



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 25, 2020 – 03:47 PM BST

PDB ID : 4DV0  
Title : Crystal structure of the *Thermus thermophilus* 30S ribosomal subunit with a 16S rRNA mutation, U20G  
Authors : Demirci, H.; Murphy IV, F.; Murphy, E.; Gregory, S.T.; Dahlberg, A.E.; Jogl, G.  
Deposited on : 2012-02-22  
Resolution : 3.85 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13

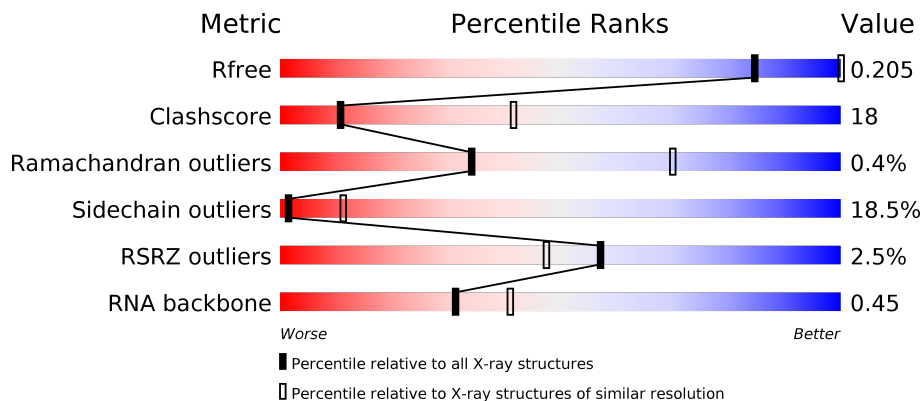
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.85 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))
$R_{free}$	130704	1048 (4.10-3.62)
Clashscore	141614	1015 (4.08-3.64)
Ramachandran outliers	138981	1069 (4.10-3.62)
Sidechain outliers	138945	1062 (4.10-3.62)
RSRZ outliers	127900	1206 (4.12-3.60)
RNA backbone	3102	1039 (4.70-3.00)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	 2% 28% 43% 23% 6%
2	B	256	 2% 47% 36% 8% 9%
3	C	239	 5% 41% 38% 8% 14%
4	D	209	 0% 49% 38% 12%

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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
22	MG	A	1696	-	-	-	X
22	MG	A	1721	-	-	-	X
22	MG	A	1722	-	-	-	X
22	MG	A	1737	-	-	-	X
22	MG	A	1743	-	-	-	X
22	MG	A	1778	-	-	-	X
22	MG	A	1792	-	-	-	X
22	MG	A	1815	-	-	-	X

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<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
22	MG	A	1827	-	-	-	X
22	MG	A	1831	-	-	-	X
22	MG	A	1836	-	-	-	X
22	MG	A	1862	-	-	-	X
22	MG	M	201	-	-	-	X

## 2 Entry composition i

There are 24 unique types of molecules in this entry. The entry contains 52453 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
			Total	C	N	O	P			
1	A	1512	32647	14541	6042	10546	1518	0	6	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	G	U	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
			Total	C	N	O	S			
2	B	234	1900	1213	341	341	5	0	0	0

- Molecule 3 is a protein called ribosomal protein S3.

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

- Molecule 4 is a protein called ribosomal protein S4.

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

- Molecule 5 is a protein called ribosomal protein S5.

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

- Molecule 6 is a protein called ribosomal protein S6.

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

- Molecule 7 is a protein called ribosomal protein S7.

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

- Molecule 8 is a protein called ribosomal protein S8.

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

- Molecule 9 is a protein called ribosomal protein S9.

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

- Molecule 10 is a protein called ribosomal protein S10.

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

- Molecule 11 is a protein called ribosomal protein S11.

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

- Molecule 12 is a protein called ribosomal protein S12.

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

- Molecule 13 is a protein called ribosomal protein S13.

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

- Molecule 14 is a protein called ribosomal protein S14.

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

- Molecule 15 is a protein called ribosomal protein S15.

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

- Molecule 16 is a protein called ribosomal protein S16.

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

- Molecule 17 is a protein called ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
17	Q	99	823	528	152	141	2	0	0	0

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
			Total	C	N	O			
18	R	70	574	367	112	95	0	0	0

- Molecule 19 is a protein called ribosomal protein S19.

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

- Molecule 20 is a protein called ribosomal protein S20.

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

- Molecule 21 is a protein called ribosomal protein THX.

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

- Molecule 22 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	P	2	Total 2	Mg 2	0	0
22	J	2	Total 2	Mg 2	0	0
22	Q	1	Total 1	Mg 1	0	0
22	D	2	Total 2	Mg 2	0	0
22	E	1	Total 1	Mg 1	0	0
22	B	3	Total 3	Mg 3	0	0
22	C	1	Total 1	Mg 1	0	0
22	A	262	Total 262	Mg 262	0	0
22	S	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	F	1	Total Mg 1 1	0	0
22	M	1	Total Mg 1 1	0	0

- Molecule 23 is ZINC ION (three-letter code: ZN) (formula: Zn).

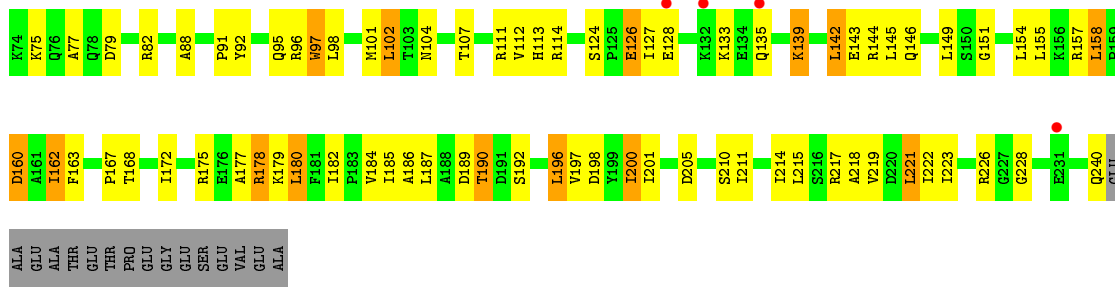
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	D	1	Total Zn 1 1	0	0
23	N	1	Total Zn 1 1	0	0

- Molecule 24 is water.

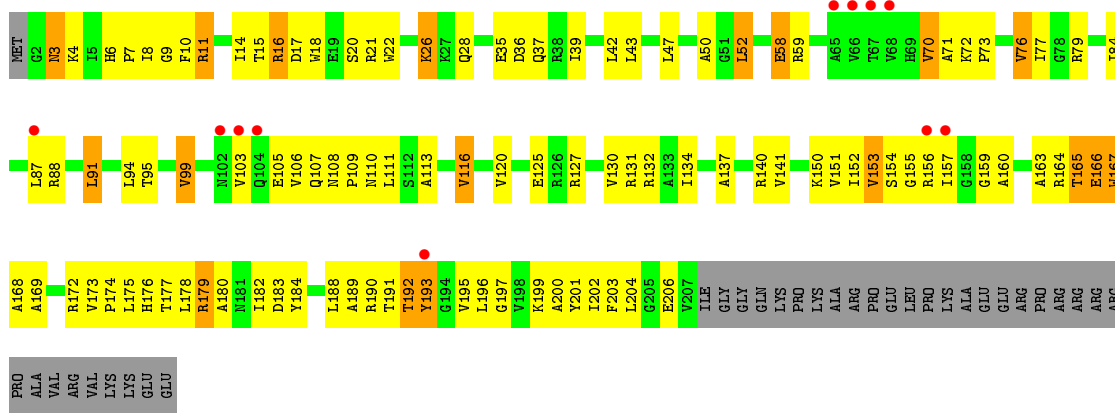
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	397	Total O 397 397	0	0
24	D	1	Total O 1 1	0	0
24	E	4	Total O 4 4	0	0
24	G	4	Total O 4 4	0	0
24	I	1	Total O 1 1	0	0
24	J	3	Total O 3 3	0	0
24	L	1	Total O 1 1	0	0
24	M	8	Total O 8 8	0	0
24	N	1	Total O 1 1	0	0
24	P	10	Total O 10 10	0	0
24	Q	2	Total O 2 2	0	0
24	S	2	Total O 2 2	0	0
24	T	5	Total O 5 5	0	0



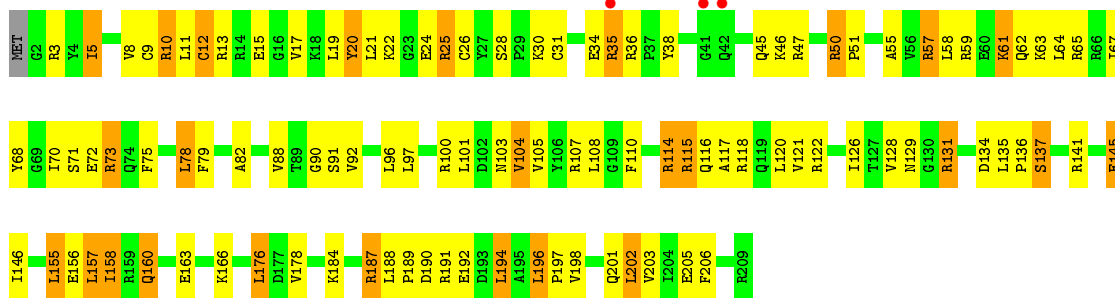




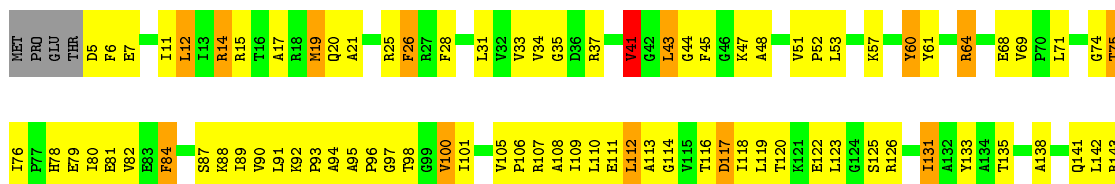
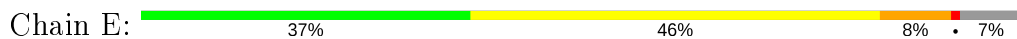
• Molecule 3: ribosomal protein S3



• Molecule 4: ribosomal protein S4



• Molecule 5: ribosomal protein S5





- Molecule 6: ribosomal protein S6



- Molecule 7: ribosomal protein S7



- Molecule 8: ribosomal protein S8

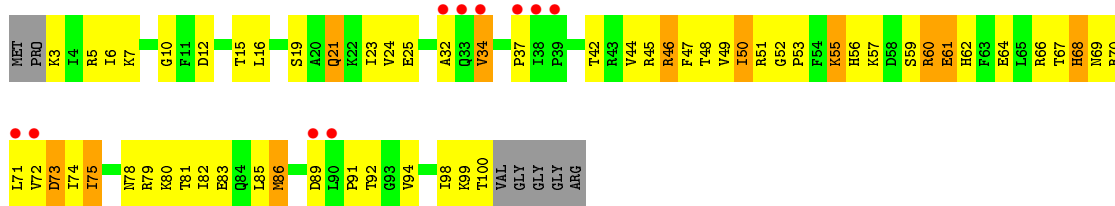


- Molecule 9: ribosomal protein S9

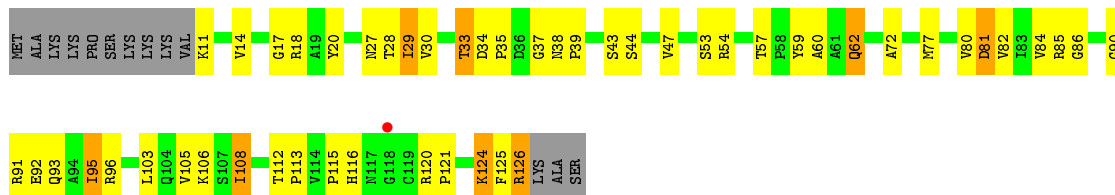


- Molecule 10: ribosomal protein S10

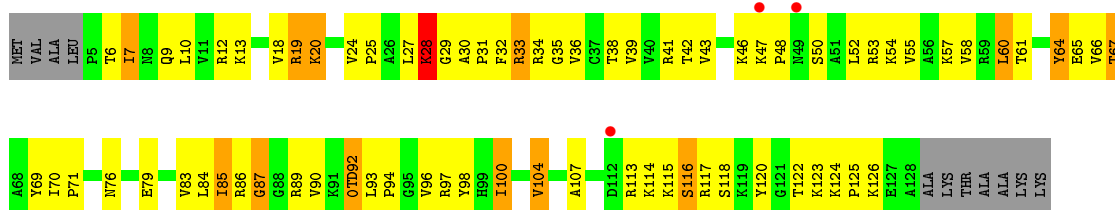




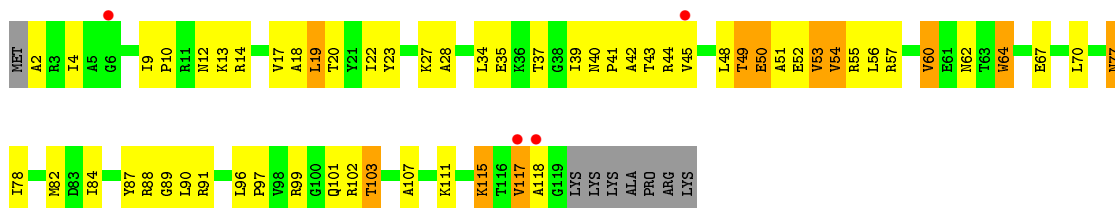
• Molecule 11: ribosomal protein S11



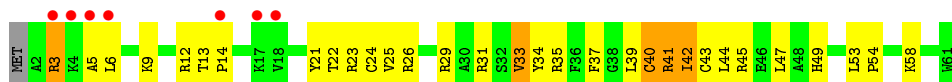
• Molecule 12: ribosomal protein S12



• Molecule 13: ribosomal protein S13

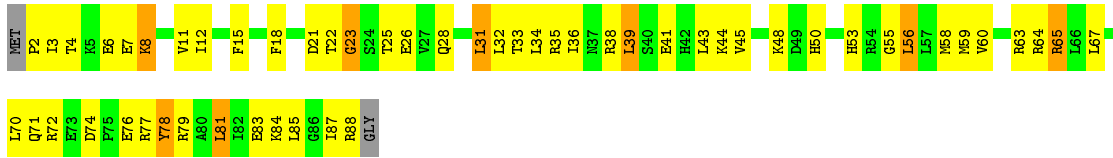


• Molecule 14: ribosomal protein S14

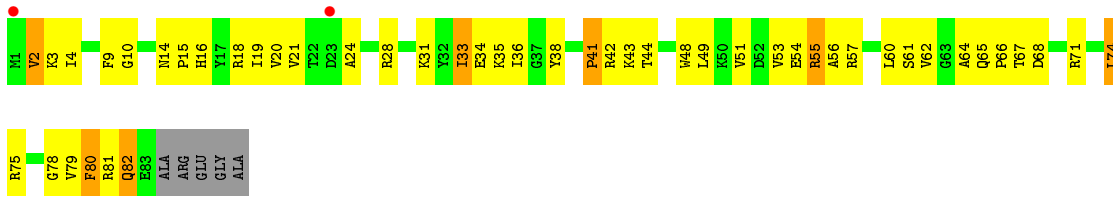


• Molecule 15: ribosomal protein S15

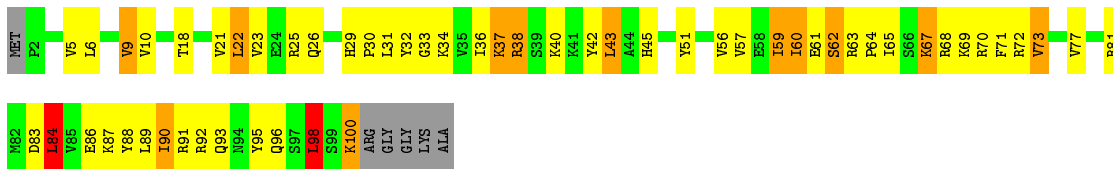




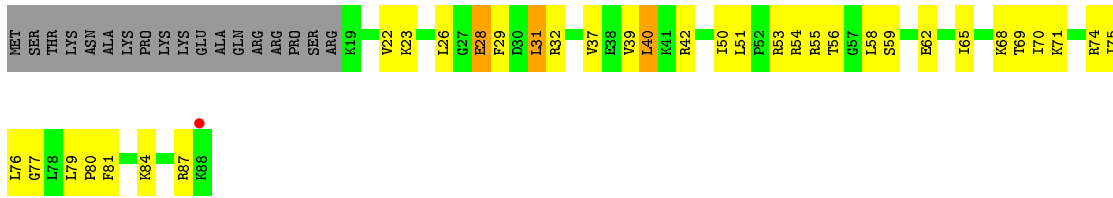
- Molecule 16: ribosomal protein S16



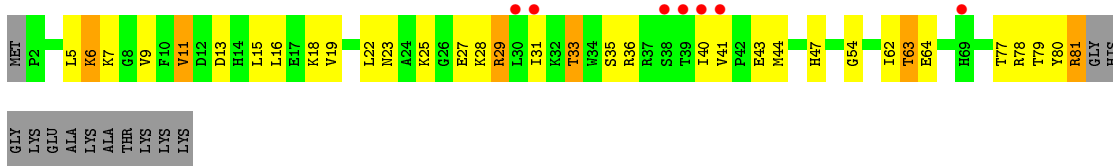
- Molecule 17: ribosomal protein S17



- Molecule 18: ribosomal protein S18

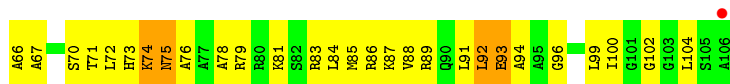


- Molecule 19: ribosomal protein S19

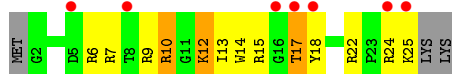
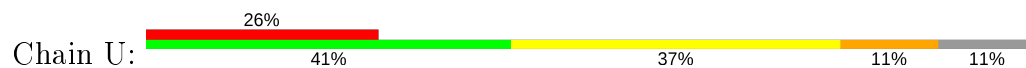


- Molecule 20: ribosomal protein S20





- 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, $\alpha$ , $\beta$ , $\gamma$	402.11Å 402.11Å 174.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.82 – 3.85 34.82 – 3.85	Depositor EDS
% Data completeness (in resolution range)	97.7 (34.82-3.85) 97.4 (34.82-3.85)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.95 (at 3.87Å)	Xtrriage
Refinement program	PHENIX dev_978	Depositor
R, $R_{free}$	0.147 , 0.206 0.148 , 0.205	Depositor DCC
$R_{free}$ test set	6511 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	164.0	Xtrriage
Anisotropy	0.173	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.23 , 130.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	52453	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	196.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.59% 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 i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MA6, 0TD, MG, 2MG, 5MC, UR3, 4OC, M2G, 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	1.01	71/36143 (0.2%)	1.67	1154/56403 (2.0%)
2	B	0.59	1/1935 (0.1%)	0.75	1/2609 (0.0%)
3	C	0.52	0/1636	0.72	0/2205
4	D	0.64	0/1733	0.85	1/2318 (0.0%)
5	E	0.86	0/1162	1.01	4/1564 (0.3%)
6	F	0.59	0/856	0.80	0/1154
7	G	0.58	0/1276	0.76	0/1709
8	H	0.88	1/1136 (0.1%)	1.06	2/1527 (0.1%)
9	I	0.51	0/1029	0.74	0/1379
10	J	0.57	0/805	0.77	0/1082
11	K	0.65	0/879	0.86	0/1187
12	L	0.72	0/977	0.94	1/1306 (0.1%)
13	M	0.54	0/947	0.72	0/1270
14	N	0.56	0/501	0.75	0/664
15	O	0.68	0/740	0.92	1/987 (0.1%)
16	P	0.76	0/716	0.96	0/963
17	Q	0.87	0/836	1.08	3/1117 (0.3%)
18	R	0.68	0/579	0.88	0/768
19	S	0.49	0/661	0.71	1/890 (0.1%)
20	T	0.71	0/765	0.97	1/1007 (0.1%)
21	U	0.59	0/212	0.77	0/277
All	All	0.90	73/55524 (0.1%)	1.47	1169/82386 (1.4%)

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
8	H	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
10	J	0	1
12	L	0	1
20	T	0	1
All	All	0	6

All (73) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	279	A	N9-C4	-11.81	1.30	1.37
1	A	1248	A	N9-C4	8.30	1.42	1.37
1	A	1509	C	N3-C4	-8.09	1.28	1.33
1	A	1504	G	N7-C5	-7.64	1.34	1.39
1	A	574	A	N9-C4	-7.46	1.33	1.37
1	A	1504	G	C5-C4	-7.37	1.33	1.38
1	A	1502	A	N9-C4	-7.28	1.33	1.37
1	A	1513	A	N9-C4	-7.25	1.33	1.37
1	A	1514	C	N3-C4	-6.90	1.29	1.33
1	A	1504	G	C6-N1	-6.74	1.34	1.39
1	A	569	C	N3-C4	-6.68	1.29	1.33
8	H	135	CYS	CB-SG	-6.49	1.71	1.82
1	A	900	A	N9-C4	-6.38	1.34	1.37
1	A	853	G	N7-C5	-6.34	1.35	1.39
1	A	279	A	N3-C4	-6.33	1.31	1.34
1	A	124	G	C6-N1	-6.30	1.35	1.39
1	A	634	C	N1-C6	-6.28	1.33	1.37
1	A	151	A	N9-C4	-6.21	1.34	1.37
1	A	574	A	C5-C6	-6.21	1.35	1.41
1	A	322	C	N1-C6	-6.20	1.33	1.37
1	A	1346	A	C3'-O3'	6.12	1.50	1.42
1	A	1502	A	N3-C4	-6.05	1.31	1.34
1	A	574	A	C6-N1	-6.03	1.31	1.35
1	A	856	C	N1-C6	-5.98	1.33	1.37
1	A	1504	G	C6-O6	-5.93	1.18	1.24
1	A	872	A	N7-C5	-5.88	1.35	1.39
1	A	289	G	N7-C5	-5.88	1.35	1.39
1	A	1513	A	N3-C4	-5.85	1.31	1.34
1	A	1329	A	C5-C6	-5.78	1.35	1.41
1	A	787	A	N9-C4	-5.77	1.34	1.37
1	A	729	A	N7-C5	-5.74	1.35	1.39
1	A	875	C	N1-C6	-5.72	1.33	1.37
1	A	574	A	C5-C4	-5.72	1.34	1.38
1	A	1502	A	C5-C6	-5.62	1.35	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	655	A	N9-C4	-5.59	1.34	1.37
1	A	1526	G	C5-C4	-5.58	1.34	1.38
1	A	922	G	N7-C5	-5.53	1.35	1.39
1	A	109	A	N3-C4	-5.53	1.31	1.34
1	A	753	A	N3-C4	-5.52	1.31	1.34
1	A	1401	G	N3-C4	-5.52	1.31	1.35
1	A	1501	C	N1-C6	-5.50	1.33	1.37
1	A	116	A	N9-C4	-5.50	1.34	1.37
1	A	917	G	N3-C4	-5.48	1.31	1.35
1	A	1524	C	N1-C6	-5.47	1.33	1.37
1	A	266	G	N9-C4	-5.45	1.33	1.38
2	B	24	TRP	CB-CG	5.41	1.59	1.50
1	A	574	A	N3-C4	-5.38	1.31	1.34
1	A	1504	G	N9-C8	-5.37	1.34	1.37
1	A	900	A	N7-C5	-5.36	1.36	1.39
1	A	1510	U	C2-N3	-5.36	1.33	1.37
1	A	279	A	N7-C5	-5.36	1.36	1.39
1	A	570	G	N7-C5	-5.35	1.36	1.39
1	A	569	C	N1-C6	-5.35	1.33	1.37
1	A	1301	U	C3'-O3'	5.34	1.49	1.42
1	A	817	C	N1-C6	-5.33	1.33	1.37
1	A	596	C	N1-C6	-5.31	1.33	1.37
1	A	117	G	N1-C2	5.28	1.42	1.37
1	A	975	A	N9-C4	-5.22	1.34	1.37
1	A	1401	G	C5-C4	-5.20	1.34	1.38
1	A	382	A	N7-C5	-5.18	1.36	1.39
1	A	1529	G	N3-C4	-5.16	1.31	1.35
1	A	13	U	C2-N3	5.15	1.41	1.37
1	A	1526	G	C6-N1	-5.12	1.35	1.39
1	A	1401	G	N1-C2	-5.12	1.33	1.37
1	A	1504	G	C5-C6	-5.12	1.37	1.42
1	A	766	A	N9-C4	-5.10	1.34	1.37
1	A	1500	A	C6-N1	-5.08	1.31	1.35
1	A	130	A	N3-C4	-5.08	1.31	1.34
1	A	722	A	N7-C5	-5.07	1.36	1.39
1	A	779	C	N1-C6	-5.06	1.34	1.37
1	A	907	A	C6-N1	-5.05	1.32	1.35
1	A	828	A	N9-C4	-5.03	1.34	1.37
1	A	308	C	C4-C5	-5.01	1.39	1.43

