Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2024 – 02:31 AM EST

PDB ID	:	4JI2
Title	:	Crystal Structure of 30S ribosomal subunit from Thermus thermophilus
Authors	:	Demirci, H.; Wang, L.; Murphy IV, F.; Murphy, E.; Carr, J.; Blanchard, S.; Jogl, G.; Dahlberg, A.E.; Gregory, S.T.
Deposited on	:	2013-03-05
Resolution	:	3.64 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

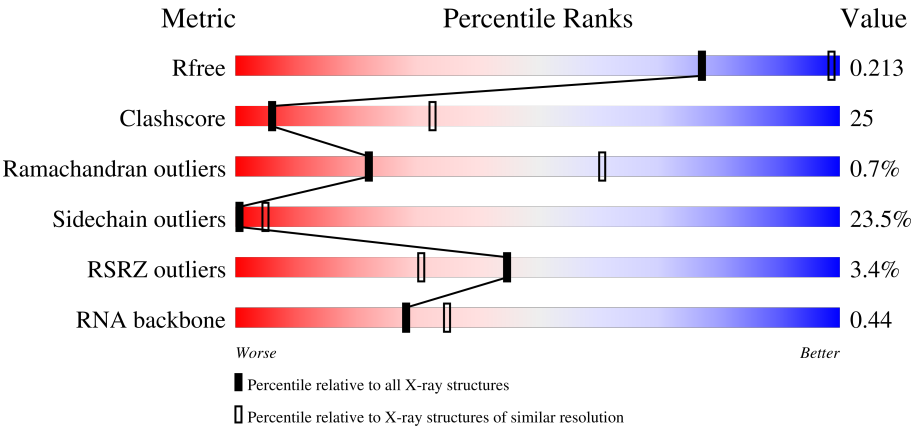
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.64 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	1341 (3.78-3.50)
Clashscore	141614	1439 (3.78-3.50)
Ramachandran outliers	138981	1391 (3.78-3.50)
Sidechain outliers	138945	1391 (3.78-3.50)
RSRZ outliers	127900	1242 (3.78-3.50)
RNA backbone	3102	1019 (4.26-3.00)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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% 16% 41% 33% 10%
2	B	256	% 37% 40% 13% 9%
3	C	239	6% 27% 44% 14% 14%
4	D	209	2% 35% 49% 14%

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Mol	Chain	Length	Quality of chain
5	E	162	38% 40% 14% 7%
6	F	101	% 39% 53% 8%
7	G	156	2% 46% 46% 8%
8	H	138	47% 40% 12%
9	I	128	12% 38% 49% 12%
10	J	105	19% 35% 40% 18% 7%
11	K	129	2% 41% 38% 11% 10%
12	L	135	2% 30% 44% 18% 8%
13	M	126	6% 27% 56% 11% 6%
14	N	61	5% 36% 52% 10%
15	O	89	44% 40% 13%
16	P	88	27% 56% 10% 6%
17	Q	105	32% 45% 16% 6%
18	R	88	27% 35% 17% 20%
19	S	93	20% 32% 43% 10% 14%
20	T	106	3% 41% 37% 16% 7%
21	U	27	11% 22% 52% 15% 11%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	PSU	A	1540	-	-	-	X
1	5MC	A	967	-	-	X	-
22	MG	A	1601	-	-	-	X
22	MG	A	1683	-	-	-	X
22	MG	A	1704	-	-	-	X
22	MG	A	1715	-	-	-	X
22	MG	A	1720	-	-	-	X
22	MG	A	1735	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	MG	A	1749	-	-	-	X
22	MG	A	1751	-	-	-	X
22	MG	A	1766	-	-	-	X
22	MG	A	1769	-	-	-	X
22	MG	A	1770	-	-	-	X
22	MG	A	1777	-	-	-	X
22	MG	A	1780	-	-	-	X
22	MG	A	1781	-	-	-	X
22	MG	A	1782	-	-	-	X
22	MG	A	1794	-	-	-	X
22	MG	A	1796	-	-	-	X
22	MG	A	1826	-	-	-	X
22	MG	A	1830	-	-	-	X
22	MG	A	1835	-	-	-	X
22	MG	A	1838	-	-	-	X
22	MG	A	1839	-	-	-	X
22	MG	A	1842	-	-	-	X
22	MG	A	1845	-	-	-	X
22	MG	A	1847	-	-	-	X
22	MG	A	1853	-	-	-	X
22	MG	A	1857	-	-	-	X
22	MG	A	1858	-	-	-	X
22	MG	A	1866	-	-	-	X
22	MG	C	301	-	-	-	X
22	MG	H	201	-	-	-	X
22	MG	P	102	-	-	-	X

