5.29	115.43	118.60
1	A	88	A	C6-N1-C2	-5.29	115.43	118.60
1	A	108	G	C1'-O4'-C4'	-5.29	105.67	109.90
1	A	317	G	N1-C6-O6	5.29	123.07	119.90
1	A	367	U	N3-C2-O2	5.29	125.90	122.20
1	A	617	G	C8-N9-C4	5.29	108.52	106.40
1	A	617	G	N1-C6-O6	5.29	123.07	119.90
1	A	783	C	C5-C4-N4	-5.29	116.50	120.20
1	A	803	G	N1-C2-N2	-5.29	111.44	116.20
1	A	942	G	C6-C5-N7	-5.29	127.23	130.40
1	A	1482	G	C2-N3-C4	5.29	114.54	111.90
1	A	647	C	C2-N1-C1'	-5.29	112.98	118.80
1	A	850	U	C5-C4-O4	5.29	129.07	125.90
1	A	570	G	N3-C4-N9	5.28	129.17	126.00
1	A	1303	C	N3-C4-C5	5.28	124.01	121.90
1	A	1355	G	C6-N1-C2	-5.28	121.93	125.10
1	A	24	U	N3-C4-O4	5.28	123.10	119.40
1	A	770	C	N3-C4-C5	5.28	124.01	121.90
1	A	886	G	N3-C4-N9	-5.28	122.83	126.00
1	A	1212	U	N1-C2-N3	-5.28	111.73	114.90
1	A	797	C	N3-C4-C5	5.28	124.01	121.90
1	A	186	C	N3-C4-N4	-5.28	114.31	118.00
1	A	315	A	N1-C2-N3	5.28	131.94	129.30
1	A	1329	A	C4-C5-N7	5.28	113.34	110.70
1	A	725	G	N7-C8-N9	5.28	115.74	113.10
1	A	923	A	C2-N3-C4	-5.28	107.96	110.60
1	A	412	A	N7-C8-N9	-5.27	111.16	113.80
1	A	1157	A	N9-C4-C5	5.27	107.91	105.80
1	A	457	C	C6-N1-C2	-5.27	118.19	120.30
1	A	904	C	N3-C4-C5	-5.27	119.79	121.90
1	A	941	G	C2-N3-C4	-5.27	109.27	111.90
1	A	351	G	C8-N9-C4	5.27	108.51	106.40
1	A	607	A	C6-C5-N7	-5.27	128.61	132.30
1	A	761	G	C4-C5-N7	5.27	112.91	110.80
1	A	190(I)	G	N9-C4-C5	-5.27	103.29	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1529	G	C4-C5-C6	5.27	121.96	118.80
1	A	867	G	C5-N7-C8	-5.26	101.67	104.30
1	A	447	G	C4-C5-N7	-5.26	108.70	110.80
1	A	825	G	C5-N7-C8	5.26	106.93	104.30
1	A	1074	G	C6-N1-C2	5.26	128.26	125.10
1	A	1496	C	C2-N3-C4	5.26	122.53	119.90
1	A	1527	C	C5-C6-N1	5.26	123.63	121.00
1	A	7	G	C6-C5-N7	5.26	133.55	130.40
1	A	229	U	N3-C4-C5	-5.26	111.45	114.60
1	A	665	A	N1-C2-N3	5.26	131.93	129.30
1	A	973	G	N9-C4-C5	-5.26	103.30	105.40
1	A	9	G	N1-C6-O6	5.25	123.05	119.90
1	A	1416	G	N7-C8-N9	5.25	115.73	113.10
1	A	6	G	C4-C5-C6	5.25	121.95	118.80
1	A	384	G	C5-C6-N1	5.25	114.13	111.50
1	A	548	G	C2-N3-C4	-5.25	109.27	111.90
1	A	774	G	C4-N9-C1'	5.25	133.33	126.50
1	A	65	U	N1-C2-O2	5.25	126.48	122.80
1	A	609	A	N7-C8-N9	5.25	116.42	113.80
1	A	1257	U	C6-N1-C2	-5.25	117.85	121.00
1	A	647	C	N1-C2-O2	-5.25	115.75	118.90
1	A	1291	G	C4-N9-C1'	5.25	133.32	126.50
1	A	1144	G	N3-C4-N9	-5.25	122.85	126.00
1	A	1467	G	C8-N9-C4	-5.25	104.30	106.40
1	A	1202	G	C6-C5-N7	5.25	133.55	130.40
1	A	1329	A	C6-C5-N7	-5.25	128.63	132.30
1	A	191	G	N1-C2-N3	5.24	127.05	123.90
1	A	257	G	N3-C4-C5	-5.24	125.98	128.60
1	A	805	C	C5-C4-N4	-5.24	116.53	120.20
1	A	142	G	C2-N3-C4	5.24	114.52	111.90
1	A	582	U	C5-C4-O4	-5.24	122.75	125.90
1	A	756	C	N3-C4-C5	5.24	124.00	121.90
1	A	1411	C	N1-C2-O2	-5.24	115.75	118.90
1	A	323	U	N1-C2-O2	-5.24	119.13	122.80
1	A	597	G	N1-C2-N3	5.24	127.05	123.90
1	A	710	G	C5-C6-N1	-5.24	108.88	111.50
1	A	1088	G	C5-C6-N1	-5.24	108.88	111.50
1	A	1353	G	C5-C6-N1	5.24	114.12	111.50
1	A	936	C	C5-C6-N1	-5.24	118.38	121.00
1	A	258	G	C5-N7-C8	-5.24	101.68	104.30
1	A	665	A	C5-C6-N1	5.24	120.32	117.70
1	A	22	G	C4-C5-N7	5.24	112.89	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	769	G	C4-C5-C6	5.24	121.94	118.80
1	A	851	G	C4-C5-C6	5.24	121.94	118.80
1	A	794	A	C5-C6-N6	5.23	127.89	123.70
1	A	1253	G	N7-C8-N9	5.23	115.72	113.10
1	A	122	G	C5-C6-O6	-5.23	125.46	128.60
1	A	270	A	C8-N9-C4	-5.23	103.71	105.80
1	A	577	G	C8-N9-C4	5.23	108.49	106.40
1	A	824	C	C5-C4-N4	-5.23	116.54	120.20
1	A	1344	C	C4-C5-C6	5.23	120.02	117.40
1	A	27	G	N1-C2-N2	-5.23	111.49	116.20
1	A	115	G	P-O3'-C3'	5.23	125.98	119.70
1	A	1328	C	N1-C2-O2	5.23	122.04	118.90
1	A	1411	C	N3-C4-C5	-5.23	119.81	121.90
1	A	656	C	C5-C6-N1	-5.23	118.39	121.00
1	A	1425	U	C4-C5-C6	5.23	122.83	119.70
1	A	484	G	C4-N9-C1'	5.22	133.29	126.50
1	A	691	G	C8-N9-C4	-5.22	104.31	106.40
1	A	701	C	C5-C6-N1	-5.22	118.39	121.00
1	A	715	A	C2-N3-C4	-5.22	107.99	110.60
1	A	1447	G	C8-N9-C4	-5.22	104.31	106.40
1	A	1498	UR3	P-O3'-C3'	5.22	125.97	119.70
1	A	665	A	N1-C6-N6	-5.22	115.47	118.60
1	A	1267	C	N3-C4-C5	-5.22	119.81	121.90
1	A	122	G	C8-N9-C4	5.22	108.49	106.40
1	A	717	C	N1-C2-O2	-5.22	115.77	118.90
1	A	1355	G	N3-C4-C5	-5.22	125.99	128.60
1	A	331	G	C2-N3-C4	-5.22	109.29	111.90
1	A	753	A	N3-C4-N9	-5.22	123.22	127.40
1	A	1265	G	C6-C5-N7	-5.22	127.27	130.40
1	A	474	G	N7-C8-N9	5.22	115.71	113.10
1	A	1451	A	N9-C4-C5	-5.22	103.71	105.80
1	A	901	A	C5-C6-N1	-5.22	115.09	117.70
1	A	130	A	C5-N7-C8	-5.21	101.29	103.90
1	A	525	C	C6-N1-C2	5.21	122.39	120.30
1	A	777	A	N3-C4-C5	-5.21	123.15	126.80
1	A	884	U	N1-C2-O2	5.21	126.45	122.80
1	A	1305	G	N7-C8-N9	5.21	115.71	113.10
1	A	1391	U	N1-C2-O2	5.21	126.45	122.80
1	A	1196	U	C3'-C2'-C1'	-5.21	97.33	101.50
1	A	53	A	N9-C4-C5	5.21	107.89	105.80
1	A	190	C	N1-C2-O2	5.21	122.03	118.90
1	A	926	G	C4-N9-C1'	5.21	133.28	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	644	G	C8-N9-C4	-5.21	104.32	106.40
1	A	308	C	C2-N1-C1'	5.21	124.53	118.80
1	A	110	C	C5-C6-N1	-5.21	118.40	121.00
1	A	418	C	C5-C6-N1	5.21	123.60	121.00
1	A	551	U	N3-C4-O4	5.21	123.05	119.40
1	A	890	G	C5-C6-O6	5.21	131.72	128.60
1	A	1172	C	N1-C2-O2	-5.21	115.78	118.90
1	A	1417	G	N3-C4-N9	5.21	129.12	126.00
1	A	1380	U	C2-N1-C1'	5.21	123.95	117.70
1	A	28	G	C4-C5-C6	5.20	121.92	118.80
1	A	594	G	C6-C5-N7	-5.20	127.28	130.40
1	A	822	C	C2-N3-C4	-5.20	117.30	119.90
1	A	1234	C	N3-C2-O2	5.20	125.54	121.90
11	K	118	GLY	N-CA-C	5.20	126.11	113.10
1	A	132	C	C2-N3-C4	-5.20	117.30	119.90
1	A	103	C	N3-C4-N4	5.20	121.64	118.00
1	A	494	G	N9-C4-C5	5.20	107.48	105.40
1	A	232	G	C8-N9-C1'	-5.20	120.24	127.00
1	A	617	G	N1-C2-N3	5.20	127.02	123.90
1	A	768	A	C2-N3-C4	-5.20	108.00	110.60
1	A	799	G	N1-C2-N3	5.20	127.02	123.90
1	A	1462	G	C5-C6-N1	-5.20	108.90	111.50
1	A	550	G	C2-N3-C4	-5.20	109.30	111.90
1	A	1531	A	C4-N9-C1'	5.20	135.65	126.30
1	A	721	G	C5-C6-O6	-5.19	125.48	128.60
1	A	824	C	C5-C6-N1	-5.19	118.40	121.00
1	A	121	C	N3-C4-C5	5.19	123.98	121.90
1	A	46	G	C4-N9-C1'	5.19	133.25	126.50
1	A	559	A	N9-C4-C5	5.19	107.88	105.80
1	A	777	A	N3-C4-N9	5.19	131.55	127.40
1	A	1088	G	C2-N3-C4	-5.19	109.31	111.90
1	A	1079	G	C4-N9-C1'	5.19	133.25	126.50
1	A	1243	C	N3-C4-C5	5.19	123.98	121.90
1	A	168	G	C4-N9-C1'	5.19	133.24	126.50
1	A	957	U	N3-C4-C5	-5.19	111.49	114.60
1	A	587	G	N1-C2-N2	-5.19	111.53	116.20
1	A	853	G	N1-C2-N2	-5.19	111.53	116.20
1	A	1355	G	C5-C6-N1	5.19	114.09	111.50
1	A	248	C	N3-C4-N4	5.18	121.63	118.00
1	A	1158	C	N3-C4-C5	-5.18	119.83	121.90
1	A	134	A	N7-C8-N9	-5.18	111.21	113.80
1	A	1425	U	N3-C4-C5	-5.18	111.49	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	269	C	C4-C5-C6	5.18	119.99	117.40
1	A	685	G	N9-C4-C5	-5.18	103.33	105.40
1	A	8	A	C4-C5-N7	-5.18	108.11	110.70
1	A	517	G	N9-C4-C5	5.18	107.47	105.40
1	A	830	G	C5-C6-N1	-5.18	108.91	111.50
1	A	917	G	N3-C4-C5	5.18	131.19	128.60
1	A	321	A	C5-C6-N1	5.18	120.29	117.70
1	A	246	A	C8-N9-C4	5.17	107.87	105.80
1	A	259	G	C6-C5-N7	-5.17	127.30	130.40
1	A	762	C	N3-C4-N4	5.17	121.62	118.00
1	A	1533	C	C6-N1-C2	-5.17	118.23	120.30
1	A	225	C	C5-C6-N1	-5.17	118.41	121.00
1	A	315	A	N7-C8-N9	5.17	116.39	113.80
1	A	1494	G	N3-C4-N9	5.17	129.10	126.00
1	A	23	C	C4-C5-C6	5.17	119.99	117.40
1	A	96	G	C6-C5-N7	-5.17	127.30	130.40
1	A	263	A	C6-N1-C2	-5.17	115.50	118.60
1	A	635	G	C5-C6-N1	-5.17	108.91	111.50
1	A	894	G	C6-C5-N7	-5.17	127.30	130.40
1	A	1135	U	C5-C6-N1	5.17	125.28	122.70
1	A	315	A	C5-N7-C8	-5.17	101.32	103.90
1	A	632	A	C6-C5-N7	-5.17	128.68	132.30
1	A	803	G	C2-N3-C4	-5.17	109.32	111.90
1	A	898	G	N1-C2-N3	5.17	127.00	123.90
1	A	1385	G	N1-C6-O6	-5.17	116.80	119.90
1	A	581	G	N3-C4-C5	5.17	131.18	128.60
1	A	1286	A	C5-C6-N1	-5.17	115.12	117.70
8	H	60	ARG	CG-CD-NE	-5.17	100.95	111.80
1	A	218	C	C4-C5-C6	-5.16	114.82	117.40
1	A	235	C	C2-N3-C4	-5.16	117.32	119.90
1	A	246	A	N1-C6-N6	-5.16	115.50	118.60
1	A	610	G	N1-C2-N3	5.16	127.00	123.90
1	A	1512	U	N3-C4-O4	5.16	123.02	119.40
1	A	132	C	N3-C2-O2	-5.16	118.29	121.90
1	A	729	A	C4-C5-N7	5.16	113.28	110.70
1	A	797	C	C2-N3-C4	-5.16	117.32	119.90
1	A	615	C	N3-C4-N4	5.16	121.61	118.00
1	A	657	G	C8-N9-C4	-5.16	104.34	106.40
1	A	569	C	C4-C5-C6	5.16	119.98	117.40
1	A	660	G	C5-C6-O6	-5.16	125.50	128.60
1	A	668	G	N1-C2-N3	5.16	127.00	123.90
1	A	872	A	C5-N7-C8	-5.16	101.32	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	289	G	N1-C6-O6	5.16	122.99	119.90
1	A	728	A	N7-C8-N9	5.15	116.38	113.80
1	A	1527	C	N3-C4-N4	5.15	121.61	118.00
1	A	203	U	C4-C5-C6	-5.15	116.61	119.70
1	A	109	A	C8-N9-C4	-5.15	103.74	105.80
1	A	1199	U	C4-C5-C6	5.15	122.79	119.70
1	A	1483	A	C6-N1-C2	-5.15	115.51	118.60
1	A	383	A	C5-N7-C8	-5.15	101.33	103.90
1	A	390	C	C4-C5-C6	5.15	119.97	117.40
1	A	600	C	C6-N1-C2	5.15	122.36	120.30
1	A	691	G	C2-N3-C4	-5.15	109.33	111.90
1	A	360	A	C2-N3-C4	-5.14	108.03	110.60
1	A	602	A	N9-C4-C5	5.14	107.86	105.80
1	A	800	G	N1-C2-N3	5.14	126.99	123.90
1	A	32	A	C8-N9-C1'	-5.14	118.44	127.70
1	A	718	G	N3-C2-N2	-5.14	116.30	119.90
1	A	895	G	C4-N9-C1'	5.14	133.19	126.50
1	A	900	A	C6-C5-N7	-5.14	128.70	132.30
1	A	1145	C	C6-N1-C1'	5.14	126.97	120.80
1	A	1229	A	C2-N3-C4	-5.14	108.03	110.60
1	A	400	C	N3-C2-O2	-5.14	118.30	121.90
1	A	1294	G	N3-C4-N9	-5.14	122.92	126.00
1	A	280	C	N3-C4-N4	-5.14	114.40	118.00
1	A	421	U	C2-N1-C1'	5.14	123.87	117.70
1	A	1035	A	C8-N9-C4	5.14	107.86	105.80
1	A	1051	C	C2-N3-C4	5.14	122.47	119.90
1	A	1191	A	N1-C6-N6	-5.14	115.52	118.60
1	A	1219	U	C5-C6-N1	5.14	125.27	122.70
1	A	233	C	N3-C4-N4	5.14	121.60	118.00
1	A	1482	G	N3-C2-N2	5.14	123.50	119.90
1	A	255	G	C5-C6-N1	-5.14	108.93	111.50
1	A	812	C	N1-C2-N3	5.13	122.79	119.20
1	A	251	G	C5-N7-C8	-5.13	101.73	104.30
1	A	383	A	C6-C5-N7	-5.13	128.71	132.30
17	Q	35	VAL	CG1-CB-CG2	5.13	119.11	110.90
1	A	627	G	N1-C2-N3	5.13	126.98	123.90
1	A	1286	A	N7-C8-N9	5.13	116.36	113.80
1	A	746	A	N1-C6-N6	5.13	121.68	118.60
1	A	825	G	N9-C4-C5	-5.13	103.35	105.40
1	A	888	G	C5-C6-N1	-5.13	108.94	111.50
1	A	492	G	C5-C6-N1	-5.13	108.94	111.50
1	A	698	G	N7-C8-N9	5.13	115.66	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1110	A	C2-N3-C4	-5.13	108.04	110.60
1	A	766	A	C6-C5-N7	-5.12	128.71	132.30
1	A	380	G	C4-C5-N7	-5.12	108.75	110.80
1	A	1323	G	C8-N9-C4	5.12	108.45	106.40
5	E	115	VAL	CB-CA-C	-5.12	101.66	111.40
1	A	43	C	N3-C4-N4	-5.12	114.42	118.00
1	A	1432	G	C2-N3-C4	-5.12	109.34	111.90
1	A	238	G	N3-C4-C5	5.12	131.16	128.60
1	A	344	A	N7-C8-N9	5.12	116.36	113.80
1	A	813	U	C2-N3-C4	-5.12	123.93	127.00
1	A	48	C	C6-N1-C2	5.12	122.35	120.30
1	A	672	U	N3-C2-O2	5.12	125.78	122.20
1	A	319	G	C4-N9-C1'	5.12	133.15	126.50
1	A	701	C	P-O3'-C3'	5.12	125.84	119.70
1	A	1496	C	C6-N1-C2	-5.12	118.25	120.30
2	B	16	HIS	N-CA-C	5.12	124.82	111.00
15	O	39	LEU	CA-CB-CG	-5.12	103.53	115.30
1	A	306	G	N3-C2-N2	-5.12	116.32	119.90
1	A	899	C	C6-N1-C2	-5.12	118.25	120.30
1	A	1426	C	C6-N1-C2	5.12	122.35	120.30
1	A	1432	G	C5-C6-O6	5.12	131.67	128.60
1	A	55	A	C8-N9-C4	-5.11	103.75	105.80
1	A	640	A	N1-C2-N3	5.11	131.86	129.30
1	A	709	G	N1-C6-O6	5.11	122.97	119.90
1	A	1064	G	C4-N9-C1'	5.11	133.15	126.50
1	A	355	C	N3-C4-C5	5.11	123.94	121.90
1	A	645	C	C6-N1-C2	-5.11	118.25	120.30
1	A	814	A	N7-C8-N9	-5.11	111.24	113.80
1	A	256	U	C5-C6-N1	5.11	125.25	122.70
1	A	451	A	C5-C6-N1	5.11	120.25	117.70
1	A	702	A	C2-N3-C4	5.11	113.15	110.60
1	A	1141	C	N3-C2-O2	-5.11	118.33	121.90
1	A	652	U	C5-C4-O4	-5.10	122.84	125.90
1	A	7	G	C6-N1-C2	-5.10	122.04	125.10
1	A	508	C	C6-N1-C1'	-5.10	114.68	120.80
1	A	638	G	C4-C5-C6	5.10	121.86	118.80
1	A	833	U	N1-C2-O2	5.10	126.37	122.80
1	A	756	C	C4-C5-C6	-5.10	114.85	117.40
1	A	1249	C	N1-C2-N3	-5.10	115.63	119.20
1	A	1251	A	C8-N9-C4	-5.10	103.76	105.80
1	A	1282	C	C2-N3-C4	5.10	122.45	119.90
1	A	1520	G	N1-C2-N3	5.10	126.96	123.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	119	LEU	CB-CG-CD1	-5.10	102.33	111.00
1	A	140	A	C8-N9-C4	-5.10	103.76	105.80
1	A	860	A	N1-C6-N6	5.10	121.66	118.60
1	A	1009	G	N3-C4-C5	-5.10	126.05	128.60
1	A	194	C	N1-C2-O2	5.09	121.96	118.90
1	A	368	U	C2-N3-C4	-5.09	123.94	127.00
1	A	587	G	N1-C2-N3	5.09	126.96	123.90
1	A	941	G	C4-C5-N7	5.09	112.84	110.80
1	A	872	A	N3-C4-C5	5.09	130.37	126.80
1	A	1482	G	C6-N1-C2	-5.09	122.04	125.10
1	A	287	U	N3-C4-C5	-5.09	111.55	114.60
1	A	575	G	C6-N1-C2	-5.09	122.05	125.10
1	A	660	G	N1-C6-O6	5.09	122.95	119.90
1	A	907	A	N9-C4-C5	5.09	107.84	105.80
1	A	1287	A	C8-N9-C4	-5.09	103.77	105.80
1	A	1254	C	C5-C6-N1	5.09	123.54	121.00
1	A	142	G	N3-C4-N9	5.08	129.05	126.00
1	A	567	G	N1-C6-O6	-5.08	116.85	119.90
1	A	700	G	C4-N9-C1'	5.08	133.11	126.50
1	A	1055	A	C6-C5-N7	5.08	135.86	132.30
1	A	1126	U	C2-N1-C1'	5.08	123.80	117.70
1	A	167	G	N1-C6-O6	-5.08	116.85	119.90
1	A	200	G	C8-N9-C4	-5.08	104.37	106.40
1	A	452	A	C5-N7-C8	5.08	106.44	103.90
1	A	638	G	C2-N3-C4	-5.08	109.36	111.90
1	A	301	G	N1-C6-O6	5.08	122.95	119.90
1	A	181	G	C4-C5-N7	5.08	112.83	110.80
1	A	577	G	C4-C5-N7	5.08	112.83	110.80
1	A	822	C	N3-C4-C5	-5.08	119.87	121.90
1	A	946	A	C4-C5-N7	-5.08	108.16	110.70
1	A	26	A	C8-N9-C4	-5.07	103.77	105.80
1	A	119	A	C5-N7-C8	5.07	106.44	103.90
1	A	15	G	N7-C8-N9	5.07	115.64	113.10
1	A	801	U	N3-C4-C5	5.07	117.64	114.60
1	A	1465	C	N3-C4-N4	5.07	121.55	118.00
1	A	698	G	N9-C4-C5	5.07	107.43	105.40
1	A	1452	C	C6-N1-C1'	-5.07	114.72	120.80
1	A	7	G	N7-C8-N9	-5.07	110.57	113.10
1	A	93	G	C8-N9-C4	5.07	108.43	106.40
1	A	612	C	C2-N1-C1'	5.07	124.37	118.80
1	A	760	G	C4-N9-C1'	-5.07	119.91	126.50
1	A	90	U	N1-C2-O2	-5.07	119.25	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1155	G	N3-C4-C5	-5.06	126.07	128.60
1	A	1329	A	C5-N7-C8	-5.06	101.37	103.90
1	A	916	G	C5-C6-O6	-5.06	125.56	128.60
1	A	1160	G	N1-C6-O6	-5.06	116.86	119.90
1	A	1279	A	C8-N9-C4	-5.06	103.78	105.80
1	A	1387	G	C2-N3-C4	-5.06	109.37	111.90
1	A	1516	G	C2-N3-C4	-5.06	109.37	111.90
1	A	1112	C	N3-C4-C5	5.06	123.92	121.90
1	A	261	U	C6-N1-C2	-5.06	117.97	121.00
1	A	1067	A	C6-N1-C2	-5.06	115.56	118.60
1	A	506	G	C2-N3-C4	-5.06	109.37	111.90
1	A	928	G	N1-C6-O6	5.06	122.93	119.90
1	A	236	G	N1-C2-N2	-5.06	111.65	116.20
1	A	839	U	C2-N1-C1'	5.06	123.77	117.70
1	A	306	G	N1-C6-O6	5.05	122.93	119.90
1	A	319	G	N1-C6-O6	5.05	122.93	119.90
4	D	97	LEU	CA-CB-CG	-5.05	103.67	115.30
1	A	595	G	C8-N9-C1'	-5.05	120.43	127.00
1	A	661	G	N7-C8-N9	5.05	115.63	113.10
1	A	866	C	N1-C2-O2	-5.05	115.87	118.90
1	A	1530	G	C2-N3-C4	-5.05	109.37	111.90
1	A	488	C	C5-C6-N1	5.05	123.52	121.00
1	A	580	U	C2-N3-C4	5.05	130.03	127.00
1	A	761	G	N9-C4-C5	-5.05	103.38	105.40
1	A	1441	G	C4-C5-N7	-5.05	108.78	110.80
1	A	1249	C	C4-C5-C6	-5.05	114.88	117.40
1	A	1303	C	C2-N1-C1'	-5.05	113.25	118.80
1	A	1403	C	N3-C2-O2	5.05	125.43	121.90
1	A	1408	A	C2-N3-C4	-5.05	108.08	110.60
1	A	1329	A	C5-C6-N6	-5.04	119.66	123.70
1	A	1108	G	N3-C4-N9	5.04	129.03	126.00
1	A	1514	C	N1-C2-N3	5.04	122.73	119.20
1	A	1470	G	N1-C6-O6	5.04	122.92	119.90
1	A	332	G	C2-N3-C4	-5.04	109.38	111.90
1	A	350	G	C5-C6-O6	5.04	131.62	128.60
1	A	773	G	C5-N7-C8	-5.04	101.78	104.30
1	A	1155	G	C4-N9-C1'	5.04	133.05	126.50
1	A	1311	G	N3-C2-N2	-5.04	116.37	119.90
1	A	1349	A	N3-C4-N9	-5.04	123.37	127.40
1	A	827	U	N3-C4-O4	5.04	122.93	119.40
1	A	728	A	C2-N3-C4	-5.04	108.08	110.60
1	A	1084	G	N9-C4-C5	5.04	107.42	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	407	G	N1-C2-N3	5.03	126.92	123.90
1	A	1380	U	P-O3'-C3'	5.03	125.74	119.70
1	A	395	C	N3-C4-C5	-5.03	119.89	121.90
1	A	771	G	N1-C2-N3	5.03	126.92	123.90
1	A	1079	G	C5-C6-O6	-5.03	125.58	128.60
1	A	699	C	N3-C2-O2	5.03	125.42	121.90
1	A	1059	C	N1-C2-N3	5.03	122.72	119.20
1	A	1060	C	C6-N1-C1'	-5.03	114.77	120.80
1	A	132	C	N3-C4-C5	-5.03	119.89	121.90
1	A	649	G	C5-C6-N1	5.03	114.01	111.50
1	A	802	A	C4-C5-N7	5.03	113.21	110.70
1	A	1083	U	N3-C4-O4	5.03	122.92	119.40
1	A	568	G	C4-N9-C1'	5.02	133.03	126.50
1	A	667	G	C6-C5-N7	-5.02	127.39	130.40
1	A	711	G	C5-C6-O6	-5.02	125.59	128.60
1	A	546	G	C6-C5-N7	-5.02	127.39	130.40
1	A	41	G	N7-C8-N9	5.02	115.61	113.10
1	A	532	A	C8-N9-C4	5.02	107.81	105.80
1	A	7	G	N9-C4-C5	5.02	107.41	105.40
1	A	17	U	C5-C6-N1	-5.02	120.19	122.70
1	A	348	G	C5-N7-C8	-5.02	101.79	104.30
1	A	451	A	C5-C6-N6	-5.02	119.69	123.70
1	A	780	A	C2-N3-C4	5.02	113.11	110.60
1	A	860	A	C6-C5-N7	-5.02	128.79	132.30
1	A	1324	A	C6-C5-N7	-5.02	128.79	132.30
1	A	175	C	C6-N1-C2	5.01	122.31	120.30
1	A	854	G	C6-N1-C2	-5.01	122.09	125.10
1	A	906	G	C6-C5-N7	-5.01	127.39	130.40
1	A	389	A	N3-C4-C5	-5.01	123.29	126.80
1	A	276	G	C8-N9-C4	5.01	108.40	106.40
1	A	906	G	C5-N7-C8	-5.01	101.80	104.30
1	A	80	G	C4-C5-C6	5.01	121.81	118.80
1	A	331	G	C4-C5-C6	5.01	121.81	118.80
1	A	651	C	C5-C4-N4	-5.01	116.69	120.20
3	C	52	LEU	CA-CB-CG	5.01	126.82	115.30
1	A	183	G	C6-C5-N7	-5.01	127.40	130.40
1	A	642	A	C5-N7-C8	-5.01	101.40	103.90
1	A	481	G	N1-C2-N2	-5.00	111.69	116.20
1	A	1087	G	C6-C5-N7	-5.00	127.40	130.40
1	A	226	G	C5-C6-N1	-5.00	109.00	111.50
1	A	232	G	C5-C6-N1	-5.00	109.00	111.50
1	A	1229	A	C5-N7-C8	-5.00	101.40	103.90

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	166	GLU	Peptide
3	C	24	ALA	Peptide
4	D	195	ALA	Peptide
7	G	154	TYR	Peptide
8	H	90	GLY	Peptide
9	I	126	SER	Peptide
10	J	3	LYS	Peptide
10	J	87	THR	Peptide
12	L	25	PRO	Peptide
17	Q	13	ASP	Peptide
20	T	93	GLU	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32508	0	16426	863	0
2	B	1900	0	1951	117	0
3	C	1612	0	1677	93	0
4	D	1703	0	1763	100	0
5	E	1146	0	1207	73	0
6	F	843	0	857	55	0
7	G	1257	0	1296	76	0
8	H	1116	0	1177	70	0
9	I	1010	0	1037	76	0
10	J	792	0	835	50	0
11	K	864	0	881	51	0
12	L	972	0	1058	67	0
13	M	937	0	995	55	0
14	N	492	0	529	49	0
15	O	729	0	768	47	0
16	P	700	0	720	48	0
17	Q	823	0	893	52	0
18	R	574	0	644	47	0
19	S	647	0	673	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	T	763	0	861	49	0
21	U	208	0	221	20	0
22	A	40	0	37	7	0
23	A	253	0	0	0	0
23	B	2	0	0	0	0
23	D	1	0	0	0	0
23	E	1	0	0	0	0
23	H	4	0	0	0	0
23	J	2	0	0	0	0
23	M	2	0	0	0	0
23	N	1	0	0	0	0
23	P	3	0	0	0	0
23	Q	1	0	0	0	0
23	S	1	0	0	0	0
23	T	2	0	0	0	0
24	D	1	0	0	0	0
24	N	1	0	0	0	0
25	A	374	0	0	14	0
25	B	1	0	0	0	0
25	D	1	0	0	0	0
25	E	7	0	0	0	0
25	L	1	0	0	0	0
25	N	1	0	0	0	0
25	P	2	0	0	0	0
25	T	2	0	0	1	0
All	All	52300	0	36506	1903	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 22.