All (1169) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1505	G	C8-N9-C4	-14.29	100.69	106.40
1	A	635	G	N1-C6-O6	13.97	128.28	119.90
1	A	117	G	N1-C6-O6	12.96	127.68	119.90
1	A	279	A	C5-N7-C8	-12.79	97.51	103.90
1	A	13	U	C2-N1-C1'	12.74	132.99	117.70
1	A	1181	G	C8-N9-C4	12.55	111.42	106.40
1	A	117	G	C6-C5-N7	-12.52	122.89	130.40
1	A	80	G	C8-N9-C4	-12.38	101.45	106.40
1	A	190(G)	G	N1-C6-O6	12.11	127.17	119.90
1	A	703	G	C4-C5-N7	-12.00	106.00	110.80
1	A	624	C	C6-N1-C2	11.43	124.87	120.30
1	A	481	G	N3-C4-N9	11.41	132.85	126.00
1	A	279	A	N7-C8-N9	11.38	119.49	113.80
1	A	873	A	C8-N9-C4	-11.38	101.25	105.80
1	A	1505	G	N7-C8-N9	11.35	118.78	113.10
1	A	117	G	C5-C6-N1	-11.19	105.91	111.50
1	A	722	A	C2-N3-C4	-10.99	105.11	110.60
1	A	638	G	N1-C6-O6	10.88	126.43	119.90
1	A	922	G	N1-C6-O6	10.75	126.35	119.90
1	A	1403	C	N1-C2-O2	-10.73	112.46	118.90
1	A	13	U	C5-C6-N1	10.54	127.97	122.70
1	A	1354	C	C6-N1-C2	-10.37	116.15	120.30
1	A	289	G	N1-C6-O6	10.29	126.08	119.90
1	A	331	G	N1-C6-O6	10.25	126.05	119.90
1	A	852	G	N1-C6-O6	10.24	126.05	119.90
1	A	852	G	C5-C6-N1	-10.24	106.38	111.50
1	A	1367	C	C6-N1-C2	-10.17	116.23	120.30
1	A	190(G)	G	C6-C5-N7	-10.14	124.31	130.40
1	A	922	G	C6-C5-N7	-10.12	124.33	130.40
1	A	309	G	C5-C6-O6	-10.06	122.56	128.60
1	A	922	G	C5-C6-O6	-10.05	122.57	128.60
1	A	964	A	C8-N9-C4	-9.94	101.82	105.80
1	A	117	G	C2-N3-C4	-9.76	107.02	111.90
1	A	928	G	N1-C6-O6	9.72	125.73	119.90
1	A	1370	G	C8-N9-C4	-9.70	102.52	106.40
1	A	128	G	N1-C6-O6	9.69	125.71	119.90
1	A	328	C	N1-C2-O2	9.57	124.64	118.90
1	A	232	G	N1-C6-O6	9.54	125.62	119.90
1	A	839	U	C2-N1-C1'	9.43	129.01	117.70
1	A	718	G	C4-N9-C1'	9.41	138.73	126.50
1	A	1502	A	C2-N3-C4	-9.38	105.91	110.60
1	A	836	G	N1-C6-O6	9.33	125.50	119.90
1	A	92	C	N3-C2-O2	-9.32	115.37	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	853	G	N3-C4-C5	-9.32	123.94	128.60
1	A	623	C	C6-N1-C2	9.30	124.02	120.30
1	A	292	G	C4-C5-N7	9.29	114.52	110.80
1	A	284	G	C5-C6-O6	-9.27	123.04	128.60
1	A	785	G	N1-C6-O6	9.24	125.44	119.90
1	A	938	A	N1-C6-N6	-9.23	113.06	118.60
1	A	117	G	C4-C5-C6	9.18	124.31	118.80
1	A	1403	C	N3-C2-O2	9.15	128.31	121.90
1	A	703	G	C5-C6-O6	9.15	134.09	128.60
1	A	719	C	N1-C2-O2	9.14	124.38	118.90
1	A	251	G	N7-C8-N9	9.11	117.66	113.10
1	A	915	A	N1-C6-N6	9.11	124.07	118.60
1	A	251	G	C6-C5-N7	-9.09	124.95	130.40
1	A	328	C	C2-N1-C1'	9.08	128.78	118.80
1	A	1502	A	C5-N7-C8	-9.05	99.38	103.90
1	A	106	C	C6-N1-C2	-9.02	116.69	120.30
1	A	1531	A	N1-C6-N6	8.98	123.99	118.60
1	A	936	C	C6-N1-C2	8.98	123.89	120.30
1	A	279	A	C8-N9-C4	-8.91	102.24	105.80
1	A	283	C	C2-N1-C1'	8.90	128.59	118.80
1	A	292	G	C6-C5-N7	-8.90	125.06	130.40
1	A	190(A)	C	C6-N1-C2	-8.89	116.74	120.30
1	A	58	C	C6-N1-C2	-8.87	116.75	120.30
1	A	15	G	N1-C6-O6	8.84	125.20	119.90
1	A	1365	G	C8-N9-C4	-8.82	102.87	106.40
1	A	1107	C	C6-N1-C2	-8.80	116.78	120.30
1	A	589	C	C5-C6-N1	-8.74	116.63	121.00
1	A	292	G	C5-C6-O6	-8.73	123.36	128.60
1	A	923	A	C2-N3-C4	-8.73	106.24	110.60
1	A	107	G	N1-C6-O6	8.73	125.14	119.90
1	A	853	G	C4-N9-C1'	8.71	137.83	126.50
1	A	851	G	C4-N9-C1'	8.71	137.82	126.50
1	A	1181	G	N7-C8-N9	-8.70	108.75	113.10
1	A	266	G	C2-N3-C4	-8.68	107.56	111.90
1	A	92	C	C6-N1-C2	-8.67	116.83	120.30
1	A	852	G	C2-N3-C4	-8.67	107.56	111.90
1	A	201	C	C6-N1-C2	-8.65	116.84	120.30
1	A	1502	A	C4-C5-N7	8.65	115.03	110.70
1	A	572	A	N9-C4-C5	8.65	109.26	105.80
1	A	789	U	N3-C2-O2	-8.64	116.15	122.20
1	A	1322	C	C6-N1-C2	-8.62	116.85	120.30
1	A	147	G	N1-C6-O6	8.60	125.06	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1303	C	N3-C4-C5	8.59	125.33	121.90
1	A	863	U	C5-C6-N1	-8.58	118.41	122.70
1	A	481	G	C8-N9-C1'	-8.58	115.85	127.00
1	A	853	G	N3-C4-N9	8.55	131.13	126.00
1	A	292	G	N1-C6-O6	8.54	125.03	119.90
1	A	907	A	C2-N3-C4	-8.54	106.33	110.60
1	A	853	G	C6-C5-N7	-8.54	125.28	130.40
1	A	878	G	C5-C6-O6	-8.53	123.48	128.60
1	A	881	G	C2-N3-C4	-8.53	107.64	111.90
1	A	283	C	N3-C4-N4	8.53	123.97	118.00
1	A	789	U	C6-N1-C2	-8.50	115.90	121.00
1	A	718	G	N3-C4-C5	-8.50	124.35	128.60
1	A	108	G	N1-C6-O6	8.49	124.99	119.90
1	A	881	G	N1-C6-O6	8.47	124.98	119.90
1	A	922	G	C4-C5-N7	8.47	114.19	110.80
1	A	703	G	N9-C4-C5	8.44	108.78	105.40
1	A	760	G	C8-N9-C4	8.44	109.77	106.40
1	A	638	G	C5-C6-N1	-8.42	107.29	111.50
1	A	1079	G	C8-N9-C4	-8.40	103.04	106.40
1	A	931	C	C5-C6-N1	-8.40	116.80	121.00
1	A	1338	G	C8-N9-C4	-8.38	103.05	106.40
1	A	871	U	N1-C2-O2	8.37	128.66	122.80
1	A	392	G	N1-C6-O6	8.37	124.92	119.90
1	A	1504	G	N1-C6-O6	-8.37	114.88	119.90
1	A	635	G	C5-C6-N1	-8.35	107.32	111.50
1	A	190(C)	C	C6-N1-C2	-8.35	116.96	120.30
1	A	1502	A	N1-C6-N6	8.31	123.58	118.60
1	A	15	G	C5-C6-N1	-8.30	107.35	111.50
1	A	266	G	C5-N7-C8	-8.28	100.16	104.30
1	A	851	G	C6-C5-N7	-8.26	125.45	130.40
1	A	1455	G	N1-C6-O6	8.24	124.84	119.90
1	A	1446	A	C8-N9-C4	8.24	109.09	105.80
1	A	146	G	N1-C6-O6	8.22	124.83	119.90
1	A	900	A	C2-N3-C4	-8.22	106.49	110.60
1	A	945	G	C5-C6-N1	8.21	115.60	111.50
1	A	805	C	C5-C4-N4	-8.20	114.46	120.20
1	A	48	C	C6-N1-C2	8.20	123.58	120.30
1	A	295	C	C6-N1-C2	8.19	123.58	120.30
1	A	13	U	C6-N1-C1'	-8.18	109.74	121.20
1	A	326	G	C4-C5-N7	-8.18	107.53	110.80
1	A	670	G	N3-C4-N9	8.15	130.89	126.00
1	A	929	G	C2-N3-C4	-8.15	107.83	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	975	A	N1-C6-N6	8.14	123.48	118.60
1	A	878	G	C4-C5-N7	8.13	114.05	110.80
1	A	785	G	C6-C5-N7	-8.12	125.53	130.40
1	A	799	G	C4-C5-N7	8.10	114.04	110.80
1	A	279	A	C2-N3-C4	-8.10	106.55	110.60
1	A	1354	C	C5-C6-N1	8.09	125.05	121.00
1	A	481	G	N9-C4-C5	-8.08	102.17	105.40
1	A	598	U	C5-C6-N1	-8.07	118.66	122.70
1	A	1238	A	N9-C4-C5	8.05	109.02	105.80
1	A	289	G	C6-C5-N7	-8.04	125.58	130.40
1	A	722	A	C5-C6-N1	-8.04	113.68	117.70
1	A	590	C	C6-N1-C2	8.03	123.51	120.30
1	A	718	G	C8-N9-C4	-8.02	103.19	106.40
1	A	284	G	N1-C6-O6	8.00	124.70	119.90
1	A	964	A	N7-C8-N9	7.99	117.80	113.80
1	A	662	G	N1-C6-O6	7.98	124.69	119.90
1	A	703	G	C5-N7-C8	7.98	108.29	104.30
1	A	482	A	C8-N9-C4	-7.97	102.61	105.80
1	A	326	G	C5-C6-O6	7.96	133.38	128.60
1	A	600	C	C5-C6-N1	-7.96	117.02	121.00
1	A	851	G	C8-N9-C4	-7.95	103.22	106.40
1	A	131	C	C5-C6-N1	-7.94	117.03	121.00
1	A	712	A	N1-C2-N3	7.94	133.27	129.30
1	A	875	C	C5-C6-N1	-7.93	117.03	121.00
1	A	799	G	C5-C6-O6	-7.93	123.84	128.60
1	A	1230	C	C6-N1-C2	-7.93	117.13	120.30
1	A	766	A	C8-N9-C4	7.92	108.97	105.80
1	A	80	G	N3-C4-C5	-7.90	124.65	128.60
1	A	382	A	C8-N9-C4	-7.90	102.64	105.80
17	Q	98	LEU	CA-CB-CG	7.89	133.46	115.30
1	A	693	G	C6-C5-N7	-7.88	125.67	130.40
1	A	1370	G	N7-C8-N9	7.88	117.04	113.10
1	A	331	G	C6-C5-N7	-7.86	125.68	130.40
1	A	898	G	N3-C4-N9	-7.86	121.28	126.00
1	A	266	G	N3-C4-C5	7.85	132.53	128.60
1	A	103	C	C6-N1-C2	-7.83	117.17	120.30
1	A	176	C	C6-N1-C2	7.82	123.43	120.30
1	A	328	C	C6-N1-C1'	-7.82	111.42	120.80
1	A	511	C	C2-N3-C4	-7.81	115.99	119.90
1	A	797	C	C6-N1-C2	7.81	123.42	120.30
1	A	693	G	N1-C6-O6	7.79	124.57	119.90
1	A	613	C	C6-N1-C2	7.78	123.41	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	150	C	C6-N1-C2	-7.78	117.19	120.30
1	A	190(G)	G	C5-C6-N1	-7.75	107.62	111.50
1	A	251	G	N1-C6-O6	7.74	124.54	119.90
1	A	576	G	N3-C4-C5	-7.72	124.74	128.60
1	A	1489	G	C8-N9-C4	-7.71	103.31	106.40
1	A	283	C	C5-C6-N1	7.71	124.85	121.00
1	A	107	G	C6-C5-N7	-7.69	125.78	130.40
1	A	569	C	C5-C6-N1	-7.68	117.16	121.00
1	A	893	C	N1-C2-O2	7.68	123.51	118.90
1	A	1377	A	N1-C6-N6	-7.68	113.99	118.60
1	A	1502	A	C6-C5-N7	-7.67	126.93	132.30
1	A	117	G	N9-C4-C5	-7.67	102.33	105.40
1	A	1338	G	N3-C4-C5	-7.66	124.77	128.60
1	A	814	A	C2-N3-C4	-7.65	106.77	110.60
1	A	907	A	N1-C2-N3	7.65	133.12	129.30
1	A	899	C	C5-C6-N1	7.65	124.82	121.00
1	A	638	G	C6-C5-N7	-7.63	125.82	130.40
1	A	839	U	N1-C2-O2	7.62	128.13	122.80
1	A	752	G	C8-N9-C4	7.62	109.45	106.40
1	A	1084	G	N1-C6-O6	-7.61	115.34	119.90
1	A	251	G	C4-C5-N7	7.60	113.84	110.80
1	A	255	G	N1-C6-O6	7.60	124.46	119.90
1	A	1282	C	C6-N1-C2	-7.60	117.26	120.30
1	A	722	A	C5-N7-C8	-7.59	100.11	103.90
1	A	482	A	N7-C8-N9	7.58	117.59	113.80
1	A	745	C	C6-N1-C2	7.56	123.33	120.30
1	A	1178	G	N9-C4-C5	7.56	108.42	105.40
1	A	1516[A]	G	C8-N9-C4	-7.55	103.38	106.40
1	A	1516[B]	G	C8-N9-C4	-7.55	103.38	106.40
1	A	600	C	C4-C5-C6	7.53	121.17	117.40
1	A	667	G	N1-C6-O6	7.53	124.42	119.90
1	A	266	G	N3-C4-N9	-7.52	121.49	126.00
1	A	292	G	N9-C4-C5	-7.51	102.40	105.40
1	A	836	G	C5-C6-N1	-7.50	107.75	111.50
1	A	1092	A	N1-C6-N6	7.48	123.09	118.60
1	A	92	C	C2-N1-C1'	7.47	127.02	118.80
1	A	1238	A	C8-N9-C4	-7.47	102.81	105.80
1	A	875	C	C2-N3-C4	-7.46	116.17	119.90
1	A	839	U	C6-N1-C1'	-7.46	110.76	121.20
1	A	853	G	C4-C5-C6	7.45	123.27	118.80
1	A	301	G	N9-C4-C5	7.44	108.38	105.40
1	A	28	G	N1-C6-O6	7.43	124.36	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1178	G	C8-N9-C4	-7.43	103.43	106.40
1	A	116	A	C8-N9-C4	7.42	108.77	105.80
1	A	1478	C	C6-N1-C2	-7.41	117.33	120.30
1	A	1084	G	N3-C4-C5	-7.41	124.90	128.60
1	A	80	G	N7-C8-N9	7.40	116.80	113.10
1	A	308	C	C5-C4-N4	-7.39	115.03	120.20
1	A	1514	C	C2-N3-C4	-7.38	116.21	119.90
1	A	1156	G	C8-N9-C4	-7.38	103.45	106.40
1	A	308	C	N1-C2-O2	7.37	123.33	118.90
1	A	543	C	C6-N1-C2	-7.37	117.35	120.30
1	A	117	G	C8-N9-C1'	-7.35	117.44	127.00
1	A	279	A	N1-C2-N3	7.35	132.97	129.30
1	A	1084	G	C4-C5-N7	-7.33	107.87	110.80
1	A	76	C	C2-N1-C1'	-7.31	110.76	118.80
1	A	78	G	N1-C6-O6	7.30	124.28	119.90
1	A	851	G	N7-C8-N9	7.29	116.75	113.10
1	A	1193	G	C8-N9-C4	7.28	109.31	106.40
1	A	1344	C	C5-C6-N1	-7.27	117.36	121.00
1	A	881	G	C5-C6-N1	-7.27	107.86	111.50
1	A	773	G	N1-C6-O6	7.26	124.25	119.90
1	A	309	G	N1-C6-O6	7.25	124.25	119.90
1	A	862	C	N3-C4-C5	7.25	124.80	121.90
1	A	331	G	C5-C6-O6	-7.24	124.25	128.60
1	A	1305	G	C5-C6-N1	-7.24	107.88	111.50
1	A	1079	G	N9-C4-C5	7.24	108.29	105.40
1	A	1239	A	C8-N9-C4	7.24	108.69	105.80
1	A	752	G	N7-C8-N9	-7.23	109.48	113.10
1	A	116	A	N1-C6-N6	7.23	122.94	118.60
1	A	481	G	N3-C4-C5	-7.23	124.99	128.60
17	Q	22	LEU	CA-CB-CG	-7.23	98.67	115.30
1	A	139	G	N1-C6-O6	7.22	124.23	119.90
1	A	266	G	N7-C8-N9	7.22	116.71	113.10
1	A	251	G	C5-N7-C8	-7.21	100.69	104.30
1	A	511	C	N3-C2-O2	-7.21	116.85	121.90
1	A	918	A	C6-N1-C2	-7.19	114.28	118.60
1	A	559	A	C6-N1-C2	-7.18	114.29	118.60
1	A	753	A	N1-C2-N3	7.17	132.89	129.30
1	A	301	G	C8-N9-C4	-7.17	103.53	106.40
1	A	1295	G	C8-N9-C4	-7.17	103.53	106.40
1	A	878	G	N1-C6-O6	7.16	124.20	119.90
1	A	1395	C	C6-N1-C2	7.16	123.17	120.30
1	A	300	A	C8-N9-C4	-7.15	102.94	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	58	C	C5-C6-N1	7.14	124.57	121.00
1	A	814	A	N1-C2-N3	7.14	132.87	129.30
1	A	328	C	N3-C2-O2	-7.12	116.92	121.90
1	A	1300	G	N7-C8-N9	-7.11	109.54	113.10
1	A	722	A	C6-C5-N7	-7.10	127.33	132.30
1	A	279	A	N1-C6-N6	7.10	122.86	118.60
1	A	975	A	C2-N3-C4	-7.10	107.05	110.60
1	A	750	G	N1-C6-O6	7.09	124.16	119.90
1	A	945	G	C4-C5-C6	-7.09	114.55	118.80
1	A	445	G	N1-C6-O6	7.08	124.15	119.90
1	A	722	A	N1-C6-N6	7.08	122.85	118.60
1	A	1200	C	N1-C2-O2	7.07	123.14	118.90
1	A	116	A	C2-N3-C4	-7.06	107.07	110.60
1	A	579	G	C8-N9-C4	7.05	109.22	106.40
1	A	576	G	C4-N9-C1'	7.04	135.66	126.50
1	A	232	G	C5-C6-N1	-7.04	107.98	111.50
1	A	1504	G	C5-C6-N1	7.04	115.02	111.50
1	A	639	G	N1-C2-N3	7.04	128.12	123.90
1	A	831	U	N3-C4-C5	-7.04	110.38	114.60
1	A	301	G	C5-C6-O6	7.02	132.81	128.60
1	A	635	G	C5-C6-O6	-7.01	124.39	128.60
1	A	400	C	C6-N1-C2	7.01	123.11	120.30
1	A	66	G	N3-C2-N2	-7.01	114.99	119.90
1	A	928	G	C5-C6-O6	-7.01	124.39	128.60
1	A	572	A	N1-C6-N6	-7.00	114.40	118.60
1	A	755	G	C4-C5-N7	7.00	113.60	110.80
1	A	635	G	C2-N3-C4	-7.00	108.40	111.90
1	A	1524	C	N3-C4-C5	-6.99	119.11	121.90
1	A	126	G	C8-N9-C4	6.98	109.19	106.40
1	A	318	G	N1-C6-O6	6.97	124.08	119.90
1	A	326	G	C5-C6-N1	-6.97	108.01	111.50
1	A	1401	G	C6-N1-C2	-6.97	120.92	125.10
1	A	1510	U	N3-C2-O2	-6.96	117.33	122.20
1	A	791	G	N3-C4-C5	-6.96	125.12	128.60
1	A	1334	G	C8-N9-C4	6.95	109.18	106.40
4	D	12	CYS	CA-CB-SG	6.94	126.49	114.00
1	A	32	A	N1-C6-N6	6.94	122.76	118.60
1	A	718	G	C8-N9-C1'	-6.93	117.99	127.00
1	A	1532	U	C5-C6-N1	6.93	126.17	122.70
1	A	1377	A	C6-N1-C2	-6.89	114.46	118.60
1	A	909	A	C6-N1-C2	-6.88	114.47	118.60
1	A	944	G	C8-N9-C4	-6.87	103.65	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	573	A	C8-N9-C4	-6.84	103.06	105.80
1	A	853	G	C8-N9-C4	-6.84	103.66	106.40
1	A	755	G	C5-C6-O6	-6.83	124.50	128.60
1	A	1347	G	C5-C6-O6	-6.83	124.50	128.60
1	A	81	U	C5-C6-N1	6.83	126.12	122.70
1	A	1469	G	N7-C8-N9	6.83	116.52	113.10
1	A	181	G	N3-C4-N9	6.83	130.10	126.00
1	A	597	G	C8-N9-C4	-6.81	103.67	106.40
1	A	753	A	C6-N1-C2	-6.81	114.51	118.60
1	A	831	U	C6-N1-C2	-6.81	116.91	121.00
1	A	1190	G	C4-N9-C1'	6.80	135.34	126.50
1	A	1379	G	C5-C6-N1	6.80	114.90	111.50
1	A	603	U	N3-C4-C5	-6.79	110.52	114.60
1	A	856	C	C5-C6-N1	-6.79	117.61	121.00
1	A	299	G	N9-C4-C5	-6.79	102.69	105.40
1	A	569	C	N1-C2-O2	-6.79	114.83	118.90
1	A	564	C	C6-N1-C2	-6.78	117.59	120.30
1	A	597	G	N3-C4-C5	-6.78	125.21	128.60
1	A	1092	A	N9-C4-C5	-6.78	103.09	105.80
1	A	461	C	N1-C2-O2	6.78	122.97	118.90
1	A	181	G	N3-C4-C5	-6.78	125.21	128.60
1	A	1446	A	N7-C8-N9	-6.77	110.41	113.80
1	A	375	U	N3-C2-O2	-6.77	117.46	122.20
1	A	791	G	C8-N9-C4	-6.76	103.70	106.40
1	A	1529	G	C4-N9-C1'	6.76	135.28	126.50
1	A	1376	U	N3-C2-O2	-6.75	117.47	122.20
1	A	23	C	C2-N3-C4	-6.75	116.53	119.90
1	A	856	C	C6-N1-C2	6.75	123.00	120.30
1	A	572	A	C8-N9-C4	-6.75	103.10	105.80
1	A	129(A)	G	C4-C5-N7	6.73	113.49	110.80
1	A	978	A	C8-N9-C4	6.73	108.49	105.80
1	A	563	A	C8-N9-C4	-6.72	103.11	105.80
1	A	1469	G	C6-C5-N7	-6.72	126.36	130.40
1	A	703	G	N3-C4-C5	-6.72	125.24	128.60
1	A	850	U	C5-C4-O4	6.72	129.93	125.90
1	A	107	G	C4-C5-N7	6.71	113.48	110.80
1	A	1348	U	C2-N1-C1'	6.71	125.75	117.70
1	A	295	C	N3-C4-C5	6.70	124.58	121.90
1	A	1365	G	N9-C4-C5	6.70	108.08	105.40
1	A	227	G	N1-C6-O6	6.70	123.92	119.90
1	A	310	G	C5-C6-O6	-6.70	124.58	128.60
1	A	779	C	N1-C2-O2	-6.70	114.88	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	929	G	N3-C4-C5	6.70	131.95	128.60
1	A	296	U	C5-C6-N1	-6.69	119.35	122.70
1	A	1067	A	N1-C6-N6	-6.69	114.59	118.60
1	A	637	G	C8-N9-C4	6.68	109.07	106.40
1	A	851	G	N3-C4-C5	-6.67	125.26	128.60
1	A	624	C	N1-C2-N3	-6.67	114.53	119.20
1	A	852	G	N3-C4-C5	6.67	131.93	128.60
1	A	1532	U	C4-C5-C6	-6.66	115.70	119.70
1	A	718	G	N7-C8-N9	6.66	116.43	113.10
1	A	243	A	N1-C2-N3	6.66	132.63	129.30
1	A	1092	A	C4-C5-N7	6.65	114.03	110.70
1	A	1200	C	C2-N1-C1'	6.65	126.12	118.80
1	A	576	G	N3-C4-N9	6.63	129.98	126.00
1	A	766	A	N3-C4-C5	6.63	131.44	126.80
1	A	839	U	C5-C6-N1	6.63	126.01	122.70
1	A	746	A	N1-C6-N6	-6.62	114.63	118.60
1	A	576	G	C4-C5-C6	6.61	122.77	118.80
1	A	103	C	N3-C4-C5	-6.61	119.26	121.90
1	A	190(G)	G	C4-C5-N7	6.61	113.44	110.80
1	A	1329	A	N1-C6-N6	6.60	122.56	118.60
1	A	874	G	C8-N9-C4	6.58	109.03	106.40
1	A	907	A	N1-C6-N6	-6.58	114.65	118.60
1	A	1181	G	N3-C4-C5	6.58	131.89	128.60
1	A	1333	A	C8-N9-C4	-6.58	103.17	105.80
1	A	626	U	N3-C2-O2	-6.57	117.60	122.20
1	A	670	G	N3-C4-C5	-6.57	125.31	128.60
1	A	881	G	C6-C5-N7	-6.57	126.46	130.40
1	A	1524	C	C4-C5-C6	6.56	120.68	117.40
1	A	1370	G	N3-C4-C5	-6.56	125.32	128.60
1	A	21	G	N3-C4-N9	6.56	129.93	126.00
1	A	76	C	C6-N1-C1'	6.55	128.66	120.80
1	A	765	G	C4-C5-N7	6.55	113.42	110.80
1	A	953	G	N3-C4-N9	6.55	129.93	126.00
1	A	181	G	C4-N9-C1'	6.55	135.01	126.50
1	A	1066	C	C2-N3-C4	-6.54	116.63	119.90
1	A	59	A	C4-C5-N7	6.54	113.97	110.70
1	A	392	G	C6-C5-N7	-6.54	126.47	130.40
1	A	576	G	C8-N9-C1'	-6.54	118.50	127.00
1	A	853	G	C8-N9-C1'	-6.54	118.50	127.00
8	H	12	ARG	NE-CZ-NH1	-6.54	117.03	120.30
1	A	117	G	C4-N9-C1'	6.53	134.99	126.50
1	A	1529	G	C8-N9-C1'	-6.53	118.51	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	T	94	ALA	N-CA-C	-6.53	93.37	111.00
1	A	8	A	C8-N9-C4	-6.53	103.19	105.80
1	A	597	G	N1-C2-N2	-6.52	110.33	116.20
1	A	722	A	C4-C5-N7	6.51	113.96	110.70
1	A	873	A	N7-C8-N9	6.50	117.05	113.80
1	A	654	G	N3-C4-N9	-6.50	122.10	126.00
1	A	281	G	C5-C6-N1	6.50	114.75	111.50
1	A	851	G	N3-C4-N9	6.49	129.89	126.00
1	A	899	C	C6-N1-C2	-6.49	117.70	120.30
1	A	283	C	N1-C2-O2	6.48	122.79	118.90
5	E	12	LEU	CA-CB-CG	6.48	130.20	115.30
1	A	190(A)	C	C5-C6-N1	6.48	124.24	121.00
1	A	1182	G	N1-C6-O6	6.47	123.78	119.90
1	A	835	U	C5-C4-O4	6.47	129.78	125.90
1	A	565	U	N1-C2-N3	-6.47	111.02	114.90
1	A	511	C	C5-C6-N1	-6.47	117.77	121.00
1	A	753	A	N9-C4-C5	6.47	108.39	105.80
1	A	120	A	C2-N3-C4	-6.46	107.37	110.60
1	A	625	G	N3-C4-C5	-6.46	125.37	128.60
1	A	21	G	C6-C5-N7	-6.46	126.52	130.40
1	A	1106	G	C2-N3-C4	-6.46	108.67	111.90
1	A	1527	C	N3-C4-C5	6.46	124.48	121.90
1	A	730	G	N9-C4-C5	6.45	107.98	105.40
1	A	279	A	C6-C5-N7	-6.45	127.78	132.30
1	A	789	U	N1-C2-N3	6.45	118.77	114.90
1	A	635	G	C6-C5-N7	-6.45	126.53	130.40
1	A	625	G	N3-C4-N9	6.44	129.87	126.00
1	A	779	C	C2-N3-C4	-6.44	116.68	119.90
1	A	1300	G	C4-C5-N7	-6.44	108.22	110.80
1	A	129	U	C5-C4-O4	6.44	129.76	125.90
1	A	251	G	C8-N9-C4	-6.44	103.83	106.40
1	A	254	G	C8-N9-C4	6.44	108.97	106.40
1	A	898	G	C5-C6-O6	6.44	132.46	128.60
1	A	59	A	C5-C6-N6	-6.43	118.56	123.70
1	A	129(A)	G	C5-N7-C8	-6.43	101.09	104.30
1	A	247	G	N1-C6-O6	6.42	123.75	119.90
1	A	218	C	C6-N1-C2	-6.42	117.73	120.30
1	A	922	G	C4-N9-C1'	6.42	134.84	126.50
1	A	1338	G	N7-C8-N9	6.42	116.31	113.10
1	A	670	G	C8-N9-C1'	-6.41	118.66	127.00
1	A	718	G	N3-C4-N9	6.41	129.84	126.00
1	A	656	C	C6-N1-C2	6.40	122.86	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	946	A	N1-C6-N6	-6.40	114.76	118.60
1	A	146	G	C5-C6-O6	-6.40	124.76	128.60
1	A	317	G	N1-C6-O6	6.39	123.74	119.90
1	A	1527	C	C5-C4-N4	-6.39	115.72	120.20
1	A	11	G	C2-N3-C4	-6.38	108.71	111.90
1	A	1343	G	C8-N9-C4	-6.38	103.85	106.40
1	A	218	C	C5-C6-N1	6.38	124.19	121.00
1	A	765	G	C5-N7-C8	-6.38	101.11	104.30
1	A	897	C	C2-N3-C4	-6.38	116.71	119.90
1	A	638	G	C4-C5-C6	6.38	122.63	118.80
1	A	896	C	C6-N1-C2	-6.37	117.75	120.30
1	A	833	U	C5-C4-O4	6.37	129.72	125.90
1	A	693	G	C8-N9-C1'	-6.36	118.73	127.00
1	A	878	G	C6-C5-N7	-6.36	126.58	130.40
1	A	703	G	C4-C5-C6	6.35	122.61	118.80
1	A	1066	C	C4-C5-C6	6.35	120.57	117.40
1	A	944	G	N7-C8-N9	6.34	116.27	113.10
1	A	1374	A	C8-N9-C4	-6.34	103.27	105.80
1	A	805	C	N3-C4-C5	6.33	124.43	121.90
1	A	484	G	C8-N9-C1'	-6.33	118.77	127.00
1	A	268	C	N3-C4-C5	-6.33	119.37	121.90
1	A	75	G	N7-C8-N9	-6.32	109.94	113.10
1	A	623	C	C5-C6-N1	-6.32	117.84	121.00
1	A	1490	C	C5-C6-N1	6.32	124.16	121.00
1	A	1300	G	C4-N9-C1'	-6.32	118.28	126.50
1	A	151	A	C2-N3-C4	-6.32	107.44	110.60
1	A	89	C	C6-N1-C2	-6.32	117.77	120.30
1	A	75	G	C8-N9-C4	6.32	108.93	106.40
1	A	625	G	C4-N9-C1'	6.32	134.71	126.50
1	A	1195	C	N1-C2-O2	-6.32	115.11	118.90
1	A	653	A	N1-C6-N6	-6.31	114.81	118.60
1	A	1300	G	C5-N7-C8	6.31	107.45	104.30
1	A	765	G	C6-C5-N7	-6.30	126.62	130.40
1	A	1200	C	C5-C6-N1	6.30	124.15	121.00
1	A	1514	C	C5-C6-N1	-6.30	117.85	121.00
1	A	656	C	C5-C6-N1	-6.29	117.85	121.00
1	A	888	G	C5-C6-N1	-6.29	108.35	111.50
1	A	1399	C	C5-C4-N4	-6.29	115.80	120.20
1	A	32	A	C5-C6-N6	-6.29	118.67	123.70
1	A	243	A	C6-N1-C2	-6.29	114.83	118.60
1	A	1148	U	N3-C2-O2	-6.29	117.80	122.20
1	A	232	G	N9-C4-C5	-6.29	102.89	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1469	G	C8-N9-C4	-6.29	103.89	106.40
1	A	558	G	N1-C6-O6	6.28	123.67	119.90
1	A	23	C	N1-C2-N3	6.27	123.59	119.20
1	A	1405	G	N1-C6-O6	6.27	123.66	119.90
1	A	597	G	N1-C2-N3	6.27	127.66	123.90
1	A	900	A	N1-C2-N3	6.26	132.43	129.30
1	A	836	G	C8-N9-C4	6.25	108.90	106.40
1	A	106	C	N1-C2-N3	6.25	123.58	119.20
1	A	481	G	C4-N9-C1'	6.25	134.62	126.50
1	A	13	U	C6-N1-C2	-6.24	117.25	121.00
1	A	1129	C	C6-N1-C2	-6.24	117.80	120.30
1	A	969	A	N1-C6-N6	6.24	122.34	118.60
1	A	1443	G	C8-N9-C4	6.23	108.89	106.40
1	A	1521	G	N3-C4-C5	-6.23	125.49	128.60
1	A	481	G	C8-N9-C4	6.23	108.89	106.40
1	A	74	C	C6-N1-C2	-6.22	117.81	120.30
1	A	788	U	N3-C4-O4	6.22	123.76	119.40
1	A	5	U	P-O3'-C3'	6.22	127.16	119.70
1	A	873	A	C5-C6-N1	6.22	120.81	117.70
1	A	511	C	N3-C4-C5	6.21	124.39	121.90
1	A	765	G	N1-C6-O6	6.21	123.63	119.90
1	A	326	G	N9-C4-C5	6.21	107.89	105.40
1	A	872	A	C6-C5-N7	-6.21	127.95	132.30
1	A	851	G	C8-N9-C1'	-6.20	118.94	127.00
1	A	945	G	C5-N7-C8	-6.20	101.20	104.30
1	A	613	C	C5-C4-N4	-6.20	115.86	120.20
1	A	299	G	C8-N9-C4	6.19	108.88	106.40
1	A	624	C	N3-C4-C5	6.19	124.38	121.90
1	A	945	G	C5-C6-O6	-6.19	124.89	128.60
1	A	1328	C	N3-C4-C5	6.19	124.38	121.90
1	A	1079	G	C5-C6-O6	6.18	132.31	128.60
1	A	1329	A	C4-C5-N7	6.18	113.79	110.70
1	A	786	G	N1-C6-O6	6.18	123.61	119.90
1	A	597	G	N7-C8-N9	6.18	116.19	113.10
1	A	1533	C	C2-N1-C1'	6.18	125.60	118.80
1	A	1346	A	P-O3'-C3'	6.17	127.11	119.70
1	A	1237	C	C6-N1-C2	-6.17	117.83	120.30
1	A	625	G	C6-C5-N7	-6.17	126.70	130.40
1	A	945	G	C4-C5-N7	6.16	113.26	110.80
1	A	881	G	C4-C5-C6	6.14	122.48	118.80
1	A	1100	C	C6-N1-C2	-6.14	117.84	120.30
1	A	907	A	C5-C6-N6	6.14	128.61	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1417	G	C5-C6-N1	-6.13	108.43	111.50
1	A	1064	G	N1-C2-N3	6.13	127.58	123.90
1	A	589	C	C2-N3-C4	-6.13	116.83	119.90
1	A	1294	G	C8-N9-C4	-6.13	103.95	106.40
1	A	181	G	C8-N9-C1'	-6.12	119.04	127.00
1	A	299	G	N1-C6-O6	6.12	123.57	119.90
1	A	1469	G	N1-C6-O6	6.12	123.57	119.90
1	A	169	C	N3-C4-C5	-6.12	119.45	121.90
1	A	730	G	N1-C2-N3	6.12	127.57	123.90
1	A	1343	G	N3-C4-N9	-6.12	122.33	126.00
1	A	1348	U	N3-C2-O2	-6.12	117.92	122.20
1	A	1499	A	C8-N9-C4	6.11	108.25	105.80
1	A	800	G	N3-C4-C5	-6.11	125.54	128.60
1	A	654	G	N3-C2-N2	-6.11	115.62	119.90
1	A	1084	G	C5-C6-O6	6.11	132.26	128.60
1	A	745	C	N3-C4-C5	6.10	124.34	121.90
1	A	128	G	C6-C5-N7	-6.10	126.74	130.40
1	A	1237	C	N3-C2-O2	-6.10	117.63	121.90
1	A	1378	C	C6-N1-C2	-6.10	117.86	120.30
1	A	1340	A	N1-C2-N3	6.09	132.35	129.30
1	A	833	U	C4-C5-C6	6.09	123.36	119.70
1	A	276	G	C8-N9-C4	6.08	108.83	106.40
1	A	1094	G	N3-C4-N9	6.08	129.65	126.00
1	A	283	C	C6-N1-C1'	-6.08	113.50	120.80
1	A	690	G	C8-N9-C4	6.07	108.83	106.40
1	A	1235	U	C6-N1-C2	-6.07	117.36	121.00
1	A	130	A	N1-C6-N6	6.07	122.24	118.60
1	A	1178	G	C4-C5-N7	-6.07	108.37	110.80
1	A	92	C	N1-C2-O2	6.07	122.54	118.90
1	A	722	A	N7-C8-N9	6.07	116.83	113.80
1	A	719	C	N3-C2-O2	-6.06	117.66	121.90
1	A	296	U	C2-N3-C4	-6.06	123.36	127.00
1	A	70	G	N3-C4-C5	6.06	131.63	128.60
1	A	1327	C	C6-N1-C2	6.06	122.72	120.30
1	A	693	G	C4-N9-C1'	6.05	134.37	126.50
1	A	368	U	N3-C4-O4	-6.05	115.17	119.40
1	A	190(B)	C	C6-N1-C2	-6.05	117.88	120.30
1	A	552	U	C2-N3-C4	-6.04	123.37	127.00
1	A	667	G	C2-N3-C4	-6.04	108.88	111.90
1	A	11	G	N1-C6-O6	6.04	123.52	119.90
1	A	21	G	C4-N9-C1'	6.04	134.35	126.50
1	A	677	U	N3-C4-C5	-6.04	110.98	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	283	C	C6-N1-C2	-6.03	117.89	120.30
1	A	601	C	C2-N3-C4	-6.03	116.89	119.90
1	A	773	G	C5-C6-O6	-6.03	124.98	128.60
1	A	544	G	N1-C6-O6	-6.03	116.28	119.90
1	A	726	C	N3-C4-C5	6.02	124.31	121.90
1	A	703	G	C5-C6-N1	-6.02	108.49	111.50
1	A	902	G	C8-N9-C4	6.02	108.81	106.40
1	A	1312	G	C4-C5-N7	-6.01	108.39	110.80
1	A	186	C	N3-C4-C5	6.01	124.30	121.90
1	A	642	A	N1-C6-N6	-6.01	115.00	118.60
1	A	1319	A	N1-C6-N6	-6.01	114.99	118.60
1	A	635	G	N3-C4-C5	6.01	131.60	128.60
1	A	1442	G	C4-N9-C1'	6.01	134.31	126.50
1	A	322	C	C6-N1-C2	6.00	122.70	120.30
1	A	923	A	N1-C2-N3	6.00	132.30	129.30
1	A	266	G	C8-N9-C4	-6.00	104.00	106.40
1	A	922	G	C5-N7-C8	-6.00	101.30	104.30
1	A	382	A	N7-C8-N9	6.00	116.80	113.80
1	A	190(B)	C	C5-C6-N1	5.99	124.00	121.00
1	A	227	G	C5-C6-O6	-5.99	125.01	128.60
1	A	485	G	C4-C5-N7	-5.99	108.41	110.80
1	A	144	G	N1-C6-O6	5.99	123.49	119.90
1	A	564	C	N3-C4-C5	-5.99	119.50	121.90
1	A	852	G	N3-C2-N2	-5.99	115.71	119.90
1	A	1140	C	C6-N1-C2	-5.99	117.91	120.30
1	A	80	G	N9-C4-C5	5.98	107.79	105.40
1	A	1455	G	C4-C5-N7	5.98	113.19	110.80
1	A	872	A	N1-C6-N6	5.97	122.18	118.60
1	A	1346	A	C6-N1-C2	-5.97	115.02	118.60
1	A	1300	G	C8-N9-C4	5.97	108.79	106.40
1	A	88	A	C8-N9-C4	-5.97	103.41	105.80
1	A	811	C	C6-N1-C2	5.97	122.69	120.30
1	A	1533	C	C5-C6-N1	5.97	123.98	121.00
1	A	1322	C	N3-C4-C5	-5.96	119.52	121.90
1	A	299	G	C5-C6-O6	-5.96	125.02	128.60
1	A	308	C	N1-C2-N3	-5.96	115.03	119.20
1	A	78	G	C5-C6-N1	-5.96	108.52	111.50
1	A	691	G	N9-C4-C5	5.96	107.78	105.40
1	A	691	G	C8-N9-C4	-5.96	104.02	106.40
1	A	1301	U	P-O3'-C3'	5.96	126.85	119.70
1	A	1098	C	C6-N1-C2	5.96	122.68	120.30
1	A	821	G	C8-N9-C4	5.95	108.78	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	650	G	C8-N9-C4	5.95	108.78	106.40
1	A	279	A	C4-C5-N7	5.95	113.67	110.70
1	A	654	G	N3-C4-C5	5.95	131.57	128.60
1	A	309	G	C4-C5-N7	5.94	113.18	110.80
1	A	625	G	C5-C6-O6	-5.94	125.04	128.60
1	A	1412	C	N3-C4-C5	5.94	124.28	121.90
1	A	651	C	C6-N1-C2	5.94	122.67	120.30
1	A	1401	G	C5-C6-O6	-5.93	125.04	128.60
1	A	1521	G	C6-N1-C2	-5.93	121.54	125.10
1	A	1094	G	N9-C4-C5	-5.93	103.03	105.40
1	A	932	C	C6-N1-C2	-5.93	117.93	120.30
1	A	673	G	N1-C6-O6	5.92	123.45	119.90
1	A	13	U	N1-C2-O2	5.92	126.94	122.80
1	A	677	U	N1-C2-N3	5.92	118.45	114.90
1	A	21	G	N3-C4-C5	-5.92	125.64	128.60
1	A	813	U	N3-C4-O4	5.92	123.54	119.40
1	A	1067	A	N9-C4-C5	5.92	108.17	105.80
1	A	1190	G	C4-C5-C6	5.91	122.35	118.80
1	A	1447	G	C4-C5-N7	5.91	113.16	110.80
1	A	975	A	C5-N7-C8	-5.91	100.95	103.90
1	A	147	G	C8-N9-C4	5.91	108.76	106.40
1	A	154	C	C6-N1-C2	5.90	122.66	120.30
1	A	308	C	C6-N1-C1'	-5.90	113.72	120.80
1	A	882	C	N1-C2-N3	5.90	123.33	119.20
1	A	815	A	C8-N9-C4	5.90	108.16	105.80
1	A	22	G	C6-C5-N7	-5.89	126.86	130.40
1	A	1312	G	C5-N7-C8	5.89	107.25	104.30
1	A	664	G	C5-C6-O6	5.89	132.13	128.60
1	A	580	U	C5-C6-N1	-5.89	119.76	122.70
1	A	28	G	C5-C6-N1	-5.89	108.56	111.50
1	A	1335	C	C2-N1-C1'	-5.89	112.32	118.80
1	A	837	G	C8-N9-C4	5.88	108.75	106.40
1	A	317	G	C6-C5-N7	-5.88	126.87	130.40
1	A	1107	C	N3-C4-C5	-5.88	119.55	121.90
1	A	1238	A	N1-C6-N6	-5.88	115.07	118.60
1	A	740	U	C5-C6-N1	-5.88	119.76	122.70
1	A	881	G	N1-C2-N3	5.87	127.42	123.90
1	A	131	C	C2-N3-C4	-5.87	116.97	119.90
1	A	1241	G	C4-C5-C6	5.87	122.32	118.80
1	A	731	G	C5-C6-O6	-5.86	125.08	128.60
1	A	730	G	C4-C5-N7	-5.86	108.46	110.80
1	A	1374	A	N7-C8-N9	5.86	116.73	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	613	C	N3-C4-C5	5.86	124.24	121.90
1	A	1379	G	N1-C6-O6	-5.86	116.39	119.90
1	A	1348	U	C6-N1-C1'	-5.85	113.00	121.20
1	A	1344	C	C6-N1-C2	5.85	122.64	120.30
1	A	300	A	N9-C4-C5	5.85	108.14	105.80
1	A	615	C	C6-N1-C2	-5.85	117.96	120.30
1	A	28	G	C6-C5-N7	-5.84	126.90	130.40
1	A	308	C	C2-N1-C1'	5.84	125.22	118.80
1	A	785	G	C5-C6-O6	-5.84	125.10	128.60
1	A	898	G	N9-C4-C5	5.84	107.73	105.40
1	A	639	G	N1-C2-N2	-5.83	110.95	116.20
1	A	676	A	C8-N9-C4	5.83	108.13	105.80
1	A	799	G	N1-C6-O6	5.83	123.40	119.90
1	A	1531	A	C6-C5-N7	-5.83	128.22	132.30
1	A	796	C	N3-C2-O2	-5.83	117.82	121.90
1	A	307	C	N1-C2-O2	5.83	122.40	118.90
1	A	917	G	C5-N7-C8	-5.83	101.39	104.30
1	A	42	G	N3-C4-C5	-5.82	125.69	128.60
1	A	331	G	C4-C5-N7	5.82	113.13	110.80
1	A	651	C	N3-C2-O2	5.82	125.97	121.90
1	A	289	G	C5-C6-N1	-5.81	108.60	111.50
1	A	928	G	C6-C5-N7	-5.81	126.92	130.40
1	A	931	C	N3-C4-N4	-5.81	113.94	118.00
1	A	454	C	N1-C2-O2	5.80	122.38	118.90
1	A	752	G	N3-C4-C5	5.80	131.50	128.60
1	A	769	G	C5-C6-O6	-5.80	125.12	128.60
1	A	1442	G	N3-C4-C5	-5.80	125.70	128.60
1	A	1367	C	N3-C2-O2	-5.80	117.84	121.90
1	A	1370	G	C4-N9-C1'	5.80	134.04	126.50
1	A	713	G	C8-N9-C4	-5.80	104.08	106.40
1	A	698	G	N3-C4-C5	-5.79	125.70	128.60
1	A	799	G	C5-N7-C8	-5.79	101.41	104.30
1	A	931	C	C4-C5-C6	5.79	120.29	117.40
1	A	635	G	N3-C2-N2	-5.78	115.85	119.90
1	A	518	C	N1-C2-O2	5.78	122.37	118.90
1	A	890	G	C4-C5-N7	-5.78	108.49	110.80
1	A	1361(A)	C	C5-C6-N1	5.78	123.89	121.00
1	A	116	A	N9-C4-C5	-5.78	103.49	105.80
1	A	731	G	C8-N9-C4	5.78	108.71	106.40
1	A	199	G	N1-C6-O6	5.77	123.36	119.90
1	A	946	A	N9-C4-C5	5.77	108.11	105.80
1	A	1066	C	C5-C6-N1	-5.77	118.12	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	771	G	N1-C6-O6	5.77	123.36	119.90
1	A	635	G	N9-C4-C5	-5.76	103.09	105.40
1	A	1078	U	C5-C6-N1	5.76	125.58	122.70
1	A	309	G	N9-C4-C5	-5.76	103.10	105.40
1	A	1377	A	N9-C4-C5	5.76	108.11	105.80
2	B	180	LEU	CA-CB-CG	-5.76	102.05	115.30
1	A	392	G	C5-C6-O6	-5.75	125.15	128.60
1	A	796	C	C5-C6-N1	-5.75	118.12	121.00
1	A	564	C	N1-C2-N3	5.74	123.22	119.20
1	A	626	U	N1-C2-N3	5.74	118.34	114.90
1	A	670	G	C4-N9-C1'	5.74	133.96	126.50
1	A	190(G)	G	C4-C5-C6	5.74	122.24	118.80
1	A	750	G	C6-C5-N7	-5.74	126.96	130.40
1	A	1224	G	C4-N9-C1'	-5.74	119.04	126.50
1	A	1528	U	N3-C2-O2	5.74	126.21	122.20
1	A	664	G	N1-C6-O6	-5.73	116.46	119.90
1	A	34	C	C2-N1-C1'	-5.73	112.50	118.80
1	A	789	U	C2-N1-C1'	5.73	124.58	117.70
1	A	700	G	N3-C4-N9	5.73	129.44	126.00
1	A	1377	A	C5-C6-N1	5.72	120.56	117.70
1	A	762	C	C5-C4-N4	-5.72	116.20	120.20
1	A	635	G	C8-N9-C4	5.72	108.69	106.40
1	A	27	G	N1-C6-O6	5.71	123.33	119.90
1	A	403	C	C4-C5-C6	5.71	120.26	117.40
1	A	1516[A]	G	N9-C4-C5	5.71	107.68	105.40
1	A	1516[B]	G	N9-C4-C5	5.71	107.68	105.40
1	A	289	G	C4-C5-C6	5.71	122.22	118.80
1	A	485	G	C8-N9-C4	5.71	108.68	106.40
1	A	1193	G	N7-C8-N9	-5.71	110.25	113.10
1	A	718	G	C6-C5-N7	-5.70	126.98	130.40
8	H	4	ASP	CB-CG-OD1	5.70	123.43	118.30
1	A	485	G	N7-C8-N9	-5.70	110.25	113.10
1	A	1502	A	N9-C4-C5	-5.70	103.52	105.80
5	E	41	VAL	CB-CA-C	-5.70	100.57	111.40
1	A	628	G	N3-C4-C5	-5.70	125.75	128.60
1	A	1190	G	C8-N9-C4	-5.69	104.12	106.40
1	A	800	G	C8-N9-C4	-5.69	104.12	106.40
1	A	815	A	N7-C8-N9	-5.69	110.95	113.80
1	A	833	U	N3-C2-O2	-5.69	118.22	122.20
1	A	909	A	C5-C6-N1	5.69	120.55	117.70
1	A	1064	G	C2-N3-C4	-5.69	109.06	111.90
1	A	128	G	C5-C6-O6	-5.69	125.19	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1469	G	C4-N9-C1'	5.69	133.90	126.50
1	A	7	G	N3-C4-C5	-5.69	125.76	128.60
1	A	1195	C	N3-C2-O2	5.68	125.88	121.90
1	A	1346	A	N9-C4-C5	5.68	108.07	105.80
1	A	66	G	N1-C6-O6	5.68	123.31	119.90
1	A	301	G	N1-C6-O6	-5.68	116.49	119.90
1	A	582	U	N3-C2-O2	-5.68	118.22	122.20
1	A	296	U	N3-C4-O4	-5.68	115.43	119.40
1	A	1528	U	C5-C6-N1	-5.68	119.86	122.70
1	A	920	U	C5-C4-O4	5.67	129.30	125.90
1	A	872	A	C4-C5-N7	5.67	113.54	110.70
1	A	328	C	N3-C4-C5	5.67	124.17	121.90
1	A	1181	G	C4-N9-C1'	-5.67	119.13	126.50
1	A	281	G	P-O3'-C3'	5.67	126.50	119.70
1	A	154	C	N3-C4-C5	5.66	124.17	121.90
1	A	61	G	C6-N1-C2	-5.66	121.70	125.10
1	A	553	A	C2-N3-C4	-5.66	107.77	110.60
1	A	576	G	N1-C2-N3	5.66	127.30	123.90
1	A	190(G)	G	C5-C6-O6	-5.66	125.20	128.60
1	A	616	G	C5-C6-N1	-5.66	108.67	111.50
1	A	975	A	C6-C5-N7	-5.66	128.34	132.30
1	A	1531	A	N7-C8-N9	5.66	116.63	113.80
1	A	20	G	C2-N3-C4	-5.66	109.07	111.90
1	A	53	A	C6-N1-C2	-5.66	115.21	118.60
1	A	283	C	C2-N3-C4	5.66	122.73	119.90
1	A	266	G	C4-C5-N7	5.65	113.06	110.80
1	A	236	G	C8-N9-C1'	-5.65	119.65	127.00
1	A	1079	G	N1-C6-O6	-5.65	116.51	119.90
1	A	251	G	C4-N9-C1'	5.65	133.84	126.50
1	A	292	G	N3-C4-N9	5.65	129.39	126.00
1	A	1505	G	C5-N7-C8	-5.64	101.48	104.30
12	L	85	ILE	CB-CA-C	-5.64	100.32	111.60
1	A	236	G	N3-C4-N9	5.64	129.38	126.00
1	A	305	G	C8-N9-C4	-5.63	104.15	106.40
1	A	1544	U	N3-C4-C5	-5.63	111.22	114.60
1	A	753	A	C4-C5-C6	5.63	119.81	117.00
1	A	553	A	N1-C2-N3	5.63	132.12	129.30
1	A	122	G	N1-C6-O6	5.62	123.28	119.90
1	A	76	C	N1-C2-O2	-5.62	115.53	118.90
1	A	391	G	N3-C4-N9	5.62	129.37	126.00
1	A	129(A)	G	N1-C6-O6	5.62	123.27	119.90
1	A	783	C	C6-N1-C2	5.62	122.55	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	771	G	C5-C6-O6	-5.62	125.23	128.60
1	A	863	U	C5-C4-O4	5.61	129.27	125.90
1	A	1045	C	C6-N1-C2	-5.61	118.05	120.30
1	A	1401	G	N1-C2-N3	5.61	127.27	123.90
1	A	790	A	C2-N3-C4	-5.61	107.79	110.60
1	A	82	U	C2-N1-C1'	5.61	124.43	117.70
1	A	1399	C	N3-C4-N4	5.61	121.93	118.00
1	A	18	C	C6-N1-C2	5.61	122.54	120.30
1	A	703	G	C8-N9-C4	-5.61	104.16	106.40
1	A	130	A	C6-C5-N7	-5.61	128.38	132.30
1	A	760	G	N7-C8-N9	-5.60	110.30	113.10
1	A	288	A	C2-N3-C4	-5.60	107.80	110.60
1	A	601	C	C5-C6-N1	-5.60	118.20	121.00
1	A	779	C	C5-C6-N1	-5.60	118.20	121.00
1	A	1367	C	C5-C6-N1	5.59	123.80	121.00
1	A	871	U	N3-C2-O2	-5.59	118.29	122.20
1	A	219	C	C6-N1-C2	-5.58	118.07	120.30
1	A	129	U	N1-C2-N3	5.58	118.25	114.90
1	A	1482	G	C4-C5-N7	-5.58	108.57	110.80
1	A	23	C	C4-C5-C6	5.58	120.19	117.40
1	A	650	G	N1-C6-O6	5.58	123.25	119.90
1	A	552	U	C5-C6-N1	-5.57	119.92	122.70
1	A	606	G	C4-C5-N7	-5.57	108.57	110.80
1	A	389	A	N1-C2-N3	5.57	132.08	129.30
1	A	397	A	N7-C8-N9	5.57	116.58	113.80
1	A	454	C	C5-C6-N1	5.57	123.78	121.00
1	A	190(G)	G	C2-N3-C4	-5.57	109.12	111.90
1	A	283	C	N3-C4-C5	-5.56	119.67	121.90
1	A	1195	C	N3-C4-N4	5.56	121.89	118.00
1	A	77	G	C5-C6-N1	5.56	114.28	111.50
1	A	522	C	C6-N1-C2	5.55	122.52	120.30
1	A	628	G	N3-C4-N9	5.55	129.33	126.00
1	A	377	G	N1-C2-N3	5.54	127.23	123.90
1	A	201	C	C5-C6-N1	5.54	123.77	121.00
1	A	171	A	C6-N1-C2	-5.54	115.28	118.60
1	A	82	U	N3-C2-O2	-5.54	118.32	122.20
1	A	1347	G	C8-N9-C4	5.54	108.61	106.40
1	A	931	C	C5-C4-N4	5.54	124.07	120.20
1	A	1181	G	N9-C4-C5	-5.54	103.19	105.40
1	A	130	A	C4-C5-C6	5.53	119.77	117.00
1	A	541	G	N1-C6-O6	5.53	123.22	119.90
1	A	541	G	N3-C4-C5	5.53	131.37	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1334	G	N9-C4-C5	-5.53	103.19	105.40
1	A	840	C	N1-C2-O2	5.53	122.22	118.90
1	A	82	U	C5-C6-N1	5.53	125.46	122.70
1	A	766	A	C2-N3-C4	-5.53	107.84	110.60
1	A	1022	G	N3-C4-C5	-5.53	125.84	128.60
1	A	1298	C	C6-N1-C2	5.53	122.51	120.30
1	A	190(G)	G	N7-C8-N9	5.52	115.86	113.10
1	A	859	A	N1-C6-N6	5.52	121.91	118.60
1	A	538	G	C8-N9-C4	5.52	108.61	106.40
1	A	560	U	N3-C2-O2	-5.52	118.34	122.20
1	A	318	G	C5-C6-N1	-5.51	108.74	111.50
1	A	1108	G	C8-N9-C4	-5.51	104.19	106.40
1	A	558	G	C8-N9-C4	-5.51	104.19	106.40
1	A	965	A	C8-N9-C4	5.51	108.00	105.80
1	A	1528	U	C6-N1-C2	5.51	124.31	121.00
1	A	484	G	C4-N9-C1'	5.51	133.66	126.50
1	A	888	G	C4-C5-N7	-5.51	108.60	110.80
1	A	1468	A	C5-C6-N6	-5.50	119.30	123.70
1	A	168	G	C5-C6-N1	-5.50	108.75	111.50
1	A	547	A	N1-C6-N6	-5.50	115.30	118.60
1	A	654	G	C2-N3-C4	-5.50	109.15	111.90
1	A	1378	C	C2-N1-C1'	5.50	124.84	118.80
1	A	283	C	C5-C4-N4	-5.49	116.36	120.20
1	A	661	G	C8-N9-C4	-5.49	104.20	106.40
1	A	677	U	C4-C5-C6	5.49	122.99	119.70
1	A	15	G	C8-N9-C4	5.48	108.59	106.40
1	A	752	G	N3-C4-N9	-5.48	122.71	126.00
1	A	831	U	N3-C4-O4	5.48	123.24	119.40
1	A	555	C	C5-C6-N1	5.48	123.74	121.00
1	A	933	G	C5-C6-O6	-5.48	125.31	128.60
1	A	765	G	N7-C8-N9	5.47	115.84	113.10
1	A	795	C	N1-C2-O2	-5.47	115.61	118.90
1	A	368	U	N3-C4-C5	5.47	117.88	114.60
1	A	568	G	C8-N9-C4	-5.47	104.21	106.40
1	A	559	A	N1-C2-N3	5.47	132.03	129.30
1	A	1182	G	C5-C6-O6	-5.47	125.32	128.60
1	A	1182	G	N7-C8-N9	5.47	115.83	113.10
1	A	1490	C	C4-C5-C6	-5.47	114.67	117.40
1	A	1182	G	C4-N9-C1'	5.47	133.61	126.50
1	A	142	G	C2-N3-C4	5.46	114.63	111.90
1	A	825	G	C5-C6-O6	-5.46	125.32	128.60
1	A	383	A	N1-C2-N3	-5.46	126.57	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	368	U	C2-N1-C1'	-5.46	111.15	117.70
1	A	579	G	N9-C4-C5	-5.46	103.22	105.40
1	A	1503	A	C8-N9-C4	5.46	107.98	105.80
1	A	773	G	C6-C5-N7	-5.45	127.13	130.40
1	A	289	G	C5-C6-O6	-5.45	125.33	128.60
1	A	75	G	C4-N9-C1'	-5.45	119.42	126.50
1	A	40	C	C5-C6-N1	5.45	123.72	121.00
1	A	484	G	N3-C4-N9	5.45	129.27	126.00
1	A	687	A	C8-N9-C4	-5.45	103.62	105.80
1	A	1447	G	C5-N7-C8	-5.45	101.58	104.30
1	A	249	U	N1-C2-N3	5.44	118.17	114.90
1	A	301	G	C4-C5-N7	-5.44	108.62	110.80
1	A	638	G	C2-N3-C4	-5.44	109.18	111.90
1	A	75	G	C6-C5-N7	5.44	133.66	130.40
1	A	239	U	N3-C2-O2	5.43	126.00	122.20
1	A	190(G)	G	C5-N7-C8	-5.43	101.59	104.30
1	A	1505	G	N9-C4-C5	5.43	107.57	105.40
1	A	160	A	N1-C6-N6	5.42	121.85	118.60
1	A	853	G	N7-C8-N9	5.42	115.81	113.10
1	A	151	A	C5-C6-N1	-5.42	114.99	117.70
1	A	1319	A	N9-C4-C5	5.42	107.97	105.80
1	A	523	A	C2-N3-C4	-5.42	107.89	110.60
17	Q	84	LEU	CA-CB-CG	-5.42	102.83	115.30
1	A	1067	A	P-O3'-C3'	5.42	126.20	119.70
1	A	975	A	C4-C5-N7	5.41	113.41	110.70
1	A	1160	G	C5-C6-O6	-5.41	125.35	128.60
1	A	8	A	N9-C4-C5	5.41	107.97	105.80
1	A	1293	G	N1-C6-O6	5.41	123.15	119.90
1	A	1376	U	N1-C2-O2	5.41	126.59	122.80
1	A	522	C	N3-C2-O2	5.41	125.69	121.90
1	A	1084	G	C2-N3-C4	5.41	114.60	111.90
1	A	154	C	C2-N3-C4	-5.41	117.20	119.90
1	A	129(A)	G	C6-C5-N7	-5.41	127.16	130.40
1	A	1398	A	N1-C6-N6	-5.41	115.36	118.60
1	A	915	A	C6-C5-N7	-5.40	128.52	132.30
1	A	853	G	N1-C2-N2	-5.40	111.34	116.20
1	A	53	A	C5-C6-N1	5.40	120.40	117.70
1	A	66	G	C8-N9-C4	-5.40	104.24	106.40
1	A	803	G	C8-N9-C4	-5.40	104.24	106.40
1	A	1358	U	N3-C2-O2	-5.40	118.42	122.20
1	A	582	U	N1-C2-N3	5.40	118.14	114.90
1	A	1299	A	C4-N9-C1'	5.40	136.01	126.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	139	G	C5-C6-O6	-5.39	125.36	128.60
1	A	637	G	N9-C4-C5	-5.39	103.24	105.40
1	A	1405	G	C5-C6-N1	-5.39	108.80	111.50
1	A	662	G	N3-C2-N2	-5.39	116.13	119.90
1	A	129(A)	G	N7-C8-N9	5.39	115.79	113.10
1	A	818	G	C5-C6-N1	-5.38	108.81	111.50
1	A	626	U	C6-N1-C2	-5.38	117.77	121.00
1	A	1513	A	N1-C6-N6	5.38	121.83	118.60
1	A	597	G	C4-N9-C1'	5.38	133.50	126.50
1	A	812	C	C5-C4-N4	5.38	123.97	120.20
1	A	890	G	N9-C4-C5	5.38	107.55	105.40
1	A	59	A	C5-N7-C8	-5.38	101.21	103.90
1	A	771	G	C4-C5-N7	5.38	112.95	110.80
1	A	780	A	N1-C6-N6	-5.38	115.37	118.60
1	A	1084	G	N9-C4-C5	5.38	107.55	105.40
1	A	1392	G	C8-N9-C1'	-5.38	120.01	127.00
1	A	1202	G	C4-C5-N7	-5.38	108.65	110.80
1	A	1239	A	N7-C8-N9	-5.37	111.11	113.80
1	A	601	C	N3-C4-C5	5.37	124.05	121.90
1	A	1178	G	C5-C6-O6	5.37	131.82	128.60
1	A	247	G	C5-C6-N1	-5.37	108.81	111.50
1	A	736	C	C5-C6-N1	-5.37	118.31	121.00
1	A	227	G	C4-C5-N7	5.37	112.95	110.80
1	A	873	A	C2-N3-C4	5.37	113.28	110.60
1	A	860	A	C4-C5-C6	5.37	119.68	117.00
1	A	916	G	C8-N9-C4	-5.37	104.25	106.40
1	A	1455	G	C6-C5-N7	-5.37	127.18	130.40
1	A	1533	C	N1-C2-O2	5.37	122.12	118.90
1	A	831	U	C5-C6-N1	5.36	125.38	122.70
1	A	1182	G	C6-C5-N7	-5.36	127.18	130.40
1	A	1190	G	C8-N9-C1'	-5.36	120.03	127.00
1	A	1300	G	C6-C5-N7	5.36	133.62	130.40
1	A	840	C	N3-C2-O2	-5.36	118.15	121.90
1	A	859	A	C5-N7-C8	-5.35	101.22	103.90
1	A	1156	G	N3-C4-C5	-5.35	125.92	128.60
1	A	255	G	C5-C6-O6	-5.35	125.39	128.60
1	A	1514	C	N3-C4-N4	-5.35	114.26	118.00
1	A	175	C	C6-N1-C2	5.34	122.44	120.30
1	A	147	G	C5-C6-N1	-5.34	108.83	111.50
1	A	873	A	N9-C4-C5	5.34	107.94	105.80
1	A	915	A	C5-C6-N1	-5.34	115.03	117.70
1	A	230	G	N1-C2-N3	5.34	127.10	123.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	829	G	N1-C2-N2	-5.34	111.40	116.20
1	A	922	G	C8-N9-C1'	-5.34	120.06	127.00
1	A	310	G	C4-C5-N7	5.33	112.93	110.80
1	A	82	U	N1-C2-O2	5.33	126.53	122.80
1	A	268	C	C6-N1-C2	-5.33	118.17	120.30
1	A	1178	G	N1-C6-O6	-5.33	116.70	119.90
1	A	866	C	C6-N1-C2	5.33	122.43	120.30
1	A	1505	G	C6-C5-N7	-5.33	127.20	130.40
1	A	1529	G	C6-C5-N7	-5.33	127.20	130.40
1	A	763	G	C8-N9-C4	-5.33	104.27	106.40
1	A	922	G	N7-C8-N9	5.33	115.76	113.10
1	A	864	A	N7-C8-N9	-5.32	111.14	113.80
1	A	1215	G	C8-N9-C4	-5.32	104.27	106.40
1	A	860	A	N1-C2-N3	5.32	131.96	129.30
1	A	375	U	N1-C2-N3	5.32	118.09	114.90
1	A	5	U	C5-C6-N1	-5.31	120.04	122.70
1	A	288	A	C8-N9-C4	5.31	107.92	105.80
1	A	877	C	N3-C4-C5	5.31	124.03	121.90
1	A	922	G	N3-C4-N9	5.31	129.19	126.00
1	A	1231	G	N3-C4-C5	5.31	131.26	128.60
1	A	182	U	C5-C6-N1	5.31	125.36	122.70
1	A	1305	G	N1-C6-O6	5.31	123.09	119.90
1	A	259	G	C6-C5-N7	-5.31	127.22	130.40
1	A	1299	A	C8-N9-C1'	-5.31	118.15	127.70
1	A	1390	U	N1-C2-N3	5.31	118.08	114.90
1	A	1491	G	N3-C4-C5	-5.30	125.95	128.60
1	A	788	U	C2-N1-C1'	5.30	124.06	117.70
1	A	637	G	C8-N9-C1'	-5.30	120.11	127.00
1	A	863	U	N3-C4-O4	-5.30	115.69	119.40
1	A	388	G	N3-C4-C5	-5.29	125.95	128.60
1	A	975	A	C5-C6-N1	-5.29	115.05	117.70
1	A	915	A	N9-C4-C5	-5.29	103.69	105.80
1	A	1478	C	C5-C6-N1	5.29	123.64	121.00
1	A	1514	C	N3-C4-C5	5.29	124.02	121.90
1	A	1202	G	N1-C6-O6	-5.29	116.73	119.90
1	A	146	G	N1-C2-N2	5.29	120.96	116.20
1	A	1524	C	C6-N1-C2	-5.29	118.19	120.30
1	A	535	A	C8-N9-C4	5.28	107.91	105.80
1	A	897	C	N3-C4-C5	5.28	124.01	121.90
1	A	1022	G	C4-N9-C1'	5.28	133.37	126.50
1	A	59	A	N1-C6-N6	5.28	121.77	118.60
1	A	228	A	C5-N7-C8	-5.28	101.26	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	693	G	C4-C5-C6	5.28	121.97	118.80
1	A	535	A	N1-C6-N6	5.27	121.76	118.60
1	A	293	G	N3-C2-N2	-5.27	116.21	119.90
1	A	52	G	N1-C2-N3	5.27	127.06	123.90
1	A	624	C	N1-C2-O2	5.27	122.06	118.90
1	A	713	G	N9-C4-C5	5.27	107.51	105.40
1	A	789	U	N3-C4-C5	-5.27	111.44	114.60
1	A	236	G	C4-N9-C1'	5.27	133.35	126.50
1	A	779	C	N1-C2-N3	5.26	122.89	119.20
1	A	872	A	C5-N7-C8	-5.26	101.27	103.90
1	A	555	C	C6-N1-C2	-5.26	118.19	120.30
1	A	305	G	N1-C2-N3	5.26	127.06	123.90
1	A	588	G	C5-C6-N1	-5.26	108.87	111.50
1	A	898	G	C4-C5-N7	-5.26	108.70	110.80
1	A	255	G	N9-C4-C5	-5.25	103.30	105.40
1	A	107	G	C5-C6-O6	-5.25	125.45	128.60
1	A	174	C	N3-C4-C5	5.25	124.00	121.90
1	A	400	C	C5-C6-N1	-5.25	118.37	121.00
1	A	575	G	C2-N3-C4	-5.25	109.27	111.90
1	A	917	G	C6-C5-N7	-5.25	127.25	130.40
1	A	1380	U	C5-C4-O4	5.25	129.05	125.90
1	A	720	C	C2-N1-C1'	5.25	124.58	118.80
1	A	474	G	C8-N9-C4	5.25	108.50	106.40
1	A	1406	U	N3-C4-O4	5.25	123.07	119.40
1	A	1513	A	N1-C2-N3	5.25	131.92	129.30
1	A	1236	A	N1-C6-N6	5.25	121.75	118.60
1	A	1544	U	N3-C4-O4	5.25	123.07	119.40
1	A	851	G	N1-C6-O6	5.24	123.05	119.90
1	A	1251	A	C8-N9-C4	-5.24	103.70	105.80
1	A	368	U	C5-C6-N1	-5.24	120.08	122.70
1	A	1160	G	N3-C4-N9	5.23	129.14	126.00
1	A	129	U	C6-N1-C1'	5.23	128.53	121.20
1	A	926	G	C4-C5-N7	-5.23	108.71	110.80
1	A	171	A	N1-C2-N3	5.23	131.91	129.30
1	A	601	C	C6-N1-C2	5.23	122.39	120.30
1	A	281	G	N3-C4-N9	5.23	129.14	126.00
1	A	818	G	N3-C4-N9	-5.23	122.86	126.00
1	A	1344	C	N3-C4-C5	5.23	123.99	121.90
1	A	1508	G	C4-C5-N7	5.23	112.89	110.80
1	A	1501	C	C2-N3-C4	-5.22	117.29	119.90
1	A	170	U	C5-C6-N1	-5.22	120.09	122.70
1	A	190(C)	C	C2-N1-C1'	5.22	124.54	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1157	A	C5-C6-N6	5.22	127.88	123.70
1	A	653	A	C5-C6-N6	5.22	127.88	123.70
1	A	993	G	C8-N9-C4	-5.22	104.31	106.40
1	A	1379	G	N3-C4-C5	-5.22	125.99	128.60
1	A	145	G	C5-C6-N1	-5.22	108.89	111.50
1	A	771	G	C2-N3-C4	-5.21	109.29	111.90
1	A	249	U	N3-C2-O2	-5.21	118.55	122.20
1	A	588	G	N1-C2-N3	5.21	127.03	123.90
1	A	852	G	N3-C4-N9	-5.21	122.87	126.00
1	A	559	A	C5-C6-N1	5.21	120.31	117.70
1	A	1329	A	C6-C5-N7	-5.21	128.65	132.30
1	A	1329	A	C5-C6-N6	-5.21	119.53	123.70
1	A	154	C	C5-C6-N1	-5.21	118.40	121.00
1	A	296	U	N3-C2-O2	-5.20	118.56	122.20
1	A	613	C	N3-C2-O2	5.20	125.54	121.90
1	A	1190	G	C6-C5-N7	-5.20	127.28	130.40
1	A	277	C	C6-N1-C2	5.20	122.38	120.30
1	A	882	C	C6-N1-C2	-5.20	118.22	120.30
1	A	934	C	C2-N1-C1'	-5.20	113.08	118.80
1	A	1401	G	C6-C5-N7	-5.20	127.28	130.40
5	E	148	VAL	CB-CA-C	-5.20	101.52	111.40
1	A	140	A	N1-C6-N6	5.20	121.72	118.60
1	A	851	G	C4-C5-C6	5.20	121.92	118.80
1	A	80	G	C4-N9-C1'	5.19	133.25	126.50
1	A	928	G	N9-C4-C5	-5.19	103.32	105.40
1	A	888	G	N3-C2-N2	-5.19	116.27	119.90
1	A	108	G	C6-C5-N7	-5.19	127.29	130.40
1	A	32	A	N3-C4-N9	5.19	131.55	127.40
1	A	1039	C	C6-N1-C2	-5.19	118.22	120.30
1	A	917	G	C4-C5-N7	5.19	112.87	110.80
1	A	1199	U	N3-C2-O2	-5.19	118.57	122.20
1	A	291	C	C5-C4-N4	-5.18	116.57	120.20
1	A	584	G	C5-C6-N1	5.18	114.09	111.50
1	A	915	A	C2-N3-C4	-5.18	108.01	110.60
1	A	682	G	C4-N9-C1'	-5.18	119.77	126.50
1	A	791	G	C4-C5-C6	5.18	121.91	118.80
1	A	1525	G	N1-C2-N3	5.18	127.01	123.90
1	A	400	C	N3-C4-C5	5.18	123.97	121.90
1	A	610	G	N1-C6-O6	-5.18	116.79	119.90
1	A	653	A	C8-N9-C4	-5.18	103.73	105.80
1	A	1303	C	C6-N1-C2	5.18	122.37	120.30
1	A	612	C	N3-C4-C5	5.17	123.97	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	485	G	C5-N7-C8	5.17	106.89	104.30
1	A	229	U	C6-N1-C2	-5.17	117.90	121.00
1	A	1240	U	C5-C4-O4	5.17	129.00	125.90
1	A	578	C	C5-C6-N1	-5.17	118.42	121.00
1	A	1443	G	N3-C4-C5	5.17	131.18	128.60
1	A	14	U	C6-N1-C2	-5.16	117.90	121.00
1	A	123	C	C6-N1-C2	-5.16	118.24	120.30
1	A	331	G	N9-C4-C5	-5.16	103.34	105.40
1	A	729	A	C4-C5-C6	5.16	119.58	117.00
1	A	514	C	C6-N1-C2	-5.16	118.24	120.30
1	A	175	C	C5-C6-N1	-5.15	118.42	121.00
1	A	1009	G	C8-N9-C4	-5.15	104.34	106.40
1	A	129	U	N3-C4-C5	-5.15	111.51	114.60
1	A	833	U	N1-C2-N3	5.15	117.99	114.90
1	A	1092	A	C5-N7-C8	-5.15	101.32	103.90
1	A	605	U	N3-C4-C5	-5.15	111.51	114.60
1	A	27	G	C6-C5-N7	-5.15	127.31	130.40
1	A	1529	G	N1-C2-N3	5.15	126.99	123.90
1	A	255	G	C6-C5-N7	-5.15	127.31	130.40
1	A	813	U	C5-C4-O4	-5.15	122.81	125.90
1	A	864	A	C5-N7-C8	5.15	106.47	103.90
1	A	43	C	C4-C5-C6	5.15	119.97	117.40
1	A	1100	C	N3-C2-O2	-5.15	118.30	121.90
1	A	7	G	C6-N1-C2	-5.14	122.01	125.10
1	A	307	C	N3-C4-C5	5.14	123.96	121.90
1	A	407	G	N3-C4-N9	-5.13	122.92	126.00
1	A	1303	C	N1-C2-O2	5.13	121.98	118.90
1	A	659	U	C2-N3-C4	-5.13	123.92	127.00
1	A	406	G	N1-C6-O6	5.13	122.98	119.90
1	A	682	G	C8-N9-C1'	5.13	133.67	127.00
1	A	1398	A	C5-C6-N6	5.13	127.81	123.70
1	A	1446	A	C4-C5-C6	-5.13	114.44	117.00
1	A	147	G	N9-C4-C5	-5.13	103.35	105.40
1	A	569	C	C2-N3-C4	-5.13	117.34	119.90
1	A	253	U	N3-C2-O2	5.12	125.79	122.20
1	A	1156	G	N7-C8-N9	5.12	115.66	113.10
1	A	726	C	C2-N3-C4	-5.12	117.34	119.90
1	A	1067	A	C4-C5-N7	-5.12	108.14	110.70
1	A	875	C	C6-N1-C2	5.12	122.35	120.30
1	A	878	G	N9-C4-C5	-5.12	103.35	105.40
1	A	1392	G	C4-N9-C1'	5.11	133.15	126.50
1	A	576	G	C6-C5-N7	-5.11	127.33	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	521	G	N1-C6-O6	-5.11	116.84	119.90
1	A	1528	U	N1-C2-O2	-5.11	119.22	122.80
1	A	28	G	C4-C5-C6	5.11	121.86	118.80
1	A	780	A	N1-C2-N3	5.10	131.85	129.30
1	A	1442	G	C8-N9-C1'	-5.10	120.37	127.00
1	A	1502	A	N7-C8-N9	5.10	116.35	113.80
1	A	1508	G	C8-N9-C4	-5.10	104.36	106.40
1	A	1376	U	C5-C4-O4	5.10	128.96	125.90
1	A	653	A	N1-C2-N3	5.10	131.85	129.30
1	A	608	A	C2-N3-C4	-5.09	108.05	110.60
1	A	1250	A	C5-C6-N6	5.09	127.77	123.70
1	A	1295	G	N7-C8-N9	5.09	115.64	113.10
1	A	1092	A	C5-C6-N6	-5.08	119.63	123.70
1	A	577	G	N3-C4-C5	5.08	131.14	128.60
1	A	791	G	C4-C5-N7	-5.08	108.77	110.80
1	A	1338	G	C6-N1-C2	-5.08	122.05	125.10
1	A	1343	G	C8-N9-C1'	5.08	133.60	127.00
1	A	1531	A	C4-C5-N7	5.08	113.24	110.70
1	A	147	G	C2-N3-C4	-5.08	109.36	111.90
1	A	505	G	C8-N9-C4	5.08	108.43	106.40
1	A	570	G	C4-N9-C1'	5.08	133.10	126.50
1	A	805	C	C4-C5-C6	-5.08	114.86	117.40
1	A	1512	U	N1-C2-O2	-5.08	119.25	122.80
1	A	93	G	C4-C5-N7	5.07	112.83	110.80
1	A	1059	C	C6-N1-C2	5.07	122.33	120.30
1	A	1417	G	N1-C6-O6	5.07	122.94	119.90
1	A	1531	A	C5-N7-C8	-5.07	101.36	103.90
1	A	48	C	N3-C2-O2	5.07	125.45	121.90
1	A	753	A	C4-C5-N7	-5.07	108.17	110.70
1	A	953	G	N3-C4-C5	-5.07	126.07	128.60
1	A	1542	U	C6-N1-C2	5.07	124.04	121.00
1	A	391	G	N3-C4-C5	-5.06	126.07	128.60
1	A	637	G	N3-C4-N9	5.06	129.04	126.00
1	A	1310	G	N1-C6-O6	5.06	122.94	119.90
1	A	20	G	C8-N9-C4	-5.06	104.38	106.40
1	A	752	G	C4-C5-N7	-5.06	108.78	110.80
1	A	82	U	C6-N1-C2	-5.06	117.97	121.00
1	A	863	U	C2-N1-C1'	-5.06	111.63	117.70
1	A	625	G	C8-N9-C1'	-5.06	120.43	127.00
15	O	23	GLY	N-CA-C	5.06	125.74	113.10
1	A	1238	A	C6-N1-C2	-5.05	115.57	118.60
1	A	232	G	C8-N9-C4	5.05	108.42	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1343	G	N9-C4-C5	5.05	107.42	105.40
1	A	820	U	N1-C2-N3	5.05	117.93	114.90
1	A	882	C	C2-N3-C4	-5.05	117.38	119.90
1	A	1378	C	C5-C6-N1	5.05	123.52	121.00
1	A	29	G	C2-N3-C4	-5.04	109.38	111.90
1	A	823	G	C5-C6-N1	5.04	114.02	111.50
5	E	69	VAL	CB-CA-C	-5.04	101.82	111.40
1	A	230	G	N1-C2-N2	-5.04	111.66	116.20
1	A	645	C	C2-N1-C1'	5.04	124.34	118.80
1	A	273	A	C8-N9-C4	-5.04	103.78	105.80
1	A	821	G	N7-C8-N9	-5.04	110.58	113.10
1	A	484	G	P-O3'-C3'	5.03	125.74	119.70
1	A	1379	G	C2-N3-C4	5.03	114.42	111.90
1	A	1489	G	N7-C8-N9	5.03	115.61	113.10
1	A	569	C	C6-N1-C2	5.03	122.31	120.30
1	A	363	A	C2-N3-C4	-5.03	108.09	110.60
1	A	1254	C	C6-N1-C2	-5.03	118.29	120.30
1	A	232	G	C6-N1-C2	5.03	128.12	125.10
1	A	238	G	C8-N9-C4	-5.03	104.39	106.40
1	A	659	U	C5-C6-N1	-5.02	120.19	122.70
1	A	388	G	C4-N9-C1'	5.02	133.02	126.50
1	A	597	G	N3-C4-N9	5.01	129.01	126.00
1	A	872	A	N7-C8-N9	5.01	116.31	113.80
1	A	264	U	N3-C2-O2	-5.01	118.69	122.20
1	A	117	G	C4-C5-N7	5.01	112.80	110.80
1	A	953	G	C8-N9-C1'	-5.01	120.49	127.00
1	A	1310	G	C8-N9-C1'	-5.01	120.49	127.00
1	A	29	G	N1-C6-O6	5.01	122.90	119.90
1	A	970	C	N3-C4-N4	-5.01	114.50	118.00
1	A	316	G	N3-C4-N9	5.00	129.00	126.00
1	A	820	U	N1-C2-O2	-5.00	119.30	122.80
1	A	821	G	N1-C2-N3	5.00	126.90	123.90
1	A	20	G	N3-C4-N9	-5.00	123.00	126.00
19	S	6	LYS	N-CA-C	5.00	124.50	111.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	166	GLU	Peptide
3	C	179	ARG	Peptide
8	H	90	GLY	Peptide