2 Entry composition (i)

There are 24 unique types of molecules in this entry. The entry contains 52307 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	32644	14540	6039	10547	1518	0	6	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1534	C	A	engineered mutation	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
6	F	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 7 is a protein called RIBOSOMAL PROTEIN S7.

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

- Molecule 8 is a protein called RIBOSOMAL PROTEIN S8.

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

- Molecule 9 is a protein called RIBOSOMAL PROTEIN S9.

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

- Molecule 10 is a protein called RIBOSOMAL PROTEIN S10.

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

- Molecule 11 is a protein called RIBOSOMAL PROTEIN S11.

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

- Molecule 12 is a protein called RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	124	Total	C	N	O	S	0	0	0
			977	617	196	163	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	94	TRP	PRO	conflict	UNP F6DEQ7

- Molecule 13 is a protein called RIBOSOMAL PROTEIN S13.

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

- Molecule 14 is a protein called RIBOSOMAL PROTEIN S14.

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

- Molecule 15 is a protein called RIBOSOMAL PROTEIN S15.

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

- Molecule 16 is a protein called RIBOSOMAL PROTEIN S16.

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

- Molecule 17 is a protein called RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

- Molecule 18 is a protein called RIBOSOMAL PROTEIN S18.

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

- Molecule 19 is a protein called RIBOSOMAL PROTEIN S19.

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

- Molecule 20 is a protein called RIBOSOMAL PROTEIN S20.

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

- Molecule 21 is a protein called RIBOSOMAL PROTEIN THX.

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	276	Total 276	Mg 276	0	0
22	B	3	Total 3	Mg 3	0	0
22	C	2	Total 2	Mg 2	0	0
22	D	3	Total 3	Mg 3	0	0
22	E	1	Total 1	Mg 1	0	0
22	F	1	Total 1	Mg 1	0	0
22	H	1	Total 1	Mg 1	0	0
22	I	1	Total 1	Mg 1	0	0
22	J	1	Total 1	Mg 1	0	0
22	N	1	Total 1	Mg 1	0	0
22	P	2	Total 2	Mg 2	0	0
22	Q	1	Total 1	Mg 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.