All (1903) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:26:LEU:HD11	18:R:42:ARG:HD3	1.46	0.98
1:A:792:A:H1'	1:A:793:U:H2'	1.47	0.96
11:K:48:ILE:HD12	11:K:63:LEU:HB2	1.45	0.96
1:A:1326:C:OP2	21:U:6:ARG:NH2	2.00	0.93
12:L:87:GLY:HA2	12:L:98:TYR:HA	1.51	0.92
3:C:129:ALA:HB1	3:C:132:ARG:HB3	1.51	0.92
3:C:27:LYS:O	3:C:30:ARG:NH2	2.05	0.89
1:A:103:C:OP1	20:T:17:ARG:NH1	2.05	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:87:ARG:HH11	6:F:87:ARG:HG3	1.36	0.89
1:A:1030:C:O2	1:A:1031:G:N2	2.05	0.89
15:O:39:LEU:HD23	15:O:56:LEU:HB2	1.53	0.89
3:C:153:VAL:HG12	3:C:166:GLU:HB2	1.55	0.89
1:A:1373:G:H5''	7:G:36:LYS:HD2	1.55	0.88
11:K:91:ARG:HD2	18:R:88:LYS:HZ3	1.36	0.88
1:A:1496:C:O2'	1:A:1497:G:O5'	1.91	0.87
1:A:1126:U:H3'	1:A:1127:G:H8	1.36	0.87
1:A:1249:C:O2'	9:I:73:GLN:NE2	2.07	0.86
3:C:188:LEU:HD11	3:C:195:VAL:HG23	1.57	0.86
7:G:69:VAL:HG21	7:G:104:LEU:HD21	1.58	0.86
6:F:36:ARG:HB3	6:F:36:ARG:HH11	1.40	0.86
3:C:58:GLU:O	3:C:59:ARG:NH1	2.09	0.86
3:C:34:LEU:HD13	3:C:38:ARG:HH21	1.40	0.86
7:G:78:ARG:HD2	7:G:156:TRP:HB2	1.58	0.86
1:A:973:G:H3'	1:A:974:A:H5''	1.57	0.85
1:A:1442:G:N2	1:A:1447:G:N7	2.22	0.85
15:O:29:VAL:HG21	15:O:67:LEU:HD23	1.59	0.85
5:E:11:ILE:HG23	5:E:31:LEU:HB3	1.59	0.84
5:E:84:PHE:HB2	5:E:134:ALA:HB2	1.59	0.84
7:G:5:ARG:HH12	7:G:8:GLU:HG3	1.41	0.84
21:U:12:LYS:O	21:U:22:ARG:NH1	2.11	0.83
1:A:235:C:N4	25:A:1963:HOH:O	2.10	0.83
19:S:31:ILE:HG21	19:S:49:ILE:HD13	1.61	0.83
11:K:65:ALA:HB1	11:K:98:LEU:HD13	1.61	0.82
1:A:1366:C:H2'	1:A:1367:C:H6	1.44	0.82
1:A:1221:G:OP2	19:S:37:ARG:NH2	2.11	0.82
3:C:121:ALA:HA	3:C:124:ILE:HD12	1.61	0.82
1:A:1255:G:N2	1:A:1259:C:O2	2.13	0.82
1:A:1357:A:H2'	1:A:1358:U:C6	2.14	0.81
15:O:38:ARG:HH11	15:O:38:ARG:HB3	1.46	0.81
1:A:1238:A:H5'	1:A:1336:C:H41	1.45	0.81
1:A:138:G:O6	1:A:225:C:N4	2.09	0.81
8:H:11:THR:OG1	8:H:14:ARG:NH1	2.11	0.81
1:A:1510:U:H2'	1:A:1511:G:C8	2.16	0.81
17:Q:27:PHE:CE1	17:Q:36:ILE:HD11	2.15	0.81
18:R:53:ARG:HG2	18:R:63:GLN:HE21	1.46	0.81
5:E:126:ARG:HH11	5:E:126:ARG:HG2	1.46	0.81
13:M:10:PRO:HB2	13:M:18:ALA:HB1	1.60	0.81
1:A:1404:5MC:H1'	1:A:1499:A:C2	2.15	0.81
1:A:996:A:N1	1:A:1046:A:O2'	2.13	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:156:ARG:NH1	3:C:160:ALA:O	2.14	0.80
2:B:12:GLU:HG3	2:B:213:LEU:HD21	1.63	0.80
12:L:47:LYS:HG3	12:L:48:PRO:HD3	1.63	0.80
7:G:17:VAL:HG12	7:G:18:TYR:HD1	1.47	0.80
13:M:75:ALA:HA	13:M:78:ILE:HD12	1.64	0.80
1:A:1009:G:H1	1:A:1020:U:H3	1.27	0.80
7:G:5:ARG:HD3	7:G:7:ALA:H	1.47	0.79
8:H:100:ILE:O	8:H:125:ARG:NH2	2.16	0.79
12:L:59:ARG:HH12	12:L:65:GLU:HG3	1.47	0.79
1:A:989:C:O2	1:A:1216:G:N2	2.13	0.79
8:H:69:ARG:NH1	8:H:75:ARG:O	2.15	0.79
1:A:1047:G:OP1	14:N:4:LYS:NZ	2.13	0.79
3:C:134:ILE:HD11	3:C:153:VAL:HB	1.65	0.79
9:I:79:LEU:HD21	9:I:104:ARG:HA	1.65	0.79
9:I:108:VAL:HG12	9:I:109:VAL:H	1.48	0.79
1:A:1280:A:O2'	25:A:2104:HOH:O	2.01	0.78
16:P:67:THR:HB	16:P:70:ALA:H	1.47	0.78
1:A:1163:C:H2'	1:A:1164:G:H8	1.49	0.78
6:F:14:LEU:HB2	6:F:19:LEU:HD12	1.64	0.78
1:A:1101:A:H4'	1:A:1102:A:O5'	1.84	0.77
20:T:12:ALA:HA	25:T:302:HOH:O	1.82	0.77
1:A:130:A:H5'	17:Q:63:ARG:HE	1.50	0.77
7:G:20:ASP:OD1	7:G:22:LEU:N	2.16	0.77
1:A:1347:G:H3'	9:I:108:VAL:O	1.85	0.77
1:A:992:U:H3	1:A:1044:A:H62	1.30	0.77
3:C:167:TRP:HE3	3:C:168:ALA:H	1.32	0.77
1:A:1246:C:H42	1:A:1291:G:H1	1.32	0.76
1:A:457:C:O2	1:A:475:G:N2	2.11	0.76
1:A:1435:G:H2'	1:A:1436:U:C6	2.21	0.76
22:A:1601:SRY:OG2	12:L:91:LYS:NZ	2.17	0.76
10:J:53:PRO:HB3	14:N:42:ILE:HD11	1.68	0.76
3:C:147:LYS:NZ	3:C:206:GLU:OE2	2.18	0.75
9:I:17:VAL:HG11	9:I:81:ILE:HA	1.68	0.75
15:O:67:LEU:HD13	15:O:78:TYR:HE1	1.51	0.75
1:A:1380:U:O2'	1:A:1381:U:OP2	2.04	0.75
8:H:17:THR:O	8:H:78:GLN:NE2	2.20	0.75
12:L:5:PRO:HB2	12:L:10:LEU:HD23	1.68	0.75
4:D:8:VAL:HG11	4:D:21:LEU:HB2	1.68	0.75
12:L:53:ARG:NH1	12:L:92:0TD:OD2	2.20	0.75
1:A:1242:C:H42	1:A:1295:G:H1	1.34	0.74
1:A:448:A:OP2	1:A:485:G:N2	2.16	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:664:G:H22	1:A:741:G:H1	1.33	0.74
1:A:1356:G:H2'	1:A:1357:A:C8	2.23	0.74
1:A:532:A:O2'	1:A:533:A:OP1	2.06	0.73
4:D:28:SER:O	4:D:30:LYS:N	2.21	0.73
1:A:1125:U:H3	10:J:5:ARG:HH21	1.36	0.73
1:A:1118:C:H1'	1:A:1179:A:C4	2.23	0.73
1:A:617:G:H1	1:A:623:C:H42	1.35	0.73
1:A:975:A:H5'	1:A:975:A:H8	1.52	0.73
7:G:38:LEU:O	7:G:42:ILE:HG13	1.89	0.73
20:T:56:MET:HG3	20:T:88:VAL:HG21	1.69	0.72
8:H:82:HIS:CE1	8:H:138:TRP:NE1	2.57	0.72
17:Q:40:LYS:HD3	17:Q:42:TYR:CZ	2.24	0.72
1:A:869:G:N7	25:A:2218:HOH:O	2.21	0.72
1:A:1195:C:H3'	1:A:1196:U:H5''	1.71	0.72
1:A:1493:A:H2'	1:A:1494:G:H8	1.53	0.72
1:A:794:A:H8	1:A:794:A:H3'	1.55	0.72
1:A:914:G:OP1	22:A:1601:SRY:HI33	1.90	0.72
7:G:111:ARG:HD2	7:G:112:PRO:HD2	1.72	0.72
11:K:79:SER:HB3	11:K:106:LYS:HE2	1.71	0.72
1:A:701:C:H4'	1:A:702:A:H5''	1.72	0.72
3:C:25:GLY:HA2	3:C:28:GLN:H	1.54	0.72
1:A:18:C:H5''	5:E:127:ASN:HD21	1.53	0.72
1:A:113:G:H1'	1:A:354:G:H5'	1.72	0.72
2:B:55:PHE:HA	2:B:58:ILE:HD12	1.71	0.72
7:G:15:ASP:OD2	7:G:44:TYR:OH	2.07	0.72
1:A:1412:C:H2'	1:A:1413:A:C8	2.24	0.71
1:A:794:A:H3'	1:A:794:A:C8	2.25	0.71
2:B:184:VAL:HG23	2:B:198:ASP:H	1.55	0.71
1:A:1125:U:OP2	1:A:1145:C:N4	2.23	0.71
2:B:17:PHE:HA	2:B:44:LEU:HD11	1.72	0.71
5:E:147:ASP:OD1	5:E:147:ASP:N	2.12	0.71
1:A:1357:A:H2'	1:A:1358:U:H6	1.56	0.71
4:D:152:SER:O	4:D:155:LEU:HG	1.90	0.71
1:A:1368:G:H5''	9:I:112:LYS:HB3	1.73	0.71
1:A:384:G:H2'	1:A:385:C:H6	1.56	0.71
1:A:74:C:O2	1:A:96:G:N2	2.20	0.71
13:M:23:TYR:CB	13:M:67:GLU:HA	2.20	0.71
1:A:1411:C:H42	1:A:1489:G:H1	1.38	0.71
1:A:73:C:H2'	1:A:74:C:H6	1.54	0.71
6:F:4:TYR:HE1	6:F:92:LYS:HG2	1.56	0.71
2:B:205:ASP:OD1	2:B:206:ASP:N	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:C:OP1	12:L:123:LYS:NZ	2.22	0.70
1:A:980:C:H5''	1:A:981:U:H5	1.56	0.70
4:D:187:ARG:HH22	4:D:188:LEU:HD12	1.56	0.70
1:A:858:G:N7	25:A:2220:HOH:O	2.24	0.70
1:A:1053:G:HO2'	1:A:1199:U:H5	1.39	0.70
1:A:200:G:H1	1:A:217:C:H42	1.38	0.70
1:A:1004:A:O2'	1:A:1005:A:O5'	2.08	0.70
9:I:48:GLU:OE2	9:I:51:ARG:NH1	2.24	0.70
2:B:73:THR:HG21	2:B:96:ARG:HD2	1.74	0.70
8:H:95:VAL:HG23	8:H:99:GLU:HB2	1.73	0.70
15:O:87:ILE:HG22	15:O:88:ARG:H	1.54	0.70
2:B:87:ARG:HH21	2:B:233:SER:HB2	1.57	0.70
1:A:1255:G:O6	1:A:1282:C:N4	2.22	0.70
1:A:1518:MA6:H93	1:A:1519:MA6:N1	2.06	0.70
21:U:10:ARG:HD3	21:U:13:ILE:HD12	1.74	0.69
1:A:1168:A:H2'	1:A:1169:A:C8	2.28	0.69
1:A:1236:A:H4'	1:A:1304:G:H4'	1.74	0.69
3:C:155:GLY:HA3	3:C:163:ALA:HB1	1.73	0.69
6:F:4:TYR:HB2	6:F:65:VAL:HG22	1.71	0.69
7:G:92:SER:OG	7:G:95:ARG:N	2.21	0.69
1:A:103:C:P	20:T:17:ARG:HH12	2.15	0.69
1:A:1358:U:H5''	14:N:35:ARG:HD2	1.73	0.69
1:A:353:A:H5'	1:A:353:A:H8	1.56	0.69
1:A:993:G:O6	1:A:1045:C:N4	2.26	0.69
2:B:185:ILE:HA	2:B:199:TYR:O	1.92	0.69
16:P:68:ASP:OD1	16:P:68:ASP:N	2.24	0.69
4:D:63:LYS:NZ	4:D:197:PRO:O	2.26	0.69
4:D:65:ARG:HG3	4:D:75:PHE:CD1	2.27	0.69
6:F:14:LEU:HD21	6:F:84:ASN:HD22	1.57	0.69
10:J:38:ILE:HG22	10:J:39:PRO:HD2	1.74	0.69
22:A:1601:SRY:O61	12:L:46:LYS:HD2	1.93	0.69
13:M:23:TYR:HB3	13:M:67:GLU:HA	1.73	0.69
19:S:22:LEU:HD11	19:S:28:LYS:HB2	1.75	0.69
1:A:250:A:H4'	1:A:251:G:O5'	1.93	0.68
1:A:827:U:H5''	1:A:828:A:OP2	1.93	0.68
3:C:120:VAL:HG12	3:C:124:ILE:HD11	1.75	0.68
1:A:36:C:H5''	12:L:123:LYS:HD3	1.75	0.68
1:A:677:U:H3	1:A:713:G:H22	1.40	0.68
1:A:1329:A:H5'	13:M:29:ARG:HD2	1.75	0.68
1:A:390:C:H4'	16:P:28:ARG:HH21	1.58	0.68
1:A:1290:G:H2'	1:A:1291:G:H8	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:40:ILE:HD11	19:S:62:ILE:HG23	1.75	0.68
1:A:1246:C:N4	1:A:1291:G:H1	1.91	0.68
1:A:1124:G:H2'	1:A:1145:C:H41	1.59	0.68
3:C:14:ILE:HB	3:C:15:THR:HG23	1.75	0.68
1:A:758:G:C8	25:A:2216:HOH:O	2.47	0.68
17:Q:84:LEU:H	17:Q:84:LEU:HD12	1.59	0.68
1:A:1022:G:N2	1:A:1023:G:O6	2.25	0.68
1:A:452:A:O2'	1:A:453:A:O5'	2.12	0.68
1:A:501:C:H2'	1:A:502:G:C8	2.28	0.68
4:D:119:GLN:HG3	4:D:123:HIS:HD2	1.59	0.68
5:E:105:VAL:HB	5:E:106:PRO:HD3	1.75	0.68
1:A:1338:G:H2'	1:A:1339:A:C8	2.28	0.68
10:J:12:ASP:HB3	10:J:15:THR:HG22	1.76	0.68
13:M:11:ARG:HA	13:M:45:VAL:HG11	1.74	0.68
1:A:505:G:H1	1:A:526:C:H42	1.40	0.67
1:A:1058:G:OP1	3:C:199:LYS:NZ	2.27	0.67
14:N:26:ARG:HD2	14:N:47:LEU:HD11	1.76	0.67
1:A:1095:U:OP1	1:A:1108:G:N2	2.20	0.67
6:F:100:ASN:HB2	18:R:23:LYS:HD2	1.74	0.67
1:A:1006:C:H42	1:A:1022:G:H1	1.39	0.67
5:E:145:LYS:O	5:E:148:VAL:HG23	1.94	0.67
10:J:34:VAL:HG13	10:J:74:ILE:HA	1.75	0.67
2:B:7:VAL:HG11	2:B:221:LEU:HD23	1.77	0.67
4:D:68:TYR:OH	4:D:98:GLU:OE1	2.09	0.67
5:E:91:LEU:HB3	5:E:118:ILE:HD11	1.75	0.67
12:L:27:LEU:C	12:L:29:GLY:H	1.97	0.67
9:I:50:LEU:HD23	9:I:85:LEU:HD13	1.76	0.67
2:B:16:HIS:CE1	2:B:210:SER:HB2	2.30	0.67
1:A:1195:C:H3'	1:A:1196:U:C5'	2.25	0.66
11:K:40:ILE:HG23	11:K:75:TYR:CD2	2.30	0.66
3:C:14:ILE:O	3:C:16:ARG:N	2.28	0.66
1:A:1147:C:O2'	9:I:16:ARG:HD3	1.94	0.66
1:A:1164:G:N2	1:A:1172:C:N3	2.42	0.66
1:A:35:G:H2'	1:A:36:C:H6	1.60	0.66
1:A:1305:G:OP1	21:U:2:GLY:N	2.28	0.66
4:D:187:ARG:NH2	4:D:188:LEU:HB2	2.10	0.66
1:A:258:G:H2'	1:A:259:G:H8	1.59	0.66
1:A:758:G:N7	25:A:2216:HOH:O	2.28	0.66
17:Q:58:GLU:HB2	17:Q:74:LEU:HB3	1.75	0.66
4:D:13:ARG:NH2	4:D:36:ARG:HH21	1.93	0.66
15:O:28:GLN:O	15:O:32:LEU:HB2	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:21:VAL:HG21	16:P:59:TRP:CD1	2.31	0.66
4:D:8:VAL:O	4:D:11:LEU:N	2.28	0.66
11:K:91:ARG:HD2	18:R:88:LYS:NZ	2.09	0.66
7:G:18:TYR:OH	7:G:58:PRO:HB2	1.96	0.66
15:O:4:THR:HG23	15:O:7:GLU:CD	2.15	0.66
1:A:1057:G:H5'	3:C:154:SER:HB2	1.78	0.66
1:A:39:G:N2	1:A:403:C:O2	2.24	0.65
4:D:163:GLU:HG3	4:D:166:LYS:HD2	1.78	0.65
1:A:21:G:N2	1:A:885:G:O3'	2.29	0.65
9:I:114:TYR:HE1	10:J:61:GLU:H	1.44	0.65
2:B:162:ILE:HG22	2:B:164:VAL:HG23	1.78	0.65
21:U:10:ARG:HA	21:U:13:ILE:HB	1.79	0.65
1:A:620:C:H2'	1:A:621:A:O4'	1.97	0.65
2:B:19:HIS:HB3	2:B:20:GLU:HG2	1.79	0.65
1:A:1240:U:OP1	7:G:119:ARG:NH2	2.28	0.65
7:G:18:TYR:HE2	7:G:59:LEU:HA	1.60	0.65
4:D:8:VAL:O	4:D:10:ARG:N	2.29	0.65
5:E:71:LEU:HD21	5:E:115:VAL:HG22	1.78	0.65
11:K:15:ALA:HA	11:K:77:MET:HA	1.79	0.65
18:R:43:PHE:HD2	18:R:56:THR:HG22	1.61	0.65
1:A:532:A:HO2'	1:A:533:A:P	2.20	0.65
4:D:13:ARG:HD2	4:D:38:TYR:O	1.97	0.65
11:K:57:THR:HG23	11:K:60:ALA:H	1.62	0.65
14:N:26:ARG:HB2	14:N:43:CYS:SG	2.37	0.65
1:A:1126:U:H3	1:A:1149:C:H1'	1.62	0.65
1:A:1413:A:H2	1:A:1487:G:H22	1.45	0.65
9:I:8:GLY:HA3	9:I:79:LEU:HB3	1.79	0.65
12:L:38:THR:HG22	12:L:39:VAL:HG13	1.78	0.65
1:A:1060:C:OP1	14:N:45:ARG:NH2	2.30	0.65
8:H:123:GLU:O	8:H:127:LEU:HB2	1.97	0.64
18:R:87:ARG:HD3	18:R:87:ARG:N	2.12	0.64
1:A:1505:G:H3'	1:A:1505:G:C8	2.32	0.64
16:P:21:VAL:HG12	16:P:33:ILE:HD12	1.78	0.64
7:G:26:PHE:HD1	7:G:101:LEU:HD22	1.62	0.64
5:E:143:ARG:HH12	8:H:77:GLU:CD	2.01	0.64
11:K:32:ILE:HD11	11:K:68:ALA:HB1	1.78	0.64
1:A:1255:G:O2'	1:A:1258:G:H1'	1.97	0.64
1:A:673:G:H2'	1:A:674:G:C8	2.33	0.64
9:I:22:GLY:N	9:I:58:HIS:O	2.25	0.64
1:A:1097:C:H2'	1:A:1098:C:C6	2.32	0.64
2:B:97:TRP:HZ2	2:B:102:LEU:HD22	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:4:TYR:CD1	9:I:88:TYR:HB2	2.33	0.64
1:A:691:G:H2'	1:A:692:U:C6	2.33	0.63
6:F:4:TYR:CE1	6:F:92:LYS:HG2	2.33	0.63
8:H:35:ILE:O	8:H:39:LEU:HD22	1.98	0.63
1:A:35:G:H2'	1:A:36:C:C6	2.33	0.63
12:L:113:ARG:HH11	12:L:113:ARG:HG3	1.61	0.63
7:G:91:VAL:HG12	7:G:95:ARG:HB3	1.78	0.63
1:A:1003(A):G:N2	1:A:1038:C:O2'	2.18	0.63
1:A:1305:G:N2	1:A:1331:G:H1'	2.14	0.63
3:C:25:GLY:HA2	3:C:28:GLN:N	2.14	0.63
12:L:27:LEU:C	12:L:29:GLY:N	2.50	0.63
2:B:95:GLN:HG3	2:B:148:TYR:HA	1.79	0.63
15:O:33:THR:HG21	15:O:85:LEU:HD13	1.81	0.63
20:T:71:THR:O	20:T:72:LEU:HD23	1.99	0.63
1:A:384:G:H2'	1:A:385:C:C6	2.33	0.63
1:A:451:A:N6	1:A:481:G:C4	2.67	0.63
5:E:17:ALA:HB2	5:E:26:PHE:HD2	1.64	0.63
4:D:107:ARG:HH21	4:D:194:LEU:HD11	1.63	0.63
13:M:40:ASN:HB3	13:M:43:THR:HG23	1.80	0.63
1:A:62:U:O2'	1:A:379:C:O2	2.15	0.62
1:A:953:G:H5'	1:A:965:A:H61	1.64	0.62
3:C:88:ARG:HE	3:C:100:ALA:HB1	1.63	0.62
9:I:51:ARG:HG2	9:I:56:LEU:HG	1.81	0.62
4:D:173:TRP:CE2	4:D:189:PRO:HB3	2.34	0.62
10:J:61:GLU:OE1	14:N:45:ARG:NH1	2.27	0.62
1:A:1183:A:O2'	1:A:1184:G:OP1	2.16	0.62
1:A:691:G:H2'	1:A:692:U:H6	1.65	0.62
2:B:97:TRP:CZ2	2:B:102:LEU:HD22	2.34	0.62
3:C:148:GLY:HA3	3:C:172:ARG:O	2.00	0.62
5:E:84:PHE:CE1	5:E:133:TYR:HB3	2.35	0.62
8:H:10:LEU:HD22	8:H:83:ILE:HD13	1.82	0.62
10:J:76:ASN:O	10:J:78:ASN:HB2	2.00	0.62
6:F:8:ILE:HD12	6:F:26:ILE:HD13	1.81	0.62
11:K:40:ILE:HG23	11:K:75:TYR:HD2	1.64	0.62
12:L:87:GLY:HA2	12:L:98:TYR:CA	2.26	0.62
12:L:82:VAL:HG12	12:L:106:ASP:OD1	2.00	0.62
1:A:413:G:O2'	1:A:428:G:N2	2.32	0.62
1:A:980:C:H5''	1:A:981:U:C5	2.34	0.62
3:C:120:VAL:O	3:C:124:ILE:HG13	2.00	0.62
7:G:68:ASN:O	7:G:138:LYS:NZ	2.28	0.62
1:A:826:C:O2	8:H:15:ASN:ND2	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:202:ILE:HG22	3:C:204:LEU:HD23	1.82	0.61
5:E:118:ILE:C	5:E:119:LEU:HD23	2.21	0.61
19:S:14:HIS:CE1	19:S:35:SER:HB2	2.35	0.61
1:A:328:C:O2	1:A:328:C:H2'	2.00	0.61
1:A:375:U:OP1	16:P:69:THR:HG21	2.00	0.61
1:A:789:U:O2'	1:A:791:G:N7	2.33	0.61
1:A:129:U:O3'	1:A:129(A):G:H3'	2.00	0.61
1:A:191:G:O2'	20:T:101:GLY:O	2.17	0.61
1:A:838:G:H2'	1:A:839:U:H5''	1.82	0.61
1:A:345:C:OP2	1:A:345:C:H6	1.84	0.61
1:A:9:G:OP1	5:E:122:GLU:HG3	2.00	0.61
5:E:80:ILE:H	5:E:80:ILE:HD12	1.65	0.61
13:M:16:ASP:OD1	13:M:16:ASP:N	2.33	0.61
2:B:87:ARG:HB3	2:B:87:ARG:HH11	1.66	0.61
9:I:51:ARG:HB2	9:I:51:ARG:NH1	2.15	0.61
15:O:26:GLU:HA	15:O:81:LEU:HD11	1.83	0.61
1:A:1300:G:O2'	1:A:1301:U:OP2	2.10	0.61
1:A:344:A:H5'	1:A:345:C:C5	2.35	0.61
1:A:560:U:H5'	1:A:566:G:N2	2.16	0.61
1:A:682:G:H1	1:A:708:C:H42	1.47	0.61
3:C:89:GLU:HG3	3:C:93:LYS:NZ	2.15	0.61
6:F:35:ALA:HA	6:F:67:MET:HB3	1.82	0.61
16:P:74:LEU:HD13	16:P:79:VAL:HG21	1.83	0.61
1:A:551:U:O2'	12:L:86:ARG:HD2	2.01	0.61
1:A:1381:U:H2'	1:A:1382:C:H6	1.66	0.60
1:A:975:A:H5'	1:A:975:A:C8	2.34	0.60
1:A:757:U:H2'	1:A:758:G:O4'	2.01	0.60
1:A:427:U:OP1	4:D:13:ARG:NH2	2.34	0.60
8:H:20:TYR:CE1	8:H:76:PRO:HG2	2.36	0.60
12:L:27:LEU:HG	12:L:28:LYS:H	1.66	0.60
18:R:43:PHE:C	18:R:51:LEU:HD12	2.22	0.60
1:A:981:U:H5'	14:N:21:TYR:CZ	2.36	0.60
1:A:695:A:OP2	11:K:53:SER:N	2.32	0.60
1:A:269:C:H2'	1:A:270:A:C8	2.36	0.60
7:G:20:ASP:OD1	7:G:21:VAL:N	2.35	0.60
1:A:21:G:O2'	1:A:22:G:OP1	2.12	0.60
1:A:671:G:H1	1:A:735:C:H42	1.49	0.60
6:F:80:ARG:NH1	6:F:88:VAL:O	2.30	0.60
8:H:9:MET:HG3	8:H:26:VAL:HG21	1.84	0.60
1:A:1238:A:H5'	1:A:1336:C:N4	2.16	0.60
2:B:61:LEU:HD11	2:B:160:ASP:HB3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:87:ARG:NH1	2:B:230:VAL:HG21	2.17	0.60
8:H:82:HIS:HE1	8:H:138:TRP:HE1	1.50	0.60
9:I:53:VAL:HG21	9:I:85:LEU:HD11	1.84	0.60
18:R:56:THR:HB	18:R:58:LEU:HG	1.84	0.60
1:A:1191:A:OP1	3:C:3:ASN:HB2	2.02	0.60
2:B:70:PHE:HE1	2:B:90:MET:HG3	1.67	0.60
18:R:53:ARG:HG2	18:R:63:GLN:NE2	2.13	0.60
6:F:7:ASN:HD21	18:R:34:TYR:HE1	1.49	0.60
7:G:70:LYS:HD3	7:G:96:GLN:HB3	1.84	0.60
13:M:23:TYR:HB2	13:M:67:GLU:HG2	1.82	0.60
1:A:1182:G:H4'	1:A:1183:A:H5''	1.81	0.60
1:A:665:A:N3	1:A:732:C:H2'	2.17	0.60
3:C:153:VAL:HG23	3:C:198:VAL:HG13	1.84	0.60
9:I:114:TYR:HD1	10:J:60:ARG:HB2	1.66	0.60
1:A:279:A:OP1	1:A:280:C:O2'	2.13	0.59
1:A:73:C:H2'	1:A:74:C:C6	2.35	0.59
2:B:117:GLU:O	2:B:120:ALA:HB3	2.01	0.59
3:C:34:LEU:HD13	3:C:38:ARG:NH2	2.15	0.59
5:E:118:ILE:O	5:E:119:LEU:HD23	2.02	0.59
16:P:43:LYS:HA	16:P:48:TRP:HB3	1.84	0.59
1:A:279:A:OP2	17:Q:95:TYR:OH	2.06	0.59
17:Q:27:PHE:CZ	17:Q:36:ILE:HD11	2.36	0.59
8:H:97:VAL:HA	8:H:100:ILE:HD11	1.83	0.59
18:R:39:VAL:HG13	18:R:40:LEU:HD23	1.84	0.59
1:A:349:A:H2'	1:A:350:G:H5''	1.85	0.59
2:B:82:ARG:HG2	2:B:92:TYR:HE1	1.65	0.59
3:C:88:ARG:CG	3:C:101:LEU:HB2	2.32	0.59
9:I:70:LYS:NZ	9:I:73:GLN:OE1	2.36	0.59
1:A:1150:U:O4	1:A:1151:A:N6	2.35	0.59
1:A:179:A:H2'	1:A:180:U:C6	2.38	0.59
15:O:26:GLU:OE1	15:O:77:ARG:HD2	2.01	0.59
20:T:14:LYS:O	20:T:18:GLN:HG2	2.03	0.59
1:A:1026:G:O2'	1:A:1027:C:OP1	2.18	0.59
1:A:1376:U:OP1	7:G:98:SER:OG	2.16	0.59
1:A:552:U:H2'	1:A:553:A:C8	2.38	0.59
2:B:82:ARG:HA	2:B:92:TYR:CE1	2.38	0.59
18:R:26:LEU:HD23	18:R:29:PHE:CE2	2.37	0.59
1:A:1121:U:H2'	1:A:1122:U:H6	1.68	0.59
1:A:200:G:H2'	1:A:201:C:O4'	2.02	0.59
1:A:1180:A:OP1	9:I:103:THR:OG1	2.21	0.59
20:T:75:ASN:OD1	20:T:75:ASN:N	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:11:VAL:HG22	17:Q:29:HIS:CD2	2.38	0.59
16:P:69:THR:HA	16:P:72:ARG:HG2	1.83	0.59
1:A:1255:G:H2'	1:A:1279:A:H61	1.68	0.58
1:A:489:C:H2'	1:A:490:G:H8	1.67	0.58
2:B:15:VAL:HG13	2:B:209:ARG:HB3	1.83	0.58
5:E:43:LEU:HD23	5:E:44:GLY:N	2.17	0.58
15:O:55:GLY:HA2	15:O:58:MET:HE2	1.85	0.58
1:A:1004:A:H4'	1:A:1005:A:OP1	2.03	0.58
1:A:1541:PSU:H6	1:A:1541:PSU:H3'	1.68	0.58
1:A:509:A:H3'	1:A:509:A:C8	2.38	0.58
1:A:5:U:H4'	1:A:6:G:O5'	2.02	0.58
4:D:170:VAL:HG22	4:D:174:LEU:HD12	1.85	0.58
9:I:26:VAL:HG12	9:I:61:ALA:HB3	1.85	0.58
11:K:124:LYS:HG3	11:K:125:PHE:CD2	2.39	0.58
18:R:43:PHE:O	18:R:51:LEU:HD12	2.03	0.58
1:A:353:A:H5'	1:A:353:A:C8	2.38	0.58
1:A:526:C:O3'	22:A:1601:SRY:HI31	2.03	0.58
7:G:122:HIS:O	7:G:126:ASP:HB2	2.02	0.58
6:F:48:LEU:HG	6:F:57:GLN:HA	1.84	0.58
12:L:42:THR:HA	12:L:53:ARG:O	2.04	0.58
14:N:39:LEU:HB3	14:N:43:CYS:HB3	1.86	0.58
1:A:1240:U:C2	7:G:32:ARG:HD2	2.37	0.58
1:A:89:C:O2'	1:A:90:U:H5'	2.02	0.58
1:A:945:G:O6	1:A:1236:A:N1	2.36	0.58
7:G:60:LYS:HZ3	7:G:63:LYS:HD2	1.68	0.58
4:D:65:ARG:HD2	4:D:72:GLU:HA	1.86	0.58
7:G:70:LYS:HG2	7:G:100:ALA:HB2	1.84	0.58
12:L:84:LEU:HD23	12:L:101:VAL:HG21	1.86	0.58
1:A:1029:C:N4	1:A:1032:G:H1	2.01	0.58
1:A:1255:G:O2'	1:A:1258:G:O2'	2.21	0.58
1:A:1474:G:H2'	1:A:1475:G:H8	1.67	0.58
4:D:30:LYS:O	4:D:32:ALA:N	2.36	0.58
4:D:55:ALA:O	4:D:59:ARG:HG2	2.04	0.58
17:Q:4:LYS:HG2	17:Q:6:LEU:HD21	1.86	0.58
2:B:18:GLY:HA3	2:B:42:ILE:H	1.69	0.58
9:I:48:GLU:N	9:I:49:PRO:HD2	2.19	0.58
15:O:38:ARG:NH1	15:O:38:ARG:HB3	2.16	0.58
1:A:1225:A:N3	1:A:1225:A:H2'	2.18	0.57
1:A:1242:C:N4	1:A:1295:G:H1	2.01	0.57
5:E:83:GLU:HG2	5:E:88:LYS:HG3	1.86	0.57
8:H:100:ILE:HG23	8:H:112:LEU:HD11	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:45:GLN:HB3	20:T:91:LEU:HD13	1.86	0.57
6:F:15:ASP:HB3	6:F:18:GLN:NE2	2.19	0.57
10:J:12:ASP:OD2	10:J:15:THR:N	2.31	0.57
16:P:28:ARG:HD2	16:P:29:ASP:OD2	2.04	0.57
1:A:1493:A:H2'	1:A:1494:G:C8	2.37	0.57
1:A:616:G:H1	1:A:624:C:H42	1.52	0.57
1:A:859:A:OP2	1:A:869:G:N1	2.33	0.57
7:G:47:CYS:HB3	7:G:58:PRO:HG2	1.85	0.57
11:K:99:GLN:NE2	11:K:105:VAL:HG21	2.19	0.57
18:R:22:VAL:HG23	18:R:56:THR:HA	1.85	0.57
21:U:6:ARG:HG2	21:U:15:ARG:HE	1.69	0.57
1:A:1223:C:H5''	1:A:1224:G:H5''	1.85	0.57
1:A:258:G:H2'	1:A:259:G:C8	2.38	0.57
5:E:15:ARG:HH11	5:E:15:ARG:HG2	1.69	0.57
1:A:1121:U:H2'	1:A:1122:U:C6	2.40	0.57
1:A:939:G:H5''	7:G:102:ARG:HH22	1.69	0.57
2:B:112:VAL:O	2:B:115:LEU:N	2.37	0.57
16:P:53:VAL:O	16:P:55:ARG:N	2.38	0.57
19:S:22:LEU:HG	19:S:28:LYS:HD2	1.85	0.57
1:A:1347:G:N2	1:A:1374:A:OP2	2.26	0.57
1:A:184:G:H2'	1:A:185:A:C8	2.39	0.57
2:B:17:PHE:HD1	2:B:18:GLY:N	2.02	0.57
2:B:189:ASP:HB3	2:B:203:GLY:O	2.05	0.57
4:D:31:CYS:SG	4:D:31:CYS:O	2.62	0.57
1:A:1510:U:H2'	1:A:1511:G:H8	1.67	0.57
2:B:92:TYR:CD2	2:B:151:GLY:HA3	2.40	0.57
11:K:121:PRO:HD2	11:K:126:ARG:HD2	1.85	0.57
16:P:53:VAL:HG23	16:P:54:GLU:H	1.70	0.57
1:A:695:A:OP2	11:K:52:GLY:HA3	2.05	0.57
11:K:82:VAL:O	11:K:109:VAL:HG23	2.04	0.57
1:A:1404:5MC:H1'	1:A:1499:A:H2	1.66	0.57
1:A:416:G:H2'	1:A:417:C:C6	2.40	0.57
1:A:83:U:O2'	1:A:84:U:H5'	2.05	0.57
2:B:29:ALA:HA	2:B:32:ILE:HG13	1.87	0.57
5:E:130:ASN:OD1	5:E:130:ASN:N	2.35	0.57
9:I:15:ALA:HA	9:I:65:VAL:HB	1.85	0.57
1:A:1329:A:P	13:M:28:ALA:HB3	2.45	0.56
1:A:254:G:OP1	17:Q:67:LYS:O	2.23	0.56
7:G:5:ARG:NH1	7:G:8:GLU:H	2.03	0.56
10:J:76:ASN:HB3	10:J:78:ASN:CG	2.26	0.56
17:Q:66:SER:O	17:Q:70:ARG:NH1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:C:H2'	1:A:402:G:H8	1.71	0.56
1:A:95:U:H2'	1:A:96:G:C8	2.39	0.56
13:M:22:ILE:HG22	13:M:23:TYR:N	2.20	0.56
17:Q:29:HIS:CG	17:Q:30:PRO:HD2	2.40	0.56
1:A:1325:C:OP1	21:U:15:ARG:HD3	2.05	0.56
1:A:1427:U:H2'	1:A:1428:A:C8	2.41	0.56
5:E:31:LEU:HD21	5:E:43:LEU:HD21	1.88	0.56
21:U:6:ARG:O	21:U:12:LYS:HE3	2.04	0.56
9:I:32:ASP:OD1	9:I:33:PHE:N	2.38	0.56
17:Q:58:GLU:CB	17:Q:74:LEU:HB3	2.34	0.56
3:C:44:GLU:HA	3:C:52:LEU:HD21	1.87	0.56
1:A:17:U:H2'	1:A:18:C:C6	2.39	0.56
3:C:22:TRP:HB3	3:C:59:ARG:HB2	1.86	0.56
13:M:5:ALA:HB2	13:M:22:ILE:HD13	1.88	0.56
1:A:1505:G:H8	1:A:1505:G:H3'	1.69	0.56
1:A:203:U:H3'	1:A:203:U:P	2.45	0.56
1:A:357:G:C2	1:A:358:U:C5	2.94	0.56
1:A:489:C:H2'	1:A:490:G:C8	2.41	0.56
1:A:837:G:C2	1:A:850:U:O2	2.59	0.56
9:I:97:LYS:N	9:I:98:PRO:HD2	2.20	0.56
14:N:37:PHE:HD1	14:N:44:LEU:HD13	1.71	0.56
6:F:50:TYR:CE1	18:R:77:GLY:HA2	2.40	0.56
1:A:1141:C:H2'	1:A:1142:G:C8	2.41	0.56
1:A:1234:C:H1'	1:A:1364:U:O2	2.05	0.56
1:A:928:G:O2'	1:A:1533:C:OP1	2.21	0.56
1:A:262:A:H5'	20:T:74:LYS:HG3	1.87	0.56
2:B:240:GLN:OE1	2:B:240:GLN:N	2.39	0.56
6:F:11:ASN:HB2	6:F:86:ARG:CZ	2.36	0.56
16:P:57:ARG:HG3	16:P:79:VAL:HG12	1.87	0.56
1:A:54:C:H42	1:A:357:G:H1	1.54	0.56
4:D:31:CYS:C	4:D:33:MET:H	2.08	0.56
5:E:146:ALA:O	5:E:149:GLU:HB2	2.05	0.56
1:A:939:G:H5''	7:G:102:ARG:NH2	2.20	0.56
10:J:78:ASN:O	10:J:82:ILE:HB	2.06	0.56
13:M:86:CYS:SG	13:M:87:TYR:N	2.78	0.56
19:S:16:LEU:O	19:S:20:LEU:HB2	2.05	0.56
1:A:1303:C:C2'	1:A:1304:G:H5'	2.36	0.56
1:A:976:G:H5''	1:A:1358:U:O2	2.06	0.56
6:F:77:ARG:O	6:F:81:ILE:HG13	2.05	0.56
12:L:60:LEU:N	12:L:64:TYR:O	2.38	0.56
19:S:19:VAL:HA	19:S:22:LEU:HB3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1190:G:OP1	3:C:4:LYS:HA	2.06	0.56
1:A:1301:U:O2'	1:A:1302:U:H3'	2.07	0.56
1:A:695:A:C2	1:A:787:A:H1'	2.41	0.56
5:E:80:ILE:N	5:E:80:ILE:HD12	2.20	0.56
18:R:43:PHE:CG	18:R:66:LEU:HD21	2.41	0.56
2:B:162:ILE:O	2:B:185:ILE:HG12	2.06	0.55
8:H:82:HIS:HE1	8:H:138:TRP:NE1	2.01	0.55
18:R:60:ALA:O	18:R:64:ARG:HG3	2.06	0.55
1:A:1366:C:H2'	1:A:1367:C:C6	2.34	0.55
1:A:420:U:H3'	1:A:422:C:H41	1.71	0.55
1:A:572:A:H5'	1:A:573:A:OP2	2.06	0.55
2:B:115:LEU:HD23	2:B:145:LEU:CB	2.36	0.55
1:A:1198:G:H2'	1:A:1199:U:C6	2.42	0.55
1:A:1531:A:O5'	1:A:1531:A:H8	1.89	0.55
2:B:54:THR:HG22	2:B:58:ILE:HD11	1.88	0.55
6:F:3:ARG:O	6:F:93:SER:HB2	2.06	0.55
12:L:62:SER:HB2	12:L:64:TYR:HB2	1.87	0.55
15:O:39:LEU:CD2	15:O:56:LEU:HB2	2.32	0.55
17:Q:81:ARG:NE	17:Q:84:LEU:HD11	2.22	0.55
1:A:481:G:O2'	1:A:482:A:H8	1.89	0.55
6:F:4:TYR:HD1	6:F:92:LYS:HA	1.72	0.55
7:G:60:LYS:HA	7:G:63:LYS:HB3	1.88	0.55
9:I:50:LEU:HD11	9:I:81:ILE:HD12	1.87	0.55
9:I:63:ILE:HG21	9:I:77:ILE:HG12	1.88	0.55
1:A:447:G:H2'	1:A:485:G:N2	2.22	0.55
1:A:665:A:C2	1:A:732:C:C2	2.94	0.55
2:B:162:ILE:CG2	2:B:164:VAL:HG23	2.37	0.55
1:A:1001:A:H2'	1:A:1002:G:H8	1.72	0.55
1:A:83:U:C2'	1:A:84:U:H5'	2.36	0.55
5:E:28:PHE:CD1	5:E:51:VAL:HG23	2.42	0.55
7:G:65:ALA:O	7:G:69:VAL:HG23	2.07	0.55
1:A:1403:C:C6	1:A:1404:5MC:HM52	2.41	0.55
1:A:653:A:OP1	8:H:56:LYS:NZ	2.39	0.55
2:B:115:LEU:HD23	2:B:145:LEU:HB3	1.89	0.55
9:I:10:ARG:HD3	9:I:105:ASP:HB3	1.88	0.55
13:M:91:ARG:HB2	13:M:98:VAL:HG22	1.89	0.55
1:A:1255:G:H2'	1:A:1279:A:N6	2.21	0.55
1:A:1138:G:O2'	1:A:1140:C:H5'	2.06	0.54
1:A:280:C:H4'	1:A:281:G:OP2	2.07	0.54
4:D:127:THR:HG23	4:D:147:ALA:O	2.07	0.54
9:I:63:ILE:HD13	9:I:77:ILE:HG23	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:53:ARG:HG2	12:L:69:TYR:HE1	1.72	0.54
16:P:17:TYR:HE1	16:P:41:PRO:HG3	1.72	0.54
1:A:1011:G:H2'	1:A:1012:U:O4'	2.08	0.54
1:A:1127:G:H2'	1:A:1127:G:N3	2.22	0.54
10:J:82:ILE:HG22	10:J:83:GLU:OE1	2.06	0.54
1:A:1163:C:C2'	1:A:1164:G:H5'	2.37	0.54
1:A:390:C:O3'	16:P:28:ARG:NH2	2.40	0.54
1:A:457:C:H2'	1:A:458:C:C6	2.42	0.54
1:A:80:G:H1	1:A:89:C:H42	1.56	0.54
2:B:142:LEU:HD13	2:B:146:GLN:NE2	2.23	0.54
3:C:11:ARG:NH1	3:C:177:THR:O	2.40	0.54
15:O:15:PHE:CZ	15:O:85:LEU:HD21	2.43	0.54
20:T:29:LYS:O	20:T:32:ALA:HB3	2.06	0.54
1:A:1303:C:H2'	1:A:1304:G:H5'	1.89	0.54
1:A:525:C:H2'	1:A:526:C:C6	2.42	0.54
2:B:134:GLU:O	2:B:138:LEU:HG	2.07	0.54
15:O:42:HIS:CD2	15:O:42:HIS:C	2.79	0.54
1:A:1048:G:H2'	1:A:1050:G:C8	2.43	0.54
1:A:1054:C:OP1	1:A:1197:G:OP1	2.25	0.54
6:F:4:TYR:CD1	6:F:92:LYS:HA	2.42	0.54
1:A:1243:C:H2'	1:A:1244:C:C6	2.43	0.54
1:A:1243:C:H2'	1:A:1244:C:H6	1.73	0.54
1:A:858:G:O2'	1:A:859:A:H5''	2.08	0.54
1:A:946:A:H2'	1:A:947:G:C8	2.42	0.54
2:B:20:GLU:OE1	2:B:23:ARG:NH2	2.41	0.54
5:E:81:GLU:HG2	5:E:90:VAL:HG13	1.90	0.54
12:L:82:VAL:O	12:L:106:ASP:HB2	2.08	0.54
15:O:82:ILE:HD12	15:O:87:ILE:HB	1.90	0.54
19:S:28:LYS:HG2	19:S:29:ARG:H	1.73	0.54
19:S:39:THR:HG23	19:S:70:LYS:HE2	1.88	0.54
21:U:5:ASP:HB3	21:U:8:THR:OG1	2.08	0.54
1:A:139:G:C2'	1:A:140:A:H5'	2.37	0.54
1:A:269:C:H2'	1:A:270:A:H8	1.71	0.54
1:A:731:G:OP1	1:A:766:A:H1'	2.07	0.54
1:A:92:C:O2'	1:A:93:G:H5'	2.07	0.54
1:A:955:U:H2'	1:A:956:U:H6	1.73	0.54
2:B:21:ARG:HG3	2:B:22:LYS:H	1.72	0.54
13:M:40:ASN:ND2	13:M:42:ALA:HB3	2.22	0.54
1:A:1000:U:H3	1:A:1041:A:H61	1.55	0.54
1:A:1179:A:H2'	1:A:1180:A:O4'	2.07	0.54
1:A:413:G:N2	1:A:429:U:OP2	2.28	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:91:VAL:HG21	7:G:96:GLN:HG3	1.90	0.54
17:Q:97:SER:OG	17:Q:98:LEU:N	2.40	0.54
1:A:912:C:O2'	1:A:913:A:H5'	2.08	0.54
2:B:92:TYR:HD2	2:B:92:TYR:H	1.55	0.54
3:C:156:ARG:H	3:C:163:ALA:HA	1.72	0.54
6:F:60:PHE:CZ	18:R:78:LEU:HD21	2.42	0.54
18:R:59:SER:O	18:R:63:GLN:N	2.35	0.54
1:A:411:A:C5	1:A:413:G:H1'	2.43	0.54
1:A:551:U:H2'	1:A:552:U:C6	2.43	0.54
4:D:52:SER:O	4:D:56:VAL:HG23	2.07	0.54
5:E:86:ALA:HB3	5:E:125:SER:HB3	1.90	0.54
5:E:11:ILE:CG2	5:E:31:LEU:HB3	2.34	0.54
1:A:1357:A:H2'	1:A:1358:U:C5	2.43	0.53
2:B:163:PHE:CD1	2:B:185:ILE:HG13	2.43	0.53
18:R:59:SER:H	18:R:62:GLU:HB2	1.72	0.53
19:S:63:THR:HB	19:S:66:MET:HG3	1.90	0.53
1:A:1185:G:C2'	1:A:1186:G:H5'	2.38	0.53
1:A:1191:A:H5''	3:C:4:LYS:HE3	1.90	0.53
1:A:1332:A:H5'	1:A:1332:A:H8	1.72	0.53
5:E:90:VAL:C	5:E:91:LEU:HD23	2.28	0.53
4:D:111:ALA:HB2	4:D:120:LEU:HD12	1.90	0.53
10:J:79:ARG:HB2	10:J:80:LYS:HD2	1.89	0.53
14:N:15:LYS:HE3	14:N:16:PHE:CE1	2.43	0.53
16:P:66:PRO:HD2	16:P:71:ARG:HH12	1.73	0.53
1:A:1403:C:H2'	1:A:1404:5MC:C6	2.43	0.53
1:A:673:G:H5''	6:F:87:ARG:NH1	2.22	0.53
9:I:29:ASN:O	9:I:29:ASN:ND2	2.41	0.53
10:J:6:ILE:HB	10:J:72:VAL:HB	1.90	0.53
1:A:1141:C:H2'	1:A:1142:G:H8	1.73	0.53
1:A:1403:C:H3'	1:A:1404:5MC:HM51	1.91	0.53
4:D:107:ARG:HH21	4:D:194:LEU:CD1	2.22	0.53
5:E:15:ARG:NH1	5:E:15:ARG:HG2	2.24	0.53
10:J:45:ARG:HD2	14:N:36:PHE:CE2	2.43	0.53
1:A:172:A:H2'	1:A:173:U:H5'	1.91	0.53
1:A:299:G:C6	1:A:300:A:C6	2.97	0.53
1:A:481:G:HO2'	1:A:482:A:H8	1.54	0.53
1:A:617:G:H1	1:A:623:C:N4	2.04	0.53
2:B:219:VAL:HA	2:B:222:ILE:HD12	1.91	0.53
7:G:151:TYR:O	7:G:154:TYR:HB2	2.09	0.53
12:L:25:PRO:HB3	12:L:27:LEU:HD13	1.91	0.53
12:L:58:VAL:O	12:L:65:GLU:HA	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:27:VAL:O	15:O:31:LEU:HB2	2.08	0.53
18:R:43:PHE:CD2	18:R:56:THR:HG22	2.43	0.53
1:A:1145:C:O2'	1:A:1146:A:O5'	2.22	0.53
1:A:1212:U:O2'	1:A:1213:A:O5'	2.21	0.53
1:A:476:G:H2'	1:A:477:G:C8	2.44	0.53
3:C:121:ALA:HB2	3:C:198:VAL:HG21	1.91	0.53
3:C:43:LEU:HA	3:C:47:LEU:HD13	1.90	0.53