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Mol	Chain	Res	Type	Group
10	J	86	MET	Peptide
12	L	87	GLY	Peptide
20	T	93	GLU	Peptide

## 5.2 Too-close contacts [i](#)

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	32647	0	16508	762	0
2	B	1900	0	1951	80	0
3	C	1612	0	1677	81	0
4	D	1703	0	1763	91	0
5	E	1146	0	1207	63	0
6	F	843	0	857	44	0
7	G	1257	0	1296	53	0
8	H	1116	0	1177	73	0
9	I	1010	0	1037	68	0
10	J	792	0	835	52	0
11	K	864	0	881	36	0
12	L	972	0	1058	65	0
13	M	937	0	995	50	0
14	N	492	0	529	30	0
15	O	729	0	768	41	0
16	P	700	0	720	36	0
17	Q	823	0	893	43	0
18	R	574	0	644	27	0
19	S	647	0	673	20	0
20	T	763	0	861	52	0
21	U	208	0	221	11	0
22	A	262	0	0	0	0
22	B	3	0	0	0	0
22	C	1	0	0	0	0
22	D	2	0	0	0	0
22	E	1	0	0	0	0
22	F	1	0	0	0	0
22	J	2	0	0	0	0
22	M	1	0	0	0	0
22	P	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	Q	1	0	0	0	0
22	S	1	0	0	0	0
23	D	1	0	0	0	0
23	N	1	0	0	0	0
24	A	397	0	0	11	0
24	D	1	0	0	0	0
24	E	4	0	0	0	0
24	G	4	0	0	0	0
24	I	1	0	0	0	0
24	J	3	0	0	1	0
24	L	1	0	0	0	0
24	M	8	0	0	3	0
24	N	1	0	0	1	0
24	P	10	0	0	4	0
24	Q	2	0	0	0	0
24	S	2	0	0	0	0
24	T	5	0	0	1	0
All	All	52453	0	36551	1587	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 18.