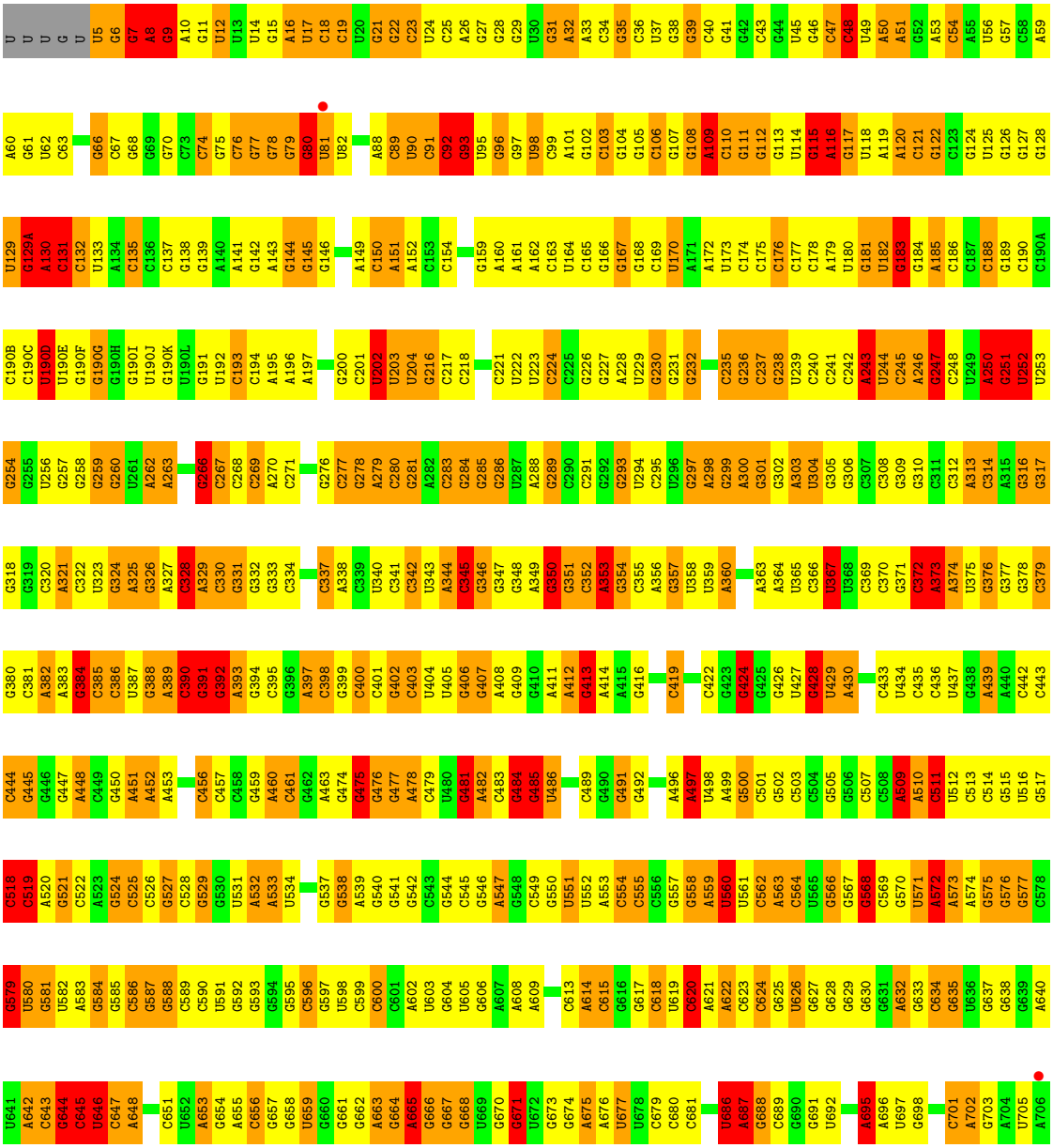
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	266	Total O 266 266	0	0
24	E	3	Total O 3 3	0	0
24	K	1	Total O 1 1	0	0
24	L	1	Total O 1 1	0	0
24	Q	2	Total O 2 2	0	0
24	T	2	Total O 2 2	0	0