15:O:36:ILE:HG13	15:O:59:MET:HE2	1.90	0.53
1:A:1270:C:OP2	21:U:24:ARG:NH2	2.42	0.53
1:A:130:A:OP2	1:A:190(E):U:O2'	2.13	0.53
1:A:981:U:H5'	14:N:21:TYR:OH	2.09	0.53
4:D:92:VAL:O	4:D:96:LEU:HD13	2.09	0.53
12:L:113:ARG:NH1	12:L:113:ARG:HG3	2.23	0.53
12:L:93:LEU:O	12:L:96:VAL:HG23	2.09	0.53
1:A:1229:A:OP1	13:M:114:ARG:HD3	2.08	0.53
1:A:328:C:O2'	1:A:329:A:OP2	2.13	0.53
5:E:126:ARG:CG	5:E:126:ARG:HH11	2.18	0.53
9:I:126:SER:OG	9:I:127:LYS:HD2	2.09	0.53
14:N:39:LEU:HB3	14:N:43:CYS:CB	2.39	0.53
1:A:1287:A:H2	1:A:1353:G:N3	2.06	0.52
1:A:299:G:H2'	1:A:300:A:C8	2.44	0.52
1:A:434:U:H2'	1:A:435:C:C6	2.44	0.52
1:A:79:G:H1	1:A:90:U:H3	1.57	0.52
1:A:902:G:H2'	1:A:903:G:H8	1.74	0.52
1:A:922:G:C6	1:A:923:A:C6	2.97	0.52
3:C:26:LYS:NZ	10:J:45:ARG:HH22	2.06	0.52
4:D:35:ARG:O	4:D:36:ARG:HG3	2.09	0.52
13:M:2:ALA:O	13:M:10:PRO:HD2	2.09	0.52
16:P:3:LYS:HD3	16:P:24:ALA:HB2	1.90	0.52
1:A:1066:C:H2'	1:A:1067:A:H5'	1.91	0.52
1:A:1426:C:H42	1:A:1474:G:H1	1.56	0.52
1:A:977:A:N6	25:A:2230:HOH:O	2.42	0.52
3:C:89:GLU:HG3	3:C:93:LYS:HZ3	1.73	0.52
6:F:67:MET:HB2	6:F:68:PRO:HD2	1.90	0.52
8:H:58:TYR:O	8:H:59:LEU:HD23	2.08	0.52
1:A:1250:A:H4'	9:I:68:GLY:N	2.24	0.52
10:J:22:LYS:O	10:J:25:GLU:HB2	2.09	0.52
17:Q:90:ILE:O	17:Q:93:GLN:HB2	2.09	0.52
1:A:1228:C:OP1	13:M:115:LYS:HG3	2.09	0.52
1:A:144:G:H1	1:A:178:C:H42	1.57	0.52
1:A:788:U:H5''	1:A:789:U:OP2	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:36:ARG:HG2	4:D:38:TYR:OH	2.09	0.52
1:A:390:C:H4'	16:P:28:ARG:NH2	2.23	0.52
16:P:38:TYR:O	16:P:49:LEU:HD12	2.10	0.52
16:P:78:GLY:C	16:P:80:PHE:N	2.59	0.52
17:Q:27:PHE:O	17:Q:36:ILE:HD13	2.09	0.52
20:T:21:LYS:O	20:T:24:LEU:HB3	2.09	0.52
1:A:1403:C:C5	1:A:1404:5MC:HM52	2.43	0.52
1:A:804:U:H5''	1:A:805:C:OP2	2.10	0.52
1:A:818:G:H3'	1:A:819:A:H5''	1.91	0.52
2:B:25:ASN:OD1	2:B:27:LYS:N	2.38	0.52
10:J:37:PRO:HA	10:J:72:VAL:H	1.74	0.52
1:A:765:G:H5''	1:A:766:A:OP1	2.08	0.52
1:A:794:A:C3'	1:A:794:A:C8	2.90	0.52
1:A:112:G:C2'	1:A:113:G:H5'	2.39	0.52
1:A:1358:U:H5''	14:N:35:ARG:CD	2.40	0.52
1:A:1502:A:H2	1:A:1505:G:H1	1.57	0.52
2:B:158:LEU:HD23	2:B:159:PRO:CD	2.40	0.52
6:F:2:ARG:O	6:F:66:GLU:HA	2.08	0.52
12:L:27:LEU:CG	12:L:28:LYS:H	2.21	0.52
12:L:28:LYS:HE2	12:L:33:ARG:NH1	2.25	0.52
15:O:87:ILE:HG22	15:O:88:ARG:N	2.23	0.52
1:A:1488:G:C2'	1:A:1489:G:H5'	2.39	0.52
1:A:788:U:H3'	1:A:789:U:O4'	2.09	0.52
4:D:20:TYR:CD1	4:D:27:TYR:HE2	2.28	0.52
12:L:28:LYS:HE2	12:L:33:ARG:HH12	1.74	0.52
1:A:835:U:OP1	18:R:64:ARG:NH2	2.43	0.52
1:A:1070:U:H2'	1:A:1071:C:H6	1.73	0.52
1:A:552:U:H2'	1:A:553:A:H8	1.74	0.52
7:G:57:GLU:O	7:G:59:LEU:N	2.43	0.52
5:E:143:ARG:NH1	8:H:77:GLU:OE1	2.37	0.52
19:S:15:LEU:O	19:S:18:LYS:HG3	2.09	0.52
1:A:909:A:H2'	1:A:910:C:O4'	2.10	0.52
7:G:26:PHE:CD1	7:G:101:LEU:HD22	2.43	0.52
1:A:335:C:O2'	1:A:1433:A:N3	2.36	0.52
1:A:539:A:H2'	1:A:540:G:C8	2.45	0.52
2:B:62:ALA:HB1	2:B:222:ILE:HG23	1.92	0.52
4:D:128:VAL:HG12	4:D:129:ASN:ND2	2.24	0.52
7:G:26:PHE:CE2	7:G:124:LEU:HD11	2.45	0.52
12:L:39:VAL:HG22	12:L:57:LYS:HB2	1.92	0.52
13:M:23:TYR:CE2	13:M:71:ARG:HB3	2.45	0.52
1:A:1095:U:H2'	1:A:1096:C:O4'	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1112:C:O2	3:C:179:ARG:HG3	2.09	0.51
1:A:1202:G:C4	14:N:42:ILE:HD13	2.46	0.51
1:A:1225:A:H5'	1:A:1226:C:OP2	2.10	0.51
1:A:22:G:H2'	1:A:23:C:H6	1.75	0.51
1:A:448:A:H2'	1:A:449:C:C6	2.45	0.51
2:B:161:ALA:O	2:B:162:ILE:HD13	2.10	0.51
1:A:653:A:P	8:H:56:LYS:HZ1	2.32	0.51
10:J:22:LYS:HA	10:J:25:GLU:HG3	1.91	0.51
19:S:5:LEU:O	19:S:6:LYS:HE3	2.10	0.51
1:A:1152:A:H5'	10:J:13:HIS:HB2	1.92	0.51
3:C:157:ILE:H	3:C:157:ILE:HD13	1.75	0.51
14:N:21:TYR:CD1	14:N:21:TYR:N	2.77	0.51
1:A:1126:U:H4'	25:A:2105:HOH:O	2.09	0.51
1:A:1229:A:H2'	1:A:1230:C:C6	2.44	0.51
1:A:373:A:H1'	1:A:481:G:N3	2.25	0.51
2:B:24:TRP:HA	2:B:191:ASP:HA	1.91	0.51
12:L:41:ARG:HH21	12:L:43:VAL:HG13	1.74	0.51
20:T:56:MET:HE2	20:T:85:MET:HA	1.93	0.51
1:A:1314:C:O2'	1:A:1315:U:H5'	2.09	0.51
1:A:1342:C:O2'	9:I:124:GLN:HB2	2.11	0.51
4:D:68:TYR:HB3	4:D:70:ILE:HG12	1.90	0.51
7:G:108:ALA:HB2	7:G:123:GLU:HG2	1.91	0.51
8:H:53:VAL:HB	8:H:58:TYR:CD1	2.45	0.51
9:I:50:LEU:O	9:I:53:VAL:HG23	2.11	0.51
12:L:113:ARG:HH12	12:L:116:SER:H	1.59	0.51
13:M:8:GLU:CD	13:M:22:ILE:HA	2.31	0.51
16:P:10:GLY:HA3	16:P:14:ASN:O	2.09	0.51
18:R:70:ILE:O	18:R:73:ALA:N	2.44	0.51
1:A:1348:U:H2'	1:A:1348:U:O2	2.10	0.51
1:A:262:A:H2'	1:A:263:A:C8	2.46	0.51
7:G:76:ARG:O	7:G:87:VAL:HG23	2.11	0.51
8:H:86:ILE:HG21	8:H:133:LEU:HD13	1.93	0.51
1:A:1278:U:H5'	1:A:1279:A:C8	2.45	0.51
1:A:379:C:H42	1:A:384:G:H1	1.59	0.51
3:C:25:GLY:O	3:C:29:TYR:HB2	2.10	0.51
4:D:110:PHE:HE2	4:D:146:ILE:HG22	1.76	0.51
9:I:53:VAL:HG11	9:I:92:TYR:CE1	2.46	0.51
21:U:10:ARG:HD3	21:U:13:ILE:CD1	2.41	0.51
1:A:502:G:H2'	1:A:503:C:O4'	2.09	0.51
1:A:921:U:O2'	5:E:18:ARG:HG3	2.11	0.51
2:B:24:TRP:CG	2:B:25:ASN:N	2.78	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:71:VAL:HG22	2:B:93:VAL:HB	1.92	0.51
1:A:1026:G:HO2'	1:A:1027:C:P	2.33	0.51
1:A:1337:G:H5''	1:A:1338:G:OP1	2.10	0.51
1:A:157:G:H1	1:A:164:U:H3	1.58	0.51
9:I:5:TYR:CD2	9:I:6:GLY:N	2.79	0.51
13:M:92:HIS:HA	13:M:110:ARG:HH22	1.75	0.51
16:P:53:VAL:O	16:P:56:ALA:N	2.44	0.51
1:A:1145:C:HO2'	1:A:1146:A:P	2.34	0.51
1:A:1229:A:H2'	1:A:1230:C:H6	1.76	0.51
1:A:1241:G:H2'	1:A:1242:C:C6	2.46	0.51
1:A:1291:G:H2'	1:A:1292:U:C6	2.46	0.51
1:A:253:U:OP1	17:Q:67:LYS:HD3	2.11	0.51
2:B:16:HIS:NE2	2:B:204:ASN:N	2.58	0.51
2:B:62:ALA:CB	2:B:222:ILE:HG23	2.41	0.51
4:D:187:ARG:CZ	4:D:188:LEU:H	2.24	0.51
4:D:76:ARG:HD2	4:D:207:TYR:CE2	2.46	0.51
9:I:25:LYS:HG2	9:I:60:ASP:OD1	2.11	0.51
1:A:974:A:OP2	14:N:41:ARG:NH1	2.42	0.51
15:O:30:ALA:HA	15:O:85:LEU:HD11	1.93	0.51
16:P:26:ARG:HD3	16:P:31:LYS:O	2.11	0.51
1:A:718:G:H5'	11:K:117:ASN:HB2	1.92	0.51
1:A:803:G:C6	1:A:804:U:C4	2.99	0.51
1:A:77:G:C2	1:A:93:G:C2	2.99	0.51
3:C:29:TYR:OH	14:N:54:PRO:HD2	2.10	0.51
5:E:46:GLY:H	5:E:58:ALA:HB2	1.76	0.51
12:L:6:THR:OG1	12:L:9:GLN:HG3	2.11	0.51
1:A:1179:A:OP2	9:I:93:ARG:NH2	2.44	0.50
1:A:1290:G:H2'	1:A:1291:G:C8	2.43	0.50
1:A:373:A:C2	1:A:374:A:C8	3.00	0.50
1:A:933:G:OP2	7:G:3:ARG:HB3	2.11	0.50
7:G:42:ILE:HG22	7:G:120:ILE:HD12	1.93	0.50
8:H:84:ARG:O	8:H:135:CYS:HB2	2.12	0.50
10:J:45:ARG:HD2	14:N:36:PHE:HE2	1.75	0.50
1:A:263:A:OP2	20:T:79:ARG:NH1	2.44	0.50
1:A:1127:G:N2	1:A:1147:C:C4	2.79	0.50
1:A:22:G:C5	1:A:23:C:C5	2.99	0.50
1:A:113:G:C1'	1:A:354:G:H5'	2.40	0.50
1:A:730:G:C5	1:A:731:G:H1'	2.46	0.50
6:F:14:LEU:HD21	6:F:84:ASN:ND2	2.26	0.50
8:H:70:GLN:OE1	8:H:70:GLN:HA	2.11	0.50
9:I:105:ASP:OD2	9:I:107:ARG:HG3	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:53:ARG:HG2	12:L:69:TYR:CE1	2.46	0.50
20:T:43:LEU:HD12	20:T:52:ALA:HA	1.94	0.50
1:A:1465:C:H2'	1:A:1466:C:O4'	2.10	0.50
1:A:1518:MA6:H102	1:A:1519:MA6:H103	1.92	0.50
16:P:3:LYS:CA	16:P:64:ALA:HB1	2.41	0.50
1:A:1521:G:H2'	1:A:1522:U:C6	2.47	0.50
1:A:18:C:H5''	5:E:127:ASN:ND2	2.25	0.50
1:A:580:U:H2'	1:A:581:G:O4'	2.12	0.50
1:A:7:G:O6	5:E:92:LYS:NZ	2.35	0.50
1:A:858:G:O6	1:A:869:G:H3'	2.10	0.50
5:E:147:ASP:HA	5:E:150:ARG:HG2	1.94	0.50
1:A:193:C:H4'	20:T:61:SER:HB2	1.93	0.50
1:A:953:G:H2'	1:A:954:G:O4'	2.11	0.50
6:F:4:TYR:HB2	6:F:65:VAL:CG2	2.42	0.50
10:J:69:ASN:O	10:J:70:ARG:HD3	2.12	0.50
1:A:1281:U:H4'	1:A:1282:C:OP2	2.11	0.50
1:A:236:G:H2'	1:A:237:C:O4'	2.11	0.50
1:A:243:A:H4'	1:A:244:U:O5'	2.12	0.50
1:A:692:U:H1'	1:A:695:A:N7	2.27	0.50
1:A:882:C:O2'	1:A:883:C:H5'	2.12	0.50
4:D:108:LEU:HD23	4:D:174:LEU:HD13	1.94	0.50
3:C:167:TRP:HE3	3:C:168:ALA:N	2.06	0.50
1:A:109:A:C6	1:A:327:A:C6	3.00	0.50
3:C:166:GLU:HA	3:C:166:GLU:OE2	2.12	0.50
8:H:104:ARG:HG3	8:H:138:TRP:CD2	2.47	0.50
1:A:1249:C:HO2'	9:I:73:GLN:NE2	2.08	0.50
15:O:30:ALA:O	15:O:33:THR:N	2.45	0.50
1:A:1218:C:H2'	1:A:1219:U:C6	2.47	0.50
1:A:812:C:OP1	1:A:903:G:H1'	2.12	0.50
4:D:173:TRP:HE3	4:D:173:TRP:H	1.58	0.50
4:D:173:TRP:NE1	4:D:189:PRO:HB3	2.27	0.50
5:E:118:ILE:HG12	5:E:119:LEU:H	1.77	0.50
12:L:47:LYS:HG3	12:L:48:PRO:CD	2.40	0.50
1:A:1403:C:H2'	1:A:1404:5MC:H6	1.77	0.49
1:A:414:A:OP2	1:A:428:G:N2	2.38	0.49
1:A:657:G:C2'	1:A:658:G:H5'	2.42	0.49
5:E:11:ILE:HD11	5:E:105:VAL:HG13	1.93	0.49
1:A:1351:U:H4'	7:G:33:ASP:CG	2.32	0.49
7:G:87:VAL:HG12	7:G:88:PRO:HD2	1.93	0.49
8:H:112:LEU:HD23	8:H:133:LEU:HA	1.93	0.49
8:H:4:ASP:OD1	8:H:85:ARG:NH1	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:111:ARG:O	9:I:119:ALA:HB2	2.12	0.49
1:A:1061:G:H1'	10:J:56:HIS:CE1	2.47	0.49
1:A:1004:A:HO2'	1:A:1005:A:P	2.34	0.49
1:A:1025:U:H4'	1:A:1025:U:OP1	2.11	0.49
1:A:665:A:H3'	1:A:725:G:H21	1.76	0.49
10:J:16:LEU:HD13	10:J:70:ARG:HG2	1.93	0.49
18:R:36:ASN:O	18:R:40:LEU:HG	2.12	0.49
20:T:100:ILE:HD12	20:T:100:ILE:H	1.76	0.49
20:T:30:LYS:HG2	20:T:34:LYS:HE2	1.93	0.49
1:A:1317:C:OP2	14:N:17:LYS:NZ	2.23	0.49
2:B:108:ILE:HG22	2:B:152:PHE:CE2	2.47	0.49
1:A:426:G:H4'	4:D:41:GLY:O	2.11	0.49
10:J:64:GLU:HG2	14:N:59:ALA:HB2	1.94	0.49
17:Q:58:GLU:O	17:Q:59:ILE:HD13	2.12	0.49
1:A:66:G:N7	1:A:104:G:N2	2.59	0.49
1:A:66:G:N3	1:A:66:G:H2'	2.27	0.49
1:A:980:C:H3'	1:A:981:U:H6	1.76	0.49
1:A:980:C:H5'	1:A:981:U:OP2	2.12	0.49
7:G:77:SER:HA	7:G:86:GLN:HA	1.94	0.49
9:I:126:SER:CB	9:I:127:LYS:HD2	2.43	0.49
14:N:12:ARG:HB3	14:N:14:PRO:HD3	1.94	0.49
1:A:1314:C:N4	19:S:4:SER:OG	2.43	0.49
1:A:690:G:C6	1:A:691:G:C6	3.01	0.49
2:B:153:ARG:HH11	2:B:153:ARG:HB2	1.78	0.49
7:G:32:ARG:O	7:G:34:GLY:N	2.45	0.49
1:A:1029:C:N4	1:A:1032:G:H22	2.09	0.49
2:B:112:VAL:HG23	2:B:149:LEU:HD13	1.94	0.49
2:B:212:GLN:O	2:B:216:SER:HB3	2.13	0.49
4:D:9:CYS:O	4:D:12:CYS:HB2	2.13	0.49
5:E:40:ARG:HG2	5:E:40:ARG:HH11	1.77	0.49
7:G:17:VAL:HB	7:G:44:TYR:OH	2.11	0.49
10:J:27:ALA:O	10:J:30:SER:OG	2.22	0.49
11:K:11:LYS:HE3	11:K:11:LYS:N	2.28	0.49
21:U:5:ASP:O	21:U:8:THR:OG1	2.30	0.49
1:A:1005:A:H5''	1:A:1006:C:C5	2.48	0.49
1:A:1067:A:HO2'	1:A:1094:G:H5'	1.77	0.49
4:D:173:TRP:CD1	4:D:189:PRO:HB3	2.46	0.49
1:A:1148:U:H2'	1:A:1149:C:O4'	2.13	0.49
1:A:1241:G:H2'	1:A:1242:C:H6	1.77	0.49
1:A:1280:A:H3'	1:A:1281:U:H5''	1.93	0.49
1:A:177:C:OP2	20:T:65:LYS:NZ	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:748:C:H4'	1:A:749:C:O5'	2.13	0.49
3:C:120:VAL:O	3:C:123:GLN:HB2	2.13	0.49
3:C:79:ARG:NH1	3:C:82:GLU:HB3	2.26	0.49
4:D:102:ASP:OD1	4:D:103:ASN:N	2.44	0.49
13:M:108:ARG:HD3	13:M:114:ARG:NH1	2.28	0.49
14:N:21:TYR:HD1	14:N:21:TYR:N	2.11	0.49
15:O:4:THR:OG1	15:O:5:LYS:N	2.46	0.49
11:K:91:ARG:HH11	18:R:88:LYS:NZ	2.11	0.49
21:U:15:ARG:HG3	21:U:15:ARG:HH11	1.77	0.49
1:A:448:A:H2'	1:A:449:C:H6	1.78	0.49
1:A:59:A:H3'	1:A:331:G:H22	1.77	0.49
1:A:676:A:H1'	11:K:115:PRO:HB3	1.95	0.49
15:O:34:LEU:O	15:O:38:ARG:HG2	2.12	0.49
13:M:84:ILE:HB	19:S:74:PHE:HE2	1.77	0.49
1:A:1370:G:C2	1:A:1371:G:N7	2.80	0.49
1:A:1474:G:H2'	1:A:1475:G:C8	2.46	0.49
1:A:273:A:N6	1:A:274:A:C6	2.81	0.49
1:A:328:C:HO2'	1:A:329:A:P	2.32	0.49
1:A:420:U:H3'	1:A:422:C:N4	2.27	0.49
2:B:185:ILE:HG22	2:B:199:TYR:HB2	1.95	0.49
5:E:118:ILE:HG12	5:E:119:LEU:N	2.28	0.49
8:H:86:ILE:HG22	8:H:87:SER:N	2.27	0.49
12:L:78:GLN:O	12:L:81:SER:HB2	2.13	0.49
1:A:376:G:OP2	16:P:67:THR:HG21	2.13	0.49
20:T:39:LYS:HD3	20:T:55:ILE:HD12	1.95	0.49
1:A:1372:U:C2'	1:A:1373:G:H5'	2.43	0.48
1:A:1419:G:H1	1:A:1481:U:H3	1.61	0.48
1:A:1505:G:C3'	1:A:1505:G:C8	2.93	0.48
1:A:44:G:H2'	1:A:45:U:O4'	2.14	0.48
7:G:17:VAL:HG12	7:G:18:TYR:CD1	2.37	0.48
7:G:92:SER:HG	7:G:95:ARG:H	1.55	0.48
7:G:9:VAL:HG12	7:G:10:ARG:O	2.13	0.48
9:I:33:PHE:CE2	9:I:43:ALA:HB1	2.48	0.48
10:J:65:LEU:HB2	14:N:56:VAL:HG22	1.95	0.48
11:K:31:THR:C	11:K:32:ILE:HD13	2.33	0.48
13:M:54:VAL:HA	13:M:57:ARG:HD3	1.94	0.48
17:Q:100:LYS:HA	17:Q:100:LYS:HE2	1.95	0.48
1:A:1029:C:H2'	1:A:1030:C:H5'	1.95	0.48
1:A:107:G:N2	1:A:108:G:H1'	2.28	0.48
1:A:1451:A:H5''	1:A:1452:C:H5	1.78	0.48
1:A:355:C:H5'	1:A:389:A:OP2	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:518:C:H5''	1:A:519:C:C6	2.49	0.48
4:D:21:LEU:HD21	4:D:66:ARG:O	2.13	0.48
5:E:137:GLU:HG3	5:E:141:GLN:HE21	1.78	0.48
13:M:11:ARG:HD2	13:M:45:VAL:CG1	2.43	0.48
16:P:26:ARG:HG2	16:P:26:ARG:HH11	1.78	0.48
16:P:20:VAL:HG13	16:P:32:TYR:CD2	2.47	0.48
17:Q:63:ARG:HG2	17:Q:64:PRO:HD2	1.94	0.48
20:T:60:GLU:HA	20:T:63:ILE:HD12	1.95	0.48
1:A:1126:U:H3'	1:A:1127:G:C8	2.29	0.48
1:A:1470:G:C2'	1:A:1471:G:H5'	2.43	0.48
1:A:1504:G:H5''	1:A:1504:G:H8	1.79	0.48
1:A:216:G:C2	1:A:217:C:C4	3.01	0.48
3:C:91:LEU:HD21	3:C:99:VAL:HG22	1.95	0.48
9:I:5:TYR:HD2	9:I:6:GLY:N	2.11	0.48
16:P:78:GLY:C	16:P:80:PHE:H	2.12	0.48
1:A:1326:C:OP1	21:U:12:LYS:HE2	2.13	0.48
1:A:1065:U:C5	1:A:1190:G:H1'	2.49	0.48
1:A:1426:C:H2'	1:A:1427:U:C6	2.48	0.48
1:A:184:G:H2'	1:A:185:A:H8	1.77	0.48
1:A:491:G:C4	1:A:492:G:C8	3.01	0.48
1:A:778:G:O5'	1:A:778:G:H8	1.96	0.48
2:B:32:ILE:CG2	2:B:40:HIS:HB3	2.44	0.48
2:B:92:TYR:N	2:B:92:TYR:CD2	2.81	0.48
3:C:112:SER:OG	3:C:112:SER:O	2.26	0.48
8:H:96:GLY:HA2	8:H:130:GLY:HA3	1.95	0.48
8:H:31:PHE:O	8:H:35:ILE:HG12	2.14	0.48
1:A:1329:A:C5'	13:M:29:ARG:HD2	2.43	0.48
16:P:53:VAL:O	16:P:54:GLU:C	2.51	0.48
1:A:277:C:H5'	17:Q:68:ARG:NH1	2.28	0.48
1:A:102:G:H2'	1:A:103:C:H6	1.79	0.48
1:A:935:A:H61	7:G:3:ARG:HG3	1.79	0.48
13:M:57:ARG:O	13:M:61:GLU:HB2	2.14	0.48
19:S:18:LYS:HD3	19:S:19:VAL:HB	1.95	0.48
1:A:1128:C:O2'	1:A:1130:A:OP2	2.23	0.48
1:A:1132:C:H2'	1:A:1133:G:H8	1.79	0.48
1:A:1196:U:H3'	1:A:1197:G:H5'	1.94	0.48
1:A:1285:A:H8	1:A:1285:A:O5'	1.97	0.48
4:D:60:GLU:HA	4:D:60:GLU:OE1	2.13	0.48
1:A:1026:G:O2'	1:A:1027:C:P	2.71	0.48
1:A:1029:C:H42	1:A:1032:G:H1	1.61	0.48
1:A:1496:C:HO2'	1:A:1497:G:P	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:U:H2'	1:A:38:G:O4'	2.14	0.48
1:A:481:G:O2'	1:A:482:A:O5'	2.27	0.48
1:A:93:G:C2	1:A:95:U:C2	3.02	0.48
2:B:60:ASP:O	2:B:64:ARG:HB2	2.13	0.48
4:D:15:GLU:HG3	4:D:63:LYS:HD3	1.95	0.48
4:D:38:TYR:CE1	4:D:45:GLN:HG2	2.48	0.48
11:K:40:ILE:HA	11:K:40:ILE:HD13	1.69	0.48
15:O:38:ARG:O	15:O:41:GLU:HB3	2.13	0.48
15:O:56:LEU:O	15:O:60:VAL:HG23	2.13	0.48
17:Q:29:HIS:ND1	17:Q:30:PRO:HD2	2.29	0.48
20:T:81:LYS:O	20:T:85:MET:HG3	2.13	0.48
1:A:1068:G:H8	1:A:1068:G:OP2	1.97	0.48
1:A:1542:U:H2'	1:A:1543:C:C6	2.49	0.48
1:A:438:G:H4'	4:D:123:HIS:ND1	2.28	0.48
1:A:597:G:H1'	1:A:644:G:N2	2.29	0.48
1:A:706:A:H1'	11:K:29:ILE:HD11	1.96	0.48
1:A:953:G:C6	1:A:954:G:C4	3.01	0.48
2:B:17:PHE:CD1	2:B:18:GLY:N	2.81	0.48
7:G:26:PHE:O	7:G:30:ILE:HD12	2.12	0.48
1:A:1361(A):C:O2	1:A:1362:C:H5	1.97	0.48
1:A:518:C:OP2	1:A:530:G:H1'	2.14	0.48
1:A:575:G:HO2'	1:A:821:G:H5'	1.79	0.48
1:A:686:U:O2'	1:A:687:A:C8	2.60	0.48
1:A:767:A:H2'	1:A:768:A:O4'	2.14	0.48
1:A:744:C:H4'	1:A:852:G:O2'	2.14	0.48
2:B:16:HIS:CD2	2:B:204:ASN:H	2.32	0.48
4:D:15:GLU:CG	4:D:63:LYS:HD3	2.43	0.48
4:D:32:ALA:O	4:D:36:ARG:N	2.47	0.48
12:L:77:LEU:HD21	12:L:107:ALA:HB2	1.96	0.48
17:Q:40:LYS:HD3	17:Q:42:TYR:OH	2.13	0.48
1:A:1157:A:H4'	1:A:1158:C:O5'	2.14	0.48
1:A:1265:G:H2'	1:A:1266:G:O4'	2.14	0.48
1:A:436:C:H2'	1:A:437:U:H6	1.78	0.48
4:D:200:GLU:HG2	4:D:201:GLN:H	1.78	0.48
5:E:107:ARG:O	5:E:111:GLU:HB2	2.14	0.48
10:J:54:PHE:O	10:J:55:LYS:HG3	2.14	0.48
11:K:19:ALA:HB2	11:K:80:VAL:HG11	1.96	0.48
1:A:1202:G:O2'	14:N:27:CYS:SG	2.66	0.48
1:A:34:C:H2'	1:A:35:G:C8	2.49	0.47
1:A:818:G:C3'	1:A:819:A:H5''	2.44	0.47
2:B:185:ILE:HG22	2:B:199:TYR:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:48:TYR:HA	8:H:60:ARG:O	2.14	0.47
17:Q:22:LEU:HA	17:Q:22:LEU:HD12	1.53	0.47
1:A:576:G:H3'	1:A:577:G:H5''	1.96	0.47
1:A:914:G:P	22:A:1601:SRV:HI33	2.53	0.47
1:A:943:U:H2'	1:A:944:G:H5'	1.97	0.47
2:B:196:LEU:HD22	2:B:196:LEU:HA	1.56	0.47
6:F:22:GLU:HA	6:F:25:ILE:HD12	1.96	0.47
8:H:96:GLY:O	8:H:97:VAL:C	2.52	0.47
9:I:111:ARG:O	9:I:113:LYS:HD2	2.14	0.47
9:I:19:LEU:HD12	9:I:84:ALA:HB3	1.97	0.47
12:L:84:LEU:HB3	12:L:101:VAL:HG23	1.96	0.47
12:L:11:VAL:HG12	12:L:12:ARG:N	2.29	0.47
6:F:99:ALA:HB1	18:R:62:GLU:OE2	2.14	0.47
20:T:92:LEU:O	20:T:96:GLY:HA2	2.13	0.47
1:A:106:C:C2'	1:A:107:G:H5'	2.43	0.47
1:A:1304:G:C6	1:A:1305:G:N1	2.82	0.47
1:A:1505:G:H4'	1:A:1506:U:H5''	1.95	0.47
4:D:194:LEU:HD12	4:D:195:ALA:H	1.77	0.47
7:G:5:ARG:NH1	7:G:8:GLU:HG3	2.20	0.47
2:B:179:LYS:HA	8:H:72:PRO:HD3	1.96	0.47
9:I:17:VAL:HG13	9:I:63:ILE:HG12	1.95	0.47
11:K:18:ARG:HB2	11:K:33:THR:CG2	2.45	0.47
16:P:66:PRO:HD2	16:P:71:ARG:NH1	2.29	0.47
20:T:57:ARG:HD3	20:T:102:GLY:HA3	1.96	0.47
1:A:1244:C:OP1	21:U:9:ARG:HB2	2.14	0.47
1:A:949:A:C2	1:A:1233:G:N3	2.82	0.47
1:A:559:A:O2'	1:A:560:U:OP2	2.24	0.47
2:B:32:ILE:HG21	2:B:40:HIS:HB3	1.95	0.47
7:G:140:ASP:O	7:G:144:MET:HG3	2.13	0.47
8:H:2:LEU:HD23	8:H:2:LEU:HA	1.68	0.47
11:K:32:ILE:N	11:K:32:ILE:HD13	2.29	0.47
20:T:53:LEU:HA	20:T:56:MET:HB3	1.96	0.47
1:A:1411:C:N4	1:A:1489:G:H1	2.10	0.47
1:A:234:C:H2'	1:A:235:C:C6	2.49	0.47
1:A:250:A:O5'	1:A:250:A:H8	1.96	0.47
1:A:405:U:O4	4:D:2:GLY:HA2	2.15	0.47
1:A:49:U:O2'	1:A:50:A:H2'	2.15	0.47
1:A:781:A:C5	1:A:802:A:C2	3.02	0.47
2:B:236:TYR:HD2	2:B:239:VAL:HG21	1.79	0.47
2:B:97:TRP:CH2	2:B:101:MET:HB2	2.50	0.47
3:C:88:ARG:HG2	3:C:101:LEU:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:114:ARG:HG3	4:D:114:ARG:HH11	1.79	0.47
5:E:143:ARG:NH1	8:H:77:GLU:OE2	2.48	0.47
14:N:4:LYS:HB3	14:N:4:LYS:HE2	1.58	0.47
17:Q:53:LEU:HD12	17:Q:85:VAL:HG21	1.96	0.47
1:A:1004:A:H5''	1:A:1025:U:N3	2.28	0.47
1:A:1210:C:HO2'	1:A:1213:A:HO2'	1.60	0.47
1:A:1460:A:OP2	20:T:27:LYS:NZ	2.47	0.47
1:A:452:A:H2'	1:A:453:A:C8	2.50	0.47
1:A:500:G:H2'	1:A:501:C:C6	2.49	0.47
1:A:835:U:H3	1:A:851:G:H1	1.62	0.47
4:D:9:CYS:SG	4:D:31:CYS:O	2.73	0.47
5:E:82:VAL:O	5:E:88:LYS:HA	2.14	0.47
7:G:116:ALA:O	7:G:120:ILE:HG13	2.15	0.47
7:G:134:ALA:O	7:G:137:LYS:N	2.47	0.47
10:J:49:VAL:HG21	14:N:44:LEU:HD23	1.96	0.47
12:L:41:ARG:NH2	12:L:43:VAL:HG13	2.28	0.47
17:Q:31:LEU:HA	17:Q:31:LEU:HD12	1.49	0.47
17:Q:38:ARG:HA	17:Q:38:ARG:HD3	1.48	0.47
1:A:1293:G:H2'	1:A:1294:G:O4'	2.14	0.47
1:A:1237:C:C4	1:A:1336:C:O2	2.68	0.47
1:A:146:G:C2	1:A:147:G:C4	3.03	0.47
1:A:766:A:P	25:A:2188:HOH:O	2.72	0.47
2:B:189:ASP:OD1	2:B:189:ASP:N	2.47	0.47
2:B:96:ARG:O	2:B:98:LEU:HD23	2.15	0.47
3:C:88:ARG:HA	3:C:91:LEU:HD22	1.97	0.47
18:R:37:VAL:CG2	18:R:78:LEU:HB3	2.45	0.47
1:A:455:C:H6	1:A:455:C:O5'	1.98	0.47
1:A:765:G:H8	1:A:765:G:O5'	1.98	0.47
1:A:954:G:C6	1:A:955:U:N3	2.83	0.47
4:D:70:ILE:HG22	4:D:71:SER:O	2.14	0.47
1:A:935:A:N6	7:G:3:ARG:HG3	2.29	0.47
8:H:104:ARG:HG2	8:H:104:ARG:HH11	1.79	0.47
1:A:1228:C:N4	13:M:104:ARG:O	2.42	0.47
18:R:26:LEU:HD12	18:R:42:ARG:HH11	1.79	0.47
1:A:1147:C:H2'	1:A:1148:U:C6	2.49	0.47
1:A:1239:A:C4	1:A:1298:C:N4	2.82	0.47
1:A:286:G:H2'	1:A:287:U:H6	1.80	0.47
1:A:289:G:P	25:A:1908:HOH:O	2.73	0.47
1:A:509:A:H4'	1:A:510:A:OP1	2.15	0.47
3:C:33:LEU:HD21	14:N:53:LEU:HD22	1.96	0.47
4:D:10:ARG:O	4:D:13:ARG:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:C:P	5:E:127:ASN:HD22	2.37	0.47
9:I:89:ASN:O	9:I:92:TYR:HB2	2.15	0.47
12:L:19:ARG:H	12:L:19:ARG:HG2	1.21	0.47
1:A:751:U:H4'	15:O:24:SER:HB3	1.97	0.47
1:A:1055:A:H1'	3:C:156:ARG:NH2	2.30	0.47
1:A:355:C:C4	1:A:356:A:N7	2.83	0.47
1:A:500:G:C6	1:A:501:C:C4	3.03	0.47
1:A:724:G:O2'	1:A:725:G:H5'	2.14	0.47
1:A:975:A:HO2'	1:A:976:G:P	2.37	0.47
5:E:98:THR:HB	5:E:117:ASP:HB3	1.96	0.47
8:H:20:TYR:CE2	8:H:75:ARG:HD2	2.50	0.47
1:A:1332:A:H2'	1:A:1333:A:H8	1.80	0.47
1:A:1347:G:O2'	1:A:1348:U:P	2.73	0.47
1:A:1518:MA6:C10	1:A:1519:MA6:H103	2.44	0.47
1:A:285:G:O2'	1:A:286:G:H5'	2.15	0.47
1:A:667:G:H4'	15:O:51:HIS:ND1	2.30	0.47
4:D:158:ILE:HA	4:D:158:ILE:HD13	1.76	0.47
4:D:176:LEU:HD21	4:D:178:VAL:HB	1.96	0.47
5:E:71:LEU:CD2	5:E:115:VAL:HG22	2.43	0.47
1:A:1298:C:OP2	7:G:114:ARG:NH2	2.48	0.47
8:H:36:LEU:HD23	8:H:39:LEU:HD23	1.97	0.47
1:A:1225:A:H5''	1:A:1226:C:H5	1.80	0.46
1:A:1498:UR3:H6	1:A:1498:UR3:O5'	2.14	0.46
1:A:701:C:H4'	1:A:702:A:C5'	2.43	0.46
1:A:996:A:C8	1:A:997:U:C5	3.03	0.46
8:H:10:LEU:HA	8:H:10:LEU:HD23	1.57	0.46
13:M:96:LEU:HD23	13:M:96:LEU:HA	1.69	0.46
15:O:49:ASP:OD2	15:O:52:SER:OG	2.26	0.46
16:P:18:ARG:HD3	16:P:35:LYS:HD2	1.97	0.46
19:S:31:ILE:CG2	19:S:49:ILE:HD13	2.39	0.46
1:A:102:G:H2'	1:A:103:C:C6	2.51	0.46
1:A:34:C:H2'	1:A:35:G:H8	1.80	0.46
1:A:519:C:OP2	12:L:50:SER:OG	2.29	0.46
1:A:833:U:H2'	1:A:834:C:C6	2.51	0.46
1:A:954:G:H5''	1:A:955:U:OP2	2.15	0.46
3:C:155:GLY:HA2	3:C:164:ARG:H	1.80	0.46
3:C:39:ILE:CG2	3:C:91:LEU:HD12	2.45	0.46
5:E:123:LEU:HA	5:E:123:LEU:HD23	1.53	0.46
10:J:19:SER:HB2	10:J:91:PRO:HB3	1.97	0.46
11:K:19:ALA:HB3	11:K:82:VAL:HG22	1.96	0.46
1:A:1293:G:C2	1:A:1294:G:C4	3.03	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:622:A:H5''	1:A:623:C:OP2	2.15	0.46
1:A:6:G:O2'	1:A:7:G:H5''	2.16	0.46
2:B:91:PRO:HG3	2:B:155:LEU:CD2	2.45	0.46
2:B:158:LEU:HD23	2:B:159:PRO:HD2	1.97	0.46
3:C:153:VAL:CG1	3:C:166:GLU:HB2	2.38	0.46
4:D:65:ARG:HG3	4:D:75:PHE:CG	2.50	0.46
7:G:75:VAL:HG11	7:G:86:GLN:HB3	1.97	0.46
1:A:1280:A:H5'	10:J:40:LEU:HD22	1.96	0.46
10:J:31:GLY:HA3	10:J:81:THR:OG1	2.15	0.46
13:M:12:ASN:H	13:M:45:VAL:CG1	2.27	0.46
15:O:67:LEU:HD13	15:O:78:TYR:CE1	2.40	0.46
17:Q:56:VAL:O	17:Q:77:VAL:N	2.41	0.46
1:A:1305:G:OP2	1:A:1305:G:C8	2.69	0.46
1:A:451:A:N7	1:A:481:G:C2	2.84	0.46
1:A:579:G:H2'	1:A:580:U:C6	2.50	0.46
1:A:668:G:O4'	15:O:49:ASP:HB2	2.16	0.46
12:L:126:LYS:HG2	12:L:128:ALA:HB2	1.97	0.46
12:L:31:PRO:O	12:L:32:PHE:CG	2.68	0.46
1:A:1311:G:H5''	1:A:1312:G:OP2	2.16	0.46
1:A:1470:G:H2'	1:A:1471:G:H5'	1.98	0.46
1:A:392:G:C2	1:A:393:A:C4	3.03	0.46
1:A:838:G:C2'	1:A:839:U:H5''	2.45	0.46
4:D:131:ARG:NH1	4:D:131:ARG:HB2	2.30	0.46
4:D:186:LEU:HD23	4:D:186:LEU:N	2.31	0.46
11:K:82:VAL:HG11	11:K:95:ILE:HD11	1.97	0.46
1:A:976:G:OP1	14:N:32:SER:HA	2.15	0.46
20:T:63:ILE:O	20:T:66:ALA:HB3	2.15	0.46
1:A:1014:A:C2	19:S:34:TRP:CD1	3.04	0.46
1:A:1174:G:H2'	1:A:1175:G:C8	2.51	0.46
1:A:927:G:H4'	1:A:1503:A:N7	2.30	0.46
1:A:448:A:C2	1:A:449:C:C4	3.04	0.46
1:A:463:A:H2'	1:A:474:G:C8	2.51	0.46
1:A:614:A:P	4:D:86:LYS:HZ1	2.39	0.46
1:A:686:U:O2'	1:A:687:A:O5'	2.34	0.46
1:A:89:C:C2'	1:A:90:U:H5'	2.46	0.46
1:A:954:G:N2	1:A:1227:A:H62	2.13	0.46
8:H:113:SER:HB2	8:H:134:ILE:HD11	1.97	0.46
19:S:6:LYS:HB3	19:S:7:LYS:H	1.33	0.46
1:A:1067:A:O5'	1:A:1067:A:H8	1.98	0.46
1:A:1495:U:O2'	1:A:1496:C:H5'	2.16	0.46
2:B:132:LYS:O	2:B:136:VAL:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:155:GLY:HA2	3:C:164:ARG:O	2.15	0.46
6:F:33:TYR:HE2	6:F:74:ASP:CB	2.29	0.46
12:L:120:TYR:O	12:L:122:THR:HG22	2.16	0.46
13:M:23:TYR:CZ	13:M:71:ARG:HB3	2.50	0.46
15:O:29:VAL:HG11	15:O:81:LEU:HD13	1.97	0.46
1:A:1152:A:H2'	1:A:1153:C:O4'	2.16	0.46
7:G:108:ALA:O	7:G:119:ARG:HB3	2.16	0.46
8:H:101:PRO:HG3	8:H:133:LEU:HD11	1.97	0.46
9:I:80:GLY:HA2	9:I:83:ARG:HG3	1.97	0.46
11:K:99:GLN:HE21	11:K:105:VAL:HG21	1.80	0.46
1:A:1228:C:H5''	1:A:1228:C:H6	1.81	0.46
1:A:1447:G:C6	1:A:1460:A:C2	3.04	0.46
1:A:1542:U:H2'	1:A:1543:C:C5	2.50	0.46
1:A:216:G:O2'	1:A:217:C:O5'	2.34	0.46
1:A:279:A:H8	1:A:279:A:H5'	1.81	0.46
1:A:78:G:N1	1:A:92:C:C4	2.84	0.46
2:B:24:TRP:HB3	2:B:40:HIS:CE1	2.51	0.46
8:H:20:TYR:HE2	8:H:75:ARG:HD2	1.80	0.46
11:K:18:ARG:HB2	11:K:33:THR:HG23	1.98	0.46
11:K:29:ILE:C	11:K:29:ILE:HD12	2.37	0.46
11:K:85:ARG:CD	11:K:111:ASP:HB3	2.46	0.46
13:M:67:GLU:O	13:M:71:ARG:HG2	2.16	0.46
13:M:67:GLU:HB3	13:M:68:GLY:H	1.55	0.46
13:M:82:MET:HA	13:M:89:GLY:HA3	1.97	0.46
10:J:62:HIS:HB2	14:N:59:ALA:HB3	1.97	0.46
17:Q:81:ARG:HB2	17:Q:84:LEU:CD1	2.46	0.46
19:S:26:GLY:O	19:S:27:GLU:HG2	2.16	0.46
1:A:1097:C:C4	1:A:1098:C:N4	2.84	0.46
1:A:1392:G:N2	1:A:1502:A:H8	2.12	0.46
1:A:1399:C:O2	1:A:1401:G:C5	2.69	0.46
1:A:369:C:OP2	1:A:388:G:N2	2.45	0.46
1:A:616:G:H1'	1:A:625:G:N2	2.31	0.46
6:F:47:ARG:HA	6:F:57:GLN:HB3	1.98	0.46
6:F:79:LEU:HD23	6:F:79:LEU:HA	1.50	0.46
8:H:36:LEU:HA	8:H:36:LEU:HD23	1.63	0.46
10:J:6:ILE:HG22	10:J:7:LYS:N	2.31	0.46
11:K:65:ALA:HB1	11:K:98:LEU:CD1	2.38	0.46
1:A:324:G:OP1	20:T:22:ARG:HD2	2.15	0.45
1:A:344:A:H4'	1:A:345:C:OP2	2.15	0.45
1:A:475:G:C4	1:A:476:G:C8	3.04	0.45
1:A:657:G:H2'	1:A:658:G:H5'	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:661:G:H1	1:A:744:C:H42	1.63	0.45
3:C:202:ILE:CG2	3:C:204:LEU:HD23	2.45	0.45
3:C:22:TRP:CH2	3:C:32:LEU:HB2	2.51	0.45
3:C:21:ARG:NH2	3:C:56:ASP:HB3	2.31	0.45
8:H:28:ALA:HB3	8:H:57:PRO:HB2	1.98	0.45
17:Q:8:GLY:O	17:Q:56:VAL:HG13	2.16	0.45
1:A:1323:G:N7	19:S:3:ARG:HD2	2.31	0.45
1:A:1081:G:H5''	1:A:1081:G:H8	1.81	0.45
1:A:1221:G:H2'	1:A:1222:G:O4'	2.16	0.45
1:A:1277:C:O2'	1:A:1279:A:H1'	2.16	0.45
1:A:1374:A:OP1	7:G:36:LYS:NZ	2.49	0.45
1:A:446:G:H2'	1:A:447:G:H5'	1.98	0.45
2:B:223:ILE:O	2:B:227:GLY:N	2.50	0.45
4:D:110:PHE:HD1	4:D:162:LEU:HD21	1.80	0.45
5:E:151:LEU:HD23	5:E:151:LEU:HA	1.64	0.45
11:K:85:ARG:HD3	11:K:111:ASP:HB3	1.97	0.45
15:O:14:GLU:HB3	15:O:15:PHE:CD1	2.51	0.45
15:O:34:LEU:HD23	15:O:35:ARG:N	2.31	0.45
20:T:53:LEU:HB2	20:T:100:ILE:HD13	1.97	0.45
1:A:397:A:H5'	1:A:398:C:OP1	2.15	0.45
1:A:474:G:H4'	16:P:81:ARG:NH2	2.31	0.45
1:A:532:A:O2'	1:A:533:A:P	2.72	0.45
1:A:653:A:P	8:H:56:LYS:NZ	2.89	0.45
1:A:974:A:C8	14:N:31:ARG:HG2	2.50	0.45
2:B:44:LEU:HD23	2:B:44:LEU:HA	1.64	0.45
3:C:87:LEU:O	3:C:91:LEU:HB3	2.17	0.45
7:G:45:ASP:O	7:G:49:ILE:HG13	2.15	0.45
8:H:124:ALA:O	8:H:128:GLY:N	2.49	0.45
9:I:63:ILE:CG2	9:I:77:ILE:HG12	2.46	0.45
1:A:1358:U:H5'	14:N:35:ARG:H	1.81	0.45
16:P:60:LEU:HD23	16:P:60:LEU:HA	1.40	0.45
1:A:721:G:C6	1:A:733:A:C2	3.05	0.45
1:A:858:G:C5	25:A:2220:HOH:O	2.68	0.45
4:D:172:PRO:HD2	4:D:173:TRP:CZ3	2.52	0.45
7:G:3:ARG:HH11	7:G:3:ARG:HG2	1.81	0.45
7:G:40:ALA:CB	9:I:41:VAL:HG21	2.47	0.45
10:J:12:ASP:HB3	10:J:15:THR:CG2	2.46	0.45
15:O:18:PHE:CZ	15:O:21:ASP:HB2	2.51	0.45
16:P:40:ASP:HA	16:P:41:PRO:HD3	1.84	0.45
17:Q:43:LEU:HD23	17:Q:43:LEU:HA	1.51	0.45
21:U:18:TYR:CG	21:U:24:ARG:HG2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1174:G:C2	1:A:1175:G:C5	3.05	0.45
1:A:1372:U:O2'	1:A:1373:G:H5'	2.17	0.45
1:A:1442:G:N1	1:A:1446:A:N7	2.64	0.45
1:A:1527:C:O2'	1:A:1528:U:H5'	2.16	0.45
1:A:284:G:H2'	1:A:285:G:H8	1.81	0.45
1:A:350:G:C5'	1:A:350:G:H8	2.29	0.45
1:A:690:G:H2'	1:A:691:G:O4'	2.16	0.45
1:A:837:G:N2	1:A:850:U:O2	2.49	0.45
3:C:35:GLU:O	3:C:39:ILE:HG13	2.16	0.45
1:A:983:A:P	14:N:3:ARG:HH22	2.40	0.45
16:P:53:VAL:HG23	16:P:54:GLU:N	2.31	0.45
20:T:10:LEU:HD13	20:T:11:SER:N	2.30	0.45
1:A:1021:G:H2'	1:A:1021:G:N3	2.32	0.45
1:A:991:U:O4	1:A:1212:U:H1'	2.16	0.45
1:A:192:U:H2'	1:A:193:C:H6	1.81	0.45
1:A:757:U:H5''	1:A:822:C:O2	2.17	0.45
1:A:82:U:O2'	1:A:83:U:H5'	2.16	0.45
2:B:92:TYR:CD1	2:B:94:ASN:HB2	2.52	0.45
4:D:194:LEU:HD13	4:D:194:LEU:HA	1.47	0.45
6:F:14:LEU:HB3	6:F:18:GLN:HB2	1.97	0.45
6:F:40:VAL:HG23	6:F:63:TYR:CD1	2.51	0.45
8:H:86:ILE:HD13	8:H:86:ILE:HA	1.59	0.45
14:N:53:LEU:O	14:N:56:VAL:HB	2.17	0.45
15:O:45:VAL:HB	15:O:46:HIS:ND1	2.32	0.45
15:O:70:LEU:HD12	15:O:78:TYR:HA	1.97	0.45
15:O:70:LEU:HD22	15:O:70:LEU:HA	1.58	0.45
1:A:1300:G:O5'	1:A:1335:C:N4	2.50	0.45
1:A:1418:A:H2'	1:A:1419:G:O4'	2.17	0.45
1:A:200:G:H1	1:A:217:C:N4	2.10	0.45