All (1587) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1377:A:HO2'	7:G:2:ALA:N	1.58	1.00
1:A:481:G:HO2'	1:A:482:A:H8	1.06	0.96
13:M:10:PRO:HB2	13:M:18:ALA:HB1	1.48	0.96
1:A:103:C:OP1	20:T:17:ARG:NH1	2.01	0.93
8:H:83:ILE:HG12	8:H:137:VAL:HG22	1.52	0.90
1:A:1144:G:N2	1:A:1145:C:O2	2.05	0.89
1:A:1338:G:H2'	1:A:1339:A:C8	2.07	0.89
20:T:100:ILE:HG22	20:T:102:GLY:H	1.39	0.87
6:F:23:LYS:NZ	6:F:42:GLU:OE2	2.08	0.86
1:A:1368:G:H5''	9:I:112:LYS:HB3	1.57	0.85
7:G:69:VAL:HG23	7:G:135:VAL:HG22	1.56	0.85
21:U:10:ARG:HD3	21:U:13:ILE:HD12	1.58	0.84
1:A:1195:C:H3'	1:A:1196:U:H5''	1.60	0.83
1:A:1417:G:O2'	1:A:1483:A:N6	2.11	0.83
1:A:1152:A:OP1	10:J:68:HIS:ND1	2.11	0.83
13:M:34:LEU:HD12	13:M:41:PRO:HA	1.61	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1326:C:OP2	21:U:6:ARG:NH2	2.12	0.83
18:R:58:LEU:HB3	18:R:62:GLU:HB3	1.59	0.82
1:A:263:A:OP2	20:T:79:ARG:NH1	2.11	0.82
8:H:64:LYS:HG2	8:H:79:VAL:HG21	1.61	0.82
3:C:6:HIS:CD2	3:C:9:GLY:H	1.98	0.81
15:O:70:LEU:HB3	15:O:78:TYR:HB2	1.63	0.81
12:L:87:GLY:HA2	12:L:98:TYR:HA	1.63	0.81
1:A:1316:G:N2	1:A:1319:A:OP2	2.14	0.80
2:B:91:PRO:HG3	2:B:154:LEU:HB2	1.62	0.80
7:G:5:ARG:HG3	7:G:7:ALA:H	1.47	0.80
12:L:47:LYS:HG3	12:L:48:PRO:HD3	1.63	0.80
6:F:22:GLU:OE1	6:F:82:ARG:NH1	2.15	0.80
1:A:1243:C:H42	1:A:1294:G:H1	1.27	0.79
11:K:82:VAL:HG11	11:K:95:ILE:HD11	1.64	0.79
11:K:57:THR:HG23	11:K:60:ALA:H	1.48	0.78
15:O:8:LYS:HE3	15:O:31:LEU:HD21	1.66	0.78
10:J:47:PHE:HB3	14:N:34:TYR:HE2	1.48	0.78
1:A:1191:A:H5''	3:C:4:LYS:HE3	1.66	0.78
12:L:89:ARG:HG2	12:L:97:ARG:HA	1.66	0.78
5:E:11:ILE:HB	5:E:31:LEU:HB3	1.65	0.77
1:A:738:C:OP2	6:F:92:LYS:NZ	2.18	0.77
1:A:384:G:H2'	1:A:385:C:C6	2.19	0.77
1:A:1057:G:H5''	3:C:154:SER:HB2	1.67	0.77
1:A:1404:5MC:H1'	1:A:1499:A:C2	2.20	0.77
1:A:1406:U:O2'	1:A:1517[B]:G:N2	2.17	0.76
1:A:1004:A:O2'	1:A:1005:A:OP1	2.04	0.76
1:A:1240:U:OP1	7:G:119:ARG:NH2	2.17	0.76
1:A:1435:G:H2'	1:A:1436:U:C6	2.19	0.76
4:D:155:LEU:HD23	4:D:157:LEU:H	1.51	0.76
1:A:1426:C:H42	1:A:1474:G:H1	1.30	0.76
11:K:72:ALA:HB1	11:K:77:MET:HG3	1.66	0.76
10:J:61:GLU:OE1	14:N:45:ARG:NH1	2.19	0.76
1:A:279:A:OP2	17:Q:95:TYR:OH	2.04	0.76
1:A:1202:G:C4	14:N:42:ILE:HD12	2.20	0.75
5:E:17:ALA:HA	5:E:26:PHE:HB3	1.67	0.75
1:A:298:A:N6	24:A:2036:HOH:O	2.16	0.75
2:B:223:ILE:HG22	2:B:228:GLY:HA3	1.69	0.74
1:A:115:G:O2'	1:A:116:A:OP2	2.06	0.74
1:A:677:U:H3	1:A:713:G:H22	1.35	0.74
1:A:1414:U:H2'	1:A:1415:G:H8	1.51	0.74
1:A:130:A:H5'	17:Q:63:ARG:HE	1.51	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:74:LEU:HD13	16:P:79:VAL:HG21	1.69	0.74
3:C:174:PRO:HB2	3:C:177:THR:HG22	1.70	0.73
8:H:2:LEU:HD23	8:H:3:THR:N	2.02	0.73
1:A:1278:U:H5'	1:A:1279:A:H5'	1.69	0.73
2:B:24:TRP:CZ3	2:B:26:PRO:HA	2.23	0.73
7:G:16:LEU:HD21	9:I:45:ALA:HB2	1.70	0.73
1:A:217:C:H2'	1:A:218:C:H6	1.53	0.73
1:A:411:A:H62	1:A:413:G:H21	1.33	0.73
4:D:64:LEU:HD23	4:D:198:VAL:HG21	1.68	0.73
1:A:337:C:H2'	1:A:338:A:H8	1.54	0.72
10:J:19:SER:HB2	10:J:91:PRO:HG2	1.71	0.72
1:A:1376:U:OP1	7:G:98:SER:OG	2.06	0.72
2:B:157:ARG:HG3	2:B:158:LEU:HD12	1.71	0.72
1:A:190(E):U:O2'	17:Q:63:ARG:NH2	2.23	0.72
3:C:150:LYS:HB3	3:C:201:TYR:HB2	1.69	0.72
14:N:47:LEU:HB3	14:N:53:LEU:HD21	1.70	0.72
2:B:73:THR:HG21	2:B:96:ARG:HD3	1.72	0.72
1:A:1128:C:O2'	1:A:1130:A:N7	2.23	0.72
1:A:1366:C:O2'	10:J:60:ARG:NH2	2.21	0.72
1:A:584:G:OP2	17:Q:87:LYS:NZ	2.17	0.72
4:D:78:LEU:HD21	4:D:96:LEU:HB3	1.72	0.72
1:A:84:U:H2'	1:A:88:A:H8	1.55	0.71
1:A:1441:G:H5''	1:A:1442:G:H5'	1.72	0.71
1:A:918:A:H2'	1:A:919:A:C8	2.25	0.71
15:O:74:ASP:HB2	15:O:77:ARG:HH21	1.53	0.71
10:J:61:GLU:HA	24:J:303:HOH:O	1.90	0.71
12:L:27:LEU:O	12:L:29:GLY:N	2.23	0.71
7:G:70:LYS:O	7:G:72:ARG:NH1	2.23	0.71
9:I:24:GLY:HA3	9:I:56:LEU:HD23	1.72	0.71
1:A:1300:G:OP2	1:A:1335:C:N4	2.24	0.71
2:B:98:LEU:HB2	2:B:101:MET:HG3	1.72	0.71
12:L:9:GLN:HA	12:L:12:ARG:HG3	1.73	0.71
1:A:262:A:H5'	20:T:74:LYS:HD3	1.73	0.71
13:M:4:ILE:HG23	13:M:57:ARG:HA	1.74	0.70
17:Q:40:LYS:HD3	17:Q:42:TYR:CZ	2.26	0.70
1:A:1143:G:H2'	1:A:1144:G:H8	1.55	0.70
1:A:390:C:O3'	16:P:28:ARG:NH2	2.25	0.70
1:A:184:G:H2'	1:A:185:A:H8	1.54	0.70
15:O:6:GLU:OE2	15:O:6:GLU:N	2.25	0.70
20:T:83:ARG:NH2	24:T:203:HOH:O	2.25	0.70
1:A:935:A:N6	7:G:3:ARG:HG3	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:83:VAL:HG23	12:L:107:ALA:HB2	1.75	0.69
14:N:24:CYS:HB2	14:N:39:LEU:HA	1.74	0.69
1:A:1225:A:N3	1:A:1225:A:H2'	2.07	0.69
1:A:839:U:H5'	1:A:840:C:C5	2.27	0.69
1:A:946:A:H2'	1:A:947:G:C8	2.27	0.69
2:B:167:PRO:HG2	2:B:192:SER:HB2	1.74	0.69
5:E:75:THR:OG1	5:E:76:ILE:N	2.25	0.69
1:A:1347:G:O2'	1:A:1348:U:OP2	2.07	0.69
2:B:178:ARG:NH1	2:B:198:ASP:OD2	2.23	0.69
5:E:100:VAL:HG12	5:E:118:ILE:HG22	1.73	0.69
1:A:337:C:H2'	1:A:338:A:C8	2.28	0.69
6:F:42:GLU:OE1	6:F:59:TYR:OH	2.11	0.69
1:A:1347:G:H3'	9:I:108:VAL:O	1.92	0.69
1:A:411:A:H62	1:A:413:G:N2	1.91	0.69
3:C:36:ASP:HA	3:C:39:ILE:HD12	1.75	0.69
12:L:57:LYS:HD3	12:L:67:THR:HG23	1.74	0.69
3:C:130:VAL:HG12	3:C:134:ILE:HD11	1.76	0.68
1:A:250:A:H4'	1:A:251:G:O5'	1.92	0.68
11:K:120:ARG:HG2	11:K:120:ARG:HH11	1.57	0.68
1:A:1498:UR3:O4'	1:A:1519[A]:MA6:H2	1.94	0.68
4:D:163:GLU:HG2	4:D:166:LYS:HE3	1.75	0.68
9:I:42:ARG:NH2	9:I:71:SER:OG	2.26	0.68
1:A:962:C:O2'	24:A:2118:HOH:O	2.11	0.68
1:A:113:G:H1'	1:A:354:G:H5'	1.75	0.68
4:D:57:ARG:HG3	4:D:202:LEU:HD13	1.74	0.68
8:H:36:LEU:HA	8:H:39:LEU:HD12	1.75	0.68
1:A:1133:G:H1	1:A:1141:C:H42	1.41	0.67
3:C:137:ALA:HA	3:C:140:ARG:HD2	1.76	0.67
1:A:933:G:O6	7:G:3:ARG:NH2	2.27	0.67
1:A:1347:G:N2	1:A:1373:G:H2'	2.10	0.67
2:B:178:ARG:HD3	2:B:196:LEU:HD22	1.76	0.67
1:A:1474:G:H2'	1:A:1475:G:H8	1.60	0.67
1:A:129(A):G:N3	1:A:190(E):U:H5''	2.10	0.67
3:C:58:GLU:HB3	10:J:92:THR:HG21	1.76	0.67
10:J:50:ILE:H	10:J:50:ILE:HD12	1.59	0.67
1:A:1124:G:N2	1:A:1126:U:O4	2.28	0.67
1:A:551:U:O2'	12:L:86:ARG:HD2	1.95	0.67
2:B:60:ASP:O	2:B:64:ARG:NH1	2.28	0.67
1:A:1065:U:H5''	1:A:1190:G:N2	2.10	0.66
1:A:1305:G:N2	1:A:1331:G:H1'	2.10	0.66
1:A:1029:C:N3	1:A:1033:G:N2	2.44	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:C:O2'	1:A:621:A:N3	2.23	0.66
1:A:36:C:OP1	12:L:123:LYS:NZ	2.29	0.66
3:C:42:LEU:HD12	3:C:94:LEU:HD13	1.76	0.66
5:E:109:ILE:HG22	5:E:110:LEU:HD23	1.78	0.66
1:A:633:G:H2'	1:A:634:C:C6	2.31	0.66
8:H:6:ILE:HB	8:H:85:ARG:NH2	2.11	0.66
10:J:6:ILE:HB	10:J:72:VAL:HB	1.75	0.66
13:M:117:VAL:HG12	13:M:118:ALA:H	1.61	0.66
1:A:1310:G:OP1	13:M:77:ASN:ND2	2.27	0.66
1:A:1250:A:H2'	1:A:1251:A:C8	2.30	0.66
3:C:152:ILE:HB	3:C:199:LYS:HB2	1.78	0.66
1:A:1267:C:N3	1:A:1327:C:O2'	2.29	0.66
1:A:664:G:H22	1:A:741:G:H1	1.43	0.66
1:A:957:U:O2'	1:A:959:A:N7	2.27	0.66
1:A:1504:G:OP1	1:A:1507:A:H4'	1.96	0.66
4:D:3:ARG:HH22	4:D:100:ARG:NH2	1.94	0.66
11:K:18:ARG:HG3	11:K:33:THR:HG23	1.78	0.66
9:I:89:ASN:O	9:I:92:TYR:HB2	1.96	0.66
13:M:4:ILE:HD13	13:M:56:LEU:HB3	1.77	0.65
15:O:26:GLU:HA	15:O:81:LEU:HD11	1.78	0.65
1:A:1028:C:H42	1:A:1033:G:H22	1.42	0.65
1:A:1241:G:H2'	1:A:1242:C:H6	1.61	0.65
7:G:108:ALA:O	7:G:119:ARG:HB3	1.96	0.65
15:O:36:ILE:HD13	15:O:59:MET:HE3	1.79	0.65
19:S:11:VAL:HG12	19:S:15:LEU:HD11	1.78	0.65
12:L:25:PRO:C	12:L:27:LEU:H	1.95	0.65
1:A:1300:G:O2'	1:A:1301:U:P	2.55	0.65
8:H:51:VAL:HG11	8:H:60:ARG:HG3	1.78	0.65
1:A:99:C:H2'	1:A:101:A:C8	2.31	0.65
2:B:240:GLN:N	2:B:240:GLN:OE1	2.30	0.65
6:F:80:ARG:NH2	6:F:88:VAL:O	2.30	0.65
5:E:122:GLU:O	5:E:126:ARG:NH1	2.29	0.65
16:P:2:VAL:O	16:P:64:ALA:HA	1.97	0.65
1:A:767:A:H2'	1:A:768:A:O4'	1.97	0.64
1:A:707:C:H4'	11:K:20:TYR:CD1	2.31	0.64
14:N:23:ARG:HA	14:N:29:ARG:O	1.96	0.64
14:N:6:LEU:HD12	14:N:23:ARG:HH21	1.63	0.64
1:A:992:U:O2'	1:A:993:G:OP2	2.11	0.64
3:C:167:TRP:HE3	3:C:168:ALA:H	1.46	0.64
11:K:33:THR:HB	11:K:39:PRO:HA	1.78	0.64
8:H:10:LEU:HD22	8:H:83:ILE:HD13	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1391:U:H2'	1:A:1392:G:C8	2.33	0.64
3:C:150:LYS:HG3	3:C:169:ALA:HB2	1.78	0.64
9:I:3:GLN:OE1	9:I:20:ARG:NH2	2.30	0.64
10:J:48:THR:HA	10:J:62:HIS:HB3	1.79	0.64
1:A:1347:G:HO2'	1:A:1373:G:H1	1.44	0.64
2:B:24:TRP:HZ3	2:B:29:ALA:HB2	1.63	0.64
1:A:1198:G:H2'	1:A:1199:U:C6	2.33	0.64
1:A:1520[A]:G:H2'	1:A:1521:G:H8	1.63	0.64
4:D:13:ARG:HD2	4:D:38:TYR:O	1.98	0.64
4:D:8:VAL:O	4:D:11:LEU:N	2.29	0.64
7:G:27:ILE:HA	7:G:30:ILE:HD12	1.79	0.64
8:H:17:THR:HB	8:H:78:GLN:HE22	1.63	0.64
1:A:1301:U:O2'	1:A:1302:U:O5'	2.12	0.64
1:A:427:U:OP1	4:D:13:ARG:NH2	2.30	0.64
1:A:1343:G:H1'	9:I:121:ARG:HH12	1.63	0.64
9:I:20:ARG:HB2	9:I:20:ARG:HH11	1.62	0.64
17:Q:29:HIS:CG	17:Q:30:PRO:HD2	2.32	0.64
20:T:70:SER:HA	20:T:73:HIS:CD2	2.32	0.64
1:A:81:U:H6	1:A:83:U:OP2	1.81	0.64
11:K:84:VAL:HG11	11:K:91:ARG:HD3	1.80	0.64
13:M:115:LYS:H	13:M:115:LYS:HD3	1.63	0.64
1:A:748:C:H4'	1:A:749:C:O5'	1.98	0.63
13:M:34:LEU:HD13	13:M:39:ILE:HD13	1.79	0.63
1:A:839:U:H5'	1:A:840:C:H5	1.62	0.63
12:L:85:ILE:CG2	12:L:98:TYR:HB3	2.28	0.63
13:M:14:ARG:HE	13:M:42:ALA:HA	1.62	0.63
1:A:329:A:H5''	24:A:2232:HOH:O	1.98	0.63
3:C:88:ARG:HA	3:C:91:LEU:HD22	1.81	0.63
2:B:69:LEU:HD12	2:B:155:LEU:HD11	1.81	0.63
6:F:95:GLU:HG3	6:F:96:PRO:HD2	1.79	0.63
15:O:26:GLU:OE1	15:O:77:ARG:HD2	1.98	0.63
6:F:70:ASP:N	6:F:70:ASP:OD1	2.32	0.63
1:A:1300:G:H4'	1:A:1301:U:H5'	1.80	0.63
1:A:673:G:H2'	1:A:674:G:C8	2.33	0.63
3:C:26:LYS:HD2	3:C:26:LYS:H	1.62	0.63
1:A:217:C:H2'	1:A:218:C:C6	2.33	0.63
1:A:512:U:O2	1:A:540:G:N2	2.31	0.63
7:G:152:ALA:O	7:G:155:ARG:HG2	1.99	0.63
1:A:1379:G:OP2	7:G:6:ARG:NH2	2.31	0.63
2:B:142:LEU:HD13	2:B:146:GLN:NE2	2.14	0.63
2:B:7:VAL:HG21	2:B:221:LEU:HD23	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:179:ARG:HG3	3:C:179:ARG:HH11	1.64	0.63
1:A:130:A:H1'	1:A:263:A:O2'	1.99	0.62
16:P:21:VAL:O	16:P:33:ILE:HG12	1.99	0.62
3:C:156:ARG:NE	3:C:160:ALA:O	2.28	0.62
1:A:1119:C:H42	1:A:1154:G:H1	1.47	0.62
2:B:97:TRP:CH2	2:B:101:MET:HB2	2.35	0.62
1:A:166:G:H5''	1:A:167:G:OP2	1.98	0.62
4:D:25:ARG:HH21	4:D:30:LYS:HD3	1.64	0.62
20:T:27:LYS:HA	20:T:30:LYS:HE3	1.80	0.62
4:D:68:TYR:CE2	4:D:97:LEU:HB3	2.33	0.62
1:A:1505:G:H3'	1:A:1505:G:C8	2.34	0.62
1:A:951:G:OP2	13:M:102:ARG:NH1	2.33	0.62
4:D:22:LYS:HB2	4:D:26:CYS:SG	2.40	0.62
1:A:1225:A:H5'	1:A:1226:C:OP2	1.99	0.62
1:A:1435:G:H2'	1:A:1436:U:H6	1.62	0.62
2:B:167:PRO:HG2	2:B:192:SER:CB	2.30	0.62
4:D:55:ALA:O	4:D:59:ARG:HG2	1.99	0.62
18:R:40:LEU:HD11	18:R:69:THR:HG22	1.80	0.62
1:A:1158:C:N3	1:A:1181:G:N2	2.43	0.62
3:C:179:ARG:HD3	3:C:206:GLU:HG3	1.82	0.62
6:F:99:ALA:HB2	18:R:31:LEU:HD12	1.82	0.62
1:A:77:G:H2'	1:A:78:G:H8	1.65	0.61
6:F:6:VAL:HG13	6:F:90:VAL:HG22	1.82	0.61
1:A:1347:G:O2'	1:A:1348:U:P	2.58	0.61
2:B:97:TRP:HH2	2:B:102:LEU:HD22	1.65	0.61
3:C:131:ARG:HA	3:C:134:ILE:HD12	1.81	0.61
3:C:180:ALA:HB1	3:C:203:PHE:CE1	2.35	0.61
3:C:180:ALA:HB1	3:C:203:PHE:HE1	1.64	0.61
1:A:949:A:OP1	13:M:101:GLN:HB3	2.00	0.61
1:A:77:G:H2'	1:A:78:G:C8	2.34	0.61
16:P:19:ILE:HG22	16:P:36:ILE:HG13	1.82	0.61
1:A:902:G:H2'	1:A:903:G:H8	1.66	0.61
3:C:164:ARG:HG2	3:C:165:THR:H	1.64	0.61
1:A:1049:U:H4'	1:A:1050:G:O5'	2.00	0.61
1:A:84:U:H2'	1:A:88:A:C8	2.34	0.61
7:G:38:LEU:O	7:G:42:ILE:HG13	1.99	0.61
11:K:81:ASP:OD1	11:K:106:LYS:HD3	2.00	0.61
1:A:939:G:H5''	7:G:102:ARG:HH12	1.65	0.61
1:A:1414:U:H3	1:A:1486:G:H1	1.47	0.61
2:B:16:HIS:ND1	2:B:210:SER:HB2	2.15	0.61
1:A:1188:A:H5''	24:A:2229:HOH:O	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:5:ARG:HA	10:J:73:ASP:OD1	2.01	0.61
11:K:80:VAL:HG21	11:K:103:LEU:HD13	1.81	0.61
1:A:518:C:H1'	12:L:50:SER:HB3	1.83	0.61
1:A:1392:G:H21	1:A:1502:A:H8	1.47	0.60
1:A:973:G:H3'	1:A:974:A:H5''	1.81	0.60
8:H:127:LEU:HB3	8:H:129:VAL:HG23	1.83	0.60
1:A:129:U:O3'	1:A:129(A):G:H3'	2.01	0.60
1:A:1511:G:H2'	1:A:1512:U:O4'	2.01	0.60
5:E:105:VAL:HG11	5:E:131:ILE:HG22	1.83	0.60
1:A:1087:G:N2	1:A:1099:G:H1'	2.17	0.60
1:A:1213:A:N6	1:A:1215:G:N3	2.49	0.60
1:A:1356:G:H2'	1:A:1357:A:C8	2.37	0.60
1:A:5:U:H4'	1:A:6:G:O5'	2.01	0.60
8:H:4:ASP:OD2	8:H:85:ARG:NH1	2.34	0.60
19:S:33:THR:HG22	19:S:35:SER:H	1.65	0.60
1:A:970:C:OP1	10:J:57:LYS:NZ	2.34	0.60
6:F:80:ARG:HH12	6:F:88:VAL:H	1.49	0.60
16:P:74:LEU:O	16:P:79:VAL:HG23	2.00	0.60
8:H:114:THR:HG22	8:H:130:GLY:O	2.02	0.60
9:I:26:VAL:HG13	9:I:61:ALA:HB3	1.82	0.60
1:A:954:G:N2	1:A:1228:C:N3	2.50	0.60
9:I:111:ARG:NH1	9:I:112:LYS:O	2.35	0.60
1:A:1218:C:H2'	1:A:1219:U:C6	2.37	0.60
1:A:413:G:H2'	1:A:428:G:N2	2.17	0.60
1:A:1342:C:H2'	1:A:1343:G:C8	2.36	0.60
1:A:81:U:H2'	1:A:83:U:OP2	2.01	0.60
1:A:916:G:H2'	1:A:917:G:H8	1.65	0.60
4:D:3:ARG:CG	4:D:118:ARG:HH11	2.13	0.60
5:E:74:GLY:HA3	5:E:116:THR:HG22	1.84	0.60
1:A:1379:G:N7	7:G:2:ALA:HB3	2.17	0.60
9:I:118:LYS:O	9:I:120:ARG:N	2.32	0.60
9:I:50:LEU:HB3	9:I:55:ALA:HB3	1.83	0.60
1:A:1498:UR3:O2'	1:A:1499:A:OP2	2.10	0.60
1:A:264:U:H2'	1:A:265:G:O4'	2.02	0.60
6:F:50:TYR:HE1	18:R:77:GLY:HA2	1.67	0.60
1:A:1227:A:O3'	13:M:115:LYS:HE2	2.02	0.59
1:A:1301:U:HO2'	1:A:1302:U:P	2.25	0.59
16:P:74:LEU:HB3	16:P:79:VAL:HG21	1.84	0.59
1:A:19:C:H2'	1:A:20:G:H8	1.67	0.59
10:J:7:LYS:HG3	10:J:71:LEU:HD13	1.83	0.59
12:L:27:LEU:C	12:L:29:GLY:H	2.06	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:707:C:H2'	1:A:708:C:C6	2.37	0.59
8:H:120:THR:HG23	8:H:123:GLU:CD	2.23	0.59
6:F:50:TYR:CE1	18:R:77:GLY:HA2	2.38	0.59
1:A:1070:U:H2'	1:A:1071:C:H6	1.68	0.59
1:A:946:A:H2'	1:A:947:G:H8	1.67	0.59
12:L:46:LYS:HG2	12:L:47:LYS:HG2	1.84	0.59
1:A:1076:C:OP1	2:B:179:LYS:NZ	2.36	0.59
1:A:1300:G:O2'	1:A:1301:U:OP2	2.18	0.59
1:A:1399:C:H4'	1:A:1400:5MC:H5''	1.83	0.59
2:B:124:SER:HB2	2:B:126:GLU:HB2	1.84	0.59
15:O:56:LEU:O	15:O:60:VAL:HG23	2.03	0.59
1:A:1414:U:H2'	1:A:1415:G:C8	2.37	0.59
1:A:1520[B]:G:H2'	1:A:1521:G:H8	1.67	0.59
1:A:665:A:H1'	1:A:733:A:O4'	2.02	0.59
11:K:92:GLU:HB3	11:K:96:ARG:HH21	1.66	0.59
1:A:1125:U:OP2	1:A:1145:C:N4	2.35	0.59
7:G:139:GLU:O	7:G:143:ARG:HB2	2.03	0.59
8:H:97:VAL:HG23	8:H:129:VAL:O	2.03	0.59
1:A:1349:A:OP1	9:I:120:ARG:HB2	2.03	0.59
1:A:1490:C:H5'	1:A:1491:G:OP2	2.02	0.59
1:A:935:A:H61	7:G:3:ARG:HG3	1.68	0.59
1:A:939:G:H5''	7:G:102:ARG:NH1	2.18	0.59
9:I:50:LEU:HD11	9:I:81:ILE:HD13	1.84	0.59
13:M:96:LEU:HB3	13:M:97:PRO:HD2	1.84	0.59
18:R:59:SER:H	18:R:62:GLU:HB2	1.68	0.59
1:A:1342:C:H2'	1:A:1343:G:H8	1.67	0.58
20:T:20:LEU:O	20:T:23:ARG:HB3	2.03	0.58
1:A:928:G:H1	1:A:1389:C:H42	1.51	0.58
1:A:1510:U:H2'	1:A:1511:G:C8	2.37	0.58
2:B:25:ASN:O	2:B:27:LYS:N	2.35	0.58
12:L:53:ARG:HH11	12:L:93:LEU:HD21	1.69	0.58
1:A:1070:U:H2'	1:A:1071:C:C6	2.38	0.58
1:A:1488:G:H2'	1:A:1489:G:H8	1.69	0.58
2:B:187:LEU:HA	2:B:201:ILE:HG13	1.83	0.58
8:H:25:ASP:OD1	8:H:25:ASP:N	2.35	0.58
1:A:112:G:O2'	1:A:113:G:H5'	2.04	0.58
1:A:1143:G:H2'	1:A:1144:G:C8	2.38	0.58
9:I:86:VAL:HG21	9:I:102:LEU:HD11	1.86	0.58
1:A:1195:C:H3'	1:A:1196:U:C5'	2.32	0.58
1:A:836:G:C6	1:A:851:G:C6	2.92	0.58
4:D:3:ARG:HG2	4:D:118:ARG:HH11	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:952:U:H2'	1:A:953:G:H8	1.67	0.58
15:O:85:LEU:HD23	15:O:85:LEU:N	2.18	0.58
15:O:87:ILE:HG22	15:O:88:ARG:HD3	1.84	0.58
1:A:1488:G:H2'	1:A:1489:G:C8	2.39	0.58
1:A:281:G:O2'	1:A:282:A:OP2	2.15	0.58
1:A:527:7MG:H5''	1:A:527:7MG:C8	2.38	0.58
14:N:26:ARG:HD3	14:N:47:LEU:HD21	1.86	0.58
5:E:98:THR:N	5:E:117:ASP:OD1	2.36	0.58
1:A:656:C:O2'	15:O:28:GLN:NE2	2.31	0.58
11:K:43:SER:HA	11:K:47:VAL:HG21	1.85	0.58
1:A:411:A:N7	1:A:413:G:N3	2.51	0.57
1:A:1497:G:C2'	1:A:1498:UR3:H5'	2.35	0.57
1:A:1145:C:O2'	1:A:1146:A:O5'	2.22	0.57
1:A:1305:G:H22	1:A:1331:G:H1'	1.69	0.57
15:O:18:PHE:CE2	15:O:21:ASP:HB2	2.39	0.57
10:J:3:LYS:N	10:J:75:ILE:HG23	2.19	0.57
10:J:52:GLY:O	14:N:41:ARG:NH2	2.37	0.57
11:K:27:ASN:OD1	11:K:28:THR:N	2.33	0.57
1:A:1452:C:H4'	1:A:1453:G:O5'	2.05	0.57
17:Q:62:SER:OG	17:Q:72:ARG:HG2	2.05	0.57
1:A:1441:G:O2'	1:A:1442:G:N2	2.38	0.57
1:A:1497:G:H2'	1:A:1498:UR3:H5'	1.86	0.57
12:L:24:VAL:HG13	12:L:98:TYR:CE2	2.39	0.57
15:O:11:VAL:HG21	15:O:34:LEU:HD12	1.87	0.57
1:A:411:A:C8	1:A:413:G:H1'	2.39	0.57
3:C:174:PRO:O	3:C:177:THR:HG22	2.05	0.57
1:A:448:A:P	1:A:485:G:H22	2.27	0.57
1:A:576:G:N2	24:A:2214:HOH:O	2.38	0.57
1:A:757:U:H2'	1:A:758:G:O4'	2.04	0.57
3:C:47:LEU:HD22	3:C:52:LEU:HD13	1.87	0.57
5:E:93:PRO:HD2	8:H:105:ARG:NH2	2.19	0.57
12:L:19:ARG:HA	12:L:20:LYS:NZ	2.19	0.57
1:A:1192:C:O2	5:E:25:ARG:NH2	2.38	0.57
1:A:1299:A:O2'	1:A:1300:G:O5'	2.20	0.57
1:A:80:G:H3'	1:A:81:U:H5''	1.86	0.57
3:C:141:VAL:HG11	3:C:202:ILE:HD12	1.87	0.57
12:L:36:VAL:O	12:L:58:VAL:HG13	2.05	0.57
1:A:1412:C:H2'	1:A:1413:A:C8	2.40	0.56
1:A:1371:G:O3'	9:I:69:GLY:HA3	2.05	0.56
1:A:1366:C:H2'	1:A:1367:C:H6	1.70	0.56
6:F:27:GLN:O	6:F:31:GLU:HG3	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:19:ILE:HD12	16:P:38:TYR:N	2.20	0.56
1:A:1248:A:H2'	1:A:1249:C:H6	1.70	0.56
1:A:164:U:H2'	1:A:165:C:C6	2.40	0.56
9:I:118:LYS:O	9:I:118:LYS:HD3	2.05	0.56
10:J:51:ARG:HG3	10:J:59:SER:O	2.05	0.56
12:L:97:ARG:HB2	12:L:98:TYR:CE1	2.40	0.56
20:T:63:ILE:HG21	20:T:81:LYS:HG3	1.86	0.56
1:A:1391:U:H2'	1:A:1392:G:H8	1.71	0.56
1:A:1465:C:H2'	1:A:1466:C:O4'	2.05	0.56
1:A:76:C:H42	1:A:95:U:H3	1.53	0.56
10:J:24:VAL:HG13	10:J:34:VAL:HG11	1.87	0.56
1:A:372:C:H4'	1:A:373:A:O5'	2.05	0.56
1:A:445:G:H2'	1:A:446:G:H8	1.70	0.56
1:A:859:A:OP2	1:A:869:G:N1	2.30	0.56
2:B:88:ALA:HB2	2:B:219:VAL:HG13	1.86	0.56
1:A:129(A):G:C2	1:A:190(E):U:H5''	2.39	0.56
1:A:1413:A:H2	1:A:1487:G:H22	1.52	0.56
1:A:309:G:H2'	1:A:310:G:H8	1.70	0.56
9:I:17:VAL:HG21	9:I:80:GLY:HA3	1.87	0.56
1:A:392:G:H2'	1:A:393:A:C8	2.41	0.56
1:A:1392:G:N2	1:A:1502:A:H8	2.02	0.56
1:A:908:A:C2	1:A:909:A:C4	2.93	0.56
1:A:949:A:N6	24:A:2221:HOH:O	2.39	0.56
3:C:91:LEU:HD21	3:C:99:VAL:HG22	1.88	0.56
4:D:65:ARG:HG3	4:D:75:PHE:CD1	2.41	0.56
11:K:121:PRO:HG2	11:K:126:ARG:HG3	1.88	0.56
1:A:512:U:OP1	4:D:46:LYS:NZ	2.39	0.56
4:D:79:PHE:O	4:D:82:ALA:N	2.38	0.56
3:C:116:VAL:O	3:C:120:VAL:HG23	2.06	0.56
15:O:15:PHE:CE2	15:O:85:LEU:HD21	2.41	0.56
17:Q:59:ILE:HG23	17:Q:71:PHE:HB3	1.88	0.56
1:A:1004:A:HO2'	1:A:1005:A:P	2.28	0.56
1:A:1369:C:H2'	1:A:1370:G:C8	2.41	0.56
1:A:1474:G:H2'	1:A:1475:G:C8	2.41	0.56
2:B:21:ARG:HA	2:B:39:ILE:HA	1.88	0.56
5:E:87:SER:HB3	5:E:131:ILE:HD13	1.88	0.56
7:G:16:LEU:HD12	9:I:44:VAL:HB	1.87	0.56
21:U:12:LYS:HB3	21:U:22:ARG:HD3	1.88	0.56
1:A:1148:U:H2'	1:A:1149:C:O4'	2.06	0.55
1:A:627:G:H2'	1:A:628:G:H8	1.70	0.55
10:J:78:ASN:N	10:J:78:ASN:OD1	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:39:LEU:HD13	15:O:56:LEU:HB2	1.87	0.55
1:A:968:A:C8	1:A:1062:U:H4'	2.41	0.55
1:A:975:A:H5'	1:A:975:A:H8	1.70	0.55
7:G:152:ALA:HA	7:G:155:ARG:HE	1.71	0.55
1:A:519:C:H2'	1:A:520:A:C8	2.41	0.55
5:E:33:VAL:HG11	5:E:109:ILE:HA	1.89	0.55
8:H:38:ILE:HG13	8:H:41:ARG:HH12	1.70	0.55
12:L:24:VAL:HG13	12:L:98:TYR:HE2	1.70	0.55
1:A:1206:G:O2'	3:C:192:THR:O	2.24	0.55
1:A:824:C:H2'	1:A:825:G:H8	1.72	0.55
1:A:1425:U:H2'	1:A:1426:C:H6	1.70	0.55
1:A:130:A:H5'	17:Q:63:ARG:NE	2.20	0.55
1:A:1197:G:H5''	24:A:2044:HOH:O	2.06	0.55
5:E:118:ILE:HG12	5:E:119:LEU:N	2.22	0.55
16:P:18:ARG:O	16:P:20:VAL:HG23	2.06	0.55
20:T:50:GLU:HA	20:T:100:ILE:HG13	1.88	0.55
1:A:91:C:H2'	1:A:92:C:C6	2.42	0.55
1:A:976:G:OP2	1:A:1358:U:H1'	2.07	0.55
3:C:6:HIS:NE2	3:C:8:ILE:HB	2.22	0.55
8:H:20:TYR:CE1	8:H:76:PRO:HG2	2.42	0.55
11:K:124:LYS:HG3	11:K:125:PHE:CD1	2.42	0.55
17:Q:26:GLN:HG2	17:Q:37:LYS:HB2	1.88	0.55
1:A:501:C:H2'	1:A:502:G:H8	1.71	0.55
1:A:627:G:H2'	1:A:628:G:C8	2.41	0.55
2:B:142:LEU:HD13	2:B:146:GLN:HE22	1.72	0.55
2:B:48:MET:HA	2:B:51:LEU:HB2	1.89	0.55
18:R:22:VAL:HG23	18:R:56:THR:HA	1.88	0.55
1:A:1137:C:H5''	1:A:1138:G:OP1	2.07	0.55
1:A:1367:C:H5'	10:J:60:ARG:CZ	2.37	0.55
1:A:1411:C:H2'	1:A:1412:C:H6	1.72	0.55
1:A:1425:U:H2'	1:A:1426:C:C6	2.42	0.55
1:A:1130:A:H4'	9:I:3:GLN:HE22	1.72	0.55
3:C:20:SER:O	14:N:54:PRO:HB3	2.06	0.54
14:N:40:CYS:O	14:N:44:LEU:N	2.30	0.54
17:Q:9:VAL:HB	17:Q:56:VAL:HG22	1.88	0.54
1:A:131:C:H2'	1:A:132:C:C6	2.42	0.54
3:C:130:VAL:HG21	3:C:157:ILE:HG23	1.87	0.54
1:A:1358:U:H5''	14:N:35:ARG:HD3	1.88	0.54
1:A:230:G:H2'	1:A:231:G:O4'	2.07	0.54
1:A:686:U:HO2'	1:A:687:A:H8	1.54	0.54
1:A:737:A:H2'	1:A:738:C:C6	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:913:A:H4'	1:A:914:A:O5'	2.06	0.54
1:A:1338:G:H2'	1:A:1339:A:H8	1.63	0.54
1:A:254:G:H2'	1:A:255:G:C8	2.42	0.54
1:A:316:G:OP2	1:A:351:G:O2'	2.25	0.54
3:C:182:ILE:HG12	3:C:203:PHE:HB2	1.89	0.54
3:C:87:LEU:O	3:C:91:LEU:HB3	2.06	0.54
16:P:79:VAL:N	24:P:210:HOH:O	2.39	0.54
9:I:126:SER:OG	9:I:127:LYS:N	2.39	0.54
12:L:39:VAL:HG12	12:L:41:ARG:HG3	1.90	0.54
15:O:4:THR:H	15:O:7:GLU:CD	2.10	0.54
1:A:881:G:H2'	1:A:882:C:O4'	2.07	0.54
10:J:49:VAL:O	10:J:61:GLU:N	2.38	0.54
11:K:85:ARG:HG2	11:K:113:PRO:HD3	1.90	0.54
1:A:411:A:C5	1:A:413:G:H1'	2.42	0.54
1:A:830:G:N2	1:A:857:C:C2	2.76	0.54
1:A:936:C:H2'	1:A:937:A:O4'	2.08	0.54
2:B:97:TRP:CZ3	2:B:101:MET:HB2	2.43	0.54
9:I:8:GLY:HA2	9:I:79:LEU:HD13	1.90	0.54
15:O:70:LEU:HD13	15:O:78:TYR:HA	1.89	0.54
6:F:10:LEU:HD23	6:F:85:VAL:HG22	1.89	0.54
18:R:74:ARG:HB3	18:R:81:PHE:CE1	2.43	0.54
9:I:8:GLY:HA3	9:I:79:LEU:HB3	1.90	0.54
13:M:23:TYR:HE2	13:M:70:LEU:HD22	1.72	0.54
1:A:1250:A:H4'	9:I:68:GLY:N	2.23	0.53
2:B:201:ILE:HD12	2:B:214:ILE:HG21	1.90	0.53
4:D:61:LYS:HE3	4:D:206:PHE:CE2	2.43	0.53
6:F:44:GLY:HA2	6:F:59:TYR:CE2	2.43	0.53
9:I:23:ASN:HB3	9:I:25:LYS:HG2	1.90	0.53
13:M:23:TYR:CE2	13:M:70:LEU:HD22	2.43	0.53
14:N:39:LEU:HD22	14:N:43:CYS:HB3	1.90	0.53
16:P:4:ILE:HG12	16:P:21:VAL:HG22	1.90	0.53
1:A:47:C:C6	1:A:365:U:H2'	2.44	0.53
1:A:1441:G:HO2'	1:A:1442:G:N2	2.06	0.53
1:A:1499:A:H1'	1:A:1520[A]:G:H5'	1.91	0.53
1:A:781:A:C4	1:A:802:A:C2	2.97	0.53
10:J:55:LYS:HB2	10:J:55:LYS:NZ	2.23	0.53
10:J:99:LYS:HG2	10:J:100:THR:H	1.73	0.53
1:A:1001:A:H2'	1:A:1002:G:C8	2.42	0.53
1:A:253:U:H2'	1:A:254:G:H8	1.72	0.53
1:A:840:C:H5''	1:A:841:U:OP1	2.09	0.53
1:A:372:C:H1'	1:A:373:A:OP2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:G:C2'	1:A:81:U:OP1	2.57	0.53
5:E:7:GLU:HB2	5:E:112:LEU:HD11	1.90	0.53
10:J:42:THR:HG23	10:J:67:THR:O	2.09	0.53
12:L:31:PRO:HB2	12:L:32:PHE:CD2	2.44	0.53
1:A:109:A:H2'	1:A:326:G:N2	2.23	0.53
1:A:459:G:H1'	1:A:463:A:H61	1.74	0.53
1:A:620:C:H2'	1:A:621:A:O4'	2.07	0.53
3:C:35:GLU:O	3:C:39:ILE:HG13	2.07	0.53
5:E:89:ILE:HD11	5:E:120:THR:HG23	1.90	0.53
16:P:53:VAL:O	16:P:56:ALA:N	2.42	0.53
17:Q:29:HIS:ND1	17:Q:30:PRO:HD2	2.24	0.53
1:A:324:G:OP1	20:T:22:ARG:NH1	2.41	0.53
1:A:580:U:H2'	1:A:581:G:O4'	2.08	0.53
1:A:934:C:H42	1:A:938:A:H61	1.56	0.53
11:K:92:GLU:HB3	11:K:96:ARG:NH2	2.23	0.53
15:O:36:ILE:HD12	15:O:60:VAL:HG22	1.89	0.53
1:A:1105:A:H2'	1:A:1106:G:H8	1.73	0.53
1:A:1239:A:H62	1:A:1299:A:H62	1.57	0.53
1:A:527:7MG:H81	1:A:527:7MG:H5''	1.91	0.53
1:A:582:U:OP1	15:O:64:ARG:NH2	2.41	0.53
1:A:750:G:H1'	15:O:23:GLY:H	1.74	0.53
1:A:80:G:H2'	1:A:81:U:OP1	2.08	0.53
3:C:43:LEU:HA	3:C:47:LEU:HD13	1.90	0.53
1:A:1028:C:N4	1:A:1033:G:H22	2.05	0.53
1:A:1120:G:H22	1:A:1154:G:H1'	1.74	0.53