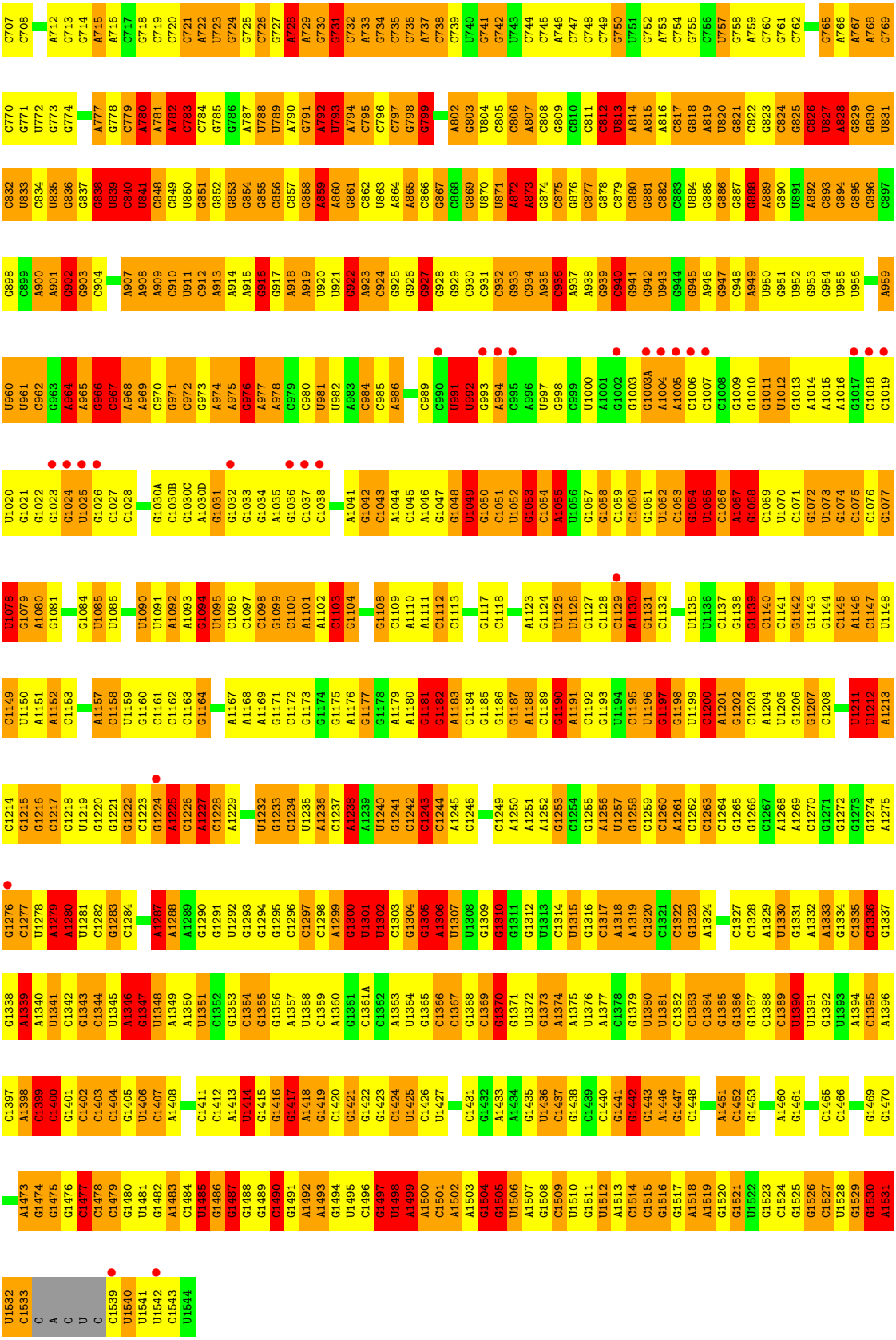
3 Residue-property plots (i)