1:A:243:A:C2	1:A:246:A:C8	3.04	0.45
1:A:74:C:H2'	1:A:75:G:C8	2.52	0.45
1:A:830:G:C6	1:A:831:U:C4	3.05	0.45
3:C:150:LYS:HB2	3:C:169:ALA:HB2	1.99	0.45
17:Q:10:VAL:O	17:Q:53:LEU:HD13	2.17	0.45
1:A:1036:G:N7	1:A:1037:C:C4	2.85	0.45
1:A:1070:U:H2'	1:A:1071:C:C6	2.52	0.45
1:A:1323:G:H2'	1:A:1324:A:C8	2.51	0.45
22:A:1601:SRY:HB11	22:A:1601:SRY:H11	1.55	0.45
1:A:35:G:C4	1:A:36:C:C5	3.05	0.45
1:A:451:A:N6	1:A:481:G:C5	2.85	0.45
1:A:778:G:H2'	1:A:779:C:O4'	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:15:VAL:HG22	2:B:209:ARG:NH1	2.32	0.45
2:B:217:ARG:HA	2:B:217:ARG:HD3	1.55	0.45
3:C:119:ARG:O	3:C:123:GLN:HG3	2.16	0.45
4:D:15:GLU:O	4:D:17:VAL:HG23	2.17	0.45
4:D:186:LEU:HD23	4:D:186:LEU:H	1.81	0.45
6:F:26:ILE:HG21	6:F:63:TYR:HE2	1.80	0.45
8:H:10:LEU:HD12	8:H:85:ARG:HB2	1.98	0.45
14:N:25:VAL:HG23	14:N:38:GLY:O	2.17	0.45
17:Q:36:ILE:HD13	17:Q:36:ILE:H	1.82	0.45
19:S:71:LEU:C	19:S:73:GLU:H	2.18	0.45
1:A:1091:U:H2'	1:A:1092:A:H5''	1.97	0.45
1:A:1112:C:C4	3:C:178:LEU:HD12	2.52	0.45
1:A:1342:C:H2'	1:A:1343:G:C8	2.52	0.45
1:A:372:C:H4'	1:A:373:A:O5'	2.16	0.45
1:A:597:G:H5''	1:A:598:U:OP2	2.17	0.45
1:A:625:G:H4'	16:P:16:HIS:ND1	2.32	0.45
1:A:89:C:H2'	1:A:90:U:O4'	2.17	0.45
2:B:68:ILE:HG12	2:B:161:ALA:HB3	1.99	0.45
3:C:152:ILE:HG22	3:C:153:VAL:N	2.32	0.45
3:C:88:ARG:HG3	3:C:101:LEU:HB2	1.97	0.45
4:D:125:HIS:O	4:D:126:ILE:HD13	2.17	0.45
6:F:9:VAL:HG13	6:F:60:PHE:CD2	2.52	0.45
10:J:24:VAL:HG21	10:J:37:PRO:HD3	1.98	0.45
1:A:1191:A:H2'	1:A:1192:C:C6	2.52	0.45
1:A:1320:C:OP1	19:S:70:LYS:NZ	2.49	0.45
1:A:139:G:H2'	1:A:140:A:H5'	1.99	0.45
2:B:219:VAL:O	2:B:223:ILE:HG12	2.17	0.45
3:C:117:ALA:HB2	3:C:200:ALA:HB2	1.99	0.45
9:I:111:ARG:HH12	9:I:113:LYS:HA	1.81	0.45
1:A:350:G:O2'	1:A:351:G:H5'	2.17	0.44
1:A:353:A:H8	1:A:353:A:C5'	2.27	0.44
1:A:38:G:N2	1:A:397:A:C4	2.85	0.44
1:A:444:C:H2'	1:A:445:G:C8	2.52	0.44
4:D:20:TYR:CE1	4:D:27:TYR:HE2	2.34	0.44
14:N:24:CYS:HB2	14:N:39:LEU:HA	1.99	0.44
18:R:50:ILE:HG12	18:R:70:ILE:HD13	1.97	0.44
20:T:39:LYS:O	20:T:43:LEU:HG	2.17	0.44
1:A:1509:C:H42	1:A:1526:G:H1	1.66	0.44
1:A:344:A:H5'	1:A:345:C:H5	1.82	0.44
1:A:687:A:O2'	1:A:688:G:OP2	2.26	0.44
1:A:821:G:H2'	1:A:822:C:H6	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:836:G:OP1	18:R:61:LYS:NZ	2.48	0.44
1:A:89:C:C2	1:A:90:U:C6	3.05	0.44
2:B:147:LYS:HD2	2:B:148:TYR:CE2	2.52	0.44
3:C:134:ILE:O	3:C:138:VAL:HG23	2.17	0.44
5:E:11:ILE:HD11	5:E:105:VAL:HA	1.99	0.44
8:H:129:VAL:HG23	8:H:130:GLY:O	2.17	0.44
10:J:51:ARG:CZ	10:J:61:GLU:HB2	2.46	0.44
10:J:63:PHE:HE1	14:N:45:ARG:HA	1.82	0.44
11:K:30:VAL:HG21	11:K:65:ALA:HA	1.99	0.44
1:A:1163:C:H2'	1:A:1164:G:C8	2.40	0.44
1:A:1275:A:H2'	1:A:1276:G:O4'	2.16	0.44
1:A:1314:C:H2'	1:A:1315:U:C6	2.52	0.44
1:A:1498:UR3:O2'	1:A:1499:A:OP2	2.31	0.44
1:A:357:G:H2'	1:A:358:U:H6	1.82	0.44
1:A:475:G:H2'	1:A:476:G:H8	1.82	0.44
1:A:695:A:H2'	1:A:696:A:C8	2.52	0.44
2:B:57:PHE:CG	2:B:199:TYR:CE1	3.05	0.44
3:C:112:SER:O	3:C:116:VAL:HG23	2.18	0.44
3:C:188:LEU:HD13	3:C:189:ALA:N	2.32	0.44
1:A:620:C:C1'	4:D:135:LEU:HD13	2.47	0.44
5:E:89:ILE:HG13	5:E:90:VAL:N	2.33	0.44
5:E:92:LYS:HA	5:E:93:PRO:HD3	1.78	0.44
6:F:11:ASN:HB2	6:F:86:ARG:NH2	2.33	0.44
7:G:48:LYS:O	7:G:52:GLU:HB2	2.17	0.44
8:H:46:LYS:HG3	8:H:64:LYS:HB3	2.00	0.44
9:I:108:VAL:HG12	9:I:109:VAL:N	2.24	0.44
9:I:47:LEU:O	9:I:50:LEU:N	2.46	0.44
13:M:22:ILE:HG21	13:M:66:LEU:HD23	1.98	0.44
13:M:59:TYR:CE1	13:M:63:THR:HG21	2.52	0.44
1:A:1000:U:H2'	1:A:1001:A:C8	2.52	0.44
1:A:1048:G:O3'	1:A:1049:U:H3'	2.17	0.44
1:A:1213:A:C6	1:A:1215:G:C4	3.05	0.44
1:A:1500:A:OP2	1:A:1505:G:OP1	2.35	0.44
1:A:1504:G:H5''	1:A:1504:G:C8	2.52	0.44
1:A:279:A:C8	1:A:279:A:H5'	2.51	0.44
1:A:303:A:H2'	1:A:304:U:O4'	2.17	0.44
2:B:91:PRO:HG3	2:B:155:LEU:HD21	2.00	0.44
3:C:88:ARG:HE	3:C:100:ALA:CB	2.28	0.44
5:E:131:ILE:HD13	5:E:131:ILE:HA	1.50	0.44
9:I:65:VAL:HG11	9:I:77:ILE:HD11	1.99	0.44
12:L:60:LEU:HA	12:L:60:LEU:HD13	1.59	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:46:LYS:N	12:L:92:0TD:O	2.48	0.44
16:P:3:LYS:HA	16:P:64:ALA:HB1	2.00	0.44
17:Q:51:TYR:CD1	17:Q:73:VAL:HG11	2.51	0.44
17:Q:8:GLY:O	17:Q:56:VAL:HA	2.18	0.44
18:R:50:ILE:CG1	18:R:70:ILE:HD13	2.48	0.44
1:A:1250:A:C6	1:A:1251:A:N1	2.86	0.44
1:A:791:G:H2'	1:A:792:A:H5''	1.99	0.44
1:A:864:A:H2'	1:A:865:A:C8	2.52	0.44
1:A:90:U:C4	1:A:91:C:N4	2.86	0.44
3:C:157:ILE:HD11	3:C:164:ARG:HB2	1.98	0.44
5:E:110:LEU:HD23	5:E:110:LEU:N	2.32	0.44
6:F:15:ASP:OD1	6:F:16:GLN:N	2.51	0.44
6:F:97:PHE:HE1	18:R:61:LYS:HE3	1.82	0.44
13:M:11:ARG:HD2	13:M:45:VAL:HG11	1.98	0.44
1:A:451:A:H8	1:A:451:A:O5'	2.00	0.44
1:A:91:C:C5	1:A:92:C:H5	2.35	0.44
2:B:97:TRP:HZ3	2:B:176:GLU:OE2	2.00	0.44
5:E:80:ILE:CD1	5:E:91:LEU:HB2	2.48	0.44
8:H:113:SER:CB	8:H:134:ILE:HD11	2.48	0.44
8:H:111:ILE:O	8:H:134:ILE:HD12	2.18	0.44
1:A:1251:A:H4'	9:I:12:GLU:OE2	2.18	0.44
10:J:48:THR:HG23	10:J:60:ARG:HB3	1.98	0.44
10:J:48:THR:OG1	10:J:62:HIS:CD2	2.71	0.44
14:N:3:ARG:HB3	14:N:6:LEU:HG	1.98	0.44
18:R:58:LEU:HD13	18:R:62:GLU:HB3	1.99	0.44
20:T:10:LEU:HD22	20:T:10:LEU:HA	1.66	0.44
20:T:30:LYS:O	20:T:34:LYS:HG2	2.17	0.44
3:C:187:ALA:O	3:C:198:VAL:HG23	2.17	0.44
8:H:63:LEU:N	8:H:63:LEU:HD13	2.33	0.44
1:A:1148:U:O3'	9:I:14:VAL:HG11	2.18	0.44
10:J:24:VAL:O	10:J:28:ARG:HB2	2.18	0.44
11:K:72:ALA:HB1	11:K:77:MET:CB	2.47	0.44
18:R:43:PHE:C	18:R:44:LEU:HD23	2.38	0.44
19:S:34:TRP:CH2	19:S:57:HIS:NE2	2.86	0.44
20:T:36:LEU:O	20:T:39:LYS:HB3	2.18	0.44
1:A:234:C:H2'	1:A:235:C:H6	1.81	0.44
1:A:671:G:H5'	6:F:77:ARG:HH21	1.83	0.44
1:A:679:C:H2'	1:A:680:C:C6	2.53	0.44
1:A:766:A:OP2	25:A:2188:HOH:O	2.21	0.44
2:B:87:ARG:HH12	2:B:230:VAL:HG21	1.81	0.44
15:O:21:ASP:OD2	15:O:21:ASP:C	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:728:A:C8	15:O:54:ARG:NH1	2.86	0.44
1:A:131:C:OP1	1:A:190(F):G:N2	2.44	0.44
1:A:1372:U:H2'	1:A:1373:G:O4'	2.18	0.44
1:A:179:A:H2'	1:A:180:U:H6	1.81	0.44
1:A:200:G:H3'	1:A:201:C:H5''	1.99	0.44
1:A:481:G:O2'	1:A:482:A:C8	2.69	0.44
1:A:695:A:N3	1:A:787:A:H1'	2.33	0.44
1:A:902:G:H2'	1:A:903:G:C8	2.53	0.44
2:B:101:MET:O	2:B:105:PHE:HD1	2.00	0.44
4:D:122:ARG:HA	4:D:134:ASP:O	2.17	0.44
4:D:187:ARG:NH2	4:D:188:LEU:HD12	2.29	0.44
5:E:110:LEU:CD1	5:E:118:ILE:HG21	2.48	0.44
7:G:71:PRO:O	7:G:91:VAL:HG21	2.18	0.44
17:Q:50:LYS:HG3	17:Q:51:TYR:CE2	2.53	0.44
20:T:104:LEU:HG	20:T:104:LEU:H	1.51	0.44
1:A:1442:G:C6	1:A:1446:A:N7	2.86	0.43
1:A:442:C:H42	1:A:492:G:H1	1.65	0.43
4:D:30:LYS:C	4:D:32:ALA:H	2.22	0.43
8:H:112:LEU:CD2	8:H:133:LEU:HA	2.47	0.43
9:I:7:THR:HG22	9:I:8:GLY:N	2.33	0.43
11:K:81:ASP:OD2	11:K:106:LYS:HE3	2.18	0.43
12:L:113:ARG:HH21	12:L:120:TYR:HE1	1.66	0.43
6:F:100:ASN:O	18:R:28:GLU:HG3	2.18	0.43
20:T:73:HIS:HB3	20:T:74:LYS:H	1.49	0.43
1:A:1279:A:H5''	1:A:1280:A:OP1	2.18	0.43
1:A:92:C:O2	1:A:93:G:C8	2.71	0.43
2:B:17:PHE:HD1	2:B:18:GLY:H	1.66	0.43
4:D:131:ARG:HB2	4:D:131:ARG:HH11	1.83	0.43
5:E:106:PRO:O	5:E:107:ARG:C	2.55	0.43
5:E:122:GLU:OE1	5:E:131:ILE:HG13	2.17	0.43
5:E:142:LEU:HA	5:E:142:LEU:HD23	1.68	0.43
6:F:74:ASP:N	6:F:74:ASP:OD1	2.51	0.43
13:M:108:ARG:NH2	13:M:112:GLY:O	2.51	0.43
13:M:5:ALA:CB	13:M:22:ILE:HD13	2.48	0.43
18:R:33:ASP:OD1	18:R:36:ASN:N	2.51	0.43
1:A:1022:G:C6	1:A:1024:G:C2	3.06	0.43
1:A:1054:C:H3'	1:A:1054:C:H6	1.83	0.43
1:A:1127:G:N2	1:A:1146:A:N6	2.67	0.43
1:A:1223:C:H5''	1:A:1224:G:C5'	2.47	0.43
1:A:1407:5MC:O2'	1:A:1408:A:H5'	2.18	0.43
1:A:1426:C:H2'	1:A:1427:U:H6	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:738:C:OP2	6:F:92:LYS:HE3	2.18	0.43
1:A:828:A:OP1	1:A:828:A:H4'	2.17	0.43
1:A:1074:G:O3'	2:B:103:THR:HG21	2.18	0.43
2:B:233:SER:HA	2:B:234:PRO:HD3	1.82	0.43
4:D:94:LEU:HD23	4:D:94:LEU:HA	1.83	0.43
11:K:54:ARG:O	11:K:57:THR:HG22	2.19	0.43
12:L:25:PRO:HB3	12:L:27:LEU:HB2	1.99	0.43
13:M:49:THR:HG22	13:M:50:GLU:H	1.83	0.43
14:N:37:PHE:HB3	14:N:39:LEU:HD12	1.99	0.43
1:A:1003:G:N2	1:A:1039:C:C2	2.86	0.43
1:A:1181:G:C2	1:A:1182:G:N2	2.86	0.43
1:A:1253:G:C5	1:A:1254:C:C4	3.06	0.43
1:A:979:C:C5	1:A:980:C:C5	3.07	0.43
2:B:157:ARG:HG2	2:B:158:LEU:N	2.32	0.43
2:B:187:LEU:HA	2:B:187:LEU:HD22	1.42	0.43
2:B:92:TYR:HD2	2:B:92:TYR:N	2.14	0.43
1:A:1152:A:C5'	10:J:13:HIS:HB2	2.48	0.43
1:A:1360:A:OP2	14:N:35:ARG:NH2	2.51	0.43
1:A:204:U:H4'	1:A:216:G:O5'	2.16	0.43
1:A:413:G:N2	1:A:428:G:H1'	2.33	0.43
1:A:491:G:C6	1:A:492:G:N7	2.86	0.43
1:A:659:U:OP2	15:O:8:LYS:NZ	2.38	0.43
1:A:939:G:H2'	1:A:940:C:C6	2.54	0.43
4:D:192:GLU:C	4:D:194:LEU:H	2.22	0.43
5:E:35:GLY:HA2	5:E:40:ARG:O	2.18	0.43
5:E:90:VAL:HG23	5:E:121:LYS:O	2.18	0.43
6:F:11:ASN:O	6:F:14:LEU:HD12	2.19	0.43
6:F:87:ARG:NH1	6:F:87:ARG:HG3	2.15	0.43
7:G:99:LEU:HA	7:G:99:LEU:HD23	1.54	0.43
9:I:89:ASN:HB3	9:I:92:TYR:CD1	2.54	0.43
10:J:4:ILE:HD13	10:J:4:ILE:HA	1.85	0.43
10:J:40:LEU:HG	10:J:71:LEU:HD21	2.00	0.43
13:M:11:ARG:HG3	13:M:12:ASN:HB2	1.99	0.43
1:A:1008:C:H6	1:A:1008:C:O5'	2.01	0.43
1:A:1120:G:C6	1:A:1121:U:C4	3.06	0.43
1:A:1163:C:O2'	1:A:1164:G:H5'	2.18	0.43
1:A:1222:G:OP2	1:A:1322:C:N4	2.51	0.43
1:A:1494:G:C2	1:A:1495:U:C6	3.07	0.43
1:A:475:G:H2'	1:A:476:G:C8	2.54	0.43
1:A:456:C:C2	1:A:477:G:N2	2.87	0.43
1:A:538:G:OP2	12:L:115:LYS:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:792:A:N7	1:A:794:A:C6	2.87	0.43
6:F:97:PHE:C	6:F:97:PHE:CD2	2.92	0.43
1:A:1358:U:H5''	14:N:35:ARG:CG	2.48	0.43
14:N:53:LEU:HA	14:N:54:PRO:HD3	1.64	0.43
15:O:76:GLU:HA	15:O:76:GLU:OE2	2.18	0.43
15:O:6:GLU:HA	15:O:9:GLN:HB2	2.00	0.43
16:P:71:ARG:O	16:P:74:LEU:HB2	2.18	0.43
17:Q:50:LYS:HG3	17:Q:51:TYR:CD2	2.54	0.43
18:R:39:VAL:HG13	18:R:40:LEU:CD2	2.47	0.43
1:A:177:C:P	20:T:65:LYS:HZ1	2.41	0.43
1:A:1065:U:H5''	1:A:1190:G:N2	2.34	0.43
1:A:106:C:H2'	1:A:107:G:O4'	2.19	0.43
1:A:117:G:O5'	1:A:117:G:H8	2.01	0.43
1:A:1064:G:H1'	1:A:1190:G:N2	2.34	0.43
1:A:1427:U:H2'	1:A:1428:A:H8	1.83	0.43
3:C:6:HIS:HA	3:C:7:PRO:HD2	1.71	0.43
7:G:32:ARG:C	7:G:34:GLY:H	2.21	0.43
9:I:17:VAL:HG11	9:I:81:ILE:CA	2.45	0.43
1:A:1202:G:C2	14:N:42:ILE:HG21	2.54	0.43
1:A:451:A:N7	1:A:481:G:N1	2.67	0.43
1:A:518:C:H4'	1:A:519:C:O5'	2.19	0.43
1:A:877:C:O2'	8:H:3:THR:HG23	2.18	0.43
2:B:142:LEU:HD13	2:B:146:GLN:HE22	1.83	0.43
2:B:167:PRO:HG2	2:B:192:SER:CB	2.48	0.43
4:D:72:GLU:O	4:D:75:PHE:HB3	2.19	0.43
8:H:27:PRO:HA	8:H:58:TYR:CD2	2.54	0.43
19:S:49:ILE:O	19:S:60:VAL:HG23	2.18	0.43
19:S:50:ALA:HA	19:S:59:PRO:HA	2.00	0.43
1:A:1071:C:C2'	1:A:1072:G:H5'	2.49	0.43
1:A:1225:A:OP1	13:M:102:ARG:HA	2.18	0.43
1:A:527:7MG:OP2	22:A:1601:SRV:O32	2.25	0.43
4:D:200:GLU:HG2	4:D:201:GLN:N	2.33	0.43
8:H:112:LEU:HD23	8:H:112:LEU:HA	1.30	0.43
12:L:27:LEU:O	12:L:29:GLY:N	2.52	0.43
1:A:279:A:C4	17:Q:98:LEU:HD23	2.53	0.43
18:R:50:ILE:HD11	18:R:70:ILE:HG21	2.01	0.43
20:T:16:HIS:CE1	20:T:20:LEU:HD23	2.54	0.43
1:A:1067:A:O2'	1:A:1094:G:H5'	2.18	0.43
1:A:1219:U:C4	1:A:1220:G:N7	2.87	0.43
1:A:1505:G:H5''	25:A:1919:HOH:O	2.18	0.43
1:A:384:G:C4	1:A:385:C:C5	3.07	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:457:C:C2	1:A:476:G:C2	3.07	0.43
1:A:500:G:C5	1:A:501:C:C4	3.07	0.43
3:C:157:ILE:N	3:C:157:ILE:HD13	2.33	0.43
1:A:923:A:OP1	5:E:21:ALA:HB2	2.18	0.43
11:K:107:SER:O	11:K:108:ILE:HD13	2.19	0.43
13:M:19:LEU:HD11	13:M:56:LEU:HD11	2.01	0.43
16:P:19:ILE:HD12	16:P:37:GLY:C	2.40	0.43
17:Q:9:VAL:HG23	17:Q:56:VAL:HG22	2.00	0.43
1:A:1332:A:H2'	1:A:1333:A:C8	2.54	0.42
1:A:1506:U:O2'	1:A:1507:A:H5'	2.18	0.42
1:A:295:C:H2'	1:A:296:U:O4'	2.19	0.42
1:A:109:A:C4	1:A:327:A:C2	3.07	0.42
1:A:392:G:C6	1:A:393:A:C6	3.07	0.42
1:A:852:G:C3'	1:A:853:G:H5''	2.49	0.42
1:A:858:G:O6	1:A:869:G:C8	2.72	0.42
2:B:115:LEU:HD23	2:B:145:LEU:HB2	2.00	0.42
2:B:73:THR:HG22	2:B:73:THR:O	2.19	0.42
4:D:22:LYS:HA	4:D:22:LYS:HD2	1.59	0.42
6:F:1:MET:HA	6:F:67:MET:O	2.18	0.42
7:G:60:LYS:NZ	7:G:63:LYS:HD2	2.34	0.42
9:I:63:ILE:HD11	9:I:81:ILE:HD11	2.01	0.42
10:J:78:ASN:ND2	10:J:79:ARG:HE	2.17	0.42
11:K:92:GLU:O	11:K:96:ARG:HD3	2.19	0.42
11:K:95:ILE:HA	11:K:95:ILE:HD13	1.85	0.42
12:L:42:THR:CG2	12:L:52:LEU:HB3	2.49	0.42
19:S:43:GLU:N	19:S:43:GLU:OE1	2.51	0.42
1:A:1056:U:O2'	1:A:1057:G:H5'	2.19	0.42
1:A:1313:U:O4	19:S:4:SER:OG	2.28	0.42
1:A:1374:A:H2'	1:A:1375:A:H8	1.84	0.42
1:A:109:A:C6	1:A:326:G:C6	3.07	0.42
1:A:946:A:H2'	1:A:947:G:H8	1.83	0.42
8:H:95:VAL:HG11	8:H:133:LEU:HG	2.01	0.42
9:I:113:LYS:H	9:I:119:ALA:HA	1.83	0.42
17:Q:61:GLU:HA	17:Q:71:PHE:CD1	2.53	0.42
18:R:48:GLY:HA3	18:R:82:THR:HA	2.01	0.42
21:U:10:ARG:O	21:U:13:ILE:HB	2.19	0.42
1:A:1125:U:O2'	1:A:1126:U:H5'	2.20	0.42
1:A:1308:U:OP2	13:M:99:ARG:HG2	2.19	0.42
1:A:1342:C:H2'	1:A:1343:G:H8	1.83	0.42
1:A:1352:C:H2'	1:A:1353:G:C8	2.54	0.42
1:A:267:C:OP2	17:Q:67:LYS:HE3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:861:G:C5	1:A:862:C:C5	3.07	0.42
3:C:92:ALA:HB2	3:C:99:VAL:O	2.20	0.42
4:D:101:LEU:O	4:D:105:VAL:HG23	2.19	0.42
6:F:25:ILE:HA	6:F:28:ARG:HD3	2.00	0.42
9:I:45:ALA:HB1	9:I:78:LYS:NZ	2.34	0.42
9:I:4:TYR:CG	9:I:88:TYR:HB2	2.53	0.42
1:A:1064:G:H1'	1:A:1190:G:H21	1.84	0.42
1:A:1366:C:C2	1:A:1367:C:C5	3.07	0.42
1:A:1374:A:N3	1:A:1375:A:C8	2.87	0.42
1:A:913:A:OP1	12:L:91:LYS:HE2	2.19	0.42
2:B:131:PRO:O	2:B:134:GLU:HG2	2.20	0.42
2:B:74:LYS:NZ	2:B:206:ASP:HB2	2.34	0.42
4:D:11:LEU:HD23	4:D:11:LEU:HA	1.68	0.42
1:A:512:U:P	4:D:46:LYS:HZ3	2.40	0.42
5:E:64:ARG:O	5:E:65:ASN:HB3	2.19	0.42
7:G:17:VAL:HB	7:G:44:TYR:CZ	2.54	0.42
7:G:85:TYR:O	7:G:87:VAL:HG22	2.19	0.42
18:R:36:ASN:OD1	18:R:39:VAL:HG12	2.19	0.42
1:A:1185:G:H2'	1:A:1186:G:H5'	2.00	0.42
1:A:1274:G:H2'	1:A:1275:A:C8	2.54	0.42
1:A:1525:G:OP1	11:K:120:ARG:NH2	2.53	0.42
1:A:243:A:C2	1:A:245:C:C2	3.07	0.42
1:A:336:C:O2'	1:A:337:C:H5'	2.19	0.42
1:A:429:U:H1'	1:A:430:A:H5''	2.00	0.42
1:A:47:C:C6	1:A:365:U:H2'	2.55	0.42
4:D:110:PHE:HA	4:D:162:LEU:HD21	2.01	0.42
5:E:119:LEU:HD23	5:E:119:LEU:N	2.35	0.42
6:F:39:LYS:NZ	6:F:64:GLN:OE1	2.51	0.42
12:L:67:THR:O	12:L:67:THR:OG1	2.34	0.42
21:U:18:TYR:CD1	21:U:24:ARG:HG2	2.53	0.42
1:A:1309:G:C6	1:A:1310:G:C5	3.07	0.42
1:A:397:A:N3	1:A:397:A:H3'	2.34	0.42
1:A:59:A:C2	1:A:354:G:C4	3.07	0.42
1:A:721:G:H4'	1:A:722:A:O4'	2.20	0.42
1:A:727:G:N2	1:A:730:G:OP2	2.47	0.42
1:A:829:G:C6	1:A:858:G:N2	2.87	0.42
1:A:836:G:C6	1:A:851:G:C6	3.08	0.42
2:B:172:ILE:H	2:B:172:ILE:HG12	1.46	0.42
2:B:21:ARG:HA	2:B:39:ILE:HA	2.01	0.42
1:A:1113:C:H4'	3:C:14:ILE:HD11	2.00	0.42
3:C:188:LEU:HD22	3:C:188:LEU:HA	1.65	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:15:THR:HG23	10:J:94:VAL:HG22	2.01	0.42
11:K:91:ARG:NH1	18:R:88:LYS:HZ1	2.18	0.42
12:L:44:THR:HA	12:L:45:PRO:HD3	1.82	0.42
17:Q:34:LYS:HG3	17:Q:35:VAL:N	2.35	0.42
1:A:1123:A:H61	1:A:1149:C:H42	1.66	0.42
1:A:1544:U:O5'	1:A:1544:U:H6	2.02	0.42
1:A:123:C:O2'	1:A:290:C:O2	2.33	0.42
1:A:454:C:N4	1:A:479:C:N3	2.67	0.42
3:C:180:ALA:O	3:C:181:ASN:HB3	2.20	0.42
5:E:41:VAL:HG13	5:E:113:ALA:HB2	2.01	0.42
8:H:97:VAL:HG12	8:H:98:LYS:N	2.35	0.42
10:J:62:HIS:CB	14:N:59:ALA:HB3	2.50	0.42
16:P:31:LYS:HG3	16:P:32:TYR:N	2.35	0.42
16:P:67:THR:HG22	16:P:68:ASP:N	2.35	0.42
18:R:33:ASP:O	18:R:40:LEU:HD11	2.20	0.42
19:S:55:LYS:HD3	19:S:56:GLN:HG2	2.02	0.42
1:A:1071:C:O2'	1:A:1072:G:H5'	2.19	0.42
1:A:1193:G:O2'	1:A:1194:U:H5'	2.20	0.42
1:A:448:A:C4	1:A:487:A:C2	3.07	0.42
1:A:45:U:H2'	1:A:46:G:C8	2.55	0.42
3:C:32:LEU:O	3:C:35:GLU:HB3	2.20	0.42
3:C:39:ILE:HD12	3:C:57:ILE:HD11	2.02	0.42
8:H:127:LEU:HA	8:H:127:LEU:HD22	1.74	0.42
8:H:137:VAL:HG12	8:H:138:TRP:N	2.33	0.42
8:H:57:PRO:O	8:H:57:PRO:HG2	2.19	0.42
9:I:111:ARG:NH1	9:I:113:LYS:HA	2.35	0.42
12:L:26:ALA:O	12:L:33:ARG:HD2	2.19	0.42
13:M:117:VAL:HG12	13:M:118:ALA:N	2.34	0.42
14:N:39:LEU:HD22	14:N:43:CYS:HB3	2.01	0.42
15:O:36:ILE:HG22	15:O:37:ASN:N	2.32	0.42
19:S:31:ILE:HD12	19:S:32:LYS:H	1.85	0.42
1:A:1284:C:OP2	1:A:1285:A:O2'	2.34	0.42
1:A:1347:G:C2'	1:A:1348:U:OP2	2.67	0.42
1:A:22:G:C5	1:A:914:G:C6	3.08	0.42
1:A:511:C:H42	1:A:540:G:H1	1.68	0.42
1:A:945:G:N1	1:A:1337:G:C2	2.88	0.42
2:B:127:ILE:H	2:B:127:ILE:HG13	1.59	0.42
2:B:224:GLN:HG3	2:B:229:VAL:HG22	2.02	0.42
3:C:54:ARG:HB3	3:C:69:HIS:HB2	2.02	0.42
8:H:104:ARG:HG3	8:H:138:TRP:CG	2.55	0.42
11:K:40:ILE:HG22	11:K:41:THR:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:59:TYR:O	11:K:63:LEU:HG	2.20	0.42
12:L:35:GLY:O	12:L:83:VAL:HG12	2.20	0.42
13:M:23:TYR:CE2	13:M:70:LEU:HD13	2.55	0.42
19:S:20:LEU:HD12	19:S:20:LEU:HA	1.87	0.42
19:S:40:ILE:HD11	19:S:62:ILE:HD12	2.01	0.42
20:T:33:ILE:CD1	20:T:63:ILE:HA	2.50	0.42
20:T:87:LYS:O	20:T:91:LEU:HG	2.20	0.42
1:A:1120:G:O6	1:A:1153:C:N4	2.53	0.42
1:A:1250:A:N1	1:A:1251:A:C2	2.88	0.42
1:A:1504:G:H4'	1:A:1505:G:H5'	2.02	0.42
1:A:358:U:H2'	1:A:359:U:H6	1.84	0.42
1:A:474:G:H2'	1:A:475:G:O4'	2.20	0.42
1:A:484:G:O2'	1:A:485:G:OP2	2.26	0.42
1:A:509:A:C3'	1:A:509:A:C8	3.03	0.42
1:A:585:G:C6	1:A:586:C:C4	3.08	0.42
1:A:693:G:C6	1:A:694:A:C5	3.07	0.42
3:C:6:HIS:HD2	3:C:8:ILE:H	1.67	0.42
4:D:187:ARG:HD2	4:D:187:ARG:HA	1.15	0.42
6:F:30:LEU:HD23	6:F:75:LEU:HD21	2.01	0.42
6:F:98:LEU:HB2	6:F:101:ALA:HB2	2.02	0.42
7:G:104:LEU:HD23	7:G:104:LEU:N	2.34	0.42
7:G:124:LEU:HD23	7:G:124:LEU:HA	1.60	0.42
17:Q:4:LYS:HG2	17:Q:6:LEU:CD2	2.49	0.42
1:A:1320:C:O2'	19:S:73:GLU:OE1	2.35	0.42
20:T:42:GLN:HA	20:T:42:GLN:OE1	2.13	0.42
1:A:1112:C:H1'	3:C:179:ARG:NH1	2.35	0.41
1:A:1134:G:C6	1:A:1141:C:C4	3.07	0.41
1:A:1197:G:H5''	1:A:1198:G:OP2	2.20	0.41
1:A:284:G:H2'	1:A:285:G:C8	2.54	0.41
1:A:527:7MG:O2'	1:A:535:A:N1	2.37	0.41
1:A:578:C:H2'	1:A:579:G:O4'	2.20	0.41
4:D:187:ARG:NH1	4:D:188:LEU:H	2.18	0.41
5:E:53:LEU:HA	5:E:53:LEU:HD23	1.66	0.41
5:E:80:ILE:HD12	5:E:91:LEU:HB2	2.00	0.41
6:F:23:LYS:O	6:F:27:GLN:HG2	2.20	0.41
8:H:4:ASP:OD2	8:H:85:ARG:NH1	2.53	0.41
6:F:41:GLU:OE1	18:R:35:ARG:NH2	2.53	0.41
18:R:53:ARG:HA	18:R:56:THR:OG1	2.19	0.41
1:A:1144:G:N2	1:A:1146:A:H62	2.17	0.41
1:A:1243:C:H5''	21:U:8:THR:HG22	2.02	0.41
1:A:134:A:H2'	1:A:135:C:O4'	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1399:C:H4'	1:A:1400:5MC:H5''	2.02	0.41
1:A:1435:G:H2'	1:A:1436:U:H6	1.79	0.41
1:A:940:C:H2'	1:A:941:G:O4'	2.20	0.41
2:B:124:SER:HB2	2:B:126:GLU:OE1	2.20	0.41
1:A:1250:A:H4'	9:I:68:GLY:CA	2.50	0.41
11:K:44:SER:H	11:K:47:VAL:HB	1.85	0.41
12:L:55:VAL:HG12	12:L:69:TYR:HA	2.02	0.41
18:R:22:VAL:HG23	18:R:55:ARG:O	2.20	0.41
20:T:33:ILE:O	20:T:34:LYS:C	2.58	0.41
1:A:1070:U:O2	1:A:1106:G:C2	2.73	0.41
1:A:109:A:H2'	1:A:326:G:N2	2.35	0.41
1:A:1171:G:C6	1:A:1172:C:N4	2.88	0.41
1:A:1296:C:H4'	1:A:1302:U:C5	2.54	0.41
1:A:1541:PSU:C6	1:A:1541:PSU:H3'	2.53	0.41
1:A:27:G:H1	1:A:556:C:N4	2.18	0.41
1:A:831:U:O2'	1:A:832:C:H5'	2.21	0.41
2:B:102:LEU:HB3	2:B:180:LEU:HD11	2.02	0.41
2:B:28:PHE:CD2	2:B:28:PHE:O	2.74	0.41
4:D:57:ARG:HG3	4:D:202:LEU:HD13	2.03	0.41
4:D:38:TYR:CD1	4:D:45:GLN:HG2	2.55	0.41
8:H:6:ILE:HG23	8:H:6:ILE:HD12	1.66	0.41
9:I:126:SER:O	9:I:128:ARG:N	2.53	0.41
20:T:41:ILE:O	20:T:44:ALA:HB3	2.21	0.41
1:A:1118:C:H1'	1:A:1179:A:C5	2.54	0.41
1:A:1118:C:H5'	9:I:104:ARG:HG3	2.02	0.41
1:A:141:A:H1'	1:A:182:U:O2	2.20	0.41
1:A:431:A:H2'	1:A:432:A:O4'	2.20	0.41
1:A:922:G:N2	1:A:1396:A:C5	2.89	0.41
2:B:158:LEU:HA	2:B:158:LEU:HD23	1.70	0.41
4:D:120:LEU:HA	4:D:120:LEU:HD23	1.72	0.41
7:G:58:PRO:HA	7:G:61:VAL:HB	2.03	0.41
11:K:18:ARG:O	11:K:33:THR:HG22	2.21	0.41
1:A:1226:C:C5	13:M:104:ARG:HA	2.54	0.41
13:M:23:TYR:HB3	13:M:67:GLU:CA	2.48	0.41
16:P:22:THR:HA	16:P:33:ILE:HG13	2.02	0.41
17:Q:10:VAL:HG23	17:Q:54:GLY:H	1.85	0.41
1:A:1172:C:O2'	1:A:1173:G:H5'	2.20	0.41
1:A:1053:G:O2'	1:A:1199:U:H5	2.01	0.41
1:A:1250:A:C2	1:A:1287:A:C2	3.09	0.41
1:A:1255:G:C2'	1:A:1279:A:H61	2.31	0.41
1:A:88:A:H2'	1:A:89:C:H6	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:182:ILE:HA	2:B:183:PRO:HD3	1.78	0.41
2:B:79:ASP:O	2:B:82:ARG:N	2.54	0.41
4:D:27:TYR:HE1	4:D:168:ARG:HH22	1.68	0.41
8:H:104:ARG:CZ	8:H:138:TRP:CZ2	3.04	0.41
12:L:30:ALA:HA	12:L:31:PRO:HD3	1.68	0.41
14:N:12:ARG:HB2	14:N:13:THR:H	1.61	0.41
21:U:3:LYS:HB2	21:U:3:LYS:HE3	1.75	0.41
1:A:1130:A:OP1	1:A:1131:G:N7	2.53	0.41
1:A:1351:U:H4'	7:G:33:ASP:OD2	2.20	0.41
1:A:379:C:N4	1:A:384:G:H1	2.18	0.41
1:A:491:G:C2	1:A:492:G:C8	3.07	0.41
1:A:824:C:H2'	1:A:825:G:C8	2.56	0.41
2:B:76:GLN:O	2:B:208:ILE:HD12	2.20	0.41
3:C:32:LEU:HG	3:C:32:LEU:H	1.58	0.41
4:D:62:GLN:NE2	4:D:66:ARG:HD2	2.35	0.41
5:E:148:VAL:O	5:E:152:ARG:HG3	2.20	0.41
6:F:36:ARG:NH1	6:F:36:ARG:HB3	2.21	0.41
9:I:49:PRO:HB2	9:I:81:ILE:HG22	2.02	0.41
13:M:18:ALA:O	13:M:21:TYR:HB2	2.19	0.41
16:P:8:ARG:HB3	16:P:28:ARG:NH1	2.35	0.41
19:S:21:GLU:O	19:S:25:LYS:HB2	2.21	0.41
20:T:49:ALA:O	20:T:52:ALA:HB3	2.20	0.41
1:A:1073:U:O2	2:B:104:ASN:ND2	2.54	0.41
1:A:1249:C:H5'	1:A:1250:A:OP2	2.21	0.41
1:A:147:G:H1	1:A:175:C:H42	1.69	0.41
1:A:966:M2G:N7	1:A:967:5MC:HM52	2.35	0.41
4:D:120:LEU:HD23	4:D:125:HIS:CD2	2.56	0.41
1:A:1119:C:OP1	9:I:83:ARG:NH1	2.53	0.41
9:I:94:ALA:O	9:I:98:PRO:HG3	2.21	0.41
12:L:33:ARG:HG3	12:L:61:THR:OG1	2.20	0.41
12:L:85:ILE:CG2	12:L:98:TYR:HB3	2.49	0.41
13:M:22:ILE:HG22	13:M:23:TYR:H	1.86	0.41
13:M:40:ASN:HD21	13:M:42:ALA:HB3	1.86	0.41
14:N:36:PHE:C	14:N:36:PHE:HD1	2.24	0.41
17:Q:65:ILE:HB	17:Q:69:LYS:HB3	2.03	0.41
1:A:1226:C:N4	13:M:104:ARG:HG3	2.36	0.41
1:A:268:C:H2'	1:A:269:C:H6	1.85	0.41
1:A:372:C:H1'	1:A:373:A:OP2	2.21	0.41
1:A:854:G:C2	1:A:855:G:C8	3.08	0.41
2:B:211:ILE:O	2:B:215:LEU:HB2	2.20	0.41
3:C:25:GLY:HA3	3:C:29:TYR:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:203:VAL:O	4:D:206:PHE:HB3	2.21	0.41
4:D:22:LYS:CB	4:D:26:CYS:HB2	2.51	0.41
5:E:91:LEU:N	5:E:91:LEU:HD23	2.35	0.41
7:G:58:PRO:HA	7:G:61:VAL:CG2	2.51	0.41
12:L:84:LEU:HA	12:L:84:LEU:HD12	1.91	0.41
16:P:19:ILE:HD12	16:P:38:TYR:N	2.36	0.41
17:Q:12:SER:HB3	17:Q:20:THR:HB	2.02	0.41
17:Q:24:GLU:HG3	17:Q:39:SER:HB3	2.03	0.41
17:Q:20:THR:CG2	17:Q:41:LYS:HG2	2.51	0.41
18:R:37:VAL:O	18:R:40:LEU:N	2.54	0.41
20:T:58:LYS:HG3	20:T:58:LYS:O	2.19	0.41
1:A:1133:G:C2	1:A:1134:G:C8	3.08	0.41
1:A:861:G:C6	1:A:862:C:C4	3.08	0.41
1:A:922:G:C2	1:A:1396:A:C6	3.09	0.41
1:A:965:A:OP1	1:A:1198:G:H5'	2.20	0.41
2:B:155:LEU:HA	2:B:155:LEU:HD23	1.64	0.41
2:B:46:LYS:HA	2:B:49:GLU:OE2	2.20	0.41
3:C:182:ILE:HA	3:C:202:ILE:O	2.20	0.41
4:D:20:TYR:CD2	4:D:20:TYR:N	2.88	0.41
1:A:8:A:H5'	5:E:101:ILE:HG23	2.02	0.41
6:F:91:VAL:HG12	6:F:92:LYS:O	2.21	0.41
12:L:98:TYR:CD1	12:L:98:TYR:N	2.89	0.41
13:M:54:VAL:HA	13:M:57:ARG:CD	2.50	0.41
15:O:21:ASP:OD2	15:O:23:GLY:N	2.54	0.41
16:P:4:ILE:O	16:P:66:PRO:HA	2.21	0.41
1:A:1164:G:C2	1:A:1165:C:C2	3.09	0.41
1:A:1285:A:H5'	1:A:1286:A:C5	2.56	0.41
1:A:1295:G:C6	1:A:1296:C:C4	3.08	0.41
1:A:976:G:C8	1:A:1358:U:O2	2.74	0.41
1:A:1375:A:N1	1:A:1376:U:C2	2.89	0.41
1:A:458:C:H2'	1:A:459:G:O4'	2.21	0.41
1:A:519:C:H2'	1:A:520:A:C8	2.55	0.41
1:A:738:C:OP1	6:F:92:LYS:HD3	2.21	0.41
3:C:113:ALA:HB3	3:C:114:PRO:HD3	2.03	0.41
4:D:192:GLU:O	4:D:194:LEU:N	2.54	0.41
7:G:42:ILE:HG21	7:G:42:ILE:HD13	1.88	0.41
8:H:86:ILE:HG21	8:H:133:LEU:HB3	2.02	0.41
9:I:111:ARG:HG2	9:I:112:LYS:N	2.36	0.41
10:J:24:VAL:HG12	10:J:24:VAL:O	2.21	0.41
12:L:7:ILE:HG23	17:Q:34:LYS:HE2	2.02	0.41
1:A:24:U:H2'	1:A:25:C:C6	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:686:U:HO2'	1:A:687:A:H8	1.59	0.41
1:A:70:G:C6	1:A:73:C:C4	3.09	0.41
1:A:95:U:H2'	1:A:96:G:H8	1.85	0.41
1:A:974:A:H4'	1:A:975:A:H3'	2.03	0.41
1:A:976:G:OP2	1:A:1358:U:H1'	2.21	0.41
2:B:236:TYR:HD2	2:B:236:TYR:HA	1.78	0.41
3:C:137:ALA:HA	3:C:140:ARG:CZ	2.51	0.41
4:D:196:LEU:HA	4:D:197:PRO:HD3	1.65	0.41
9:I:5:TYR:CE1	9:I:18:PHE:HE2	2.39	0.41
11:K:25:TYR:CZ	11:K:88:GLY:HA2	2.56	0.41
17:Q:67:LYS:O	17:Q:68:ARG:HB3	2.21	0.41
1:A:1150:U:H2'	1:A:1151:A:H5'	2.03	0.40
1:A:1172:C:H2'	1:A:1173:G:C8	2.55	0.40
1:A:1182:G:H4'	1:A:1183:A:C5'	2.49	0.40
1:A:132:C:O3'	20:T:74:LYS:NZ	2.50	0.40
1:A:349:A:H2'	1:A:350:G:C5'	2.50	0.40
2:B:188:ALA:O	2:B:202:PRO:HA	2.21	0.40
4:D:199:ASN:HD22	4:D:202:LEU:HG	1.86	0.40
5:E:55:VAL:HG12	5:E:56:GLN:N	2.35	0.40
7:G:37:ASN:HB3	7:G:38:LEU:HD12	2.03	0.40
1:A:1368:G:OP2	9:I:112:LYS:HD3	2.21	0.40
11:K:120:ARG:HA	11:K:121:PRO:HD3	1.86	0.40
11:K:58:PRO:HB2	11:K:93:GLN:HG3	2.02	0.40
15:O:36:ILE:HA	15:O:59:MET:HE2	2.03	0.40
19:S:18:LYS:HD2	19:S:31:ILE:HG12	2.03	0.40
1:A:1126:U:H6	1:A:1126:U:C5'	2.35	0.40
1:A:1213:A:N1	1:A:1215:G:H1'	2.36	0.40
1:A:1513:A:H2'	1:A:1514:C:C6	2.55	0.40
1:A:1528:U:H2'	1:A:1528:U:H6	1.65	0.40
1:A:266:G:P	25:A:2234:HOH:O	2.79	0.40
1:A:245:C:O2	1:A:283:C:N3	2.55	0.40
1:A:393:A:O2'	1:A:394:G:H5'	2.21	0.40
1:A:575:G:O2'	1:A:821:G:H5'	2.21	0.40
1:A:782:A:H2'	1:A:783:C:O4'	2.21	0.40
1:A:830:G:C5	1:A:831:U:C5	3.10	0.40
1:A:981:U:O4	1:A:1222:G:O6	2.40	0.40
2:B:97:TRP:CZ2	2:B:101:MET:HB2	2.57	0.40
1:A:1112:C:O2'	3:C:179:ARG:NH1	2.54	0.40
3:C:114:PRO:HG3	3:C:185:GLY:HA3	2.04	0.40
5:E:105:VAL:HG11	5:E:131:ILE:HG22	2.03	0.40
5:E:86:ALA:CB	5:E:125:SER:HB3	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:151:TYR:N	7:G:151:TYR:CD1	2.89	0.40
8:H:103:VAL:HG12	8:H:108:GLY:HA3	2.03	0.40
9:I:51:ARG:HH11	9:I:51:ARG:HB2	1.86	0.40
9:I:53:VAL:C	9:I:55:ALA:H	2.24	0.40
13:M:36:LYS:HD2	13:M:59:TYR:OH	2.21	0.40
16:P:3:LYS:HG3	16:P:65:GLN:O	2.21	0.40
20:T:74:LYS:HD3	20:T:74:LYS:HA	1.72	0.40
1:A:1003:G:C2	1:A:1003(A):G:C5	3.09	0.40
1:A:1066:C:C2'	1:A:1067:A:H5'	2.50	0.40
1:A:1476:G:H2'	1:A:1477:C:C6	2.57	0.40
1:A:1402:4OC:O2	1:A:1500:A:N1	2.55	0.40
1:A:1527:C:C2'	1:A:1528:U:H5'	2.52	0.40
1:A:287:U:C2'	1:A:288:A:H5'	2.52	0.40
1:A:325:A:N6	1:A:326:G:C2	2.90	0.40
1:A:631:G:H2'	1:A:632:A:C8	2.57	0.40
1:A:88:A:C4	1:A:89:C:C6	3.09	0.40
2:B:23:ARG:O	2:B:24:TRP:HD1	2.05	0.40
4:D:30:LYS:C	4:D:32:ALA:N	2.73	0.40
8:H:6:ILE:HG13	8:H:31:PHE:HE2	1.86	0.40
1:A:943:U:H1'	9:I:124:GLN:HE22	1.86	0.40
1:A:779:C:H5''	11:K:122:LYS:HB3	2.02	0.40
14:N:23:ARG:HD3	14:N:28:GLY:O	2.20	0.40
15:O:21:ASP:OD1	15:O:24:SER:OG	2.25	0.40
15:O:39:LEU:HA	15:O:39:LEU:HD12	1.77	0.40
16:P:9:PHE:HD1	16:P:9:PHE:HA	1.64	0.40
17:Q:22:LEU:HD12	17:Q:40:LYS:O	2.21	0.40
1:A:1081:G:H5''	1:A:1081:G:C8	2.57	0.40
1:A:1422:G:C2	1:A:1423:G:C8	3.10	0.40
1:A:1540:PSU:H3'	1:A:1540:PSU:C6	2.57	0.40
1:A:428:G:C6	1:A:430:A:C6	3.09	0.40
1:A:820:U:H4'	1:A:821:G:OP2	2.22	0.40
3:C:6:HIS:CD2	3:C:8:ILE:HB	2.56	0.40
4:D:152:SER:HA	4:D:155:LEU:HD21	2.03	0.40
10:J:22:LYS:NZ	10:J:90:LEU:HD12	2.37	0.40
13:M:54:VAL:HG23	13:M:57:ARG:HH11	1.87	0.40
19:S:50:ALA:HA	19:S:58:VAL:O	2.20	0.40
20:T:62:LEU:HD22	20:T:62:LEU:O	2.21	0.40
20:T:80:ARG:NH1	20:T:80:ARG:HG3	2.37	0.40
1:A:1164:G:C8	1:A:1164:G:OP2	2.74	0.40
1:A:987:G:N2	1:A:1219:U:O2	2.54	0.40
1:A:1321:C:C5	1:A:1322:C:C2	3.08	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1539:C:C4	1:A:1540:PSU:C2	3.09	0.40
1:A:20:U:H3'	1:A:20:U:C6	2.56	0.40
1:A:418:C:H1'	1:A:540:G:O2'	2.22	0.40
1:A:943:U:C2'	1:A:944:G:H5'	2.51	0.40
1:A:990:C:H42	1:A:1215:G:H1	1.68	0.40
3:C:51:GLY:O	3:C:115:LEU:HG	2.21	0.40
12:L:10:LEU:HA	12:L:10:LEU:HD22	1.75	0.40
1:A:227:G:H21	16:P:62:VAL:HG12	1.86	0.40
19:S:64:GLU:O	19:S:67:VAL:HG23	2.22	0.40