1:A:299:G:H2'	1:A:300:A:C8	2.43	0.53
2:B:9:GLU:O	2:B:10:LEU:HD23	2.09	0.53
8:H:87:SER:OG	8:H:93:VAL:N	2.32	0.53
10:J:80:LYS:H	10:J:80:LYS:HD2	1.73	0.53
1:A:392:G:H2'	1:A:393:A:H8	1.72	0.53
1:A:656:C:H42	1:A:750:G:H1	1.57	0.53
4:D:61:LYS:NZ	4:D:62:GLN:OE1	2.42	0.53
1:A:538:G:OP2	12:L:115:LYS:HB2	2.09	0.53
3:C:150:LYS:HB2	3:C:173:VAL:HG21	1.90	0.52
5:E:95:ALA:HB1	5:E:96:PRO:HD2	1.90	0.52
12:L:27:LEU:HG	12:L:28:LYS:H	1.74	0.52
1:A:501:C:H2'	1:A:502:G:C8	2.44	0.52
2:B:139:LYS:O	2:B:143:GLU:HG2	2.10	0.52
3:C:71:ALA:HA	3:C:106:VAL:HB	1.91	0.52
1:A:1000:U:H2'	1:A:1001:A:C8	2.45	0.52
1:A:665:A:H2'	1:A:732:C:O2	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:53:PRO:HA	14:N:41:ARG:HH22	1.74	0.52
16:P:57:ARG:NE	16:P:79:VAL:O	2.27	0.52
6:F:94:GLN:HB3	18:R:32:ARG:HH11	1.75	0.52
1:A:1123:A:H2'	1:A:1124:G:O4'	2.10	0.52
1:A:633:G:H2'	1:A:634:C:H6	1.75	0.52
8:H:20:TYR:HA	8:H:65:TYR:CE2	2.45	0.52
19:S:77:THR:HG22	19:S:78:ARG:HD3	1.90	0.52
20:T:100:ILE:HG22	20:T:102:GLY:N	2.18	0.52
1:A:359:U:H2'	1:A:360:A:C8	2.45	0.52
1:A:778:G:H2'	1:A:779:C:O4'	2.10	0.52
4:D:70:ILE:HG22	4:D:71:SER:H	1.75	0.52
1:A:19:C:H2'	1:A:20:G:C8	2.44	0.52
1:A:1188:A:H4'	24:N:201:HOH:O	2.08	0.52
1:A:1393:U:O2'	1:A:1501:C:O2'	2.27	0.52
11:K:59:TYR:O	11:K:62:GLN:HB3	2.08	0.52
1:A:1132:C:N4	1:A:1142:G:H1	2.08	0.52
1:A:1439:C:OP2	20:T:38:LYS:NZ	2.43	0.52
2:B:162:ILE:HD12	2:B:177:ALA:HB2	1.92	0.52
3:C:6:HIS:HD2	3:C:9:GLY:H	1.52	0.52
5:E:142:LEU:O	5:E:143:ARG:HD3	2.10	0.52
1:A:1347:G:O6	9:I:10:ARG:NH2	2.43	0.52
1:A:1123:A:H4'	10:J:37:PRO:HD2	1.92	0.52
11:K:90:GLY:HA2	11:K:93:GLN:H	1.75	0.52
1:A:1124:G:H3'	1:A:1145:C:H41	1.75	0.52
1:A:1255:G:N2	1:A:1259:C:O2	2.43	0.52
1:A:1407:5MC:H5'	1:A:1517[B]:G:H21	1.75	0.52
1:A:284:G:H2'	1:A:285:G:H8	1.74	0.52
1:A:540:G:H2'	1:A:541:G:O4'	2.10	0.52
1:A:858:G:O2'	1:A:859:A:H5''	2.10	0.52
4:D:156:GLU:O	4:D:160:GLN:HB2	2.10	0.52
9:I:48:GLU:HA	9:I:51:ARG:HD3	1.91	0.52
13:M:13:LYS:O	13:M:45:VAL:HG23	2.09	0.52
1:A:1035:A:H2'	1:A:1036:G:C8	2.45	0.52
1:A:955:U:H1'	1:A:1227:A:H61	1.75	0.52
5:E:109:ILE:HG21	5:E:135:THR:CG2	2.39	0.52
5:E:82:VAL:O	5:E:88:LYS:HA	2.10	0.52
1:A:1381:U:N1	7:G:156:TRP:HH2	2.08	0.52
13:M:37:THR:HG23	13:M:55:ARG:HG2	1.92	0.52
1:A:1037:C:H2'	1:A:1038:C:C6	2.45	0.51
1:A:665:A:H3'	1:A:725:G:N2	2.25	0.51
1:A:959:A:O2'	1:A:984:C:O2'	2.27	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:190:ARG:HA	3:C:195:VAL:HG22	1.92	0.51
1:A:1001:A:H2'	1:A:1002:G:H8	1.75	0.51
1:A:1196:U:OP1	1:A:1197:G:H5'	2.10	0.51
1:A:1257:U:H4'	1:A:1258:G:O5'	2.09	0.51
1:A:21:G:H2'	1:A:22:G:C8	2.45	0.51
1:A:254:G:H2'	1:A:255:G:H8	1.73	0.51
1:A:552:U:H2'	1:A:553:A:C8	2.46	0.51
1:A:1056:U:H5'	3:C:163:ALA:HB2	1.91	0.51
1:A:1222:G:OP1	19:S:77:THR:HG21	2.10	0.51
1:A:1129:C:OP1	9:I:62:TYR:OH	2.26	0.51
1:A:1505:G:H8	1:A:1505:G:H3'	1.72	0.51
1:A:371:G:O2'	1:A:372:C:H5'	2.10	0.51
1:A:824:C:H2'	1:A:825:G:C8	2.46	0.51
1:A:833:U:H2'	1:A:834:C:H6	1.75	0.51
15:O:12:ILE:HG12	15:O:31:LEU:HD11	1.92	0.51
1:A:1022:G:H22	1:A:1024:G:N2	2.09	0.51
1:A:1040:U:H2'	1:A:1041:A:H8	1.76	0.51
1:A:106:C:C2'	1:A:107:G:H5'	2.39	0.51
1:A:646:U:H2'	1:A:647:C:C6	2.45	0.51
1:A:679:C:H2'	1:A:680:C:C6	2.45	0.51
4:D:36:ARG:HG2	4:D:38:TYR:CZ	2.45	0.51
6:F:100:ASN:HA	18:R:23:LYS:HE2	1.92	0.51
18:R:22:VAL:HG23	18:R:55:ARG:O	2.10	0.51
18:R:59:SER:N	18:R:62:GLU:OE1	2.44	0.51
18:R:40:LEU:HD12	18:R:79:LEU:HD11	1.92	0.51
1:A:1201:A:H4'	1:A:1202:G:O5'	2.10	0.51
5:E:122:GLU:C	5:E:123:LEU:HD23	2.31	0.51
10:J:47:PHE:HB3	14:N:34:TYR:CE2	2.37	0.51
1:A:247:G:OP2	17:Q:100:LYS:HB2	2.11	0.51
1:A:75:G:C2	1:A:96:G:C2	2.99	0.51
1:A:945:G:O6	1:A:1236:A:N1	2.43	0.51
8:H:104:ARG:CZ	8:H:138:TRP:CZ2	2.93	0.51
8:H:87:SER:HG	8:H:93:VAL:H	1.54	0.51
9:I:25:LYS:HG3	9:I:60:ASP:OD1	2.11	0.51
9:I:69:GLY:O	9:I:73:GLN:HG3	2.10	0.51
10:J:55:LYS:HB2	10:J:55:LYS:HZ2	1.75	0.51
13:M:20:THR:HG22	24:M:308:HOH:O	2.10	0.51
1:A:322:C:OP2	1:A:328:C:N4	2.44	0.51
1:A:376:G:N3	1:A:389:A:C2	2.79	0.51
1:A:456:C:H2'	1:A:457:C:C6	2.46	0.51
4:D:187:ARG:NE	4:D:188:LEU:O	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:50:ARG:HD2	4:D:51:PRO:HD2	1.92	0.51
5:E:98:THR:HB	5:E:117:ASP:HB3	1.92	0.51
8:H:24:THR:O	8:H:60:ARG:HA	2.11	0.51
10:J:12:ASP:OD2	10:J:15:THR:HG22	2.10	0.51
1:A:1179:A:H2'	1:A:1180:A:O4'	2.11	0.51
1:A:1243:C:N4	1:A:1294:G:H1	2.04	0.51
1:A:143:A:H2	1:A:220:G:H22	1.57	0.51
1:A:953:G:H2'	1:A:954:G:O4'	2.11	0.51
6:F:69:GLU:CD	6:F:69:GLU:H	2.13	0.51
1:A:17:U:H2'	1:A:18:C:C6	2.45	0.51
4:D:187:ARG:NH2	4:D:189:PRO:O	2.44	0.51
13:M:12:ASN:H	13:M:45:VAL:HB	1.75	0.51
1:A:186:C:H5'	20:T:78:ALA:HB1	1.92	0.51
1:A:653:A:O4'	8:H:56:LYS:HE2	2.11	0.51
1:A:797:C:H2'	1:A:798:G:H8	1.75	0.51
3:C:18:TRP:CD1	14:N:54:PRO:HA	2.46	0.51
5:E:84:PHE:CD2	5:E:84:PHE:C	2.84	0.51
15:O:7:GLU:O	15:O:11:VAL:HG23	2.10	0.51
16:P:15:PRO:HG2	16:P:41:PRO:HG2	1.93	0.51
1:A:1520[A]:G:H2'	1:A:1521:G:C8	2.43	0.50
1:A:602:A:H2'	1:A:603:U:O4'	2.11	0.50
1:A:1009:G:N2	1:A:1010:G:N3	2.59	0.50
1:A:1145:C:HO2'	1:A:1146:A:P	2.33	0.50
1:A:1250:A:C6	1:A:1251:A:C6	3.00	0.50
1:A:193:C:H4'	20:T:61:SER:HB2	1.93	0.50
2:B:210:SER:OG	2:B:211:ILE:N	2.45	0.50
1:A:755:G:H1'	8:H:1:MET:CE	2.41	0.50
12:L:54:LYS:HD2	12:L:54:LYS:N	2.25	0.50
1:A:345:C:OP2	1:A:345:C:H6	1.95	0.50
1:A:463:A:OP1	16:P:75:ARG:NH2	2.44	0.50
8:H:4:ASP:OD1	8:H:6:ILE:N	2.41	0.50
1:A:538:G:P	12:L:115:LYS:HB2	2.52	0.50
13:M:40:ASN:HB3	13:M:43:THR:HG23	1.92	0.50
1:A:235:C:H5'	17:Q:70:ARG:HG2	1.94	0.50
1:A:1339:A:H5''	1:A:1340:A:OP2	2.12	0.50
1:A:826:C:H2'	1:A:827:U:H6	1.76	0.50
8:H:123:GLU:O	8:H:126:LYS:HG2	2.11	0.50
10:J:53:PRO:HA	14:N:41:ARG:NH2	2.26	0.50
19:S:63:THR:HG22	19:S:64:GLU:H	1.76	0.50
2:B:162:ILE:HG22	2:B:184:VAL:HG13	1.93	0.50
2:B:28:PHE:HD2	2:B:32:ILE:HD11	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:687:A:H4'	1:A:688:G:O5'	2.10	0.50
3:C:184:TYR:HA	3:C:200:ALA:O	2.12	0.50
7:G:20:ASP:OD1	7:G:22:LEU:HB3	2.11	0.50
1:A:1343:G:H1'	9:I:121:ARG:NH1	2.26	0.50
12:L:38:THR:HG22	12:L:39:VAL:HG23	1.93	0.50
1:A:1436:U:H2'	1:A:1437:C:H6	1.76	0.50
8:H:65:TYR:N	8:H:65:TYR:CD1	2.80	0.50
13:M:60:VAL:HG22	13:M:64:TRP:CZ3	2.45	0.50
1:A:1104:G:O5'	2:B:111:ARG:HD2	2.12	0.50
3:C:6:HIS:CD2	14:N:49:HIS:HB3	2.47	0.50
4:D:12:CYS:SG	4:D:19:LEU:O	2.70	0.50
19:S:18:LYS:O	19:S:22:LEU:HB2	2.11	0.50
1:A:191:G:O2'	20:T:102:GLY:O	2.16	0.50
1:A:22:G:H2'	1:A:23:C:C6	2.46	0.50
1:A:881:G:P	12:L:12:ARG:NH2	2.85	0.50
1:A:923:A:OP1	5:E:21:ALA:HB2	2.12	0.50
2:B:7:VAL:HG11	2:B:221:LEU:HD23	1.93	0.50
4:D:187:ARG:NH1	4:D:188:LEU:HD12	2.27	0.50
1:A:279:A:C6	17:Q:98:LEU:HD13	2.46	0.50
19:S:16:LEU:HA	19:S:19:VAL:HG12	1.94	0.50
4:D:88:VAL:HG12	4:D:90:GLY:N	2.27	0.49
6:F:10:LEU:HD12	6:F:59:TYR:HB3	1.94	0.49
1:A:253:U:H2'	1:A:254:G:C8	2.47	0.49
1:A:803:G:C6	1:A:804:U:C4	3.01	0.49
1:A:857:C:H5'	24:A:2174:HOH:O	2.11	0.49
5:E:84:PHE:O	5:E:87:SER:HB2	2.12	0.49
8:H:114:THR:OG1	8:H:117:GLY:O	2.27	0.49
9:I:96:LEU:O	9:I:100:GLY:N	2.36	0.49
13:M:48:LEU:HD13	13:M:53:VAL:HG23	1.93	0.49
20:T:39:LYS:HG2	20:T:55:ILE:HD13	1.93	0.49
21:U:6:ARG:HD2	21:U:15:ARG:HH12	1.76	0.49
1:A:1303:C:H2'	1:A:1304:G:H5'	1.94	0.49
1:A:1412:C:H2'	1:A:1413:A:H8	1.75	0.49
7:G:87:VAL:HG12	7:G:88:PRO:HD2	1.95	0.49
9:I:16:ARG:HB2	9:I:64:THR:HG23	1.94	0.49
13:M:62:ASN:OD1	13:M:62:ASN:N	2.44	0.49
15:O:55:GLY:HA2	15:O:58:MET:HE2	1.94	0.49
17:Q:29:HIS:O	17:Q:33:GLY:HA2	2.11	0.49
18:R:51:LEU:HB2	18:R:56:THR:HG23	1.94	0.49
1:A:1064:G:N2	1:A:1190:G:H2'	2.26	0.49
1:A:14:U:O2	1:A:16:A:C8	2.65	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:940:C:H2'	1:A:941:G:O4'	2.11	0.49
13:M:37:THR:HB	13:M:39:ILE:HD11	1.93	0.49
17:Q:63:ARG:HG2	17:Q:64:PRO:HD2	1.95	0.49
20:T:92:LEU:O	20:T:96:GLY:HA2	2.12	0.49
1:A:426:G:OP1	4:D:38:TYR:OH	2.27	0.49
1:A:642:A:H2'	1:A:643:C:C6	2.47	0.49
1:A:665:A:H3'	1:A:725:G:H21	1.76	0.49
2:B:102:LEU:H	2:B:102:LEU:HD22	1.77	0.49
3:C:14:ILE:HG22	3:C:15:THR:HG23	1.94	0.49
5:E:97:GLY:N	5:E:117:ASP:OD1	2.45	0.49
9:I:5:TYR:HD2	9:I:18:PHE:CE2	2.30	0.49
9:I:93:ARG:HD3	9:I:97:LYS:NZ	2.27	0.49
11:K:120:ARG:HG2	11:K:120:ARG:NH1	2.21	0.49
11:K:29:ILE:HG23	11:K:44:SER:CB	2.42	0.49
1:A:1003:G:C2	1:A:1003(A):G:C5	3.01	0.49
1:A:509:A:H3'	1:A:509:A:C8	2.47	0.49
1:A:828:A:H4'	1:A:828:A:OP1	2.13	0.49
17:Q:95:TYR:HA	17:Q:98:LEU:HD11	1.95	0.49
1:A:807:A:OP1	15:O:48:LYS:NZ	2.46	0.49
1:A:902:G:H2'	1:A:903:G:C8	2.48	0.49
7:G:88:PRO:HG2	7:G:155:ARG:HH21	1.78	0.49
1:A:1120:G:C2	1:A:1154:G:N3	2.81	0.49
1:A:1531:A:O5'	1:A:1531:A:H8	1.96	0.49
1:A:376:G:C2	1:A:389:A:C2	3.01	0.49
1:A:462:G:H21	16:P:82:GLN:HE21	1.61	0.49
1:A:451:A:N6	1:A:481:G:C4	2.80	0.49
8:H:17:THR:O	8:H:78:GLN:NE2	2.46	0.49
1:A:1328:C:H2'	1:A:1329:A:H8	1.78	0.49
4:D:3:ARG:HH22	4:D:100:ARG:HH22	1.61	0.49
19:S:40:ILE:HD13	19:S:62:ILE:HD11	1.95	0.49
1:A:1048:G:O3'	1:A:1049:U:H3'	2.13	0.49
1:A:384:G:H2'	1:A:385:C:H6	1.76	0.49
3:C:110:ASN:ND2	3:C:140:ARG:HB3	2.28	0.49
16:P:9:PHE:N	16:P:16:HIS:O	2.42	0.49
1:A:110:C:H2'	1:A:111:G:O4'	2.12	0.48
1:A:451:A:H2	1:A:480:U:C5	2.30	0.48
1:A:91:C:H2'	1:A:92:C:H6	1.78	0.48
5:E:90:VAL:O	5:E:91:LEU:HD23	2.13	0.48
9:I:63:ILE:HG21	9:I:77:ILE:HG12	1.94	0.48
11:K:54:ARG:O	11:K:57:THR:HG22	2.12	0.48
1:A:299:G:C6	1:A:300:A:C6	3.02	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:533:A:O2'	1:A:535:A:OP2	2.30	0.48
1:A:636:U:H2'	1:A:637:G:C8	2.48	0.48
1:A:833:U:H2'	1:A:834:C:C6	2.48	0.48
1:A:422:C:H4'	1:A:423:G:O5'	2.12	0.48
1:A:914:A:H2'	1:A:915:A:C8	2.48	0.48
1:A:97:G:H2'	1:A:98:U:O4'	2.13	0.48
7:G:155:ARG:HA	7:G:155:ARG:HD3	1.54	0.48
11:K:17:GLY:HA2	11:K:35:PRO:HD3	1.94	0.48
17:Q:67:LYS:HA	17:Q:70:ARG:HH12	1.78	0.48
6:F:33:TYR:CD1	6:F:75:LEU:HA	2.48	0.48
7:G:88:PRO:HG2	7:G:155:ARG:NH2	2.28	0.48
10:J:45:ARG:O	10:J:64:GLU:HA	2.14	0.48
20:T:64:ASP:O	20:T:67:ALA:HB3	2.12	0.48
1:A:1063:C:H2'	1:A:1064:G:C8	2.47	0.48
1:A:1101:A:H4'	1:A:1102:A:O5'	2.14	0.48
1:A:1347:G:H22	1:A:1374:A:P	2.37	0.48
1:A:260:G:H2'	1:A:261:U:C6	2.49	0.48
1:A:411:A:C6	1:A:429:U:C4	3.01	0.48
1:A:736:C:H2'	1:A:737:A:C8	2.49	0.48
3:C:77:ILE:HD11	3:C:103:VAL:HG21	1.96	0.48
1:A:437:U:H5''	4:D:155:LEU:HD11	1.95	0.48
8:H:17:THR:CB	8:H:78:GLN:HE22	2.25	0.48
7:G:40:ALA:HB3	9:I:41:VAL:HG21	1.95	0.48
1:A:114:U:O2'	1:A:115:G:H5'	2.14	0.48
1:A:1499:A:H1'	1:A:1520[A]:G:OP1	2.12	0.48
1:A:1502:A:C2	1:A:1504:G:C2	3.01	0.48
1:A:284:G:H2'	1:A:285:G:C8	2.48	0.48
1:A:50:A:H4'	1:A:51:A:H5'	1.94	0.48
1:A:794:A:C5	1:A:795:C:C4	3.02	0.48
1:A:938:A:N6	24:A:1937:HOH:O	2.47	0.48
2:B:64:ARG:NH1	2:B:64:ARG:HB2	2.28	0.48
1:A:1159:U:OP1	2:B:133:LYS:NZ	2.37	0.48
1:A:250:A:O4'	1:A:252:U:C6	2.67	0.48
1:A:676:A:H1'	11:K:115:PRO:HB3	1.95	0.48
9:I:33:PHE:O	9:I:37:PHE:HB2	2.14	0.48
1:A:1309:G:H5'	13:M:78:ILE:HD11	1.95	0.48
1:A:1180:A:OP1	9:I:103:THR:OG1	2.25	0.48
1:A:279:A:H5''	1:A:281:G:H5'	1.95	0.48
1:A:89:C:H2'	1:A:90:U:C2	2.49	0.48
1:A:960:U:H4'	1:A:961:U:C5'	2.44	0.48
4:D:121:VAL:O	4:D:134:ASP:HA	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:28:SER:O	4:D:30:LYS:N	2.42	0.48
4:D:35:ARG:N	4:D:35:ARG:HD2	2.28	0.48
5:E:138:ALA:O	5:E:141:GLN:HB2	2.14	0.48
5:E:151:LEU:HD21	8:H:79:VAL:HA	1.96	0.48
8:H:65:TYR:HA	8:H:79:VAL:HG23	1.96	0.48
9:I:9:ARG:HG2	9:I:14:VAL:HG22	1.95	0.48
12:L:28:LYS:HB3	12:L:30:ALA:HB2	1.94	0.48
1:A:1489:G:H2'	1:A:1490:C:C6	2.49	0.48
1:A:77:G:C6	1:A:93:G:N1	2.82	0.48
3:C:26:LYS:CD	3:C:26:LYS:H	2.26	0.48
19:S:27:GLU:H	19:S:27:GLU:CD	2.16	0.48
1:A:1289:A:H2'	1:A:1290:G:H5'	1.95	0.48
1:A:1518[B]:MA6:H93	1:A:1519[B]:MA6:C2	2.44	0.48
1:A:428:G:H1'	1:A:429:U:OP2	2.14	0.48
1:A:75:G:C2	1:A:76:C:C2	3.02	0.48
2:B:219:VAL:O	2:B:223:ILE:HG13	2.14	0.48
3:C:10:PHE:CE2	3:C:178:LEU:HD12	2.49	0.48
5:E:35:GLY:HA3	5:E:112:LEU:HD12	1.96	0.48
5:E:45:PHE:CE2	5:E:47:LYS:HE3	2.49	0.48
8:H:83:ILE:HG12	8:H:137:VAL:CG2	2.37	0.48
15:O:25:THR:HG21	15:O:70:LEU:HG	1.96	0.48
20:T:31:SER:HA	20:T:34:LYS:HG3	1.94	0.48
1:A:1113:C:H4'	3:C:14:ILE:HD12	1.95	0.47
1:A:1411:C:H2'	1:A:1412:C:C6	2.49	0.47
1:A:77:G:C4	1:A:93:G:N2	2.82	0.47
1:A:674:G:H5'	6:F:50:TYR:CE2	2.48	0.47
1:A:881:G:P	12:L:12:ARG:HH22	2.37	0.47
1:A:1027:C:H42	1:A:1035:A:N6	2.12	0.47
1:A:1087:G:H22	1:A:1099:G:H1'	1.78	0.47
2:B:31:TYR:CE1	2:B:200:ILE:HD11	2.48	0.47
2:B:54:THR:O	2:B:58:ILE:HG13	2.13	0.47
1:A:619:U:N3	4:D:134:ASP:OD2	2.45	0.47
10:J:49:VAL:HG13	14:N:41:ARG:HB2	1.95	0.47
11:K:29:ILE:HG23	11:K:44:SER:HB3	1.96	0.47
14:N:3:ARG:NH2	14:N:5:ALA:HB3	2.28	0.47
1:A:1498:UR3:C4'	1:A:1519[A]:MA6:H2	2.44	0.47
1:A:280:C:C2	17:Q:38:ARG:HG3	2.48	0.47
1:A:642:A:H2'	1:A:643:C:H6	1.79	0.47
5:E:105:VAL:HB	5:E:106:PRO:HD3	1.95	0.47
5:E:84:PHE:C	5:E:84:PHE:HD2	2.17	0.47
13:M:14:ARG:NE	13:M:42:ALA:HA	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:G:OP1	17:Q:25:ARG:NH2	2.47	0.47
1:A:988:G:H1'	1:A:1015:A:N1	2.29	0.47
1:A:1513:A:H2'	1:A:1514:C:C6	2.49	0.47
1:A:190(K):G:H2'	1:A:190(L):U:C6	2.48	0.47
1:A:24:U:H2'	1:A:25:C:C6	2.49	0.47
2:B:135:GLN:O	2:B:139:LYS:HB2	2.14	0.47
4:D:21:LEU:CD2	4:D:114:ARG:HB2	2.45	0.47
1:A:113:G:H2'	1:A:114:U:H6	1.80	0.47
1:A:1239:A:H62	1:A:1299:A:N6	2.11	0.47
1:A:164:U:H2'	1:A:165:C:H6	1.78	0.47
1:A:184:G:H2'	1:A:185:A:C8	2.41	0.47
1:A:459:G:H1'	1:A:463:A:N6	2.29	0.47
1:A:708:C:H2'	1:A:709:G:C8	2.49	0.47
1:A:765:G:C6	1:A:812:C:C2	3.03	0.47
1:A:766:A:H2'	1:A:767:A:O4'	2.14	0.47
4:D:19:LEU:HA	4:D:19:LEU:HD23	1.56	0.47
8:H:87:SER:HA	8:H:93:VAL:HG12	1.97	0.47
15:O:33:THR:HG23	15:O:63:ARG:HH12	1.79	0.47
20:T:16:HIS:CE1	20:T:20:LEU:HD21	2.49	0.47
1:A:1097:C:H2'	1:A:1098:C:C6	2.49	0.47
1:A:1255:G:O2'	1:A:1258:G:H1'	2.15	0.47
1:A:1399:C:O2	1:A:1401:G:C5	2.68	0.47
2:B:186:ALA:HB3	2:B:197:VAL:HG11	1.96	0.47
4:D:116:GLN:O	4:D:120:LEU:HG	2.15	0.47
4:D:131:ARG:N	4:D:131:ARG:HD2	2.29	0.47
4:D:190:ASP:OD1	4:D:191:ARG:N	2.48	0.47
1:A:1329:A:P	13:M:28:ALA:HB3	2.54	0.47
14:N:13:THR:N	14:N:14:PRO:HD3	2.29	0.47
1:A:708:C:H2'	1:A:709:G:H8	1.80	0.47
2:B:97:TRP:CE3	2:B:98:LEU:O	2.68	0.47
4:D:63:LYS:O	4:D:67:ILE:HG13	2.14	0.47
4:D:9:CYS:O	4:D:12:CYS:HB2	2.14	0.47
12:L:27:LEU:C	12:L:29:GLY:N	2.67	0.47
16:P:34:GLU:OE1	16:P:55:ARG:HD2	2.15	0.47
6:F:100:ASN:ND2	6:F:100:ASN:O	2.47	0.47
6:F:19:LEU:O	6:F:23:LYS:HG3	2.14	0.47
15:O:84:LYS:C	15:O:85:LEU:HD23	2.35	0.47
20:T:89:ARG:O	20:T:92:LEU:HB2	2.15	0.47
1:A:1093:A:N3	1:A:1109:C:O2'	2.42	0.47
1:A:355:C:H5'	1:A:389:A:OP2	2.14	0.47
1:A:451:A:H2	1:A:480:U:C4	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:740:U:O2'	1:A:741:G:H5'	2.14	0.47
1:A:922:G:H4'	5:E:20:GLN:HA	1.97	0.47
7:G:149:ARG:NH1	7:G:149:ARG:HB3	2.30	0.47
7:G:70:LYS:HD3	7:G:96:GLN:HB3	1.96	0.47
1:A:1027:C:H2'	1:A:1028:C:C6	2.50	0.47
1:A:1357:A:H2'	1:A:1358:U:C6	2.50	0.47
1:A:1518[B]:MA6:H102	1:A:1519[B]:MA6:H103	1.97	0.47
1:A:865:A:O5'	1:A:865:A:H8	1.97	0.47
4:D:91:SER:OG	4:D:92:VAL:N	2.48	0.47
7:G:15:ASP:HB3	7:G:19:GLY:H	1.79	0.47
13:M:39:ILE:HA	13:M:52:GLU:OE2	2.14	0.47
1:A:1384:C:H2'	1:A:1385:G:C8	2.50	0.47
1:A:1481:U:H2'	1:A:1482:G:O4'	2.15	0.47
1:A:397:A:H5'	1:A:398:C:OP1	2.14	0.47
1:A:420:U:H2'	1:A:422:C:H5	1.80	0.47
1:A:78:G:H2'	1:A:79:G:H5''	1.96	0.47
1:A:620:C:N1	4:D:135:LEU:HD13	2.29	0.47
8:H:20:TYR:HE1	8:H:76:PRO:HG2	1.80	0.47
15:O:39:LEU:CD1	15:O:56:LEU:HB2	2.45	0.47
1:A:1516[A]:G:H2'	1:A:1518[A]:MA6:OP2	2.15	0.46
1:A:255:G:H2'	1:A:256:U:C6	2.50	0.46
1:A:349:A:H2'	1:A:350:G:O4'	2.14	0.46
1:A:707:C:H2'	1:A:708:C:H6	1.78	0.46
1:A:973:G:C3'	1:A:974:A:H5''	2.45	0.46
6:F:67:MET:HB2	6:F:68:PRO:HD2	1.96	0.46
14:N:12:ARG:HD3	14:N:12:ARG:HA	1.78	0.46
14:N:24:CYS:HB3	14:N:33:VAL:HG12	1.96	0.46
20:T:75:ASN:N	20:T:75:ASN:OD1	2.48	0.46
2:B:92:TYR:CD2	2:B:151:GLY:HA3	2.50	0.46
3:C:134:ILE:HD11	3:C:153:VAL:HG21	1.98	0.46
1:A:542:G:OP1	4:D:10:ARG:NH2	2.47	0.46
1:A:1118:C:H2'	1:A:1119:C:C6	2.50	0.46
1:A:1254:C:OP1	10:J:45:ARG:HD3	2.15	0.46
1:A:130:A:OP2	1:A:190(E):U:H2'	2.16	0.46
1:A:601:C:H2'	1:A:602:A:C8	2.50	0.46
1:A:620:C:C1'	4:D:135:LEU:HD13	2.45	0.46
1:A:77:G:C6	1:A:93:G:C6	3.04	0.46
2:B:180:LEU:HD23	2:B:180:LEU:HA	1.55	0.46
3:C:125:GLU:O	3:C:127:ARG:HG3	2.14	0.46
5:E:148:VAL:O	5:E:152:ARG:HG3	2.16	0.46
10:J:50:ILE:HA	10:J:60:ARG:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:37:THR:HB	13:M:39:ILE:CD1	2.45	0.46
18:R:71:LYS:O	18:R:75:ILE:HG12	2.16	0.46
1:A:106:C:O2'	1:A:107:G:H5'	2.16	0.46
1:A:1206:G:C6	1:A:1207:2MG:C5	3.03	0.46
1:A:1505:G:C3'	1:A:1505:G:C8	2.98	0.46
1:A:262:A:H5'	20:T:74:LYS:CD	2.44	0.46
1:A:691:G:H2'	1:A:692:U:H6	1.80	0.46
2:B:55:PHE:CD2	2:B:58:ILE:HD12	2.50	0.46
9:I:10:ARG:NH1	9:I:75:ASP:OD2	2.49	0.46
12:L:10:LEU:HB3	17:Q:32:TYR:CD1	2.51	0.46
14:N:24:CYS:SG	14:N:40:CYS:HB3	2.55	0.46
15:O:3:ILE:HD11	15:O:35:ARG:HG3	1.95	0.46
1:A:1195:C:C4	1:A:1197:G:C8	3.04	0.46
1:A:1370:G:H5''	9:I:109:VAL:HG21	1.96	0.46
1:A:695:A:H2'	1:A:696:A:C8	2.51	0.46
1:A:881:G:OP2	12:L:12:ARG:NH2	2.48	0.46
2:B:18:GLY:HA3	2:B:42:ILE:H	1.81	0.46
3:C:28:GLN:HG2	3:C:28:GLN:H	1.49	0.46
7:G:47:CYS:HA	7:G:50:ILE:HG22	1.97	0.46
1:A:975:A:N6	10:J:60:ARG:HH21	2.14	0.46
17:Q:60:ILE:HG23	17:Q:60:ILE:HD12	1.67	0.46
17:Q:65:ILE:HB	17:Q:69:LYS:HB2	1.97	0.46
1:A:445:G:H2'	1:A:446:G:C8	2.51	0.46
4:D:157:LEU:HD22	4:D:157:LEU:HA	1.67	0.46
4:D:20:TYR:HA	4:D:26:CYS:SG	2.55	0.46
2:B:178:ARG:HE	8:H:74:PRO:HG3	1.81	0.46
9:I:53:VAL:HB	9:I:92:TYR:CE2	2.51	0.46
1:A:1172:C:H2'	1:A:1173:G:H8	1.81	0.46
1:A:1326:C:OP1	21:U:12:LYS:NZ	2.33	0.46
1:A:781:A:C5	1:A:802:A:C2	3.04	0.46
2:B:30:ARG:HD2	2:B:31:TYR:CE2	2.51	0.46
1:A:1112:C:H42	3:C:178:LEU:H	1.63	0.46
3:C:7:PRO:O	3:C:11:ARG:HD2	2.15	0.46
5:E:31:LEU:HA	5:E:31:LEU:HD23	1.53	0.46
13:M:49:THR:HG22	13:M:50:GLU:H	1.80	0.46
20:T:60:GLU:HA	20:T:63:ILE:HD12	1.98	0.46
1:A:1328:C:H2'	1:A:1329:A:C8	2.51	0.46
1:A:231:G:C2	1:A:232:G:C8	3.04	0.46
1:A:325:A:H2'	1:A:326:G:O4'	2.15	0.46
1:A:457:C:H2'	1:A:458:C:C6	2.51	0.46
1:A:601:C:H2'	1:A:602:A:H8	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:974:A:H4'	1:A:975:A:H3'	1.97	0.46
6:F:8:ILE:HG23	6:F:85:VAL:HG13	1.98	0.46
8:H:104:ARG:HG2	8:H:138:TRP:CE3	2.50	0.46
9:I:53:VAL:HB	9:I:92:TYR:CZ	2.51	0.46
13:M:23:TYR:HB2	13:M:67:GLU:OE2	2.16	0.46
17:Q:61:GLU:HA	17:Q:71:PHE:CD1	2.51	0.46
19:S:80:TYR:CG	19:S:81:ARG:N	2.84	0.46
1:A:113:G:H2'	1:A:114:U:C6	2.51	0.46
1:A:1211:U:H1'	1:A:1213:A:C2	2.50	0.46
1:A:1223:C:H3'	1:A:1224:G:C5'	2.45	0.46
1:A:1283:G:H2'	1:A:1284:C:H6	1.80	0.46
1:A:251:G:H4'	1:A:252:U:OP1	2.15	0.46
1:A:411:A:N7	1:A:413:G:H1'	2.31	0.46
2:B:222:ILE:HG22	2:B:226:ARG:HH12	1.81	0.46
2:B:40:HIS:HD1	2:B:190:THR:HG21	1.81	0.46
4:D:146:ILE:HD12	4:D:146:ILE:N	2.30	0.46
8:H:31:PHE:CE2	8:H:35:ILE:HD11	2.51	0.46
9:I:9:ARG:HG3	9:I:14:VAL:HG13	1.97	0.46
1:A:1152:A:P	10:J:70:ARG:HH22	2.39	0.46
15:O:2:PRO:HB2	15:O:3:ILE:H	1.57	0.46
16:P:43:LYS:HA	16:P:48:TRP:HB3	1.98	0.46
1:A:1347:G:O2'	1:A:1373:G:N1	2.49	0.46
1:A:1504:G:C3'	1:A:1505:G:H5'	2.46	0.46
1:A:255:G:O6	1:A:266:G:O6	2.34	0.46
1:A:518:C:H4'	1:A:519:C:O5'	2.16	0.46
1:A:607:A:N3	1:A:607:A:H2'	2.31	0.46
1:A:79:G:C2	1:A:80:G:C8	3.04	0.46
1:A:877:C:O2'	8:H:3:THR:HG23	2.15	0.46
12:L:60:LEU:HB2	12:L:64:TYR:O	2.16	0.46
1:A:1269:A:N1	1:A:1312:G:O2'	2.41	0.45
1:A:321:A:C2	1:A:333:G:C2	3.04	0.45
9:I:102:LEU:HA	9:I:102:LEU:HD23	1.78	0.45
1:A:1061:G:H1'	10:J:56:HIS:CE1	2.51	0.45
1:A:293:G:C6	1:A:294:U:C4	3.04	0.45
4:D:61:LYS:HA	4:D:203:VAL:HG22	1.98	0.45
9:I:108:VAL:HG12	9:I:109:VAL:H	1.82	0.45
1:A:1130:A:OP2	1:A:1130:A:H8	1.99	0.45
1:A:1181:G:C2	1:A:1182:G:N2	2.84	0.45
1:A:393:A:C2	1:A:394:G:C8	3.04	0.45
1:A:755:G:H1'	8:H:1:MET:HE3	1.99	0.45
4:D:201:GLN:O	4:D:205:GLU:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:11:ILE:HB	5:E:31:LEU:CB	2.43	0.45
8:H:127:LEU:HD13	8:H:127:LEU:HA	1.70	0.45
1:A:949:A:C4	1:A:1233:G:N2	2.85	0.45
1:A:564:C:C5	17:Q:31:LEU:HD21	2.51	0.45
1:A:575:G:O2'	1:A:821:G:H5'	2.16	0.45
2:B:73:THR:HG23	2:B:95:GLN:O	2.16	0.45
3:C:155:GLY:O	3:C:196:LEU:HG	2.17	0.45
4:D:101:LEU:HA	4:D:104:VAL:HB	1.97	0.45
4:D:196:LEU:HA	4:D:197:PRO:HD3	1.85	0.45
8:H:119:LEU:HD22	8:H:123:GLU:HB3	1.99	0.45
8:H:86:ILE:HG21	8:H:133:LEU:HD22	1.97	0.45
1:A:1188:A:O2'	14:N:58:LYS:NZ	2.50	0.45
1:A:1193:G:O2'	1:A:1194:U:H5'	2.17	0.45
1:A:1281:U:H5'	1:A:1282:C:C5	2.52	0.45
1:A:500:G:C6	1:A:546:G:C2	3.05	0.45
4:D:26:CYS:HA	4:D:31:CYS:HB2	1.99	0.45
5:E:14:ARG:O	5:E:28:PHE:HD2	1.99	0.45
5:E:51:VAL:HB	5:E:52:PRO:HD3	1.99	0.45
5:E:60:TYR:HE1	5:E:64:ARG:HE	1.63	0.45
6:F:48:LEU:HD13	6:F:52:ILE:HG13	1.99	0.45
8:H:48:TYR:HA	8:H:60:ARG:O	2.16	0.45
9:I:32:ASP:OD2	9:I:33:PHE:N	2.49	0.45
15:O:18:PHE:CZ	15:O:21:ASP:HB2	2.51	0.45
15:O:43:LEU:HD11	15:O:53:HIS:HA	1.98	0.45
17:Q:88:TYR:HA	17:Q:91:ARG:NH1	2.31	0.45
1:A:1302:U:C5	13:M:17:VAL:HG21	2.51	0.45
1:A:224:C:H2'	1:A:225:C:H6	1.82	0.45
1:A:424:G:H2'	1:A:425:G:C8	2.51	0.45
1:A:585:G:C6	1:A:586:C:C4	3.04	0.45
8:H:120:THR:N	8:H:123:GLU:OE1	2.44	0.45
19:S:22:LEU:HD21	19:S:28:LYS:H	1.82	0.45
1:A:1111:A:N1	3:C:177:THR:OG1	2.37	0.45
1:A:328:C:O2	1:A:328:C:H2'	2.16	0.45
1:A:958:A:O2'	1:A:985:C:O2'	2.32	0.45
4:D:145:GLU:HG3	4:D:184:LYS:HD3	1.98	0.45
16:P:66:PRO:HG2	16:P:71:ARG:HG3	1.99	0.45
1:A:1112:C:O2	3:C:179:ARG:HB2	2.17	0.45
1:A:1349:A:C2	1:A:1374:A:C4	3.05	0.45
1:A:1520[B]:G:H2'	1:A:1521:G:C8	2.50	0.45
1:A:923:A:H2'	1:A:924:C:O4'	2.16	0.45
5:E:109:ILE:HG21	5:E:135:THR:HG21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:673:G:O3'	6:F:87:ARG:NH2	2.49	0.45
12:L:42:THR:CG2	12:L:52:LEU:HB3	2.47	0.45
1:A:187:C:H4'	20:T:86:ARG:HG3	1.99	0.45
1:A:1420:C:H2'	1:A:1421:G:H8	1.81	0.45
1:A:1499:A:C1'	1:A:1520[A]:G:H5'	2.47	0.45
1:A:642:A:N3	8:H:113:SER:OG	2.41	0.45
1:A:866:C:C4	1:A:867:G:H1'	2.52	0.45
4:D:114:ARG:O	4:D:117:ALA:HB3	2.17	0.45
16:P:10:GLY:HA3	16:P:14:ASN:O	2.17	0.45
20:T:62:LEU:HD23	20:T:62:LEU:HA	1.76	0.45
20:T:60:GLU:HG3	20:T:81:LYS:HE3	1.99	0.45
1:A:741:G:H2'	1:A:742:G:O4'	2.17	0.45
2:B:102:LEU:HD11	2:B:162:ILE:HD11	1.99	0.45
15:O:84:LYS:HG2	15:O:85:LEU:HD23	1.98	0.45
17:Q:86:GLU:O	17:Q:90:ILE:HG12	2.17	0.45
1:A:1066:C:H5	1:A:1067:A:C6	2.35	0.44
1:A:1078:U:C5	1:A:1079:G:C5	3.05	0.44
1:A:1381:U:C2	7:G:156:TRP:HH2	2.34	0.44
1:A:1508:G:C5	1:A:1509:C:C5	3.05	0.44
1:A:263:A:P	20:T:79:ARG:HH11	2.39	0.44
1:A:115:G:O2'	1:A:289:G:H5''	2.17	0.44
1:A:560:U:H5'	1:A:566:G:N2	2.32	0.44
1:A:83:U:C4	1:A:84:U:C5	3.05	0.44
1:A:959:A:H3'	1:A:960:U:H5''	1.99	0.44
4:D:88:VAL:HG12	4:D:90:GLY:H	1.81	0.44
9:I:45:ALA:O	9:I:48:GLU:HB2	2.17	0.44
10:J:55:LYS:HZ2	10:J:56:HIS:N	2.14	0.44
16:P:78:GLY:N	24:P:208:HOH:O	2.46	0.44
1:A:21:G:C2	1:A:22:G:C6	3.05	0.44
1:A:353:A:H5'	1:A:353:A:H8	1.82	0.44
1:A:532:A:N6	3:C:159:GLY:O	2.50	0.44
4:D:3:ARG:HG3	4:D:118:ARG:HH11	1.82	0.44
6:F:14:LEU:HD13	6:F:18:GLN:HB3	1.99	0.44
7:G:145:ALA:C	7:G:147:ALA:H	2.19	0.44
9:I:79:LEU:O	9:I:83:ARG:HG2	2.17	0.44
19:S:16:LEU:O	19:S:19:VAL:HG12	2.17	0.44
1:A:501:C:OP1	12:L:117:ARG:NH2	2.46	0.44
7:G:109:ASN:OD1	7:G:119:ARG:NH2	2.50	0.44
8:H:124:ALA:O	8:H:128:GLY:N	2.47	0.44
1:A:1066:C:C5	1:A:1067:A:C6	3.06	0.44
1:A:604:G:C5	1:A:605:U:C5	3.05	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:C:H2'	1:A:92:C:O2	2.17	0.44
2:B:177:ALA:HB1	2:B:182:ILE:HB	1.98	0.44
3:C:70:VAL:HG21	3:C:76:VAL:HG21	1.99	0.44
4:D:25:ARG:HH21	4:D:30:LYS:HB3	1.83	0.44
1:A:921:U:O2'	5:E:19:MET:O	2.35	0.44
1:A:1291:G:OP1	7:G:41:ARG:NH2	2.50	0.44
1:A:1148:U:H4'	9:I:14:VAL:HG11	2.00	0.44
14:N:3:ARG:HH21	14:N:5:ALA:HB3	1.81	0.44
16:P:18:ARG:HD3	16:P:35:LYS:HD2	1.99	0.44
20:T:33:ILE:HD11	20:T:63:ILE:HA	1.99	0.44
20:T:74:LYS:HB2	20:T:76:ALA:H	1.81	0.44
2:B:189:ASP:OD1	2:B:205:ASP:HB3	2.16	0.44
2:B:21:ARG:HD3	2:B:22:LYS:H	1.83	0.44
4:D:57:ARG:HG3	4:D:202:LEU:CD1	2.46	0.44
7:G:76:ARG:HD2	7:G:89:MET:SD	2.58	0.44
10:J:55:LYS:HZ2	10:J:56:HIS:H	1.66	0.44
13:M:2:ALA:N	13:M:9:ILE:HG23	2.33	0.44
1:A:1010:G:N2	1:A:1019:C:O2	2.37	0.44
1:A:1105:A:H2'	1:A:1106:G:C8	2.53	0.44
1:A:134:A:H2'	1:A:135:C:O4'	2.18	0.44
1:A:922:G:C2	1:A:1396:A:C6	3.06	0.44
1:A:243:A:C2	1:A:246:A:C8	3.05	0.44
1:A:691:G:H2'	1:A:692:U:C6	2.52	0.44
1:A:942:G:N2	1:A:943:U:C2	2.86	0.44
4:D:19:LEU:HD21	4:D:67:ILE:HG12	1.99	0.44
5:E:28:PHE:HB2	5:E:48:ALA:O	2.18	0.44
7:G:18:TYR:CE2	7:G:59:LEU:HB2	2.53	0.44
8:H:119:LEU:HD13	8:H:124:ALA:HA	1.98	0.44
8:H:123:GLU:HG2	8:H:126:LYS:NZ	2.33	0.44
1:A:538:G:OP1	12:L:115:LYS:N	2.51	0.44
20:T:49:ALA:HB3	20:T:99:LEU:HD12	1.99	0.44
1:A:391:G:C6	1:A:392:G:C5	3.05	0.44
1:A:413:G:O6	4:D:36:ARG:NH1	2.51	0.44
4:D:72:GLU:O	4:D:75:PHE:HB3	2.17	0.44
6:F:1:MET:HB3	6:F:67:MET:O	2.18	0.44
7:G:86:GLN:HB2	7:G:148:ASN:ND2	2.32	0.44
12:L:70:ILE:HA	12:L:71:PRO:HD3	1.84	0.44
13:M:97:PRO:HB2	13:M:101:GLN:OE1	2.17	0.44
16:P:51:VAL:HG12	16:P:53:VAL:N	2.33	0.44
17:Q:22:LEU:HA	17:Q:22:LEU:HD12	1.24	0.44
1:A:224:C:H2'	1:A:225:C:C6	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:215:LEU:HD23	2:B:215:LEU:HA	1.81	0.44
3:C:166:GLU:HA	3:C:166:GLU:OE1	2.18	0.44
4:D:114:ARG:HG3	4:D:114:ARG:HH11	1.82	0.44
6:F:80:ARG:NH1	6:F:88:VAL:H	2.16	0.44
8:H:82:HIS:ND1	8:H:138:TRP:NE1	2.65	0.44
8:H:86:ILE:HG22	8:H:133:LEU:O	2.18	0.44
3:C:59:ARG:H	10:J:92:THR:HG23	1.83	0.44
12:L:124:LYS:HD3	12:L:125:PRO:HD2	2.00	0.44
12:L:46:LYS:HE2	12:L:94:PRO:HG2	2.00	0.44
20:T:41:ILE:HA	20:T:41:ILE:HD12	1.69	0.44
21:U:6:ARG:O	21:U:12:LYS:HE2	2.17	0.44
1:A:1226:C:OP1	13:M:91:ARG:NH1	2.49	0.44
1:A:937:A:N6	1:A:1345:U:O4	2.49	0.44
1:A:971:G:H1'	1:A:1365:G:O2'	2.17	0.44
1:A:1366:C:H2'	1:A:1367:C:C6	2.51	0.44
1:A:9:G:C2	1:A:26:A:N1	2.86	0.44
1:A:502:G:P	12:L:118:SER:HG	2.41	0.44
1:A:624:C:H2'	1:A:625:G:C8	2.53	0.44
1:A:1368:G:OP2	9:I:112:LYS:HD3	2.18	0.44
12:L:25:PRO:C	12:L:27:LEU:N	2.64	0.44
1:A:502:G:H2'	1:A:503:C:O4'	2.17	0.43
1:A:1073:U:OP2	5:E:57:LYS:HE2	2.18	0.43
16:P:43:LYS:HG2	16:P:48:TRP:CG	2.53	0.43
17:Q:51:TYR:CD1	17:Q:73:VAL:HG11	2.53	0.43
17:Q:59:ILE:HA	17:Q:59:ILE:HD13	1.67	0.43
20:T:53:LEU:HD22	20:T:53:LEU:HA	1.52	0.43
1:A:1324:A:H2'	1:A:1325:C:O4'	2.17	0.43
1:A:721:G:C6	1:A:733:A:C2	3.05	0.43
4:D:107:ARG:HH21	4:D:194:LEU:HD11	1.83	0.43
7:G:70:LYS:HG2	7:G:100:ALA:HB2	2.00	0.43
17:Q:5:VAL:HG22	17:Q:60:ILE:HD11	2.00	0.43
1:A:1118:C:H1'	1:A:1179:A:C4	2.53	0.43
1:A:1202:G:C6	14:N:42:ILE:HG21	2.53	0.43
1:A:624:C:H2'	1:A:625:G:H8	1.82	0.43
1:A:960:U:H1'	1:A:1223:C:H5'	1.99	0.43
2:B:61:LEU:HD21	2:B:160:ASP:HB2	1.99	0.43
2:B:82:ARG:HA	2:B:92:TYR:CE1	2.53	0.43
3:C:125:GLU:HG2	3:C:189:ALA:HB1	1.99	0.43
3:C:11:ARG:HB3	3:C:16:ARG:HB2	1.99	0.43
4:D:10:ARG:O	4:D:13:ARG:HB2	2.18	0.43
6:F:28:ARG:HA	6:F:31:GLU:CD	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:86:ARG:H	6:F:86:ARG:HG2	1.59	0.43
1:A:1232:U:OP1	9:I:126:SER:HB3	2.18	0.43
1:A:975:A:H62	10:J:60:ARG:NH2	2.17	0.43
11:K:38:ASN:HA	11:K:39:PRO:HD3	1.69	0.43
17:Q:18:THR:HG23	17:Q:69:LYS:HE3	2.00	0.43
20:T:43:LEU:HG	20:T:55:ILE:CD1	2.48	0.43
1:A:1064:G:H21	1:A:1190:G:H2'	1.84	0.43
1:A:1190:G:H5''	1:A:1190:G:H8	1.83	0.43
1:A:1202:G:H2'	1:A:1203:C:O4'	2.19	0.43
1:A:345:C:C6	1:A:345:C:OP2	2.71	0.43
1:A:31:G:N2	1:A:48:C:OP1	2.46	0.43
1:A:561:U:O2'	1:A:562:C:OP1	2.32	0.43
2:B:21:ARG:HG3	2:B:21:ARG:H	1.55	0.43
3:C:10:PHE:CZ	3:C:178:LEU:HD12	2.53	0.43
5:E:84:PHE:CE1	5:E:133:TYR:HB3	2.53	0.43
8:H:104:ARG:HD2	8:H:104:ARG:HA	1.67	0.43
9:I:97:LYS:HA	9:I:97:LYS:HD3	1.78	0.43
1:A:1358:U:H5''	14:N:35:ARG:CD	2.48	0.43
15:O:3:ILE:HA	15:O:7:GLU:OE1	2.18	0.43
1:A:626:U:H5''	16:P:38:TYR:CD2	2.53	0.43
16:P:68:ASP:OD1	16:P:68:ASP:N	2.50	0.43
16:P:82:GLN:H	16:P:82:GLN:HG2	1.65	0.43
17:Q:93:GLN:HG2	17:Q:96:GLN:HE22	1.83	0.43
18:R:54:ARG:HE	18:R:54:ARG:HB2	1.33	0.43
1:A:1010:G:H2'	1:A:1011:G:H8	1.84	0.43
1:A:1128:C:H42	1:A:1143:G:H1	1.67	0.43
1:A:1436:U:H2'	1:A:1437:C:C6	2.54	0.43
1:A:1517[A]:G:H2'	1:A:1518[A]:MA6:H8	2.00	0.43
1:A:1516[B]:G:H2'	1:A:1518[B]:MA6:OP2	2.18	0.43
1:A:409:G:OP1	4:D:24:GLU:O	2.36	0.43
1:A:429:U:H1'	1:A:430:A:H5''	2.01	0.43
1:A:445:G:C2	1:A:490:G:C2	3.07	0.43
8:H:105:ARG:HA	8:H:105:ARG:HD3	1.72	0.43
8:H:35:ILE:HG12	8:H:35:ILE:H	1.22	0.43
13:M:103:THR:HG23	24:M:304:HOH:O	2.18	0.43
13:M:19:LEU:HD22	13:M:22:ILE:HD13	2.01	0.43
20:T:85:MET:HG2	20:T:104:LEU:HD21	2.00	0.43
20:T:44:ALA:HB1	20:T:91:LEU:HB3	2.01	0.43
21:U:14:TRP:HZ3	21:U:15:ARG:HH21	1.65	0.43
1:A:115:G:H5''	24:A:2264:HOH:O	2.17	0.43
1:A:1182:G:H8	1:A:1182:G:H2'	1.74	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1197:G:H2'	1:A:1197:G:N3	2.33	0.43
1:A:401:C:H2'	1:A:402:G:C8	2.52	0.43
1:A:501:C:O3'	12:L:118:SER:OG	2.35	0.43
3:C:22:TRP:CD1	3:C:59:ARG:HG3	2.53	0.43
4:D:70:ILE:HG22	4:D:71:SER:N	2.33	0.43
5:E:145:LYS:O	5:E:148:VAL:HG23	2.19	0.43
5:E:76:ILE:HG23	5:E:142:LEU:HD11	2.00	0.43
9:I:27:THR:CG2	9:I:62:TYR:HA	2.49	0.43
11:K:54:ARG:HH11	11:K:54:ARG:HB3	1.84	0.43
12:L:76:ASN:OD1	12:L:76:ASN:N	2.48	0.43
17:Q:89:LEU:HD23	17:Q:89:LEU:HA	1.63	0.43
18:R:31:LEU:HD22	18:R:65:ILE:HG22	2.01	0.43
19:S:5:LEU:HD13	19:S:9:VAL:HG13	2.01	0.43
20:T:52:ALA:HA	20:T:55:ILE:HD12	2.01	0.43
20:T:88:VAL:O	20:T:92:LEU:HD23	2.18	0.43
1:A:190(E):U:C4	17:Q:72:ARG:NH2	2.87	0.43
1:A:760:G:H2'	1:A:761:G:O4'	2.18	0.43
1:A:826:C:C2	1:A:827:U:C5	3.07	0.43
3:C:36:ASP:HA	3:C:39:ILE:CD1	2.48	0.43
7:G:97:GLN:O	7:G:101:LEU:HD12	2.19	0.43
9:I:17:VAL:HA	9:I:63:ILE:HG12	2.01	0.43
1:A:553:A:O2'	12:L:29:GLY:O	2.34	0.43
12:L:41:ARG:HH21	12:L:43:VAL:HG22	1.84	0.43
13:M:34:LEU:HD13	13:M:39:ILE:HB	2.00	0.43
13:M:87:TYR:HA	13:M:90:LEU:HG	2.00	0.43
19:S:29:ARG:N	19:S:29:ARG:HD2	2.33	0.43
1:A:986:A:H1'	19:S:54:GLY:O	2.19	0.43
1:A:1007:C:H1'	1:A:1023:G:H22	1.84	0.43
1:A:1065:U:H4'	1:A:1066:C:O5'	2.17	0.43
1:A:1443:G:H4'	1:A:1446:A:O5'	2.19	0.43
1:A:786:G:C2	1:A:797:C:C2	3.06	0.43
1:A:952:U:H2'	1:A:953:G:C8	2.50	0.43
2:B:79:ASP:HA	2:B:82:ARG:HB3	2.01	0.43
3:C:155:GLY:HA2	3:C:164:ARG:H	1.84	0.43
5:E:43:LEU:HG	5:E:44:GLY:N	2.34	0.43
7:G:5:ARG:HD2	7:G:5:ARG:HA	1.79	0.43
8:H:110:ALA:HB3	8:H:121:ASP:HB3	2.00	0.43
10:J:6:ILE:HG12	10:J:98:ILE:HG12	2.00	0.43
11:K:86:GLY:H	11:K:112:THR:HG23	1.84	0.43
12:L:19:ARG:HA	12:L:20:LYS:HZ2	1.82	0.43
12:L:6:THR:N	12:L:9:GLN:HG2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:69:TYR:CD1	12:L:90:VAL:HG21	2.53	0.43
1:A:1268:A:H2'	1:A:1269:A:C8	2.54	0.43
1:A:1516[B]:G:N2	1:A:1519[B]:MA6:OP2	2.52	0.43
1:A:686:U:O2'	1:A:687:A:H8	2.02	0.43
1:A:786:G:H2'	1:A:787:A:O4'	2.18	0.43
1:A:837:G:H1	1:A:849:C:H42	1.65	0.43
1:A:955:U:H1'	1:A:1227:A:N6	2.34	0.43
4:D:115:ARG:HH11	4:D:115:ARG:HB3	1.83	0.43
4:D:128:VAL:HG12	4:D:129:ASN:ND2	2.34	0.43
12:L:7:ILE:HA	12:L:7:ILE:HD13	1.47	0.43
16:P:60:LEU:HD23	16:P:60:LEU:HA	1.60	0.43
1:A:1199:U:O5'	1:A:1199:U:H6	2.02	0.43
1:A:1500:A:OP2	1:A:1505:G:OP1	2.37	0.43
1:A:474:G:H2'	1:A:475:G:C8	2.54	0.43
1:A:544:G:C5	1:A:545:C:C5	3.07	0.43
1:A:676:A:C1'	11:K:115:PRO:HB3	2.49	0.43
1:A:907:A:C4	1:A:908:A:C8	3.07	0.43
1:A:957:U:H1'	1:A:960:U:N3	2.34	0.43
4:D:108:LEU:HD22	4:D:176:LEU:HD12	2.01	0.43
4:D:38:TYR:CE1	4:D:45:GLN:HG3	2.54	0.43
7:G:111:ARG:HG2	7:G:112:PRO:HD2	2.01	0.43
20:T:66:ALA:HB3	20:T:72:LEU:HD12	2.01	0.43
1:A:1072:G:C5	1:A:1073:U:C4	3.06	0.42
1:A:1232:U:H5''	9:I:124:GLN:O	2.19	0.42
1:A:1337:G:H5''	1:A:1338:G:OP1	2.19	0.42
1:A:390:C:H2'	1:A:391:G:C8	2.54	0.42
1:A:613:C:H42	1:A:627:G:H1	1.67	0.42
2:B:55:PHE:HE2	2:B:218:ALA:HA	1.84	0.42
5:E:45:PHE:HD2	5:E:47:LYS:HZ2	1.67	0.42
8:H:10:LEU:HA	8:H:10:LEU:HD23	1.55	0.42
10:J:46:ARG:CZ	10:J:46:ARG:HB2	2.49	0.42
16:P:3:LYS:HD3	16:P:24:ALA:HB2	2.00	0.42
19:S:22:LEU:HD22	19:S:47:HIS:CE1	2.54	0.42
19:S:41:VAL:HG22	19:S:44:MET:SD	2.59	0.42
1:A:1442:G:C5	1:A:1446:A:N6	2.87	0.42
2:B:75:LYS:HD3	2:B:75:LYS:HA	1.96	0.42
3:C:50:ALA:O	3:C:70:VAL:HG12	2.19	0.42
4:D:3:ARG:HD3	4:D:3:ARG:HA	1.86	0.42
5:E:31:LEU:HD23	5:E:44:GLY:O	2.19	0.42
6:F:62:TRP:CH2	6:F:64:GLN:HB2	2.54	0.42
13:M:102:ARG:HA	24:M:304:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:U:H4'	17:Q:63:ARG:HD3	2.01	0.42
1:A:954:G:C5	1:A:955:U:C4	3.07	0.42
5:E:37:ARG:O	5:E:114:GLY:HA3	2.19	0.42
8:H:111:ILE:HG22	8:H:134:ILE:HD12	2.01	0.42
8:H:21:LYS:O	8:H:65:TYR:OH	2.26	0.42
10:J:32:ALA:O	10:J:34:VAL:HG23	2.19	0.42
12:L:28:LYS:HG3	12:L:33:ARG:NH2	2.34	0.42
12:L:42:THR:HG23	12:L:52:LEU:HB3	2.00	0.42
1:A:522:C:H41	12:L:53:ARG:HH22	1.67	0.42
13:M:17:VAL:O	13:M:20:THR:HB	2.19	0.42
17:Q:43:LEU:HD23	17:Q:43:LEU:HA	1.58	0.42
20:T:18:GLN:O	20:T:21:LYS:HB2	2.19	0.42
20:T:56:MET:HE2	20:T:56:MET:HB3	1.71	0.42
1:A:1126:U:H6	1:A:1126:U:O5'	2.01	0.42
1:A:115:G:H8	1:A:115:G:O5'	2.02	0.42
1:A:1265:G:C6	1:A:1266:G:C6	3.07	0.42
1:A:1308:U:OP2	13:M:99:ARG:HG2	2.19	0.42
1:A:1530:G:OP1	1:A:1530:G:H4'	2.18	0.42
1:A:272:C:H2'	1:A:273:A:H8	1.84	0.42
1:A:517:G:N1	1:A:533:A:OP2	2.45	0.42
1:A:61:G:H2'	1:A:62:U:O4'	2.18	0.42
1:A:945:G:N1	1:A:1337:G:C2	2.87	0.42
1:A:954:G:C6	1:A:955:U:N3	2.87	0.42
2:B:77:ALA:HB2	2:B:211:ILE:HD13	2.01	0.42
3:C:182:ILE:HG22	3:C:183:ASP:O	2.19	0.42
3:C:95:THR:O	3:C:95:THR:OG1	2.35	0.42
5:E:101:ILE:O	5:E:120:THR:HB	2.19	0.42
7:G:136:LYS:HB3	7:G:136:LYS:HE3	1.82	0.42
10:J:79:ARG:NH2	10:J:82:ILE:HB	2.34	0.42
12:L:69:TYR:O	12:L:100:ILE:HB	2.19	0.42
16:P:38:TYR:O	16:P:49:LEU:HD12	2.20	0.42
6:F:94:GLN:HB3	18:R:32:ARG:NH1	2.34	0.42
1:A:1047:G:O2'	1:A:1048:G:H5'	2.19	0.42
1:A:1119:C:N4	1:A:1154:G:H1	2.15	0.42
1:A:1287:A:H2'	1:A:1288:A:C8	2.55	0.42
1:A:1420:C:H2'	1:A:1421:G:C8	2.55	0.42
1:A:1419:G:H1	1:A:1481:U:H3	1.68	0.42
1:A:22:G:H2'	1:A:23:C:H6	1.83	0.42
1:A:359:U:H2'	1:A:360:A:H8	1.84	0.42
1:A:544:G:C6	1:A:545:C:C4	3.07	0.42
1:A:75:G:C2	1:A:76:C:N3	2.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:G:C2	1:A:80:G:N7	2.87	0.42
1:A:1190:G:O3'	3:C:3:ASN:HB2	2.19	0.42
4:D:31:CYS:SG	4:D:31:CYS:O	2.78	0.42
1:A:939:G:H5''	7:G:102:ARG:NH2	2.34	0.42
7:G:86:GLN:HB2	7:G:148:ASN:HD22	1.84	0.42
1:A:1329:A:OP1	13:M:28:ALA:HB3	2.20	0.42
1:A:1374:A:C4	1:A:1375:A:C8	3.08	0.42
1:A:1516[A]:G:N2	1:A:1519[A]:MA6:OP2	2.26	0.42
1:A:179:A:H2'	1:A:180:U:H6	1.84	0.42
1:A:7:G:H5'	1:A:298:A:O4'	2.19	0.42
1:A:788:U:H2'	1:A:789:U:H6	1.85	0.42
1:A:918:A:H2'	1:A:919:A:H8	1.82	0.42
1:A:1130:A:H5''	9:I:20:ARG:HH21	1.83	0.42
20:T:88:VAL:HG12	20:T:89:ARG:N	2.34	0.42
1:A:1258:G:H1	1:A:1277:C:H42	1.65	0.42
1:A:1285:A:H4'	1:A:1286:A:O5'	2.19	0.42
1:A:313:A:H2'	1:A:314:C:C6	2.55	0.42
1:A:393:A:O2'	1:A:394:G:H5'	2.20	0.42
1:A:75:G:N1	1:A:96:G:C6	2.87	0.42
1:A:975:A:H4'	1:A:976:G:O5'	2.20	0.42
8:H:11:THR:O	8:H:14:ARG:N	2.53	0.42
8:H:87:SER:HB2	8:H:133:LEU:O	2.19	0.42
12:L:19:ARG:HA	12:L:20:LYS:HZ3	1.84	0.42
13:M:56:LEU:HD23	13:M:56:LEU:HA	1.73	0.42
20:T:87:LYS:O	20:T:91:LEU:HB2	2.19	0.42
1:A:122:G:C2	1:A:123:C:C2	3.08	0.42
1:A:976:G:N2	1:A:1362:C:OP2	2.46	0.42
1:A:853:G:H2'	1:A:854:G:H5'	2.01	0.42
3:C:108:ASN:HA	3:C:109:PRO:HD2	1.85	0.42
3:C:6:HIS:HA	3:C:7:PRO:HD3	1.72	0.42
4:D:15:GLU:OE1	4:D:59:ARG:NH2	2.52	0.42
5:E:122:GLU:O	5:E:123:LEU:HD23	2.20	0.42
5:E:41:VAL:HG13	5:E:113:ALA:HA	2.01	0.42
7:G:47:CYS:O	7:G:50:ILE:HG22	2.19	0.42
9:I:50:LEU:HD11	9:I:81:ILE:HG21	2.01	0.42
12:L:60:LEU:HD13	12:L:60:LEU:HA	1.69	0.42
13:M:60:VAL:HG22	13:M:64:TRP:HZ3	1.82	0.42
18:R:76:LEU:HA	18:R:76:LEU:HD23	1.50	0.42
20:T:25:ARG:HB2	20:T:25:ARG:HE	1.28	0.42
21:U:15:ARG:HG2	21:U:17:THR:OG1	2.20	0.42
1:A:413:G:H2'	1:A:428:G:H22	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:768:A:N3	1:A:1512:U:O2'	2.53	0.42
1:A:424:G:H2'	1:A:425:G:H8	1.84	0.42
1:A:512:U:O2	1:A:540:G:C2	2.73	0.42
1:A:673:G:H5''	6:F:87:ARG:CZ	2.50	0.42
2:B:97:TRP:CH2	2:B:102:LEU:HD22	2.51	0.42
4:D:105:VAL:HG13	4:D:110:PHE:HB2	2.01	0.42
4:D:158:ILE:HG13	4:D:158:ILE:H	1.40	0.42
4:D:196:LEU:O	4:D:196:LEU:HD12	2.20	0.42
4:D:19:LEU:HD11	4:D:67:ILE:HG12	2.02	0.42
8:H:127:LEU:HB3	8:H:129:VAL:CG2	2.50	0.42
15:O:44:LYS:HB3	15:O:44:LYS:HE3	1.59	0.42
1:A:1093:A:N3	1:A:1095:U:H5'	2.34	0.41
1:A:1283:G:H2'	1:A:1284:C:C6	2.55	0.41
1:A:1315:U:OP2	19:S:6:LYS:NZ	2.53	0.41
1:A:39:G:N1	1:A:40:C:C4	2.88	0.41
1:A:78:G:H2'	1:A:79:G:C5'	2.50	0.41
1:A:949:A:H1'	1:A:1364:U:H3	1.85	0.41
11:K:54:ARG:NH1	11:K:54:ARG:HB3	2.35	0.41
12:L:20:LYS:CD	12:L:20:LYS:H	2.33	0.41
13:M:107:ALA:HB3	13:M:111:LYS:HE3	2.02	0.41
15:O:76:GLU:O	15:O:79:ARG:N	2.53	0.41
17:Q:40:LYS:HD3	17:Q:42:TYR:OH	2.19	0.41
1:A:112:G:C2	1:A:113:G:C8	3.08	0.41
1:A:1343:G:H4'	9:I:122:ALA:HB3	2.02	0.41
1:A:244:U:C6	1:A:894:G:N2	2.88	0.41
1:A:66:G:N3	1:A:66:G:H2'	2.35	0.41
1:A:77:G:O2'	1:A:78:G:H5'	2.20	0.41
2:B:64:ARG:HB2	2:B:64:ARG:CZ	2.50	0.41
7:G:18:TYR:CD2	7:G:59:LEU:HB2	2.55	0.41
8:H:11:THR:O	8:H:12:ARG:C	2.57	0.41
14:N:37:PHE:HB3	14:N:39:LEU:HB2	2.01	0.41
16:P:34:GLU:HG2	16:P:36:ILE:HG23	2.02	0.41
16:P:81:ARG:N	24:P:207:HOH:O	2.53	0.41
20:T:48:LYS:HE2	20:T:48:LYS:HB3	1.95	0.41
1:A:1062:U:H2'	1:A:1063:C:C6	2.55	0.41
1:A:1092:A:H5''	1:A:1093:A:OP2	2.20	0.41
1:A:445:G:H1	1:A:489:C:H42	1.67	0.41
1:A:966:M2G:HM13	1:A:967:5MC:H1'	2.01	0.41
4:D:25:ARG:HE	4:D:30:LYS:HB2	1.86	0.41
5:E:122:GLU:OE2	5:E:131:ILE:HG21	2.20	0.41
8:H:116:LYS:NZ	8:H:127:LEU:HD12	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:2:LEU:HD23	8:H:2:LEU:C	2.40	0.41
13:M:23:TYR:HB3	13:M:67:GLU:H	1.85	0.41
11:K:108:ILE:HB	18:R:87:ARG:O	2.21	0.41
1:A:1222:G:P	19:S:77:THR:HG21	2.61	0.41
20:T:34:LYS:HB3	20:T:38:LYS:HE3	2.02	0.41
1:A:1073:U:O2	2:B:104:ASN:ND2	2.54	0.41
1:A:1394:A:N6	1:A:1501:C:H5'	2.35	0.41
1:A:815:A:N6	1:A:1509:C:H1'	2.35	0.41
1:A:1530:G:H2'	1:A:1531:A:C8	2.56	0.41
1:A:582:U:H2'	1:A:583:A:C8	2.54	0.41
1:A:755:G:OP2	15:O:65:ARG:HG2	2.21	0.41
5:E:142:LEU:HA	5:E:142:LEU:HD23	1.45	0.41
20:T:25:ARG:O	20:T:28:ALA:HB3	2.20	0.41
1:A:1063:C:C2	1:A:1064:G:N7	2.88	0.41
1:A:1430:C:C2	1:A:1471:G:N2	2.88	0.41
1:A:297:G:N2	1:A:300:A:OP2	2.52	0.41
1:A:554:C:O2'	1:A:555:C:H5'	2.20	0.41
1:A:789:U:O2	1:A:791:G:C8	2.74	0.41
3:C:154:SER:OG	3:C:197:GLY:N	2.50	0.41
3:C:59:ARG:H	10:J:92:THR:CG2	2.33	0.41
4:D:100:ARG:NH1	4:D:137:SER:HA	2.35	0.41
6:F:46:ARG:HH22	18:R:37:VAL:HG21	1.84	0.41
12:L:20:LYS:H	12:L:20:LYS:CE	2.33	0.41
18:R:50:ILE:HD11	18:R:70:ILE:HG21	2.02	0.41
18:R:79:LEU:HA	18:R:80:PRO:HD3	1.72	0.41
1:A:1015:A:H2'	1:A:1016:A:C8	2.55	0.41
1:A:1144:G:N2	1:A:1145:C:C2	2.84	0.41
1:A:1157:A:C2	1:A:1181:G:N3	2.89	0.41
1:A:445:G:C2	1:A:490:G:N1	2.88	0.41
1:A:631:G:H2'	1:A:632:A:C8	2.55	0.41
1:A:644:G:C5	1:A:645:C:C5	3.08	0.41
1:A:964:A:N6	24:A:2280:HOH:O	2.53	0.41
2:B:55:PHE:HD2	2:B:58:ILE:HD12	1.85	0.41
4:D:88:VAL:HG12	4:D:91:SER:H	1.85	0.41
5:E:118:ILE:O	5:E:119:LEU:HD23	2.21	0.41
6:F:14:LEU:HD21	6:F:84:ASN:OD1	2.21	0.41
6:F:44:GLY:HA2	6:F:59:TYR:CD2	2.56	0.41
6:F:38:GLU:HB2	6:F:64:GLN:HG2	2.03	0.41
9:I:19:LEU:HD23	9:I:60:ASP:O	2.19	0.41
18:R:26:LEU:HD23	18:R:29:PHE:CE2	2.55	0.41
21:U:18:TYR:HB2	21:U:24:ARG:HH21	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1018:C:H2'	1:A:1019:C:O4'	2.21	0.41
1:A:1063:C:OP2	1:A:1064:G:O2'	2.37	0.41
1:A:1014:A:C2	1:A:1219:U:H1'	2.56	0.41
1:A:142:G:H2'	1:A:143:A:H8	1.85	0.41
1:A:200:G:H2'	1:A:201:C:O4'	2.20	0.41
4:D:155:LEU:HD23	4:D:156:GLU:N	2.35	0.41
5:E:78:HIS:ND1	8:H:104:ARG:HG3	2.36	0.41
7:G:89:MET:HA	7:G:155:ARG:NH1	2.36	0.41
8:H:2:LEU:HD23	8:H:3:THR:H	1.81	0.41
8:H:59:LEU:HA	8:H:59:LEU:HD23	1.65	0.41
7:G:40:ALA:CB	9:I:41:VAL:HG21	2.51	0.41
10:J:21:GLN:O	10:J:25:GLU:HG3	2.20	0.41
10:J:81:THR:O	10:J:85:LEU:HD13	2.20	0.41
12:L:114:LYS:HB3	12:L:114:LYS:HE2	1.78	0.41
12:L:46:LYS:HB3	12:L:92:0TD:H8	2.03	0.41
13:M:82:MET:HA	13:M:89:GLY:HA3	2.02	0.41
17:Q:5:VAL:C	17:Q:6:LEU:HD23	2.40	0.41
17:Q:5:VAL:HG22	17:Q:60:ILE:CD1	2.51	0.41
1:A:1005:A:C2	1:A:1026:G:N3	2.89	0.41
1:A:1181:G:HO2'	1:A:1182:G:C5'	2.34	0.41
1:A:77:G:C5	1:A:93:G:C2	3.09	0.41
3:C:151:VAL:C	3:C:152:ILE:HG13	2.41	0.41
3:C:18:TRP:O	3:C:21:ARG:NH1	2.54	0.41
3:C:73:PRO:O	3:C:76:VAL:HB	2.20	0.41
5:E:107:ARG:O	5:E:111:GLU:HB2	2.20	0.41
6:F:74:ASP:OD2	6:F:74:ASP:N	2.54	0.41
14:N:39:LEU:HA	14:N:39:LEU:HD23	1.71	0.41
16:P:2:VAL:HG22	16:P:64:ALA:HB2	2.03	0.41
17:Q:83:ASP:OD1	17:Q:84:LEU:HD12	2.21	0.41
19:S:23:ASN:ND2	19:S:43:GLU:O	2.48	0.41
1:A:1168:A:H2'	1:A:1169:A:C8	2.56	0.41
1:A:1491:G:N2	1:A:1492:A:C8	2.89	0.41
1:A:422:C:H5"	1:A:423:G:C4	2.56	0.41
1:A:809:G:C6	1:A:810:C:C5	3.09	0.41
1:A:91:C:H5"	1:A:92:C:OP2	2.21	0.41
1:A:737:A:OP1	6:F:91:VAL:HG13	2.20	0.41
7:G:35:LYS:HD3	7:G:38:LEU:HD13	2.02	0.41
15:O:38:ARG:HD3	15:O:38:ARG:HA	1.84	0.41
18:R:70:ILE:HG22	18:R:71:LYS:N	2.35	0.41
1:A:1310:G:C2	1:A:1328:C:N3	2.89	0.41
1:A:448:A:C4	1:A:487:A:C2	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:A:N1	1:A:107:G:O2'	2.41	0.41
1:A:789:U:O2	1:A:789:U:H2'	2.21	0.41
1:A:794:A:N6	1:A:795:C:N4	2.68	0.41
1:A:951:G:H1	1:A:1230:C:H42	1.69	0.41
8:H:6:ILE:HB	8:H:85:ARG:HH21	1.82	0.41
9:I:118:LYS:HD2	9:I:121:ARG:HB3	2.03	0.41
1:A:674:G:H21	11:K:116:HIS:HB2	1.85	0.41
12:L:84:LEU:HB2	12:L:104:VAL:HG11	2.03	0.41
20:T:51:GLU:O	20:T:54:LYS:HB3	2.21	0.41
1:A:193:C:H2'	1:A:194:C:H6	1.85	0.41
1:A:407:G:OP1	4:D:115:ARG:NH1	2.53	0.41
1:A:854:G:H3'	1:A:871:U:O4	2.21	0.41
1:A:986:A:H2'	1:A:987:G:O4'	2.21	0.41
4:D:121:VAL:HG11	4:D:136:PRO:HA	2.03	0.41
4:D:50:ARG:HA	4:D:51:PRO:HD2	1.94	0.41
6:F:31:GLU:HG3	6:F:31:GLU:H	1.75	0.41
8:H:56:LYS:HA	8:H:57:PRO:HD3	1.71	0.41
8:H:81:HIS:N	8:H:81:HIS:ND1	2.69	0.41
8:H:83:ILE:HG21	8:H:83:ILE:HD13	1.68	0.41
11:K:34:ASP:O	11:K:37:GLY:N	2.37	0.41
12:L:46:LYS:NZ	12:L:47:LYS:HE2	2.35	0.41
15:O:12:ILE:O	15:O:15:PHE:N	2.54	0.41
16:P:42:ARG:HB2	16:P:44:THR:HG23	2.03	0.41
16:P:80:PHE:N	24:P:210:HOH:O	2.30	0.41
1:A:113:G:H1	1:A:314:C:H42	1.69	0.40
1:A:16:A:N1	1:A:919:A:H2	2.20	0.40
1:A:236:G:H2'	1:A:237:C:O4'	2.21	0.40
1:A:45:U:H2'	1:A:46:G:C8	2.57	0.40
1:A:582:U:H2'	1:A:583:A:H8	1.87	0.40
1:A:77:G:C4	1:A:93:G:C2	3.09	0.40
2:B:112:VAL:HG22	2:B:149:LEU:HD13	2.02	0.40
2:B:162:ILE:CG2	2:B:184:VAL:HG13	2.51	0.40
2:B:172:ILE:H	2:B:172:ILE:HG13	1.64	0.40
3:C:179:ARG:HG3	3:C:179:ARG:NH1	2.33	0.40
4:D:187:ARG:HH12	4:D:188:LEU:HD12	1.86	0.40
8:H:120:THR:H	8:H:123:GLU:HB2	1.86	0.40
13:M:48:LEU:HD23	13:M:49:THR:N	2.36	0.40
15:O:76:GLU:N	15:O:79:ARG:HH21	2.19	0.40
17:Q:23:VAL:HG21	17:Q:42:TYR:CD1	2.56	0.40
20:T:36:LEU:O	20:T:39:LYS:HB3	2.20	0.40
21:U:17:THR:HG22	21:U:18:TYR:H	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:C:OP1	4:D:73:ARG:NH1	2.54	0.40
1:A:765:G:N1	1:A:812:C:O2'	2.44	0.40
2:B:163:PHE:HA	2:B:185:ILE:O	2.21	0.40
2:B:196:LEU:HA	2:B:196:LEU:HD23	1.74	0.40
2:B:187:LEU:HD22	2:B:201:ILE:O	2.21	0.40
2:B:31:TYR:HA	2:B:46:LYS:NZ	2.35	0.40
3:C:159:GLY:HA2	3:C:193:TYR:CG	2.55	0.40
5:E:81:GLU:OE1	5:E:88:LYS:HD2	2.22	0.40
5:E:94:ALA:HB2	5:E:119:LEU:HG	2.03	0.40
9:I:34:ASN:N	9:I:34:ASN:OD1	2.54	0.40
10:J:50:ILE:CD1	10:J:50:ILE:H	2.24	0.40
11:K:33:THR:OG1	11:K:34:ASP:N	2.55	0.40
11:K:95:ILE:HA	11:K:95:ILE:HD13	1.49	0.40
1:A:108:G:C6	20:T:15:ARG:HG3	2.57	0.40
1:A:1144:G:N2	1:A:1146:A:H62	2.19	0.40
1:A:1245:A:N1	1:A:1293:G:C2	2.89	0.40
1:A:232:G:H2'	1:A:233:C:H6	1.86	0.40
1:A:689:C:OP1	11:K:27:ASN:ND2	2.45	0.40
1:A:729:A:H2'	1:A:730:G:O4'	2.21	0.40
1:A:578:C:H42	1:A:763:G:H1	1.70	0.40
1:A:939:G:H5''	7:G:102:ARG:HH22	1.86	0.40
1:A:992:U:H3	1:A:1044:A:H62	1.68	0.40
3:C:113:ALA:O	3:C:116:VAL:HG23	2.21	0.40
5:E:108:ALA:O	5:E:112:LEU:HB2	2.20	0.40
6:F:101:ALA:HB2	18:R:28:GLU:HG3	2.03	0.40
1:A:932:C:H4'	7:G:4:ARG:NH2	2.37	0.40
9:I:7:THR:HG22	9:I:8:GLY:N	2.36	0.40
10:J:10:GLY:O	10:J:67:THR:HA	2.21	0.40
15:O:50:HIS:O	15:O:53:HIS:HB3	2.21	0.40
1:A:1163:C:H2'	1:A:1164:G:C8	2.56	0.40
1:A:1185:G:O2'	1:A:1186:G:H5''	2.21	0.40
1:A:1431:C:H42	1:A:1469:G:H1	1.68	0.40
1:A:688:G:H2'	1:A:689:C:C6	2.57	0.40
2:B:144:ARG:HG3	2:B:145:LEU:N	2.37	0.40
2:B:28:PHE:CD2	2:B:32:ILE:HD11	2.55	0.40
9:I:10:ARG:HG2	9:I:75:ASP:HB2	2.02	0.40
10:J:69:ASN:O	10:J:70:ARG:HD3	2.21	0.40
12:L:120:TYR:CD2	12:L:120:TYR:N	2.90	0.40
12:L:35:GLY:HA3	12:L:60:LEU:HD13	2.03	0.40
1:A:736:C:OP1	18:R:68:LYS:HD3	2.21	0.40
21:U:6:ARG:CD	21:U:15:ARG:HH12	2.33	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1007:C:O2	1:A:1023:G:C2	2.74	0.40
1:A:1022:G:N2	1:A:1024:G:C2	2.89	0.40
1:A:807:A:C6	1:A:808:C:C4	3.09	0.40
4:D:105:VAL:HG21	4:D:126:ILE:HG12	2.03	0.40
4:D:5:ILE:H	4:D:5:ILE:HD12	1.87	0.40
5:E:92:LYS:HA	5:E:93:PRO:HD3	1.88	0.40
6:F:8:ILE:HG22	6:F:10:LEU:HG	2.04	0.40
8:H:102:ARG:NH1	8:H:105:ARG:HD2	2.36	0.40
9:I:117:HIS:NE2	9:I:123:PRO:HB3	2.37	0.40
10:J:6:ILE:HG12	10:J:98:ILE:CD1	2.52	0.40
12:L:113:ARG:HH12	12:L:116:SER:H	1.69	0.40
13:M:51:ALA:HA	13:M:54:VAL:HG12	2.04	0.40
20:T:29:LYS:O	20:T:32:ALA:HB3	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	232/256 (91%)	209 (90%)	22 (10%)	1 (0%)	34	70
3	C	204/239 (85%)	180 (88%)	23 (11%)	1 (0%)	29	66
4	D	206/209 (99%)	195 (95%)	11 (5%)	0	100	100
5	E	148/162 (91%)	135 (91%)	13 (9%)	0	100	100
6	F	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
7	G	153/156 (98%)	136 (89%)	17 (11%)	0	100	100
8	H	136/138 (99%)	130 (96%)	6 (4%)	0	100	100
9	I	125/128 (98%)	113 (90%)	11 (9%)	1 (1%)	19	56
10	J	96/105 (91%)	80 (83%)	14 (15%)	2 (2%)	7	38
11	K	114/129 (88%)	101 (89%)	13 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	L	121/135 (90%)	108 (89%)	12 (10%)	1 (1%)	19	56
13	M	116/126 (92%)	100 (86%)	15 (13%)	1 (1%)	17	53
14	N	58/61 (95%)	48 (83%)	9 (16%)	1 (2%)	9	42
15	O	85/89 (96%)	77 (91%)	8 (9%)	0	100	100
16	P	81/88 (92%)	79 (98%)	2 (2%)	0	100	100
17	Q	97/105 (92%)	86 (89%)	11 (11%)	0	100	100
18	R	68/88 (77%)	59 (87%)	9 (13%)	0	100	100
19	S	78/93 (84%)	70 (90%)	7 (9%)	1 (1%)	12	46
20	T	97/106 (92%)	79 (81%)	18 (19%)	0	100	100
21	U	22/27 (82%)	18 (82%)	4 (18%)	0	100	100
All	All	2336/2541 (92%)	2097 (90%)	230 (10%)	9 (0%)	34	70