There are no symmetry-related clashes.

## 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	232/256 (91%)	199 (86%)	30 (13%)	3 (1%)	14	57
3	C	204/239 (85%)	172 (84%)	30 (15%)	2 (1%)	18	61
4	D	206/209 (99%)	186 (90%)	17 (8%)	3 (2%)	12	54
5	E	148/162 (91%)	137 (93%)	9 (6%)	2 (1%)	13	55
6	F	99/101 (98%)	96 (97%)	3 (3%)	0	100	100
7	G	153/156 (98%)	137 (90%)	15 (10%)	1 (1%)	25	68
8	H	136/138 (99%)	129 (95%)	7 (5%)	0	100	100
9	I	125/128 (98%)	112 (90%)	12 (10%)	1 (1%)	22	65
10	J	96/105 (91%)	74 (77%)	20 (21%)	2 (2%)	8	48
11	K	114/129 (88%)	98 (86%)	16 (14%)	0	100	100
12	L	121/135 (90%)	105 (87%)	14 (12%)	2 (2%)	11	52
13	M	116/126 (92%)	103 (89%)	10 (9%)	3 (3%)	6	43
14	N	58/61 (95%)	48 (83%)	10 (17%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	O	85/89 (96%)	75 (88%)	10 (12%)	0	100	100
16	P	81/88 (92%)	74 (91%)	6 (7%)	1 (1%)	15	58
17	Q	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
18	R	68/88 (77%)	60 (88%)	8 (12%)	0	100	100
19	S	78/93 (84%)	70 (90%)	5 (6%)	3 (4%)	4	35
20	T	97/106 (92%)	81 (84%)	16 (16%)	0	100	100
21	U	22/27 (82%)	20 (91%)	2 (9%)	0	100	100
All	All	2336/2541 (92%)	2066 (88%)	247 (11%)	23 (1%)	18	61