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	L	28	LYS
19	S	31	ILE
2	B	21	ARG
9	I	119	ALA
10	J	86	MET
14	N	31	ARG
10	J	34	VAL
13	M	84	ILE
3	C	76	VAL

### 5.3.2 Protein sidechains [i](#)

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%)	167 (83%)	35 (17%)	2	13
3	C	160/188 (85%)	130 (81%)	30 (19%)	1	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	180/181 (99%)	146 (81%)	34 (19%)	1	10
5	E	115/123 (94%)	87 (76%)	28 (24%)	0	5
6	F	90/90 (100%)	78 (87%)	12 (13%)	4	22
7	G	126/127 (99%)	110 (87%)	16 (13%)	4	23
8	H	119/119 (100%)	90 (76%)	29 (24%)	0	5
9	I	98/99 (99%)	84 (86%)	14 (14%)	3	20
10	J	87/92 (95%)	70 (80%)	17 (20%)	1	9
11	K	88/99 (89%)	75 (85%)	13 (15%)	3	18
12	L	103/110 (94%)	81 (79%)	22 (21%)	1	7
13	M	94/101 (93%)	79 (84%)	15 (16%)	2	16
14	N	49/50 (98%)	40 (82%)	9 (18%)	1	11
15	O	79/80 (99%)	64 (81%)	15 (19%)	1	10
16	P	72/74 (97%)	59 (82%)	13 (18%)	1	12
17	Q	94/97 (97%)	71 (76%)	23 (24%)	0	5
18	R	61/77 (79%)	54 (88%)	7 (12%)	5	26
19	S	71/80 (89%)	61 (86%)	10 (14%)	3	21
20	T	76/82 (93%)	58 (76%)	18 (24%)	1	5
21	U	19/22 (86%)	13 (68%)	6 (32%)	0	2
All	All	1983/2111 (94%)	1617 (82%)	366 (18%)	1	11

All (366) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	7	VAL
2	B	8	LYS
2	B	12	GLU
2	B	19	HIS
2	B	21	ARG
2	B	23	ARG
2	B	27	LYS
2	B	39	ILE
2	B	44	LEU
2	B	46	LYS
2	B	55	PHE
2	B	59	GLU
2	B	63	MET

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	B	67	THR
2	B	97	TRP
2	B	102	LEU
2	B	107	THR
2	B	113	HIS
2	B	114	ARG
2	B	126	GLU
2	B	127	ILE
2	B	128	GLU
2	B	139	LYS
2	B	142	LEU
2	B	158	LEU
2	B	160	ASP
2	B	162	ILE
2	B	168	THR
2	B	175	ARG
2	B	178	ARG
2	B	190	THR
2	B	196	LEU
2	B	200	ILE
2	B	217	ARG
2	B	221	LEU
3	C	3	ASN
3	C	11	ARG
3	C	16	ARG
3	C	17	ASP
3	C	26	LYS
3	C	37	GLN
3	C	52	LEU
3	C	58	GLU
3	C	70	VAL
3	C	72	LYS
3	C	79	ARG
3	C	84	ILE
3	C	91	LEU
3	C	99	VAL
3	C	105	GLU
3	C	107	GLN
3	C	111	LEU
3	C	116	VAL
3	C	132	ARG
3	C	153	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	C	165	THR
3	C	167	TRP
3	C	172	ARG
3	C	175	LEU
3	C	176	HIS
3	C	188	LEU
3	C	191	THR
3	C	192	THR
3	C	193	TYR
3	C	204	LEU
4	D	5	ILE
4	D	10	ARG
4	D	17	VAL
4	D	20	TYR
4	D	25	ARG
4	D	34	GLU
4	D	35	ARG
4	D	47	ARG
4	D	50	ARG
4	D	57	ARG
4	D	58	LEU
4	D	61	LYS
4	D	73	ARG
4	D	78	LEU
4	D	103	ASN
4	D	104	VAL
4	D	114	ARG
4	D	115	ARG
4	D	122	ARG
4	D	131	ARG
4	D	137	SER
4	D	141	ARG
4	D	145	GLU
4	D	155	LEU
4	D	157	LEU
4	D	158	ILE
4	D	160	GLN
4	D	176	LEU
4	D	178	VAL
4	D	187	ARG
4	D	192	GLU
4	D	194	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	D	196	LEU
4	D	202	LEU
5	E	5	ASP
5	E	6	PHE
5	E	12	LEU
5	E	14	ARG
5	E	15	ARG
5	E	19	MET
5	E	26	PHE
5	E	34	VAL
5	E	41	VAL
5	E	43	LEU
5	E	53	LEU
5	E	60	TYR
5	E	61	TYR
5	E	64	ARG
5	E	68	GLU
5	E	71	LEU
5	E	75	THR
5	E	79	GLU
5	E	80	ILE
5	E	84	PHE
5	E	100	VAL
5	E	112	LEU
5	E	117	ASP
5	E	125	SER
5	E	131	ILE
5	E	144	THR
5	E	148	VAL
5	E	150	ARG
6	F	1	MET
6	F	10	LEU
6	F	26	ILE
6	F	31	GLU
6	F	40	VAL
6	F	59	TYR
6	F	70	ASP
6	F	74	ASP
6	F	75	LEU
6	F	79	LEU
6	F	82	ARG
6	F	84	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
7	G	3	ARG
7	G	6	ARG
7	G	38	LEU
7	G	41	ARG
7	G	69	VAL
7	G	85	TYR
7	G	87	VAL
7	G	89	MET
7	G	92	SER
7	G	94	ARG
7	G	113	GLU
7	G	115	ARG
7	G	126	ASP
7	G	136	LYS
7	G	146	GLU
7	G	149	ARG
8	H	3	THR
8	H	12	ARG
8	H	14	ARG
8	H	19	VAL
8	H	25	ASP
8	H	29	SER
8	H	35	ILE
8	H	50	ARG
8	H	51	VAL
8	H	54	ASP
8	H	63	LEU
8	H	65	TYR
8	H	68	ARG
8	H	77	GLU
8	H	81	HIS
8	H	85	ARG
8	H	86	ILE
8	H	87	SER
8	H	88	LYS
8	H	91	ARG
8	H	92	ARG
8	H	95	VAL
8	H	97	VAL
8	H	104	ARG
8	H	109	ILE
8	H	127	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
8	H	129	VAL
8	H	133	LEU
8	H	137	VAL
9	I	20	ARG
9	I	34	ASN
9	I	35	GLU
9	I	56	LEU
9	I	64	THR
9	I	91	ASP
9	I	92	TYR
9	I	104	ARG
9	I	108	VAL
9	I	109	VAL
9	I	111	ARG
9	I	118	LYS
9	I	121	ARG
9	I	124	GLN
10	J	16	LEU
10	J	21	GLN
10	J	23	ILE
10	J	44	VAL
10	J	46	ARG
10	J	50	ILE
10	J	55	LYS
10	J	60	ARG
10	J	61	GLU
10	J	66	ARG
10	J	68	HIS
10	J	73	ASP
10	J	74	ILE
10	J	75	ILE
10	J	83	GLU
10	J	89	ASP
10	J	94	VAL
11	K	11	LYS
11	K	14	VAL
11	K	29	ILE
11	K	30	VAL
11	K	33	THR
11	K	53	SER
11	K	62	GLN
11	K	81	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
11	K	95	ILE
11	K	105	VAL
11	K	108	ILE
11	K	124	LYS
11	K	126	ARG
12	L	7	ILE
12	L	13	LYS
12	L	18	VAL
12	L	19	ARG
12	L	20	LYS
12	L	28	LYS
12	L	33	ARG
12	L	34	ARG
12	L	55	VAL
12	L	60	LEU
12	L	61	THR
12	L	64	TYR
12	L	65	GLU
12	L	66	VAL
12	L	67	THR
12	L	79	GLU
12	L	96	VAL
12	L	100	ILE
12	L	104	VAL
12	L	116	SER
12	L	122	THR
12	L	126	LYS
13	M	19	LEU
13	M	27	LYS
13	M	35	GLU
13	M	44	ARG
13	M	49	THR
13	M	50	GLU
13	M	53	VAL
13	M	54	VAL
13	M	60	VAL
13	M	64	TRP
13	M	77	ASN
13	M	88	ARG
13	M	103	THR
13	M	115	LYS
13	M	117	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
14	N	3	ARG
14	N	9	LYS
14	N	21	TYR
14	N	22	THR
14	N	25	VAL
14	N	33	VAL
14	N	40	CYS
14	N	41	ARG
14	N	42	ILE
15	O	8	LYS
15	O	22	THR
15	O	31	LEU
15	O	32	LEU
15	O	39	LEU
15	O	41	GLU
15	O	45	VAL
15	O	56	LEU
15	O	65	ARG
15	O	67	LEU
15	O	71	GLN
15	O	72	ARG
15	O	78	TYR
15	O	81	LEU
15	O	83	GLU
16	P	2	VAL
16	P	31	LYS
16	P	33	ILE
16	P	41	PRO
16	P	54	GLU
16	P	55	ARG
16	P	61	SER
16	P	62	VAL
16	P	65	GLN
16	P	67	THR
16	P	74	LEU
16	P	80	PHE
16	P	82	GLN
17	Q	9	VAL
17	Q	10	VAL
17	Q	21	VAL
17	Q	34	LYS
17	Q	36	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
17	Q	37	LYS
17	Q	38	ARG
17	Q	43	LEU
17	Q	45	HIS
17	Q	57	VAL
17	Q	59	ILE
17	Q	60	ILE
17	Q	62	SER
17	Q	67	LYS
17	Q	68	ARG
17	Q	73	VAL
17	Q	77	VAL
17	Q	81	ARG
17	Q	84	LEU
17	Q	90	ILE
17	Q	92	ARG
17	Q	98	LEU
17	Q	100	LYS
18	R	28	GLU
18	R	31	LEU
18	R	39	VAL
18	R	40	LEU
18	R	42	ARG
18	R	53	ARG
18	R	84	LYS
19	S	7	LYS
19	S	11	VAL
19	S	13	ASP
19	S	25	LYS
19	S	29	ARG
19	S	33	THR
19	S	36	ARG
19	S	63	THR
19	S	79	THR
19	S	81	ARG
20	T	9	ASN
20	T	18	GLN
20	T	19	SER
20	T	25	ARG
20	T	36	LEU
20	T	37	SER
20	T	41	ILE

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Mol	Chain	Res	Type
20	T	46	GLU
20	T	53	LEU
20	T	57	ARG
20	T	62	LEU
20	T	64	ASP
20	T	71	THR
20	T	74	LYS
20	T	75	ASN
20	T	84	LEU
20	T	92	LEU
20	T	93	GLU
21	U	7	ARG
21	U	9	ARG
21	U	10	ARG
21	U	12	LYS
21	U	17	THR
21	U	25	LYS

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

Mol	Chain	Res	Type
2	B	19	HIS
2	B	135	GLN
2	B	204	ASN
3	C	6	HIS
8	H	78	GLN
9	I	73	GLN
10	J	62	HIS
15	O	28	GLN
15	O	42	HIS
16	P	82	GLN
20	T	18	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1504/1522 (98%)	334 (22%)	50 (3%)

All (334) 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	13	U
1	A	32	A
1	A	39	G
1	A	40	C
1	A	47	C
1	A	48	C
1	A	49	U
1	A	50	A
1	A	51	A
1	A	79	G
1	A	80	G
1	A	81	U
1	A	82	U
1	A	91	C
1	A	92	C
1	A	101	A
1	A	108	G
1	A	115	G
1	A	116	A
1	A	117	G
1	A	121	C
1	A	129(A)	G
1	A	130	A
1	A	131	C
1	A	163	C
1	A	166	G
1	A	182	U
1	A	183	G
1	A	190(D)	U
1	A	190(E)	U
1	A	195	A
1	A	197	A
1	A	202	U
1	A	203	U
1	A	216	G
1	A	220	G
1	A	231	G
1	A	246	A
1	A	247	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	251	G
1	A	252	U
1	A	254	G
1	A	265	G
1	A	266	G
1	A	267	C
1	A	269	C
1	A	279	A
1	A	281	G
1	A	282	A
1	A	289	G
1	A	292	G
1	A	301	G
1	A	319	G
1	A	321	A
1	A	328	C
1	A	329	A
1	A	331	G
1	A	332	G
1	A	344	A
1	A	345	C
1	A	346	G
1	A	351	G
1	A	352	C
1	A	353	A
1	A	354	G
1	A	365	U
1	A	366	C
1	A	367	U
1	A	371	G
1	A	372	C
1	A	373	A
1	A	382	A
1	A	384	G
1	A	388	G
1	A	390	C
1	A	397	A
1	A	398	C
1	A	406	G
1	A	410	G
1	A	412	A
1	A	421	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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	452	A
1	A	460	A
1	A	461	C
1	A	481	G
1	A	482	A
1	A	483	C
1	A	484	G
1	A	485	G
1	A	497	A
1	A	498	U
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	530	G
1	A	531	U
1	A	533	A
1	A	536	C
1	A	545	C
1	A	547	A
1	A	559	A
1	A	560	U
1	A	562	C
1	A	563	A
1	A	564	C
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	596	C
1	A	615	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	618	C
1	A	624	C
1	A	649	G
1	A	653	A
1	A	665	A
1	A	670	G
1	A	686	U
1	A	687	A
1	A	688	G
1	A	701	C
1	A	702	A
1	A	703	G
1	A	718	G
1	A	721	G
1	A	723	U
1	A	724	G
1	A	731	G
1	A	740	U
1	A	741	G
1	A	749	C
1	A	751	U
1	A	755	G
1	A	761	G
1	A	766	A
1	A	777	A
1	A	781	A
1	A	782	A
1	A	789	U
1	A	792	A
1	A	793	U
1	A	794	A
1	A	799	G
1	A	813	U
1	A	815	A
1	A	817	C
1	A	818	G
1	A	821	G
1	A	828	A
1	A	838	G
1	A	839	U
1	A	840	C
1	A	841	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	848	C
1	A	851	G
1	A	855	G
1	A	859	A
1	A	869	G
1	A	873	A
1	A	876	G
1	A	889	A
1	A	902	G
1	A	914	A
1	A	926	G
1	A	927	G
1	A	934	C
1	A	935	A
1	A	941	G
1	A	942	G
1	A	950	U
1	A	954	G
1	A	960	U
1	A	961	U
1	A	966	M2G
1	A	967	5MC
1	A	968	A
1	A	969	A
1	A	971	G
1	A	974	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	979	C
1	A	989	C
1	A	991	U
1	A	992	U
1	A	993	G
1	A	994	A
1	A	1004	A
1	A	1005	A
1	A	1008	C
1	A	1017	G
1	A	1020	U
1	A	1021	G
1	A	1023	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	1026	G
1	A	1030(B)	C
1	A	1034	G
1	A	1045	C
1	A	1050	G
1	A	1052	U
1	A	1053	G
1	A	1054	C
1	A	1055	A
1	A	1060	C
1	A	1065	U
1	A	1066	C
1	A	1068	G
1	A	1078	U
1	A	1085	U
1	A	1092	A
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1124	G
1	A	1125	U
1	A	1126	U
1	A	1127	G
1	A	1129	C
1	A	1130	A
1	A	1131	G
1	A	1132	C
1	A	1138	G
1	A	1139	G
1	A	1140	C
1	A	1146	A
1	A	1147	C
1	A	1157	A
1	A	1159	U
1	A	1160	G
1	A	1171	G
1	A	1176	A
1	A	1183	A
1	A	1191	A
1	A	1196	U
1	A	1197	G
1	A	1198	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	1200	C
1	A	1201	A
1	A	1202	G
1	A	1212	U
1	A	1214	C
1	A	1224	G
1	A	1225	A
1	A	1226	C
1	A	1238	A
1	A	1241	G
1	A	1245	A
1	A	1256	A
1	A	1257	U
1	A	1258	G
1	A	1260	C
1	A	1270	C
1	A	1273	G
1	A	1278	U
1	A	1280	A
1	A	1281	U
1	A	1286	A
1	A	1287	A
1	A	1288	A
1	A	1297	C
1	A	1299	A
1	A	1300	G
1	A	1301	U
1	A	1302	U
1	A	1305	G
1	A	1310	G
1	A	1317	C
1	A	1320	C
1	A	1322	C
1	A	1327	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	1351	U
1	A	1353	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	1358	U
1	A	1359	C
1	A	1360	A
1	A	1362	C
1	A	1364	U
1	A	1365	G
1	A	1368	G
1	A	1370	G
1	A	1378	C
1	A	1379	G
1	A	1381	U
1	A	1399	C
1	A	1400	5MC
1	A	1414	U
1	A	1442	G
1	A	1443	G
1	A	1446	A
1	A	1447	G
1	A	1451	A
1	A	1452	C
1	A	1453	G
1	A	1485	U
1	A	1489	G
1	A	1490	C
1	A	1493	A
1	A	1494	G
1	A	1497	G
1	A	1498	UR3
1	A	1499	A
1	A	1503	A
1	A	1504	G
1	A	1505	G
1	A	1506	U
1	A	1507	A
1	A	1529	G
1	A	1530	G
1	A	1531	A
1	A	1532	U
1	A	1533	C

All (50) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	5	U
1	A	12	U
1	A	13	U
1	A	65	U
1	A	115	G
1	A	129(A)	G
1	A	181	G
1	A	246	A
1	A	250	A
1	A	251	G
1	A	281	G
1	A	328	C
1	A	372	C
1	A	428	G
1	A	429	U
1	A	484	G
1	A	496	A
1	A	509	A
1	A	518	C
1	A	559	A
1	A	687	A
1	A	701	C
1	A	748	C
1	A	776	G
1	A	792	A
1	A	812	C
1	A	840	C
1	A	913	A
1	A	960	U
1	A	965	A
1	A	975	A
1	A	992	U
1	A	1004	A
1	A	1049	U
1	A	1065	U
1	A	1067	A
1	A	1129	C
1	A	1145	C
1	A	1182	G
1	A	1190	G
1	A	1201	A
1	A	1257	U
1	A	1285	A

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Mol	Chain	Res	Type
1	A	1300	G
1	A	1301	U
1	A	1346	A
1	A	1347	G
1	A	1380	U
1	A	1443	G
1	A	1505	G

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

17 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	5MC	A	967	1	15,22,23	1.03	2 (13%)	19,32,35	1.02	2 (10%)
1	M2G	A	966	1	20,27,28	1.47	4 (20%)	22,40,43	2.42	5 (22%)
1	UR3	A	1498	1	14,22,23	0.87	0	15,32,35	1.23	2 (13%)
1	5MC	A	1400	1	15,22,23	1.19	2 (13%)	19,32,35	1.14	3 (15%)
1	MA6	A	1518[A]	1	19,26,27	0.98	0	18,38,41	0.99	1 (5%)
1	4OC	A	1402	1	16,23,24	1.38	2 (12%)	17,32,35	0.64	0
1	5MC	A	1404	1	15,22,23	1.28	1 (6%)	19,32,35	1.09	2 (10%)
1	5MC	A	1407	1	15,22,23	1.40	3 (20%)	19,32,35	0.99	2 (10%)
1	MA6	A	1519[A]	1	19,26,27	0.73	0	18,38,41	0.83	0
1	PSU	A	516	1	17,21,22	1.14	2 (11%)	20,30,33	3.37	8 (40%)
1	MA6	A	1519[B]	1	19,26,27	1.40	3 (15%)	18,38,41	0.70	0
1	MA6	A	1518[B]	1	19,26,27	1.38	2 (10%)	18,38,41	0.61	0
1	7MG	A	527	1,22	22,26,27	1.97	5 (22%)	28,39,42	1.60	4 (14%)
1	2MG	A	1207	1	19,26,27	3.12	4 (21%)	21,38,41	2.17	4 (19%)
1	PSU	A	1541	1	17,21,22	1.15	1 (5%)	20,30,33	3.40	6 (30%)
1	PSU	A	1540	1	17,21,22	1.02	1 (5%)	20,30,33	3.50	7 (35%)
12	0TD	L	92	12	4,9,10	0.93	0	3,11,13	3.62	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	5MC	A	967	1	-	3/5/25/26	0/2/2/2
1	M2G	A	966	1	-	3/7/29/30	0/3/3/3
1	UR3	A	1498	1	-	2/5/25/26	0/2/2/2
1	5MC	A	1400	1	-	2/5/25/26	0/2/2/2
1	MA6	A	1518[A]	1	-	0/7/29/30	0/3/3/3
1	4OC	A	1402	1	-	6/9/29/30	0/2/2/2
1	5MC	A	1404	1	-	0/5/25/26	0/2/2/2
1	5MC	A	1407	1	-	0/5/25/26	0/2/2/2
1	MA6	A	1519[A]	1	-	4/7/29/30	0/3/3/3
1	PSU	A	516	1	-	0/7/25/26	0/2/2/2
1	MA6	A	1519[B]	1	-	6/7/29/30	0/3/3/3
1	MA6	A	1518[B]	1	-	0/7/29/30	0/3/3/3
1	7MG	A	527	1,22	-	0/7/37/38	0/3/3/3
1	2MG	A	1207	1	-	3/5/27/28	0/3/3/3
1	PSU	A	1541	1	-	1/7/25/26	0/2/2/2
1	PSU	A	1540	1	-	0/7/25/26	0/2/2/2
12	0TD	L	92	12	-	1/3/12/14	-