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
19	S	31	ILE
19	S	70	LYS
2	B	21	ARG
2	B	24	TRP
3	C	15	THR
12	L	28	LYS
19	S	30	LEU
4	D	35	ARG
7	G	59	LEU
9	I	117	HIS
2	B	229	VAL
4	D	160	GLN
13	M	59	TYR
13	M	61	GLU
5	E	129	ILE
10	J	34	VAL
3	C	66	VAL
4	D	5	ILE
13	M	7	VAL
16	P	53	VAL
5	E	70	PRO
10	J	72	VAL
12	L	25	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	202/220 (92%)	146 (72%)	56 (28%)	0	4
3	C	160/188 (85%)	107 (67%)	53 (33%)	0	2
4	D	180/181 (99%)	141 (78%)	39 (22%)	1	8
5	E	115/123 (94%)	78 (68%)	37 (32%)	0	2
6	F	90/90 (100%)	66 (73%)	24 (27%)	0	4
7	G	126/127 (99%)	92 (73%)	34 (27%)	0	4
8	H	119/119 (100%)	89 (75%)	30 (25%)	0	5
9	I	98/99 (99%)	77 (79%)	21 (21%)	1	8
10	J	87/92 (95%)	71 (82%)	16 (18%)	2	13
11	K	88/99 (89%)	66 (75%)	22 (25%)	1	5
12	L	103/110 (94%)	73 (71%)	30 (29%)	0	3
13	M	94/101 (93%)	71 (76%)	23 (24%)	1	6
14	N	49/50 (98%)	41 (84%)	8 (16%)	3	19
15	O	79/80 (99%)	61 (77%)	18 (23%)	1	7
16	P	72/74 (97%)	60 (83%)	12 (17%)	2	18
17	Q	94/97 (97%)	71 (76%)	23 (24%)	1	6
18	R	61/77 (79%)	45 (74%)	16 (26%)	0	4
19	S	71/80 (89%)	50 (70%)	21 (30%)	0	3
20	T	76/82 (93%)	54 (71%)	22 (29%)	0	3
21	U	19/22 (86%)	15 (79%)	4 (21%)	1	9
All	All	1983/2111 (94%)	1474 (74%)	509 (26%)	0	5

All (509) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	8	LYS
2	B	10	LEU
2	B	12	GLU

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Mol	Chain	Res	Type
2	B	16	HIS
2	B	19	HIS
2	B	23	ARG
2	B	24	TRP
2	B	26	PRO
2	B	30	ARG
2	B	33	TYR
2	B	39	ILE
2	B	46	LYS
2	B	48	MET
2	B	49	GLU
2	B	51	LEU
2	B	53	ARG
2	B	59	GLU
2	B	69	LEU
2	B	75	LYS
2	B	84	GLU
2	B	87	ARG
2	B	92	TYR
2	B	96	ARG
2	B	97	TRP
2	B	98	LEU
2	B	102	LEU
2	B	106	LYS
2	B	121	LEU
2	B	127	ILE
2	B	129	GLU
2	B	142	LEU
2	B	144	ARG
2	B	147	LYS
2	B	150	SER
2	B	153	ARG
2	B	154	LEU
2	B	157	ARG
2	B	165	VAL
2	B	169	LYS
2	B	175	ARG
2	B	178	ARG
2	B	180	LEU
2	B	184	VAL
2	B	185	ILE
2	B	187	LEU

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Mol	Chain	Res	Type
2	B	193	ASP
2	B	196	LEU
2	B	197	VAL
2	B	200	ILE
2	B	215	LEU
2	B	216	SER
2	B	217	ARG
2	B	223	ILE
2	B	226	ARG
2	B	231	GLU
2	B	236	TYR
3	C	3	ASN
3	C	4	LYS
3	C	14	ILE
3	C	15	THR
3	C	20	SER
3	C	21	ARG
3	C	26	LYS
3	C	28	GLN
3	C	30	ARG
3	C	32	LEU
3	C	33	LEU
3	C	34	LEU
3	C	39	ILE
3	C	49	SER
3	C	57	ILE
3	C	62	ASP
3	C	63	ASN
3	C	64	VAL
3	C	75	VAL
3	C	79	ARG
3	C	86	VAL
3	C	91	LEU
3	C	94	LEU
3	C	98	ASN
3	C	101	LEU
3	C	102	ASN
3	C	112	SER
3	C	115	LEU
3	C	118	GLN
3	C	127	ARG
3	C	130	VAL

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Mol	Chain	Res	Type
3	C	131	ARG
3	C	132	ARG
3	C	135	LYS
3	C	139	GLN
3	C	147	LYS
3	C	156	ARG
3	C	157	ILE
3	C	162	GLN
3	C	165	THR
3	C	167	TRP
3	C	172	ARG
3	C	175	LEU
3	C	178	LEU
3	C	188	LEU
3	C	190	ARG
3	C	193	TYR
3	C	195	VAL
3	C	196	LEU
3	C	198	VAL
3	C	203	PHE
3	C	204	LEU
3	C	207	VAL
4	D	5	ILE
4	D	9	CYS
4	D	12	CYS
4	D	15	GLU
4	D	19	LEU
4	D	20	TYR
4	D	22	LYS
4	D	25	ARG
4	D	26	CYS
4	D	30	LYS
4	D	50	ARG
4	D	58	LEU
4	D	61	LYS
4	D	64	LEU
4	D	71	SER
4	D	73	ARG
4	D	83	SER
4	D	86	LYS
4	D	91	SER
4	D	108	LEU

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Mol	Chain	Res	Type
4	D	112	VAL
4	D	115	ARG
4	D	119	GLN
4	D	120	LEU
4	D	122	ARG
4	D	127	THR
4	D	129	ASN
4	D	137	SER
4	D	140	VAL
4	D	141	ARG
4	D	148	VAL
4	D	157	LEU
4	D	174	LEU
4	D	186	LEU
4	D	187	ARG
4	D	192	GLU
4	D	194	LEU
4	D	198	VAL
4	D	202	LEU
5	E	12	LEU
5	E	16	THR
5	E	18	ARG
5	E	19	MET
5	E	20	GLN
5	E	25	ARG
5	E	26	PHE
5	E	31	LEU
5	E	34	VAL
5	E	41	VAL
5	E	53	LEU
5	E	56	GLN
5	E	60	TYR
5	E	61	TYR
5	E	67	VAL
5	E	68	GLU
5	E	75	THR
5	E	76	ILE
5	E	79	GLU
5	E	80	ILE
5	E	84	PHE
5	E	87	SER
5	E	92	LYS

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Mol	Chain	Res	Type
5	E	100	VAL
5	E	112	LEU
5	E	116	THR
5	E	117	ASP
5	E	121	LYS
5	E	125	SER
5	E	126	ARG
5	E	130	ASN
5	E	131	ILE
5	E	144	THR
5	E	147	ASP
5	E	148	VAL
5	E	151	LEU
5	E	152	ARG
6	F	5	GLU
6	F	9	VAL
6	F	15	ASP
6	F	19	LEU
6	F	23	LYS
6	F	36	ARG
6	F	37	VAL
6	F	39	LYS
6	F	43	LEU
6	F	54	LYS
6	F	55	ASP
6	F	61	LEU
6	F	69	GLU
6	F	70	ASP
6	F	71	ARG
6	F	74	ASP
6	F	75	LEU
6	F	82	ARG
6	F	83	ASP
6	F	87	ARG
6	F	93	SER
6	F	97	PHE
6	F	98	LEU
6	F	100	ASN
7	G	3	ARG
7	G	5	ARG
7	G	6	ARG
7	G	8	GLU

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Mol	Chain	Res	Type
7	G	15	ASP
7	G	22	LEU
7	G	24	THR
7	G	30	ILE
7	G	31	MET
7	G	32	ARG
7	G	49	ILE
7	G	50	ILE
7	G	52	GLU
7	G	53	LYS
7	G	54	THR
7	G	57	GLU
7	G	67	GLU
7	G	72	ARG
7	G	80	VAL
7	G	86	GLN
7	G	87	VAL
7	G	89	MET
7	G	91	VAL
7	G	95	ARG
7	G	106	GLN
7	G	110	GLN
7	G	111	ARG
7	G	113	GLU
7	G	115	ARG
7	G	125	MET
7	G	126	ASP
7	G	129	GLU
7	G	146	GLU
7	G	155	ARG
8	H	3	THR
8	H	5	PRO
8	H	6	ILE
8	H	8	ASP
8	H	11	THR
8	H	19	VAL
8	H	26	VAL
8	H	29	SER
8	H	35	ILE
8	H	50	ARG
8	H	51	VAL
8	H	63	LEU

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Mol	Chain	Res	Type
8	H	79	VAL
8	H	81	HIS
8	H	83	ILE
8	H	85	ARG
8	H	86	ILE
8	H	88	LYS
8	H	91	ARG
8	H	92	ARG
8	H	95	VAL
8	H	98	LYS
8	H	104	ARG
8	H	105	ARG
8	H	115	SER
8	H	120	THR
8	H	122	ARG
8	H	127	LEU
8	H	129	VAL
8	H	133	LEU
9	I	4	TYR
9	I	5	TYR
9	I	20	ARG
9	I	26	VAL
9	I	27	THR
9	I	53	VAL
9	I	65	VAL
9	I	66	ARG
9	I	70	LYS
9	I	78	LYS
9	I	79	LEU
9	I	102	LEU
9	I	104	ARG
9	I	107	ARG
9	I	109	VAL
9	I	112	LYS
9	I	113	LYS
9	I	114	TYR
9	I	121	ARG
9	I	127	LYS
9	I	128	ARG
10	J	3	LYS
10	J	8	LEU
10	J	17	ASP

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Mol	Chain	Res	Type
10	J	21	GLN
10	J	30	SER
10	J	38	ILE
10	J	43	ARG
10	J	48	THR
10	J	59	SER
10	J	65	LEU
10	J	68	HIS
10	J	69	ASN
10	J	79	ARG
10	J	82	ILE
10	J	89	ASP
10	J	96	ILE
11	K	11	LYS
11	K	13	GLN
11	K	14	VAL
11	K	18	ARG
11	K	29	ILE
11	K	30	VAL
11	K	32	ILE
11	K	40	ILE
11	K	48	ILE
11	K	75	TYR
11	K	77	MET
11	K	79	SER
11	K	85	ARG
11	K	87	THR
11	K	98	LEU
11	K	101	SER
11	K	104	GLN
11	K	105	VAL
11	K	109	VAL
11	K	116	HIS
11	K	117	ASN
11	K	119	CYS
12	L	6	THR
12	L	10	LEU
12	L	11	VAL
12	L	12	ARG
12	L	18	VAL
12	L	19	ARG
12	L	20	LYS

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Mol	Chain	Res	Type
12	L	33	ARG
12	L	36	VAL
12	L	41	ARG
12	L	43	VAL
12	L	47	LYS
12	L	53	ARG
12	L	55	VAL
12	L	59	ARG
12	L	61	THR
12	L	62	SER
12	L	64	TYR
12	L	66	VAL
12	L	79	GLU
12	L	80	HIS
12	L	81	SER
12	L	97	ARG
12	L	98	TYR
12	L	101	VAL
12	L	112	ASP
12	L	115	LYS
12	L	119	LYS
12	L	122	THR
12	L	126	LYS
13	M	3	ARG
13	M	12	ASN
13	M	14	ARG
13	M	16	ASP
13	M	19	LEU
13	M	27	LYS
13	M	34	LEU
13	M	35	GLU
13	M	48	LEU
13	M	49	THR
13	M	56	LEU
13	M	60	VAL
13	M	66	LEU
13	M	67	GLU
13	M	70	LEU
13	M	71	ARG
13	M	74	VAL
13	M	80	ARG
13	M	103	THR

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Mol	Chain	Res	Type
13	M	109	THR
13	M	110	ARG
13	M	113	PRO
13	M	115	LYS
14	N	21	TYR
14	N	24	CYS
14	N	31	ARG
14	N	36	PHE
14	N	41	ARG
14	N	45	ARG
14	N	58	LYS
14	N	60	SER
15	O	4	THR
15	O	9	GLN
15	O	10	LYS
15	O	17	ARG
15	O	32	LEU
15	O	33	THR
15	O	34	LEU
15	O	38	ARG
15	O	42	HIS
15	O	45	VAL
15	O	48	LYS
15	O	52	SER
15	O	56	LEU
15	O	63	ARG
15	O	65	ARG
15	O	67	LEU
15	O	70	LEU
15	O	75	PRO
16	P	3	LYS
16	P	8	ARG
16	P	27	LYS
16	P	31	LYS
16	P	44	THR
16	P	54	GLU
16	P	55	ARG
16	P	62	VAL
16	P	68	ASP
16	P	72	ARG
16	P	74	LEU
16	P	75	ARG

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Mol	Chain	Res	Type
17	Q	6	LEU
17	Q	7	THR
17	Q	9	VAL
17	Q	10	VAL
17	Q	21	VAL
17	Q	34	LYS
17	Q	35	VAL
17	Q	36	ILE
17	Q	37	LYS
17	Q	50	LYS
17	Q	53	LEU
17	Q	57	VAL
17	Q	59	ILE
17	Q	60	ILE
17	Q	68	ARG
17	Q	74	LEU
17	Q	76	LEU
17	Q	81	ARG
17	Q	86	GLU
17	Q	87	LYS
17	Q	96	GLN
17	Q	97	SER
17	Q	99	SER
18	R	19	LYS
18	R	21	LYS
18	R	30	ASP
18	R	31	LEU
18	R	32	ARG
18	R	47	THR
18	R	50	ILE
18	R	51	LEU
18	R	55	ARG
18	R	56	THR
18	R	65	ILE
18	R	69	THR
18	R	71	LYS
18	R	84	LYS
18	R	87	ARG
18	R	88	LYS
19	S	3	ARG
19	S	5	LEU
19	S	7	LYS

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Mol	Chain	Res	Type
19	S	15	LEU
19	S	18	LYS
19	S	20	LEU
19	S	29	ARG
19	S	31	ILE
19	S	33	THR
19	S	35	SER
19	S	39	THR
19	S	41	VAL
19	S	43	GLU
19	S	49	ILE
19	S	51	VAL
19	S	55	LYS
19	S	60	VAL
19	S	64	GLU
19	S	69	HIS
19	S	70	LYS
19	S	71	LEU
20	T	18	GLN
20	T	19	SER
20	T	20	LEU
20	T	25	ARG
20	T	30	LYS
20	T	33	ILE
20	T	35	THR
20	T	42	GLN
20	T	45	GLN
20	T	50	GLU
20	T	53	LEU
20	T	56	MET
20	T	62	LEU
20	T	72	LEU
20	T	75	ASN
20	T	79	ARG
20	T	84	LEU
20	T	86	ARG
20	T	90	GLN
20	T	91	LEU
20	T	92	LEU
20	T	99	LEU
21	U	8	THR
21	U	10	ARG

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Mol	Chain	Res	Type
21	U	12	LYS
21	U	13	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
4	D	119	GLN
4	D	123	HIS
4	D	129	ASN
6	F	84	ASN
8	H	82	HIS
9	I	124	GLN
10	J	56	HIS
10	J	62	HIS
17	Q	16	GLN
18	R	63	GLN
19	S	14	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1507/1522 (99%)	422 (28%)	0

All (422) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	7	G
1	A	8	A
1	A	9	G
1	A	21	G
1	A	22	G
1	A	31	G
1	A	32	A
1	A	39	G
1	A	41	G
1	A	44	G
1	A	47	C
1	A	48	C
1	A	49	U

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Mol	Chain	Res	Type
1	A	50	A
1	A	51	A
1	A	66	G
1	A	70	G
1	A	73	C
1	A	81	U
1	A	82	U
1	A	88	A
1	A	92	C
1	A	96	G
1	A	99	C
1	A	101	A
1	A	108	G
1	A	116	A
1	A	121	C
1	A	129(A)	G
1	A	130	A
1	A	131	C
1	A	134	A
1	A	144	G
1	A	149	A
1	A	151	A
1	A	156	G
1	A	159	G
1	A	163	C
1	A	167	G
1	A	173	U
1	A	181	G
1	A	182	U
1	A	183	G
1	A	187	C
1	A	190(E)	U
1	A	190(G)	G
1	A	195	A
1	A	197	A
1	A	201	C
1	A	202	U
1	A	203	U
1	A	204	U
1	A	216	G
1	A	220	G
1	A	231	G

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Mol	Chain	Res	Type
1	A	244	U
1	A	247	G
1	A	251	G
1	A	252	U
1	A	253	U
1	A	254	G
1	A	266	G
1	A	267	C
1	A	274	A
1	A	287	U
1	A	289	G
1	A	291	C
1	A	296	U
1	A	297	G
1	A	298	A
1	A	301	G
1	A	321	A
1	A	326	G
1	A	328	C
1	A	329	A
1	A	332	G
1	A	344	A
1	A	345	C
1	A	350	G
1	A	351	G
1	A	352	C
1	A	353	A
1	A	354	G
1	A	356	A
1	A	367	U
1	A	371	G
1	A	373	A
1	A	374	A
1	A	384	G
1	A	390	C
1	A	392	G
1	A	397	A
1	A	398	C
1	A	406	G
1	A	409	G
1	A	411	A
1	A	412	A

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Mol	Chain	Res	Type
1	A	413	G
1	A	417	C
1	A	420	U
1	A	421	U
1	A	422	C
1	A	423	G
1	A	424	G
1	A	429	U
1	A	430	A
1	A	439	A
1	A	450	G
1	A	453	A
1	A	455	C
1	A	459	G
1	A	460	A
1	A	461	C
1	A	475	G
1	A	476	G
1	A	478	A
1	A	479	C
1	A	481	G
1	A	482	A
1	A	484	G
1	A	485	G
1	A	497	A
1	A	498	U
1	A	504	C
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	522	C
1	A	527	7MG
1	A	530	G
1	A	531	U
1	A	532	A
1	A	533	A
1	A	547	A
1	A	548	G
1	A	559	A

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Mol	Chain	Res	Type
1	A	560	U
1	A	562	C
1	A	563	A
1	A	566	G
1	A	568	G
1	A	572	A
1	A	573	A
1	A	576	G
1	A	577	G
1	A	579	G
1	A	588	G
1	A	597	G
1	A	608	A
1	A	616	G
1	A	622	A
1	A	631	G
1	A	634	C
1	A	641	U
1	A	651	C
1	A	652	U
1	A	653	A
1	A	658	G
1	A	665	A
1	A	670	G
1	A	684	A
1	A	686	U
1	A	687	A
1	A	688	G
1	A	693	G
1	A	695	A
1	A	701	C
1	A	702	A
1	A	703	G
1	A	714	G
1	A	722	A
1	A	723	U
1	A	724	G
1	A	731	G
1	A	733	A
1	A	734	G
1	A	741	G
1	A	749	C

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Mol	Chain	Res	Type
1	A	755	G
1	A	759	A
1	A	761	G
1	A	773	G
1	A	774	G
1	A	777	A
1	A	781	A
1	A	787	A
1	A	788	U
1	A	789	U
1	A	791	G
1	A	792	A
1	A	793	U
1	A	794	A
1	A	795	C
1	A	813	U
1	A	815	A
1	A	817	C
1	A	819	A
1	A	821	G
1	A	827	U
1	A	828	A
1	A	839	U
1	A	840	C
1	A	841	U
1	A	848	C
1	A	852	G
1	A	853	G
1	A	855	G
1	A	859	A
1	A	869	G
1	A	870	U
1	A	871	U
1	A	872	A
1	A	873	A
1	A	876	G
1	A	885	G
1	A	895	G
1	A	902	G
1	A	907	A
1	A	910	C
1	A	914	G

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Mol	Chain	Res	Type
1	A	917	G
1	A	922	G
1	A	926	G
1	A	927	G
1	A	932	C
1	A	934	C
1	A	935	A
1	A	938	A
1	A	940	C
1	A	950	U
1	A	954	G
1	A	960	U
1	A	966	M2G
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	982	U
1	A	984	C
1	A	986	A
1	A	987	G
1	A	989	C
1	A	990	C
1	A	991	U
1	A	992	U
1	A	993	G
1	A	996	A
1	A	1004	A
1	A	1005	A
1	A	1007	C
1	A	1008	C
1	A	1010	G
1	A	1023	G
1	A	1024	G
1	A	1026	G
1	A	1027	C
1	A	1030(B)	C
1	A	1031	G
1	A	1037	C
1	A	1045	C

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Mol	Chain	Res	Type
1	A	1046	A
1	A	1049	U
1	A	1050	G
1	A	1051	C
1	A	1054	C
1	A	1060	C
1	A	1064	G
1	A	1065	U
1	A	1066	C
1	A	1068	G
1	A	1072	G
1	A	1085	U
1	A	1092	A
1	A	1093	A
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1104	G
1	A	1126	U
1	A	1127	G
1	A	1128	C
1	A	1129	C
1	A	1130	A
1	A	1131	G
1	A	1137	C
1	A	1139	G
1	A	1140	C
1	A	1141	C
1	A	1142	G
1	A	1145	C
1	A	1146	A
1	A	1149	C
1	A	1152	A
1	A	1159	U
1	A	1160	G
1	A	1161	C
1	A	1162	C
1	A	1164	G
1	A	1165	C
1	A	1168	A
1	A	1171	G
1	A	1172	C

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Mol	Chain	Res	Type
1	A	1176	A
1	A	1183	A
1	A	1184	G
1	A	1190	G
1	A	1194	U
1	A	1196	U
1	A	1197	G
1	A	1198	G
1	A	1200	C
1	A	1201	A
1	A	1202	G
1	A	1206	G
1	A	1210	C
1	A	1211	U
1	A	1212	U
1	A	1214	C
1	A	1223	C
1	A	1224	G
1	A	1225	A
1	A	1226	C
1	A	1228	C
1	A	1229	A
1	A	1233	G
1	A	1238	A
1	A	1241	G
1	A	1242	C
1	A	1243	C
1	A	1245	A
1	A	1249	C
1	A	1253	G
1	A	1257	U
1	A	1258	G
1	A	1260	C
1	A	1261	A
1	A	1270	C
1	A	1273	G
1	A	1277	C
1	A	1278	U
1	A	1279	A
1	A	1280	A
1	A	1281	U
1	A	1282	C

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Mol	Chain	Res	Type
1	A	1285	A
1	A	1286	A
1	A	1287	A
1	A	1289	A
1	A	1297	C
1	A	1300	G
1	A	1301	U
1	A	1302	U
1	A	1304	G
1	A	1305	G
1	A	1306	A
1	A	1311	G
1	A	1312	G
1	A	1315	U
1	A	1319	A
1	A	1320	C
1	A	1322	C
1	A	1332	A
1	A	1335	C
1	A	1336	C
1	A	1338	G
1	A	1340	A
1	A	1346	A
1	A	1347	G
1	A	1348	U
1	A	1353	G
1	A	1358	U
1	A	1359	C
1	A	1364	U
1	A	1370	G
1	A	1376	U
1	A	1378	C
1	A	1379	G
1	A	1380	U
1	A	1381	U
1	A	1394	A
1	A	1398	A
1	A	1399	C
1	A	1403	C
1	A	1411	C
1	A	1442	G
1	A	1443	G

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Mol	Chain	Res	Type
1	A	1446	A
1	A	1447	G
1	A	1451	A
1	A	1452	C
1	A	1454	G
1	A	1463	C
1	A	1464	G
1	A	1476	G
1	A	1483	A
1	A	1487	G
1	A	1489	G
1	A	1493	A
1	A	1494	G
1	A	1497	G
1	A	1498	UR3
1	A	1499	A
1	A	1502	A
1	A	1503	A
1	A	1504	G
1	A	1505	G
1	A	1506	U
1	A	1520	G
1	A	1522	U
1	A	1529	G
1	A	1530	G
1	A	1531	A
1	A	1533	C
1	A	1540	PSU
1	A	1541	PSU
1	A	1542	U

There are no RNA pucker outliers to report.

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

15 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	19,26,27	2.88	3 (15%)	20,38,41	2.30	3 (15%)
1	5MC	A	1400	1	15,22,23	0.78	0	17,32,35	1.46	3 (17%)
1	4OC	A	1402	1	16,23,24	1.55	3 (18%)	19,32,35	0.82	1 (5%)
1	5MC	A	1404	1	15,22,23	1.08	2 (13%)	17,32,35	0.91	1 (5%)
1	5MC	A	1407	1	15,22,23	0.86	0	17,32,35	1.30	2 (11%)
1	UR3	A	1498	1,23	14,22,23	1.33	3 (21%)	16,32,35	1.10	2 (12%)
1	MA6	A	1518	1	16,26,27	1.02	1 (6%)	18,38,41	1.34	3 (16%)
1	MA6	A	1519	1	16,26,27	1.79	5 (31%)	18,38,41	1.06	3 (16%)
1	PSU	A	1540	1	16,21,22	1.17	1 (6%)	20,30,33	4.15	5 (25%)
1	PSU	A	1541	1	16,21,22	1.79	2 (12%)	20,30,33	5.39	9 (45%)
1	PSU	A	516	1,23	16,21,22	1.55	3 (18%)	20,30,33	4.32	5 (25%)
1	7MG	A	527	1	20,26,27	2.84	7 (35%)	22,39,42	1.48	4 (18%)
1	M2G	A	966	1	20,27,28	1.06	2 (10%)	21,40,43	2.42	4 (19%)
1	5MC	A	967	1	15,22,23	0.99	1 (6%)	17,32,35	0.99	2 (11%)
12	0TD	L	92	12	5,9,10	3.41	1 (20%)	3,11,13	3.92	2 (66%)

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	-	0/5/27/28	0/3/3/3
1	5MC	A	1400	1	-	0/3/25/26	0/2/2/2
1	4OC	A	1402	1	-	0/7/29/30	0/2/2/2
1	5MC	A	1404	1	-	0/3/25/26	0/2/2/2
1	5MC	A	1407	1	-	0/3/25/26	0/2/2/2
1	UR3	A	1498	1,23	-	0/3/25/26	0/2/2/2
1	MA6	A	1518	1	-	0/7/29/30	0/3/3/3
1	MA6	A	1519	1	-	0/7/29/30	0/3/3/3
1	PSU	A	1540	1	-	0/7/25/26	0/2/2/2
1	PSU	A	1541	1	-	0/7/25/26	0/2/2/2
1	PSU	A	516	1,23	-	0/7/25/26	0/2/2/2
1	7MG	A	527	1	-	0/7/37/38	0/3/3/3
1	M2G	A	966	1	-	0/7/29/30	0/3/3/3
1	5MC	A	967	1	-	0/3/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	0TD	L	92	12	-	0/2/12/14	0/0/0/0

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	527	7MG	C8-N9	-7.80	1.34	1.45
1	A	527	7MG	O5'-C5'	-3.72	1.39	1.44
1	A	527	7MG	CM7-N7	-3.65	1.39	1.46
1	A	1498	UR3	C6-N1	-2.92	1.31	1.35
1	A	1402	4OC	C4-N3	-2.86	1.28	1.34
1	A	1402	4OC	C6-N1	-2.61	1.32	1.35
1	A	527	7MG	C8-N7	-2.54	1.32	1.43
1	A	1404	5MC	C6-C5	-2.51	1.33	1.40
1	A	516	PSU	O4'-C1'	-2.21	1.41	1.44
1	A	966	M2G	O5'-C5'	-2.16	1.41	1.44
1	A	1498	UR3	C4-N3	-2.08	1.35	1.38
1	A	516	PSU	C6-C5	2.05	1.41	1.38
1	A	967	5MC	C2-N3	2.07	1.42	1.38
1	A	1519	MA6	C4-N3	2.10	1.38	1.35
1	A	1404	5MC	C2-N3	2.19	1.42	1.38
1	A	1519	MA6	C2-N3	2.40	1.36	1.32
1	A	1498	UR3	O3'-C3'	2.43	1.48	1.43
1	A	1519	MA6	C5-C4	2.48	1.46	1.40
1	A	1518	MA6	C2-N1	2.51	1.38	1.33
1	A	527	7MG	C4-N3	2.65	1.37	1.34
1	A	966	M2G	C6-N1	2.95	1.38	1.33
1	A	1207	2MG	C2-N1	3.18	1.45	1.34
1	A	1519	MA6	C2-N1	3.65	1.40	1.33
1	A	1402	4OC	CM4-N4	3.73	1.51	1.45
1	A	1540	PSU	C4-N3	3.86	1.40	1.33
1	A	1519	MA6	C9-N6	4.32	1.56	1.45
1	A	516	PSU	C4-N3	4.43	1.41	1.33
1	A	1541	PSU	C4-N3	4.48	1.41	1.33
1	A	1541	PSU	C5-C1'	4.84	1.56	1.52
1	A	527	7MG	C2-N2	4.96	1.44	1.34
1	A	527	7MG	C6-C5	4.99	1.47	1.41
1	A	1207	2MG	C6-N1	6.03	1.44	1.33
12	L	92	0TD	CA-C	7.22	1.59	1.50
1	A	1207	2MG	C2-N2	9.95	1.42	1.34

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1541	PSU	N1-C2-N3	-18.01	115.44	128.40
1	A	516	PSU	N1-C2-N3	-15.37	117.34	128.40
1	A	1540	PSU	N1-C2-N3	-12.58	119.35	128.40
1	A	1207	2MG	C5-C6-N1	-8.39	111.53	123.48
1	A	966	M2G	C5-C6-N1	-8.10	111.95	123.48
1	A	1540	PSU	C5-C4-N3	-7.82	119.02	125.43
1	A	1540	PSU	C5-C1'-C2'	-7.36	102.85	115.55
1	A	1541	PSU	C5-C4-N3	-6.69	119.94	125.43
1	A	516	PSU	C5-C4-N3	-6.42	120.16	125.43
12	L	92	0TD	CSB-SB-CB	-6.30	89.85	101.60
1	A	1541	PSU	C5-C1'-C2'	-5.33	106.35	115.55
1	A	1400	5MC	CM5-C5-C4	-4.14	117.39	121.65
1	A	527	7MG	C5-C4-N3	-3.61	120.44	126.47
1	A	1407	5MC	CM5-C5-C4	-3.19	118.38	121.65
1	A	1541	PSU	C3'-C2'-C1'	-2.97	98.51	101.93
1	A	1518	MA6	N1-C6-N6	-2.84	113.99	117.00
1	A	1518	MA6	C1'-N9-C4	-2.82	121.76	126.64
1	A	966	M2G	N1-C2-N2	-2.71	114.37	117.16
1	A	1402	4OC	CM4-N4-C4	-2.58	120.71	122.94
1	A	966	M2G	CM1-N2-C2	-2.57	118.90	121.34
12	L	92	0TD	C-CA-N	-2.43	104.95	109.86
1	A	967	5MC	CM5-C5-C4	-2.25	119.34	121.65
1	A	1207	2MG	C1'-N9-C4	-2.21	122.82	126.64
1	A	1541	PSU	O4'-C4'-C3'	-2.20	100.80	105.17
1	A	1404	5MC	C5-C4-N3	2.00	124.47	121.22
1	A	1498	UR3	C2'-C3'-C4'	2.04	106.59	102.62
1	A	1400	5MC	C5-C4-N3	2.06	124.56	121.22
1	A	527	7MG	C6-N1-C2	2.14	119.14	116.06
1	A	1407	5MC	CM5-C5-C6	2.17	123.01	118.67
1	A	1498	UR3	C4'-O4'-C1'	2.23	112.15	109.77
1	A	1519	MA6	C2-N1-C6	2.28	117.41	111.82
1	A	1519	MA6	N1-C6-N6	2.29	119.43	117.00
1	A	1519	MA6	N3-C2-N1	2.29	130.85	128.86
1	A	1518	MA6	N3-C2-N1	2.41	130.95	128.86
1	A	527	7MG	C2-N3-C4	2.44	120.80	113.95
1	A	967	5MC	CM5-C5-C6	2.44	123.54	118.67
1	A	1540	PSU	C6-N1-C2	2.63	119.58	115.36
1	A	1541	PSU	C4-C5-C1'	2.66	126.31	121.15
1	A	516	PSU	C5-C1'-C2'	2.90	120.55	115.55
1	A	1400	5MC	CM5-C5-C6	3.14	124.94	118.67
1	A	516	PSU	C6-N1-C2	3.42	120.83	115.36
1	A	527	7MG	N3-C4-N9	3.54	131.50	126.98
1	A	1541	PSU	C6-N1-C2	3.91	121.62	115.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1207	2MG	C6-N1-C2	4.36	122.98	115.18
1	A	966	M2G	C6-N1-C2	5.66	122.92	116.18
1	A	1541	PSU	O4'-C1'-C5	6.15	119.45	109.93
1	A	1540	PSU	C4-N3-C2	6.89	121.18	115.16
1	A	516	PSU	C4-N3-C2	7.95	122.11	115.16
1	A	1541	PSU	C4-N3-C2	9.80	123.73	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