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1207	2MG	C2-N2	10.03	1.42	1.34
1	A	1207	2MG	C6-N1	7.53	1.46	1.33
1	A	527	7MG	C2-N2	4.69	1.43	1.33
1	A	1518[B]	MA6	C6-N1	4.03	1.39	1.33
1	A	966	M2G	C6-N1	3.98	1.40	1.33
1	A	527	7MG	C8-N9	-3.95	1.36	1.45
1	A	1404	5MC	C5-C4	3.89	1.47	1.41
1	A	527	7MG	C4-N3	3.83	1.39	1.34
1	A	1407	5MC	C5-C4	3.61	1.47	1.41
1	A	1207	2MG	C4-N3	3.59	1.41	1.35
1	A	1541	PSU	C4-N3	3.58	1.39	1.33
1	A	1519[B]	MA6	C2-N3	3.52	1.37	1.32
1	A	1540	PSU	C4-N3	3.50	1.39	1.33
1	A	516	PSU	C4-N3	3.48	1.39	1.33
1	A	527	7MG	C6-C5	3.40	1.46	1.41
1	A	966	M2G	C4-N3	3.07	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1402	4OC	C2-N3	3.01	1.44	1.38
1	A	1519[B]	MA6	C6-N1	2.97	1.37	1.33
1	A	1207	2MG	C2-N1	2.93	1.43	1.34
1	A	1519[B]	MA6	C2-N1	2.84	1.39	1.33
1	A	1400	5MC	C2-N3	2.83	1.43	1.38
1	A	1402	4OC	C4-N4	2.82	1.42	1.36
1	A	1518[B]	MA6	C4-N3	2.79	1.39	1.35
1	A	966	M2G	C2-N1	2.52	1.39	1.34
1	A	1407	5MC	C4-N4	2.39	1.40	1.34
1	A	966	M2G	C6-C5	2.29	1.45	1.41
1	A	967	5MC	C2-N3	2.21	1.42	1.38
1	A	1407	5MC	CM5-C5	2.20	1.55	1.51
1	A	516	PSU	O4'-C1'	-2.09	1.41	1.44
1	A	1400	5MC	C4-N4	2.09	1.39	1.34
1	A	527	7MG	C5-N7	2.02	1.43	1.39
1	A	967	5MC	C4-N4	2.01	1.39	1.34

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1540	PSU	N1-C2-N3	-12.28	118.67	128.43
1	A	1541	PSU	N1-C2-N3	-11.98	118.90	128.43
1	A	516	PSU	N1-C2-N3	-11.22	119.51	128.43
1	A	966	M2G	C5-C6-N1	-7.99	112.51	123.43
1	A	1207	2MG	C5-C6-N1	-7.77	112.81	123.43
1	A	516	PSU	C4-N3-C2	6.69	120.79	115.14
1	A	1541	PSU	C4-N3-C2	6.35	120.50	115.14
1	A	1540	PSU	C4-N3-C2	6.27	120.43	115.14
12	L	92	0TD	CSB-SB-CB	-5.64	90.77	101.85
1	A	966	M2G	C6-N1-C2	5.63	122.88	116.18
1	A	527	7MG	N3-C4-N9	4.34	132.48	126.91
1	A	516	PSU	C5-C4-N3	-4.33	119.79	125.36
1	A	527	7MG	C5-C4-N3	-4.17	119.67	126.49
1	A	1207	2MG	C6-N1-C2	4.07	122.46	115.18
1	A	527	7MG	N7-C8-N9	3.95	109.03	103.38
1	A	966	M2G	N1-C2-N2	-3.81	113.34	117.19
1	A	1541	PSU	C5-C4-N3	-3.65	120.65	125.36
1	A	1540	PSU	C5-C4-N3	-3.65	120.66	125.36
1	A	1540	PSU	C6-N1-C2	3.62	121.33	115.36
1	A	1541	PSU	C6-N1-C2	3.61	121.32	115.36
1	A	1207	2MG	C4-C5-N7	2.98	112.50	109.40
1	A	1540	PSU	O4'-C1'-C5	2.97	114.53	109.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	516	PSU	C6-N1-C2	2.96	120.23	115.36
1	A	1540	PSU	C5-C6-N1	-2.83	120.97	124.44
1	A	966	M2G	N3-C2-N2	2.81	120.03	117.18
1	A	516	PSU	C5-C6-N1	-2.70	121.12	124.44
1	A	1404	5MC	N4-C4-N3	-2.69	113.23	117.03
1	A	1400	5MC	CM5-C5-C4	-2.62	119.07	121.72
1	A	516	PSU	C5-C1'-C2'	-2.55	110.76	115.32
1	A	1518[A]	MA6	N1-C6-N6	-2.54	114.38	117.06
1	A	1498	UR3	C3'-C2'-C1'	2.49	104.72	100.98
1	A	1400	5MC	C2-N3-C4	2.45	118.97	116.02
1	A	1541	PSU	C5-C6-N1	-2.41	121.47	124.44
1	A	1400	5MC	CM5-C5-C6	2.39	123.73	118.68
1	A	1407	5MC	N4-C4-N3	-2.38	113.67	117.03
1	A	1541	PSU	C5-C1'-C2'	2.31	119.44	115.32
1	A	527	7MG	C2-N3-C4	2.31	120.26	113.89
1	A	516	PSU	O4'-C1'-C5	2.25	113.41	109.93
1	A	1207	2MG	N2-C2-N3	2.25	119.12	116.96
1	A	967	5MC	C2-N3-C4	2.18	118.64	116.02
1	A	1407	5MC	C2-N3-C4	2.17	118.64	116.02
1	A	967	5MC	CM5-C5-C6	2.16	123.25	118.68
1	A	516	PSU	O4'-C1'-C2'	2.14	108.13	104.66
12	L	92	0TD	CB-CA-N	-2.14	104.54	109.10
1	A	1498	UR3	C6-N1-C2	-2.09	117.86	121.23
1	A	1404	5MC	C5-C4-N3	2.05	124.50	121.26
1	A	1540	PSU	O4'-C1'-C2'	2.04	107.96	104.66
1	A	966	M2G	C2-N3-C4	-2.01	113.00	115.28

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	967	5MC	O4'-C4'-C5'-O5'
1	A	967	5MC	C3'-C4'-C5'-O5'
1	A	967	5MC	C2'-C1'-N1-C6
1	A	1207	2MG	N1-C2-N2-CM2
1	A	1207	2MG	N3-C2-N2-CM2
1	A	1402	4OC	O4'-C4'-C5'-O5'
1	A	1402	4OC	C3'-C4'-C5'-O5'
1	A	1402	4OC	O4'-C1'-N1-C6
1	A	1402	4OC	C2'-C1'-N1-C6
1	A	1402	4OC	N3-C4-N4-CM4
1	A	1402	4OC	C5-C4-N4-CM4

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Mol	Chain	Res	Type	Atoms
1	A	1519[B]	MA6	C3'-C4'-C5'-O5'
1	A	1519[B]	MA6	C5-C6-N6-C9
1	A	1519[B]	MA6	C5-C6-N6-C10
1	A	1519[B]	MA6	N1-C6-N6-C9
1	A	1519[A]	MA6	O4'-C4'-C5'-O5'
1	A	1519[A]	MA6	C5-C6-N6-C9
12	L	92	0TD	CG-CB-SB-CSB
1	A	1400	5MC	O4'-C4'-C5'-O5'
1	A	1519[B]	MA6	O4'-C4'-C5'-O5'
1	A	1519[A]	MA6	C3'-C4'-C5'-O5'
1	A	1400	5MC	C3'-C4'-C5'-O5'
1	A	1519[B]	MA6	N1-C6-N6-C10
1	A	966	M2G	C3'-C4'-C5'-O5'
1	A	966	M2G	O4'-C4'-C5'-O5'
1	A	1498	UR3	O4'-C4'-C5'-O5'
1	A	1498	UR3	C3'-C4'-C5'-O5'
1	A	966	M2G	C4'-C5'-O5'-P
1	A	1519[A]	MA6	C5-C6-N6-C10
1	A	1541	PSU	O4'-C1'-C5-C4
1	A	1207	2MG	C3'-C4'-C5'-O5'

There are no ring outliers.

13 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	967	5MC	1	0
1	A	966	M2G	1	0
1	A	1498	UR3	5	0
1	A	1400	5MC	1	0
1	A	1518[A]	MA6	2	0
1	A	1404	5MC	1	0
1	A	1407	5MC	1	0
1	A	1519[A]	MA6	3	0
1	A	1519[B]	MA6	3	0
1	A	1518[B]	MA6	3	0
1	A	527	7MG	2	0
1	A	1207	2MG	1	0
12	L	92	0TD	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 279 ligands modelled in this entry, 279 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data i

### 6.1 Protein, DNA and RNA chains i

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%)	-0.38	24 (1%) 72 63	104, 178, 309, 393	0
2	B	234/256 (91%)	-0.45	4 (1%) 70 61	145, 220, 326, 363	0
3	C	206/239 (86%)	-0.10	11 (5%) 26 22	190, 245, 287, 310	0
4	D	208/209 (99%)	-0.35	3 (1%) 75 67	120, 190, 253, 287	0
5	E	150/162 (92%)	-0.52	0 100 100	101, 152, 195, 248	0
6	F	101/101 (100%)	-0.69	0 100 100	139, 213, 251, 291	0
7	G	155/156 (99%)	-0.31	7 (4%) 33 27	162, 218, 283, 328	0
8	H	138/138 (100%)	-0.62	0 100 100	94, 136, 183, 228	0
9	I	127/128 (99%)	-0.17	3 (2%) 59 49	205, 246, 296, 310	0
10	J	98/105 (93%)	0.34	10 (10%) 6 6	194, 256, 344, 406	0
11	K	116/129 (89%)	-0.45	1 (0%) 84 78	134, 176, 225, 241	0
12	L	123/135 (91%)	-0.31	3 (2%) 59 49	99, 180, 223, 243	0
13	M	118/126 (93%)	-0.22	4 (3%) 45 36	158, 213, 251, 306	0
14	N	60/61 (98%)	0.28	7 (11%) 4 4	187, 237, 295, 326	0
15	O	87/89 (97%)	-0.41	0 100 100	110, 167, 217, 231	0
16	P	83/88 (94%)	-0.39	2 (2%) 59 49	130, 172, 227, 272	0
17	Q	99/105 (94%)	-0.55	0 100 100	115, 152, 216, 241	0
18	R	70/88 (79%)	-0.52	1 (1%) 75 67	128, 177, 240, 273	0
19	S	80/93 (86%)	0.31	7 (8%) 10 8	223, 271, 315, 328	0
20	T	99/106 (93%)	-0.68	1 (1%) 82 75	129, 173, 233, 280	0
21	U	24/27 (88%)	1.60	7 (29%) 0 0	198, 224, 253, 260	0
All	All	3874/4063 (95%)	-0.33	95 (2%) 57 47	94, 194, 292, 406	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
10	J	34	VAL	8.5
1	A	993	G	7.5
1	A	994	A	6.5
10	J	39	PRO	6.5
21	U	17	THR	6.4
14	N	18	VAL	5.1
21	U	18	TYR	5.1
14	N	4	LYS	4.8
1	A	1018	C	4.7
21	U	8	THR	4.3
4	D	41	GLY	4.3
10	J	33	GLN	4.3
14	N	5	ALA	4.2
7	G	80	VAL	4.2
10	J	38	ILE	4.2
1	A	1006	C	4.1
3	C	66	VAL	4.0
1	A	1019	C	4.0
1	A	202	U	3.9
21	U	24	ARG	3.8
14	N	3	ARG	3.8
1	A	1035	A	3.8
21	U	5	ASP	3.7
1	A	1036	G	3.6
13	M	117	VAL	3.6
3	C	193	TYR	3.5
1	A	1322	C	3.5
2	B	231	GLU	3.3
10	J	37	PRO	3.3
3	C	103	VAL	3.3
21	U	25	LYS	3.2
1	A	1047	G	3.1
7	G	81	GLY	3.1
3	C	102	ASN	3.0
1	A	1321	C	3.0
16	P	23	ASP	3.0
3	C	67	THR	2.9
19	S	41	VAL	2.9
19	S	40	ILE	2.9
4	D	35	ARG	2.9
9	I	15	ALA	2.9
1	A	1050	G	2.9
10	J	71	LEU	2.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
7	G	2	ALA	2.8
9	I	119	ALA	2.8
16	P	1	MET	2.8
10	J	89	ASP	2.7
14	N	6	LEU	2.7
13	M	118	ALA	2.7
20	T	106	ALA	2.7
1	A	1048	G	2.7
1	A	1037	C	2.6
3	C	65	ALA	2.6
12	L	112	ASP	2.6
19	S	31	ILE	2.5
7	G	78	ARG	2.5
19	S	69	HIS	2.5
10	J	72	VAL	2.5
1	A	1007	C	2.5
10	J	90	LEU	2.4
1	A	1005	A	2.4
2	B	135	GLN	2.3
18	R	88	LYS	2.3
1	A	992	U	2.3
7	G	79	ARG	2.3
3	C	68	VAL	2.3
13	M	45	VAL	2.3
3	C	156	ARG	2.3
1	A	1211	U	2.3
19	S	38	SER	2.3
1	A	979	C	2.3
13	M	6	GLY	2.3
7	G	82	GLY	2.3
4	D	42	GLN	2.3
3	C	104	GLN	2.2
7	G	156	TRP	2.2
9	I	125	TYR	2.2
3	C	157	ILE	2.2
14	N	14	PRO	2.2
19	S	30	LEU	2.2
2	B	128	GLU	2.2
21	U	16	GLY	2.2
1	A	995	C	2.2
1	A	1129	C	2.1
3	C	87	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	132	LYS	2.1
1	A	1020	U	2.1
11	K	118	GLY	2.1
1	A	1257	U	2.1
1	A	1222	G	2.0
14	N	17	LYS	2.0
12	L	47	LYS	2.0
10	J	32	ALA	2.0
12	L	49	ASN	2.0
19	S	39	THR	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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
1	PSU	A	1540	20/21	0.85	0.46	262,265,277,283	0
1	PSU	A	1541	20/21	0.92	0.30	239,247,262,263	0
1	PSU	A	516	20/21	0.94	0.09	161,204,223,224	0
1	5MC	A	967	21/22	0.94	0.16	183,190,208,211	0
1	UR3	A	1498	21/22	0.94	0.22	155,172,189,197	0
1	4OC	A	1402	22/23	0.95	0.20	148,156,171,187	0
1	5MC	A	1404	21/22	0.95	0.19	141,170,203,221	0
1	M2G	A	966	25/26	0.95	0.16	192,203,210,221	0
1	2MG	A	1207	24/25	0.95	0.12	211,231,295,300	0
1	5MC	A	1400	21/22	0.95	0.17	141,159,171,180	0
1	7MG	A	527	24/25	0.96	0.14	141,171,178,185	0
1	MA6	A	1519[A]	24/25	0.96	0.31	136,142,149,152	24
1	5MC	A	1407	21/22	0.96	0.18	157,205,219,224	0
1	MA6	A	1519[B]	24/25	0.96	0.31	136,148,164,167	24
1	MA6	A	1518[A]	24/25	0.97	0.25	145,163,168,171	24
1	MA6	A	1518[B]	24/25	0.97	0.25	143,163,180,183	24
12	0TD	L	92	10/11	0.97	0.54	158,180,208,372	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides 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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
22	MG	A	1713	1/1	0.26	0.30	155,155,155,155	0
22	MG	A	1722	1/1	0.26	0.82	130,130,130,130	0
22	MG	A	1845	1/1	0.31	0.27	137,137,137,137	0
22	MG	A	1686	1/1	0.43	0.24	135,135,135,135	0
22	MG	A	1862	1/1	0.57	0.57	129,129,129,129	0
22	MG	A	1654	1/1	0.57	0.40	111,111,111,111	0
22	MG	P	101	1/1	0.58	0.36	102,102,102,102	0
22	MG	M	201	1/1	0.60	0.61	160,160,160,160	0
22	MG	Q	201	1/1	0.63	0.13	158,158,158,158	0
22	MG	A	1836	1/1	0.64	0.90	207,207,207,207	0
22	MG	A	1737	1/1	0.65	0.46	139,139,139,139	0
22	MG	A	1849	1/1	0.66	0.26	141,141,141,141	0
22	MG	A	1837	1/1	0.66	0.28	179,179,179,179	0
22	MG	A	1827	1/1	0.66	0.42	507,507,507,507	0
22	MG	A	1778	1/1	0.67	1.46	164,164,164,164	0
22	MG	A	1696	1/1	0.69	0.55	151,151,151,151	0
22	MG	A	1850	1/1	0.70	0.18	140,140,140,140	0
22	MG	A	1712	1/1	0.72	0.39	171,171,171,171	0
22	MG	A	1815	1/1	0.72	0.57	218,218,218,218	0
22	MG	A	1650	1/1	0.72	0.38	161,161,161,161	0
22	MG	S	101	1/1	0.74	0.14	234,234,234,234	0
22	MG	P	102	1/1	0.75	0.33	360,360,360,360	0
22	MG	A	1721	1/1	0.75	0.54	166,166,166,166	0
22	MG	A	1736	1/1	0.76	0.35	110,110,110,110	0
22	MG	A	1844	1/1	0.77	0.32	138,138,138,138	0
22	MG	A	1743	1/1	0.77	1.02	159,159,159,159	0
22	MG	A	1846	1/1	0.77	0.35	163,163,163,163	0
22	MG	A	1856	1/1	0.77	0.40	132,132,132,132	0
22	MG	A	1792	1/1	0.77	0.53	229,229,229,229	0
22	MG	A	1791	1/1	0.78	0.34	444,444,444,444	0
22	MG	A	1831	1/1	0.79	0.42	322,322,322,322	0
22	MG	A	1748	1/1	0.79	0.32	149,149,149,149	0
22	MG	A	1617	1/1	0.79	0.21	140,140,140,140	0
22	MG	A	1859	1/1	0.80	0.68	161,161,161,161	0
22	MG	A	1789	1/1	0.80	0.34	259,259,259,259	0
22	MG	A	1621	1/1	0.81	0.31	132,132,132,132	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
22	MG	A	1728	1/1	0.81	0.20	129,129,129,129	0
22	MG	A	1734	1/1	0.82	0.24	129,129,129,129	0
22	MG	A	1638	1/1	0.83	0.29	155,155,155,155	0
22	MG	A	1667	1/1	0.84	0.47	128,128,128,128	0
22	MG	A	1622	1/1	0.84	0.48	71,71,71,71	0
22	MG	A	1746	1/1	0.84	0.39	157,157,157,157	0
22	MG	A	1679	1/1	0.84	0.28	146,146,146,146	0
22	MG	A	1838	1/1	0.84	0.15	198,198,198,198	0
22	MG	A	1765	1/1	0.85	0.33	149,149,149,149	0
22	MG	A	1853	1/1	0.85	0.31	171,171,171,171	0
22	MG	A	1788	1/1	0.85	0.33	288,288,288,288	0
22	MG	A	1793	1/1	0.85	0.32	189,189,189,189	0
22	MG	A	1659	1/1	0.86	0.29	154,154,154,154	0
22	MG	A	1672	1/1	0.86	0.15	163,163,163,163	0
22	MG	A	1802	1/1	0.86	0.19	225,225,225,225	0
22	MG	A	1807	1/1	0.86	0.24	500,500,500,500	0
22	MG	A	1653	1/1	0.87	0.37	129,129,129,129	0
22	MG	A	1834	1/1	0.87	0.58	113,113,113,113	0
22	MG	A	1840	1/1	0.87	0.29	153,153,153,153	0
22	MG	A	1602	1/1	0.87	0.31	237,237,237,237	0
22	MG	A	1766	1/1	0.87	0.21	171,171,171,171	0
22	MG	A	1695	1/1	0.87	0.21	386,386,386,386	0
22	MG	A	1655	1/1	0.88	0.26	136,136,136,136	0
22	MG	A	1626	1/1	0.88	0.35	127,127,127,127	0
22	MG	A	1745	1/1	0.88	0.20	126,126,126,126	0
22	MG	A	1824	1/1	0.88	0.21	424,424,424,424	0
22	MG	A	1741	1/1	0.88	0.47	145,145,145,145	0
22	MG	A	1857	1/1	0.88	0.45	189,189,189,189	0
22	MG	A	1848	1/1	0.88	0.25	173,173,173,173	0
22	MG	A	1738	1/1	0.88	0.33	167,167,167,167	0
22	MG	A	1706	1/1	0.88	0.67	131,131,131,131	0
22	MG	A	1784	1/1	0.88	0.38	250,250,250,250	0
22	MG	A	1699	1/1	0.88	0.41	126,126,126,126	0
22	MG	A	1773	1/1	0.89	0.23	121,121,121,121	0
22	MG	A	1776	1/1	0.89	0.22	159,159,159,159	0
22	MG	A	1710	1/1	0.89	0.31	157,157,157,157	0
22	MG	A	1811	1/1	0.89	0.29	317,317,317,317	0
22	MG	A	1673	1/1	0.90	0.48	175,175,175,175	0
22	MG	A	1671	1/1	0.90	0.26	171,171,171,171	0
22	MG	A	1641	1/1	0.90	0.26	139,139,139,139	0
22	MG	A	1702	1/1	0.90	0.09	165,165,165,165	0
22	MG	A	1781	1/1	0.90	0.21	247,247,247,247	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
22	MG	A	1798	1/1	0.90	0.26	514,514,514,514	0
22	MG	A	1794	1/1	0.90	0.19	173,173,173,173	0
22	MG	A	1733	1/1	0.90	0.18	102,102,102,102	0
22	MG	A	1775	1/1	0.91	0.08	120,120,120,120	0
22	MG	A	1725	1/1	0.91	0.39	131,131,131,131	0
22	MG	A	1735	1/1	0.91	0.55	157,157,157,157	0
22	MG	A	1852	1/1	0.91	0.14	152,152,152,152	0
22	MG	A	1828	1/1	0.91	0.17	281,281,281,281	0
22	MG	A	1829	1/1	0.91	0.25	317,317,317,317	0
22	MG	A	1801	1/1	0.91	0.33	465,465,465,465	0
22	MG	A	1632	1/1	0.91	0.32	109,109,109,109	0
22	MG	A	1666	1/1	0.91	0.25	155,155,155,155	0
22	MG	A	1805	1/1	0.91	0.31	450,450,450,450	0
22	MG	A	1767	1/1	0.91	0.14	136,136,136,136	0
22	MG	A	1861	1/1	0.91	0.25	155,155,155,155	0
22	MG	A	1732	1/1	0.92	0.17	127,127,127,127	0
22	MG	A	1822	1/1	0.92	0.23	202,202,202,202	0
22	MG	A	1755	1/1	0.92	0.19	192,192,192,192	0
22	MG	A	1756	1/1	0.92	0.38	126,126,126,126	0
22	MG	A	1642	1/1	0.92	0.22	129,129,129,129	0
22	MG	A	1684	1/1	0.92	0.18	222,222,222,222	0
22	MG	A	1803	1/1	0.92	0.45	413,413,413,413	0
22	MG	A	1690	1/1	0.92	0.25	154,154,154,154	0
22	MG	A	1670	1/1	0.92	0.11	209,209,209,209	0
22	MG	A	1704	1/1	0.92	0.23	105,105,105,105	0
22	MG	A	1753	1/1	0.92	0.26	128,128,128,128	0
22	MG	A	1780	1/1	0.93	0.41	380,380,380,380	0
22	MG	A	1683	1/1	0.93	0.09	310,310,310,310	0
22	MG	A	1744	1/1	0.93	0.10	158,158,158,158	0
22	MG	A	1608	1/1	0.93	0.17	150,150,150,150	0
22	MG	A	1742	1/1	0.93	0.14	148,148,148,148	0
22	MG	A	1619	1/1	0.93	0.48	179,179,179,179	0
22	MG	C	301	1/1	0.93	0.12	166,166,166,166	0
22	MG	A	1707	1/1	0.93	0.25	131,131,131,131	0
22	MG	A	1832	1/1	0.93	0.74	435,435,435,435	0
22	MG	B	302	1/1	0.93	0.14	219,219,219,219	0
22	MG	A	1709	1/1	0.94	0.23	157,157,157,157	0
22	MG	A	1631	1/1	0.94	0.52	175,175,175,175	0
22	MG	D	303	1/1	0.94	0.15	138,138,138,138	0
22	MG	A	1806	1/1	0.94	0.65	279,279,279,279	0
22	MG	A	1754	1/1	0.94	0.52	115,115,115,115	0
22	MG	A	1624	1/1	0.94	0.19	146,146,146,146	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
22	MG	B	303	1/1	0.94	1.19	260,260,260,260	0
22	MG	A	1777	1/1	0.94	0.20	119,119,119,119	0
22	MG	A	1660	1/1	0.94	0.35	135,135,135,135	0
22	MG	A	1604	1/1	0.94	0.98	120,120,120,120	0
22	MG	A	1697	1/1	0.94	0.28	119,119,119,119	0
22	MG	A	1763	1/1	0.94	0.20	358,358,358,358	0
22	MG	A	1830	1/1	0.94	0.52	321,321,321,321	0
22	MG	A	1779	1/1	0.94	0.62	137,137,137,137	0
22	MG	A	1723	1/1	0.94	0.20	163,163,163,163	0
22	MG	A	1685	1/1	0.94	0.30	247,247,247,247	0
22	MG	A	1813	1/1	0.94	0.16	460,460,460,460	0
22	MG	A	1664	1/1	0.94	0.31	120,120,120,120	0
22	MG	A	1812	1/1	0.94	0.24	450,450,450,450	0
22	MG	A	1770	1/1	0.94	0.20	185,185,185,185	0
22	MG	A	1797	1/1	0.94	0.35	387,387,387,387	0
22	MG	A	1783	1/1	0.94	0.19	404,404,404,404	0
22	MG	A	1669	1/1	0.94	0.07	306,306,306,306	0
22	MG	A	1796	1/1	0.94	0.23	271,271,271,271	0
22	MG	A	1649	1/1	0.95	0.19	235,235,235,235	0
22	MG	A	1782	1/1	0.95	0.04	517,517,517,517	0
22	MG	A	1606	1/1	0.95	0.18	174,174,174,174	0
22	MG	A	1689	1/1	0.95	0.11	223,223,223,223	0
22	MG	A	1787	1/1	0.95	0.23	254,254,254,254	0
22	MG	A	1750	1/1	0.95	0.19	152,152,152,152	0
22	MG	A	1818	1/1	0.95	0.62	432,432,432,432	0
22	MG	A	1658	1/1	0.95	0.44	210,210,210,210	0
22	MG	A	1708	1/1	0.95	0.38	135,135,135,135	0
22	MG	A	1752	1/1	0.95	0.15	149,149,149,149	0
22	MG	A	1682	1/1	0.95	0.56	123,123,123,123	0
22	MG	A	1614	1/1	0.95	0.81	194,194,194,194	0
22	MG	A	1663	1/1	0.95	0.09	315,315,315,315	0
22	MG	A	1760	1/1	0.95	0.18	189,189,189,189	0
22	MG	A	1616	1/1	0.95	0.37	190,190,190,190	0
22	MG	A	1644	1/1	0.95	0.13	143,143,143,143	0
22	MG	A	1860	1/1	0.95	0.27	151,151,151,151	0
22	MG	A	1751	1/1	0.95	0.34	160,160,160,160	0
22	MG	A	1718	1/1	0.95	0.47	145,145,145,145	0
22	MG	A	1640	1/1	0.95	0.92	165,165,165,165	0
22	MG	A	1636	1/1	0.96	0.36	114,114,114,114	0
22	MG	A	1676	1/1	0.96	0.21	173,173,173,173	0
22	MG	A	1826	1/1	0.96	0.11	178,178,178,178	0
22	MG	A	1607	1/1	0.96	0.33	130,130,130,130	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
22	MG	A	1817	1/1	0.96	0.26	489,489,489,489	0
22	MG	A	1687	1/1	0.96	0.33	325,325,325,325	0
22	MG	A	1668	1/1	0.96	0.59	153,153,153,153	0
22	MG	A	1747	1/1	0.96	0.16	134,134,134,134	0
22	MG	A	1730	1/1	0.96	0.28	149,149,149,149	0
22	MG	A	1785	1/1	0.96	0.16	243,243,243,243	0
22	MG	A	1774	1/1	0.96	0.09	154,154,154,154	0
22	MG	A	1623	1/1	0.96	0.27	185,185,185,185	0
22	MG	A	1629	1/1	0.96	0.11	154,154,154,154	0
22	MG	A	1680	1/1	0.96	0.12	165,165,165,165	0
22	MG	A	1821	1/1	0.96	0.09	449,449,449,449	0
22	MG	A	1651	1/1	0.96	0.25	141,141,141,141	0
22	MG	A	1674	1/1	0.96	0.13	153,153,153,153	0
22	MG	A	1657	1/1	0.96	0.07	190,190,190,190	0
22	MG	A	1786	1/1	0.96	0.15	449,449,449,449	0
22	MG	A	1647	1/1	0.96	0.18	132,132,132,132	0
22	MG	A	1698	1/1	0.96	0.14	180,180,180,180	0
22	MG	A	1611	1/1	0.96	0.06	234,234,234,234	0
22	MG	A	1661	1/1	0.96	0.10	136,136,136,136	0
22	MG	A	1703	1/1	0.96	0.06	237,237,237,237	0
22	MG	A	1625	1/1	0.96	0.12	114,114,114,114	0
22	MG	J	202	1/1	0.96	0.39	501,501,501,501	0
22	MG	A	1790	1/1	0.96	0.13	307,307,307,307	0
22	MG	E	201	1/1	0.96	0.18	171,171,171,171	0
22	MG	A	1847	1/1	0.96	0.14	147,147,147,147	0
22	MG	D	302	1/1	0.97	0.41	140,140,140,140	0
22	MG	A	1610	1/1	0.97	0.14	206,206,206,206	0
22	MG	A	1858	1/1	0.97	0.20	127,127,127,127	0
22	MG	F	201	1/1	0.97	0.16	170,170,170,170	0
22	MG	A	1720	1/1	0.97	0.36	171,171,171,171	0
22	MG	A	1855	1/1	0.97	0.11	133,133,133,133	0
22	MG	A	1729	1/1	0.97	0.21	169,169,169,169	0
22	MG	A	1800	1/1	0.97	0.13	237,237,237,237	0
22	MG	A	1675	1/1	0.97	0.19	269,269,269,269	0
22	MG	A	1833	1/1	0.97	0.17	338,338,338,338	0
22	MG	A	1726	1/1	0.97	0.15	132,132,132,132	0
22	MG	A	1808	1/1	0.97	0.36	359,359,359,359	0
22	MG	A	1841	1/1	0.97	0.12	196,196,196,196	0
22	MG	A	1694	1/1	0.97	0.19	346,346,346,346	0
22	MG	A	1758	1/1	0.97	0.12	172,172,172,172	0
22	MG	A	1795	1/1	0.97	0.20	416,416,416,416	0
22	MG	A	1814	1/1	0.97	0.18	336,336,336,336	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
22	MG	A	1705	1/1	0.97	0.16	129,129,129,129	0
22	MG	A	1662	1/1	0.97	0.08	182,182,182,182	0
22	MG	A	1634	1/1	0.97	0.14	118,118,118,118	0
22	MG	A	1842	1/1	0.97	0.19	173,173,173,173	0
22	MG	A	1693	1/1	0.97	0.35	394,394,394,394	0
22	MG	A	1843	1/1	0.97	0.19	156,156,156,156	0
22	MG	A	1639	1/1	0.97	0.28	227,227,227,227	0
22	MG	A	1757	1/1	0.97	0.06	162,162,162,162	0
22	MG	B	301	1/1	0.97	0.37	173,173,173,173	0
22	MG	A	1711	1/1	0.97	0.37	101,101,101,101	0
22	MG	A	1851	1/1	0.97	0.15	182,182,182,182	0
22	MG	A	1601	1/1	0.97	0.35	210,210,210,210	0
22	MG	A	1810	1/1	0.97	0.46	344,344,344,344	0
22	MG	A	1771	1/1	0.97	0.20	139,139,139,139	0
22	MG	A	1761	1/1	0.97	0.12	205,205,205,205	0
22	MG	A	1731	1/1	0.97	0.36	106,106,106,106	0
22	MG	A	1656	1/1	0.98	0.15	146,146,146,146	0
22	MG	A	1678	1/1	0.98	0.10	180,180,180,180	0
22	MG	A	1688	1/1	0.98	0.16	145,145,145,145	0
23	ZN	D	301	1/1	0.98	0.28	147,147,147,147	0
22	MG	J	201	1/1	0.98	0.30	138,138,138,138	0
22	MG	A	1854	1/1	0.98	0.16	172,172,172,172	0
22	MG	A	1635	1/1	0.98	0.38	177,177,177,177	0
22	MG	A	1618	1/1	0.98	0.21	137,137,137,137	0
22	MG	A	1769	1/1	0.98	0.27	161,161,161,161	0
22	MG	A	1823	1/1	0.98	0.26	256,256,256,256	0
22	MG	A	1772	1/1	0.98	0.16	150,150,150,150	0
22	MG	A	1691	1/1	0.98	0.41	197,197,197,197	0
22	MG	A	1819	1/1	0.98	0.09	407,407,407,407	0
22	MG	A	1820	1/1	0.98	0.59	437,437,437,437	0
22	MG	A	1839	1/1	0.98	0.26	170,170,170,170	0
22	MG	A	1620	1/1	0.98	0.12	107,107,107,107	0
22	MG	A	1633	1/1	0.98	0.09	368,368,368,368	0
22	MG	A	1714	1/1	0.98	0.33	118,118,118,118	0
22	MG	A	1715	1/1	0.98	0.11	155,155,155,155	0
22	MG	A	1717	1/1	0.98	0.10	137,137,137,137	0
22	MG	A	1652	1/1	0.98	0.16	188,188,188,188	0
22	MG	A	1762	1/1	0.98	0.29	365,365,365,365	0
22	MG	A	1816	1/1	0.98	0.09	357,357,357,357	0
22	MG	A	1692	1/1	0.98	0.07	148,148,148,148	0
22	MG	A	1681	1/1	0.98	0.08	154,154,154,154	0
22	MG	A	1740	1/1	0.98	0.69	138,138,138,138	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
22	MG	A	1835	1/1	0.98	0.17	161,161,161,161	0
22	MG	A	1612	1/1	0.98	0.17	172,172,172,172	0
22	MG	A	1646	1/1	0.98	0.35	205,205,205,205	0
22	MG	A	1768	1/1	0.98	0.45	164,164,164,164	0
22	MG	A	1739	1/1	0.98	0.13	158,158,158,158	0
23	ZN	N	101	1/1	0.98	0.18	258,258,258,258	0
22	MG	A	1719	1/1	0.98	0.33	136,136,136,136	0
22	MG	A	1799	1/1	0.98	0.25	224,224,224,224	0
22	MG	A	1809	1/1	0.98	0.33	249,249,249,249	0
22	MG	A	1764	1/1	0.99	0.20	298,298,298,298	0
22	MG	A	1605	1/1	0.99	0.08	153,153,153,153	0
22	MG	A	1727	1/1	0.99	0.07	113,113,113,113	0
22	MG	A	1648	1/1	0.99	0.17	139,139,139,139	0
22	MG	A	1716	1/1	0.99	0.11	131,131,131,131	0
22	MG	A	1665	1/1	0.99	0.15	180,180,180,180	0
22	MG	A	1628	1/1	0.99	0.42	189,189,189,189	0
22	MG	A	1825	1/1	0.99	0.17	264,264,264,264	0
22	MG	A	1630	1/1	0.99	0.12	104,104,104,104	0
22	MG	A	1700	1/1	0.99	0.16	143,143,143,143	0
22	MG	A	1613	1/1	0.99	0.09	144,144,144,144	0
22	MG	A	1615	1/1	0.99	0.17	104,104,104,104	0
22	MG	A	1603	1/1	0.99	0.27	170,170,170,170	0
22	MG	A	1804	1/1	0.99	0.12	228,228,228,228	0
22	MG	A	1609	1/1	0.99	0.20	151,151,151,151	0
22	MG	A	1701	1/1	0.99	0.14	101,101,101,101	0
22	MG	A	1645	1/1	0.99	0.21	87,87,87,87	0
22	MG	A	1677	1/1	0.99	0.09	189,189,189,189	0
22	MG	A	1749	1/1	0.99	0.06	113,113,113,113	0
22	MG	A	1724	1/1	0.99	0.39	127,127,127,127	0
22	MG	A	1759	1/1	0.99	0.30	167,167,167,167	0
22	MG	A	1643	1/1	0.99	0.10	113,113,113,113	0
22	MG	A	1637	1/1	0.99	0.19	283,283,283,283	0
22	MG	A	1627	1/1	0.99	0.14	113,113,113,113	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.