13 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1400	5MC	1	0
1	A	1402	4OC	1	0
1	A	1404	5MC	7	0
1	A	1407	5MC	1	0
1	A	1498	UR3	2	0
1	A	1518	MA6	3	0
1	A	1519	MA6	3	0
1	A	1540	PSU	2	0
1	A	1541	PSU	2	0
1	A	527	7MG	2	0
1	A	966	M2G	1	0
1	A	967	5MC	1	0
12	L	92	0TD	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 276 ligands modelled in this entry, 275 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	$\# Z  > 2$
22	SRY	A	1601	-	39,42,42	2.39	9 (23%)	45,63,63	2.53	21 (46%)

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
22	SRY	A	1601	-	-	0/20/87/87	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	1601	SRY	O53-C53	-4.20	1.34	1.44
22	A	1601	SRY	C11-N11	-3.13	1.40	1.45
22	A	1601	SRY	O51-C51	-2.64	1.36	1.43
22	A	1601	SRY	C21-C31	-2.42	1.48	1.53
22	A	1601	SRY	C23-N23	-2.30	1.43	1.47
22	A	1601	SRY	CD1-NE1	2.58	1.45	1.34
22	A	1601	SRY	CA1-NB1	2.83	1.46	1.34
22	A	1601	SRY	CA1-N11	5.94	1.43	1.33
22	A	1601	SRY	CD1-N31	9.72	1.50	1.33

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1601	SRY	C13-O13-C22	-6.27	105.15	116.29
22	A	1601	SRY	C12-O42-C42	-5.63	99.45	108.48
22	A	1601	SRY	O41-C12-O42	-4.27	106.80	111.43
22	A	1601	SRY	O51-C51-C61	-4.00	101.65	110.36
22	A	1601	SRY	C13-O53-C53	-3.19	107.70	113.72
22	A	1601	SRY	C12-O41-C41	-2.53	111.82	118.00
22	A	1601	SRY	O61-C61-C51	-2.38	105.17	110.36
22	A	1601	SRY	C43-C33-C23	-2.28	106.95	110.33
22	A	1601	SRY	O13-C13-O53	-2.23	105.29	110.70
22	A	1601	SRY	C61-C11-N11	-2.21	106.38	110.61
22	A	1601	SRY	C51-C61-C11	-2.07	107.25	110.33
22	A	1601	SRY	O43-C43-C33	2.15	115.03	110.36
22	A	1601	SRY	O41-C41-C51	2.46	113.11	107.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1601	SRY	O32-C32-C22	2.51	117.42	111.57
22	A	1601	SRY	O51-C51-C41	2.81	116.26	109.87
22	A	1601	SRY	C13-C23-N23	2.93	116.23	111.03
22	A	1601	SRY	O21-C21-C11	2.99	115.67	109.61
22	A	1601	SRY	O13-C22-C32	3.20	118.98	111.59
22	A	1601	SRY	O61-C61-C11	3.58	116.86	109.61
22	A	1601	SRY	C41-C31-N31	4.20	118.39	111.00
22	A	1601	SRY	O13-C13-C23	5.84	119.64	108.23

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	1601	SRY	7	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	1498/1522 (98%)	-0.44	18 (1%) 79 66	74, 131, 262, 364	0
2	B	234/256 (91%)	-0.63	1 (0%) 92 87	82, 143, 231, 264	0
3	C	206/239 (86%)	-0.20	10 (4%) 30 21	123, 191, 239, 272	0
4	D	208/209 (99%)	-0.50	1 (0%) 90 84	85, 134, 177, 200	0
5	E	150/162 (92%)	-0.61	0 100 100	73, 106, 144, 182	0
6	F	101/101 (100%)	-0.75	0 100 100	106, 153, 181, 203	0
7	G	155/156 (99%)	-0.38	5 (3%) 48 35	128, 180, 226, 251	0
8	H	138/138 (100%)	-0.70	0 100 100	68, 96, 145, 159	0
9	I	127/128 (99%)	-0.31	2 (1%) 72 58	126, 199, 236, 258	0
10	J	98/105 (93%)	0.28	9 (9%) 10 7	165, 229, 278, 305	0
11	K	116/129 (89%)	-0.62	0 100 100	94, 131, 177, 219	0
12	L	123/135 (91%)	-0.51	0 100 100	71, 124, 172, 206	0
13	M	118/126 (93%)	-0.37	2 (1%) 70 57	122, 164, 204, 231	0
14	N	60/61 (98%)	0.29	5 (8%) 12 9	133, 189, 234, 267	0
15	O	87/89 (97%)	-0.54	0 100 100	74, 122, 165, 180	0
16	P	83/88 (94%)	-0.60	0 100 100	92, 125, 166, 203	0
17	Q	99/105 (94%)	-0.67	0 100 100	84, 107, 140, 168	0
18	R	70/88 (79%)	-0.71	0 100 100	92, 129, 180, 220	0
19	S	80/93 (86%)	0.17	5 (6%) 21 14	174, 217, 268, 283	0
20	T	99/106 (93%)	-0.65	1 (1%) 82 71	95, 130, 179, 210	0
21	U	24/27 (88%)	1.39	8 (33%) 0 1	151, 187, 219, 221	0
All	All	3874/4063 (95%)	-0.43	67 (1%) 70 57	68, 141, 239, 364	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	103	VAL	6.2
3	C	193	TYR	5.9
10	J	34	VAL	4.5
10	J	37	PRO	4.5
1	A	793	U	4.5
3	C	102	ASN	4.3
1	A	994	A	4.3
10	J	33	GLN	4.2
19	S	40	ILE	4.2
21	U	18	TYR	4.0
1	A	1129	C	4.0
1	A	1037	C	3.9
21	U	17	THR	3.8
20	T	106	ALA	3.8
14	N	11	LYS	3.8
1	A	993	G	3.7
21	U	24	ARG	3.7
10	J	90	LEU	3.6
21	U	25	LYS	3.6
1	A	81	U	3.5
1	A	1539	C	3.5
19	S	41	VAL	3.5
10	J	36	GLY	3.3
7	G	7	ALA	3.3
2	B	231	GLU	3.3
14	N	18	VAL	3.2
3	C	65	ALA	3.2
10	J	74	ILE	3.2
1	A	995	C	3.1
7	G	2	ALA	3.1
3	C	156	ARG	3.1
14	N	3	ARG	3.0
3	C	66	VAL	3.0
19	S	4	SER	3.0
7	G	8	GLU	2.9
3	C	68	VAL	2.9
9	I	8	GLY	2.8
1	A	1036	G	2.7
10	J	38	ILE	2.7
13	M	117	VAL	2.7
4	D	45	GLN	2.7
1	A	1018	C	2.7
7	G	5	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
7	G	79	ARG	2.6
21	U	11	GLY	2.6
1	A	792	A	2.6
21	U	8	THR	2.6
1	A	1020	U	2.6
14	N	4	LYS	2.5
13	M	6	GLY	2.5
3	C	146	ALA	2.5
21	U	5	ASP	2.5
14	N	2	ALA	2.4
1	A	202	U	2.4
1	A	1019	C	2.4
3	C	161	GLU	2.3
9	I	102	LEU	2.3
10	J	89	ASP	2.3
10	J	73	ASP	2.2
19	S	69	HIS	2.2
3	C	104	GLN	2.1
1	A	1007	C	2.1
19	S	79	THR	2.1
1	A	1257	U	2.1
21	U	9	ARG	2.1
1	A	789	U	2.0
1	A	1144	G	2.0

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

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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
1	5MC	A	1400	21/22	0.95	0.19	-	95,124,131,135	0
1	UR3	A	1498	21/22	0.96	0.18	-	112,123,141,146	0
1	7MG	A	527	24/25	0.98	0.14	-	103,112,124,131	0
1	PSU	A	1540	20/21	0.79	0.75	-	207,241,323,324	0
1	M2G	A	966	25/26	0.94	0.20	-	123,141,169,173	0
1	4OC	A	1402	22/23	0.97	0.18	-	108,117,120,127	0
12	0TD	L	92	10/11	0.97	0.37	-	87,120,138,251	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
1	MA6	A	1519	24/25	0.96	0.19	-	105,122,132,134	0
1	5MC	A	1407	21/22	0.95	0.16	-	136,148,157,159	0
1	2MG	A	1207	24/25	0.90	0.28	-	175,210,229,233	0
1	MA6	A	1518	24/25	0.98	0.10	-	121,127,148,148	0
1	5MC	A	1404	21/22	0.96	0.19	-	114,124,129,132	0
1	PSU	A	516	20/21	0.95	0.12	-	110,141,152,153	0
1	PSU	A	1541	20/21	0.81	0.44	-	159,231,317,318	0
1	5MC	A	967	21/22	0.96	0.17	-	129,133,145,149	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
23	MG	A	1784	1/1	0.86	0.79	73.40	93,93,93,93	0
23	MG	A	1700	1/1	0.84	0.32	12.15	107,107,107,107	0
23	MG	A	1846	1/1	0.99	0.29	10.67	399,399,399,399	0
23	MG	B	301	1/1	0.86	0.34	8.94	110,110,110,110	0
23	MG	A	1766	1/1	0.92	0.43	7.41	146,146,146,146	0
23	MG	H	203	1/1	0.92	0.41	6.79	124,124,124,124	0
23	MG	A	1830	1/1	0.92	0.33	6.05	322,322,322,322	0
23	MG	M	202	1/1	0.97	0.54	5.82	111,111,111,111	0
23	MG	A	1701	1/1	0.98	0.25	5.55	87,87,87,87	0
23	MG	T	202	1/1	0.95	0.32	5.51	267,267,267,267	0
23	MG	A	1728	1/1	0.91	0.28	4.80	82,82,82,82	0
23	MG	A	1771	1/1	0.95	0.21	4.49	77,77,77,77	0
23	MG	A	1760	1/1	0.83	0.28	4.22	105,105,105,105	0
23	MG	A	1725	1/1	0.88	0.38	3.96	91,91,91,91	0
23	MG	A	1786	1/1	0.88	0.22	3.83	78,78,78,78	0
23	MG	A	1810	1/1	0.88	0.26	3.55	85,85,85,85	0
23	MG	A	1738	1/1	0.90	0.25	3.45	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
23	MG	A	1743	1/1	0.87	0.24	3.36	113,113,113,113	0
23	MG	A	1711	1/1	0.96	0.23	3.31	93,93,93,93	0
23	MG	A	1609	1/1	0.99	0.22	2.70	108,108,108,108	0
23	MG	A	1640	1/1	0.98	0.20	2.52	96,96,96,96	0
23	MG	A	1724	1/1	0.95	0.18	2.15	71,71,71,71	0
23	MG	A	1606	1/1	0.99	0.29	2.14	96,96,96,96	0
23	MG	A	1637	1/1	0.96	0.28	2.02	127,127,127,127	0
23	MG	A	1849	1/1	0.92	0.17	1.65	296,296,296,296	0
23	MG	A	1675	1/1	0.98	0.18	1.64	79,79,79,79	0
23	MG	A	1754	1/1	0.92	0.22	1.60	177,177,177,177	0
23	MG	A	1809	1/1	0.97	0.18	1.41	96,96,96,96	0
23	MG	A	1722	1/1	0.99	0.14	1.29	71,71,71,71	0
23	MG	A	1726	1/1	0.86	0.29	1.19	91,91,91,91	0
23	MG	A	1851	1/1	0.97	0.16	1.05	208,208,208,208	0
23	MG	A	1708	1/1	0.97	0.18	0.96	135,135,135,135	0
23	MG	A	1746	1/1	0.91	0.24	0.94	123,123,123,123	0
23	MG	A	1757	1/1	0.99	0.16	0.84	106,106,106,106	0
23	MG	T	201	1/1	0.92	0.22	0.77	92,92,92,92	0
23	MG	N	102	1/1	0.81	0.35	0.63	112,112,112,112	0
23	MG	A	1716	1/1	0.98	0.15	0.47	86,86,86,86	0
22	SRY	A	1601	40/40	0.96	0.22	0.34	85,115,145,148	0
23	MG	A	1617	1/1	0.98	0.15	0.31	75,75,75,75	0
23	MG	A	1614	1/1	0.92	0.25	0.28	83,83,83,83	0
23	MG	A	1845	1/1	0.97	0.21	0.26	159,159,159,159	0
23	MG	A	1628	1/1	0.98	0.16	0.23	171,171,171,171	0
23	MG	A	1732	1/1	0.94	0.12	0.14	114,114,114,114	0
23	MG	A	1800	1/1	0.96	0.28	0.12	108,108,108,108	0
24	ZN	D	301	1/1	1.00	0.32	-0.03	127,127,127,127	0
23	MG	A	1742	1/1	0.95	0.12	-0.21	77,77,77,77	0
23	MG	A	1645	1/1	0.92	0.13	-0.21	138,138,138,138	0
23	MG	A	1704	1/1	0.96	0.18	-0.27	105,105,105,105	0
23	MG	J	202	1/1	0.98	0.17	-0.28	105,105,105,105	0
23	MG	A	1683	1/1	0.98	0.22	-0.37	159,159,159,159	0
23	MG	D	302	1/1	0.77	0.16	-0.41	123,123,123,123	0
23	MG	A	1768	1/1	0.90	0.22	-0.41	112,112,112,112	0
23	MG	A	1633	1/1	0.96	0.15	-0.42	88,88,88,88	0
23	MG	A	1749	1/1	0.98	0.10	-0.55	99,99,99,99	0
23	MG	A	1776	1/1	0.98	0.13	-0.60	299,299,299,299	0
23	MG	A	1688	1/1	0.99	0.12	-0.69	99,99,99,99	0
23	MG	A	1827	1/1	0.94	0.18	-0.69	200,200,200,200	0
24	ZN	N	101	1/1	0.99	0.15	-0.70	168,168,168,168	0
23	MG	A	1752	1/1	0.94	0.10	-0.76	110,110,110,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
23	MG	A	1751	1/1	0.99	0.11	-0.90	108,108,108,108	0
23	MG	A	1791	1/1	0.97	0.11	-0.93	74,74,74,74	0
23	MG	A	1829	1/1	0.99	0.14	-1.04	93,93,93,93	0
23	MG	A	1844	1/1	0.96	0.13	-1.07	383,383,383,383	0
23	MG	A	1686	1/1	0.93	0.12	-1.22	130,130,130,130	0
23	MG	A	1625	1/1	0.98	0.12	-1.25	179,179,179,179	0
23	MG	A	1672	1/1	0.99	0.10	-1.33	123,123,123,123	0
23	MG	A	1646	1/1	0.99	0.10	-1.86	99,99,99,99	0
23	MG	A	1649	1/1	0.99	0.12	-2.00	162,162,162,162	0
23	MG	A	1764	1/1	0.97	0.10	-2.79	118,118,118,118	0
23	MG	A	1635	1/1	0.99	0.04	-4.34	62,62,62,62	0
23	MG	A	1689	1/1	0.97	0.10	-5.34	75,75,75,75	0
23	MG	A	1705	1/1	0.92	0.21	-	97,97,97,97	0
23	MG	A	1676	1/1	0.94	0.23	-	81,81,81,81	0
23	MG	A	1782	1/1	0.84	0.19	-	108,108,108,108	0
23	MG	A	1814	1/1	0.96	0.26	-	360,360,360,360	0
23	MG	A	1678	1/1	0.97	0.24	-	149,149,149,149	0
23	MG	A	1658	1/1	0.75	0.63	-	120,120,120,120	0
23	MG	A	1854	1/1	0.87	0.23	-	103,103,103,103	0
23	MG	A	1654	1/1	0.99	0.14	-	143,143,143,143	0
23	MG	A	1706	1/1	0.96	0.32	-	97,97,97,97	0
23	MG	M	201	1/1	0.86	0.54	-	101,101,101,101	0
23	MG	A	1621	1/1	0.97	0.19	-	87,87,87,87	0
23	MG	A	1813	1/1	0.94	0.28	-	228,228,228,228	0
23	MG	A	1817	1/1	0.88	0.98	-	312,312,312,312	0
23	MG	A	1610	1/1	0.97	0.18	-	129,129,129,129	0
23	MG	H	201	1/1	0.91	0.35	-	83,83,83,83	0
23	MG	A	1602	1/1	0.95	0.15	-	144,144,144,144	0
23	MG	A	1681	1/1	0.95	0.07	-	208,208,208,208	0
23	MG	A	1670	1/1	0.97	0.27	-	113,113,113,113	0
23	MG	A	1842	1/1	1.00	0.15	-	73,73,73,73	0
23	MG	A	1674	1/1	0.94	0.27	-	94,94,94,94	0
23	MG	A	1603	1/1	0.92	0.23	-	126,126,126,126	0
23	MG	A	1803	1/1	0.98	0.24	-	123,123,123,123	0
23	MG	A	1644	1/1	0.97	0.26	-	117,117,117,117	0
23	MG	A	1739	1/1	0.77	0.45	-	92,92,92,92	0
23	MG	A	1788	1/1	0.97	0.88	-	99,99,99,99	0
23	MG	A	1604	1/1	0.96	0.30	-	92,92,92,92	0
23	MG	A	1707	1/1	0.97	0.14	-	113,113,113,113	0
23	MG	A	1770	1/1	0.95	0.21	-	108,108,108,108	0
23	MG	A	1650	1/1	0.93	0.31	-	127,127,127,127	0
23	MG	A	1794	1/1	0.66	0.54	-	127,127,127,127	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
23	MG	A	1759	1/1	0.90	0.38	-	96,96,96,96	0
23	MG	A	1680	1/1	0.89	0.44	-	104,104,104,104	0
23	MG	A	1643	1/1	0.99	0.10	-	90,90,90,90	0
23	MG	Q	201	1/1	0.73	0.12	-	115,115,115,115	0
23	MG	A	1720	1/1	0.76	0.57	-	112,112,112,112	0
23	MG	A	1805	1/1	0.97	0.06	-	93,93,93,93	0
23	MG	A	1691	1/1	0.86	0.28	-	163,163,163,163	0
23	MG	A	1828	1/1	0.94	0.61	-	289,289,289,289	0
23	MG	A	1666	1/1	0.96	0.17	-	136,136,136,136	0
23	MG	P	103	1/1	0.70	0.23	-	102,102,102,102	0
23	MG	A	1795	1/1	0.93	0.75	-	107,107,107,107	0
23	MG	E	201	1/1	0.94	0.06	-	228,228,228,228	0
23	MG	A	1789	1/1	0.97	0.06	-	118,118,118,118	0
23	MG	A	1796	1/1	0.81	0.49	-	107,107,107,107	0
23	MG	A	1769	1/1	0.81	0.24	-	112,112,112,112	0
23	MG	A	1661	1/1	0.43	0.60	-	89,89,89,89	0
23	MG	A	1804	1/1	0.84	0.55	-	77,77,77,77	0
23	MG	A	1616	1/1	0.92	0.46	-	90,90,90,90	0
23	MG	A	1679	1/1	0.98	0.07	-	116,116,116,116	0
23	MG	A	1834	1/1	0.96	0.28	-	130,130,130,130	0
23	MG	A	1615	1/1	0.92	0.43	-	94,94,94,94	0
23	MG	A	1821	1/1	0.97	0.16	-	338,338,338,338	0
23	MG	A	1799	1/1	0.80	0.49	-	109,109,109,109	0
23	MG	S	101	1/1	0.75	0.19	-	93,93,93,93	0
23	MG	A	1669	1/1	0.98	0.39	-	102,102,102,102	0
23	MG	A	1781	1/1	0.90	0.47	-	101,101,101,101	0
23	MG	A	1699	1/1	0.93	0.30	-	221,221,221,221	0
23	MG	A	1717	1/1	0.99	0.20	-	106,106,106,106	0
23	MG	A	1712	1/1	0.94	0.23	-	91,91,91,91	0
23	MG	A	1761	1/1	0.75	0.23	-	97,97,97,97	0
23	MG	A	1753	1/1	0.84	0.18	-	168,168,168,168	0
23	MG	A	1723	1/1	0.93	0.34	-	92,92,92,92	0
23	MG	A	1848	1/1	0.94	0.24	-	336,336,336,336	0
23	MG	A	1772	1/1	0.90	0.51	-	117,117,117,117	0
23	MG	A	1620	1/1	0.98	0.32	-	128,128,128,128	0
23	MG	A	1709	1/1	0.55	0.31	-	117,117,117,117	0
23	MG	A	1665	1/1	0.96	0.13	-	176,176,176,176	0
23	MG	A	1697	1/1	0.94	0.24	-	145,145,145,145	0
23	MG	A	1715	1/1	0.87	0.08	-	120,120,120,120	0
23	MG	A	1783	1/1	0.91	0.13	-	133,133,133,133	0
23	MG	A	1662	1/1	0.97	0.12	-	141,141,141,141	0
23	MG	A	1816	1/1	0.99	0.10	-	282,282,282,282	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
23	MG	A	1668	1/1	0.92	0.35	-	149,149,149,149	0
23	MG	A	1607	1/1	0.86	0.11	-	156,156,156,156	0
23	MG	A	1626	1/1	0.92	0.25	-	146,146,146,146	0
23	MG	A	1638	1/1	0.97	0.18	-	96,96,96,96	0
23	MG	A	1823	1/1	0.86	0.23	-	317,317,317,317	0
23	MG	A	1693	1/1	0.85	0.18	-	104,104,104,104	0
23	MG	A	1775	1/1	0.95	0.10	-	235,235,235,235	0
23	MG	A	1785	1/1	0.93	0.28	-	74,74,74,74	0
23	MG	P	101	1/1	0.94	0.30	-	77,77,77,77	0
23	MG	A	1735	1/1	0.94	0.25	-	95,95,95,95	0
23	MG	A	1792	1/1	0.94	0.13	-	111,111,111,111	0
23	MG	A	1847	1/1	0.97	0.15	-	296,296,296,296	0
23	MG	A	1684	1/1	0.50	0.38	-	133,133,133,133	0
23	MG	A	1729	1/1	0.74	0.37	-	102,102,102,102	0
23	MG	A	1822	1/1	0.97	0.04	-	157,157,157,157	0
23	MG	A	1826	1/1	0.97	0.10	-	304,304,304,304	0
23	MG	A	1853	1/1	0.88	0.33	-	338,338,338,338	0
23	MG	A	1656	1/1	0.92	0.23	-	152,152,152,152	0
23	MG	H	202	1/1	0.94	0.15	-	83,83,83,83	0
23	MG	A	1730	1/1	0.96	0.20	-	91,91,91,91	0
23	MG	A	1682	1/1	0.94	0.13	-	171,171,171,171	0
23	MG	A	1652	1/1	0.98	0.11	-	114,114,114,114	0
23	MG	A	1629	1/1	0.99	0.32	-	138,138,138,138	0
23	MG	A	1663	1/1	0.76	0.11	-	109,109,109,109	0
23	MG	A	1660	1/1	0.94	0.13	-	173,173,173,173	0
23	MG	A	1622	1/1	0.95	0.13	-	86,86,86,86	0
23	MG	A	1695	1/1	0.79	0.32	-	121,121,121,121	0
23	MG	A	1820	1/1	0.97	0.10	-	313,313,313,313	0
23	MG	A	1819	1/1	0.93	0.11	-	286,286,286,286	0
23	MG	A	1642	1/1	0.98	0.15	-	105,105,105,105	0
23	MG	A	1639	1/1	0.94	0.14	-	116,116,116,116	0
23	MG	A	1793	1/1	0.74	1.41	-	105,105,105,105	0
23	MG	A	1744	1/1	0.86	0.27	-	99,99,99,99	0
23	MG	A	1671	1/1	0.70	1.25	-	125,125,125,125	0
23	MG	A	1702	1/1	0.92	0.17	-	106,106,106,106	0
23	MG	A	1733	1/1	0.84	0.28	-	111,111,111,111	0
23	MG	A	1627	1/1	0.93	0.39	-	97,97,97,97	0
23	MG	A	1833	1/1	0.90	0.12	-	98,98,98,98	0
23	MG	A	1774	1/1	0.97	0.21	-	272,272,272,272	0
23	MG	A	1747	1/1	0.83	0.35	-	111,111,111,111	0
23	MG	A	1605	1/1	0.99	0.09	-	123,123,123,123	0
23	MG	A	1703	1/1	0.99	0.05	-	109,109,109,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
23	MG	A	1762	1/1	0.96	0.28	-	122,122,122,122	0
23	MG	A	1736	1/1	0.98	0.13	-	84,84,84,84	0
23	MG	A	1839	1/1	0.96	0.12	-	137,137,137,137	0
23	MG	A	1818	1/1	0.94	0.08	-	266,266,266,266	0
23	MG	A	1740	1/1	0.88	0.33	-	123,123,123,123	0
23	MG	A	1659	1/1	0.83	0.20	-	108,108,108,108	0
23	MG	A	1667	1/1	0.80	0.22	-	100,100,100,100	0
23	MG	A	1750	1/1	0.88	0.41	-	115,115,115,115	0
23	MG	A	1673	1/1	0.69	0.52	-	73,73,73,73	0
23	MG	A	1634	1/1	0.94	0.37	-	82,82,82,82	0
23	MG	A	1631	1/1	1.00	0.10	-	71,71,71,71	0
23	MG	A	1664	1/1	0.88	0.24	-	133,133,133,133	0
23	MG	A	1734	1/1	0.97	0.30	-	108,108,108,108	0
23	MG	A	1831	1/1	0.97	0.13	-	168,168,168,168	0
23	MG	A	1714	1/1	0.95	0.15	-	130,130,130,130	0
23	MG	A	1797	1/1	0.72	0.79	-	127,127,127,127	0
23	MG	A	1727	1/1	0.97	0.24	-	95,95,95,95	0
23	MG	B	302	1/1	0.86	0.26	-	89,89,89,89	0
23	MG	A	1780	1/1	0.97	0.15	-	107,107,107,107	0
23	MG	A	1838	1/1	0.98	0.23	-	126,126,126,126	0
23	MG	A	1636	1/1	0.98	0.35	-	176,176,176,176	0
23	MG	A	1777	1/1	0.98	0.07	-	485,485,485,485	0
23	MG	A	1756	1/1	0.98	0.07	-	203,203,203,203	0
23	MG	A	1763	1/1	0.98	0.14	-	93,93,93,93	0
23	MG	A	1802	1/1	0.79	0.34	-	86,86,86,86	0
23	MG	A	1808	1/1	0.98	0.19	-	107,107,107,107	0
23	MG	A	1687	1/1	0.98	0.07	-	210,210,210,210	0
23	MG	A	1713	1/1	0.79	0.38	-	96,96,96,96	0
23	MG	A	1694	1/1	0.96	0.06	-	95,95,95,95	0
23	MG	A	1612	1/1	0.98	0.14	-	75,75,75,75	0
23	MG	A	1698	1/1	0.98	0.05	-	170,170,170,170	0
23	MG	A	1836	1/1	0.95	0.10	-	175,175,175,175	0
23	MG	A	1835	1/1	0.90	0.56	-	128,128,128,128	0
23	MG	A	1721	1/1	0.94	0.23	-	115,115,115,115	0
23	MG	A	1837	1/1	0.47	0.50	-	103,103,103,103	0
23	MG	A	1778	1/1	0.97	0.14	-	129,129,129,129	0
23	MG	A	1832	1/1	0.82	0.26	-	109,109,109,109	0
23	MG	A	1840	1/1	0.96	0.27	-	386,386,386,386	0
23	MG	J	201	1/1	0.88	0.37	-	107,107,107,107	0
23	MG	A	1824	1/1	0.98	0.13	-	168,168,168,168	0
23	MG	A	1843	1/1	1.00	0.10	-	55,55,55,55	0
23	MG	A	1710	1/1	0.82	0.54	-	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
23	MG	A	1765	1/1	0.92	0.51	-	124,124,124,124	0
23	MG	A	1641	1/1	0.98	0.15	-	87,87,87,87	0
23	MG	A	1608	1/1	0.99	0.27	-	80,80,80,80	0
23	MG	A	1841	1/1	0.83	0.47	-	392,392,392,392	0
23	MG	A	1677	1/1	0.90	0.32	-	97,97,97,97	0
23	MG	A	1648	1/1	0.97	0.09	-	227,227,227,227	0
23	MG	A	1624	1/1	0.86	0.33	-	97,97,97,97	0
23	MG	A	1619	1/1	0.97	0.20	-	141,141,141,141	0
23	MG	A	1630	1/1	0.99	0.21	-	145,145,145,145	0
23	MG	A	1755	1/1	0.93	0.11	-	159,159,159,159	0
23	MG	A	1692	1/1	0.96	0.17	-	170,170,170,170	0
23	MG	A	1801	1/1	0.93	0.41	-	111,111,111,111	0
23	MG	A	1790	1/1	0.93	0.17	-	129,129,129,129	0
23	MG	A	1651	1/1	0.96	0.56	-	108,108,108,108	0
23	MG	A	1657	1/1	0.96	0.22	-	116,116,116,116	0
23	MG	A	1647	1/1	0.92	0.20	-	115,115,115,115	0
23	MG	A	1798	1/1	0.82	0.65	-	122,122,122,122	0
23	MG	A	1745	1/1	0.90	0.38	-	85,85,85,85	0
23	MG	A	1737	1/1	0.76	0.30	-	128,128,128,128	0
23	MG	A	1807	1/1	0.99	0.06	-	111,111,111,111	0
23	MG	A	1811	1/1	0.94	0.12	-	87,87,87,87	0
23	MG	H	204	1/1	0.68	0.65	-	105,105,105,105	0
23	MG	A	1690	1/1	0.97	0.31	-	324,324,324,324	0
23	MG	A	1623	1/1	0.96	0.09	-	146,146,146,146	0
23	MG	A	1825	1/1	0.98	0.14	-	272,272,272,272	0
23	MG	A	1758	1/1	0.81	1.09	-	98,98,98,98	0
23	MG	A	1685	1/1	0.87	0.16	-	269,269,269,269	0
23	MG	A	1850	1/1	0.95	0.17	-	270,270,270,270	0
23	MG	A	1611	1/1	0.96	0.05	-	127,127,127,127	0
23	MG	A	1812	1/1	0.94	0.27	-	183,183,183,183	0
23	MG	A	1718	1/1	0.90	0.17	-	95,95,95,95	0
23	MG	A	1696	1/1	0.99	0.10	-	141,141,141,141	0
23	MG	A	1779	1/1	0.83	0.34	-	91,91,91,91	0
23	MG	A	1719	1/1	0.81	0.20	-	113,113,113,113	0
23	MG	A	1655	1/1	0.92	0.32	-	137,137,137,137	0
23	MG	A	1773	1/1	0.97	0.15	-	135,135,135,135	0
23	MG	A	1815	1/1	0.89	0.25	-	355,355,355,355	0
23	MG	A	1852	1/1	0.97	0.13	-	404,404,404,404	0
23	MG	A	1613	1/1	0.83	0.45	-	98,98,98,98	0
23	MG	A	1767	1/1	0.38	0.46	-	93,93,93,93	0
23	MG	A	1632	1/1	0.84	0.24	-	105,105,105,105	0
23	MG	A	1806	1/1	0.98	0.23	-	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
23	MG	A	1731	1/1	0.59	0.55	-	95,95,95,95	0
23	MG	P	102	1/1	0.96	0.24	-	100,100,100,100	0
23	MG	A	1787	1/1	0.90	0.17	-	81,81,81,81	0
23	MG	A	1748	1/1	0.68	0.16	-	143,143,143,143	0
23	MG	A	1618	1/1	0.99	0.22	-	108,108,108,108	0
23	MG	A	1741	1/1	0.83	0.27	-	113,113,113,113	0
23	MG	A	1653	1/1	0.95	0.20	-	145,145,145,145	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.