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

- Molecule 1: 16S rRNA

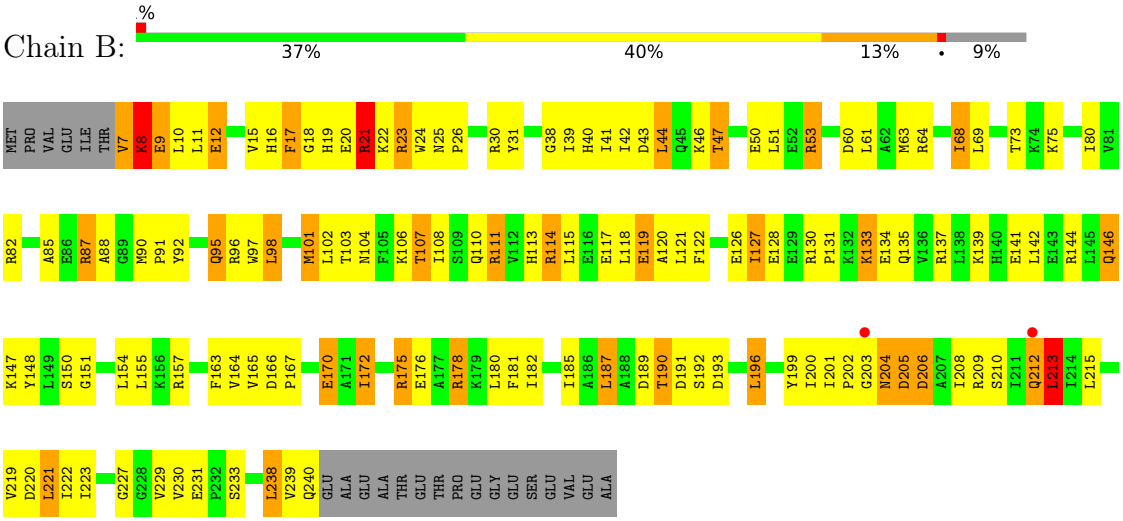
Chain A: 2% 16% 41% 33% 10%





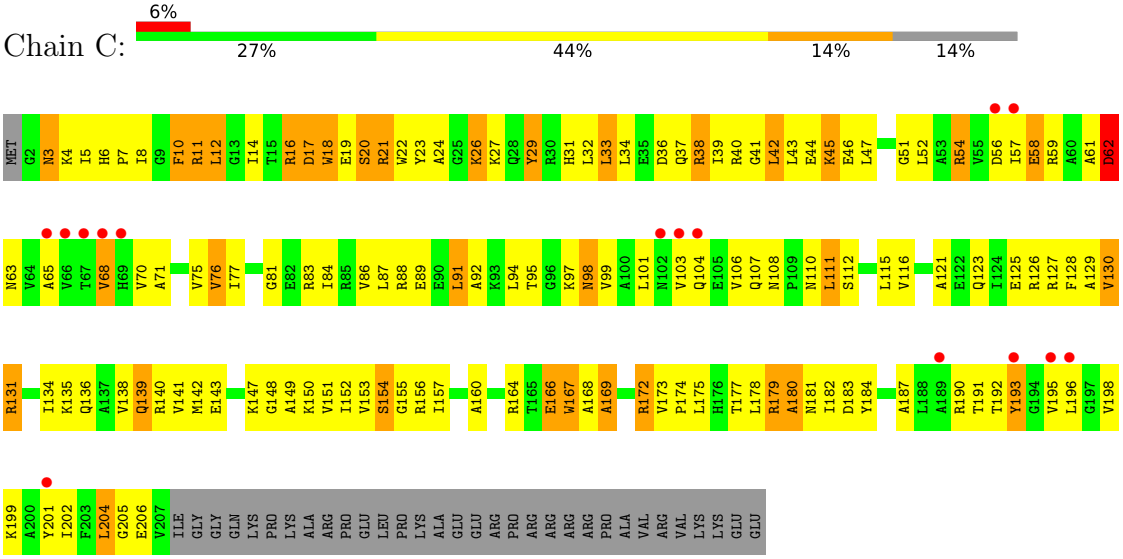
• Molecule 2: RIBOSOMAL PROTEIN S2

Chain B:



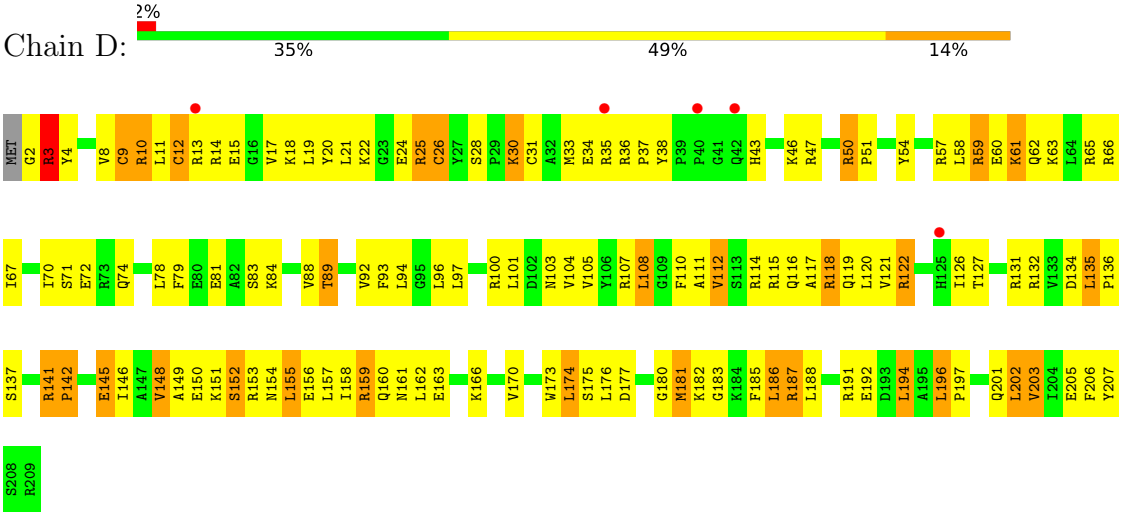
• Molecule 3: RIBOSOMAL PROTEIN S3

Chain C:



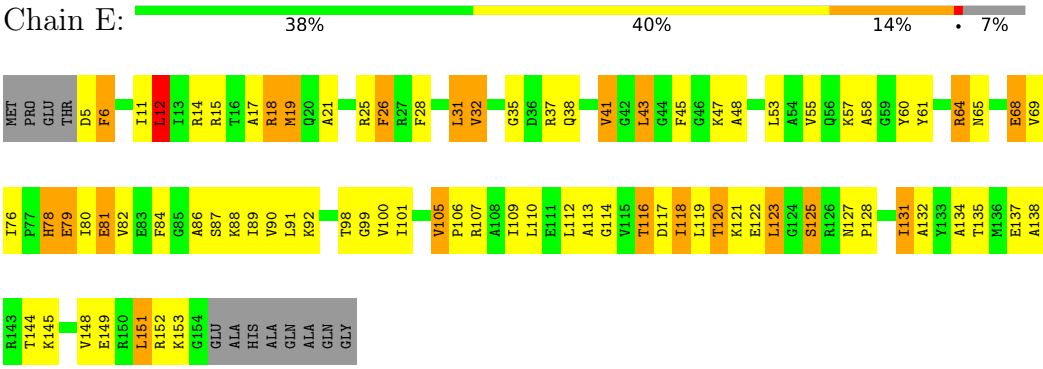
• Molecule 4: RIBOSOMAL PROTEIN S4

Chain D:



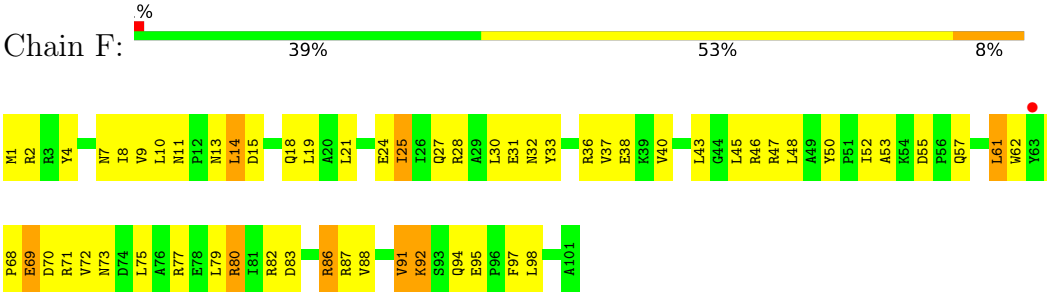
• Molecule 5: RIBOSOMAL PROTEIN S5

Chain E:



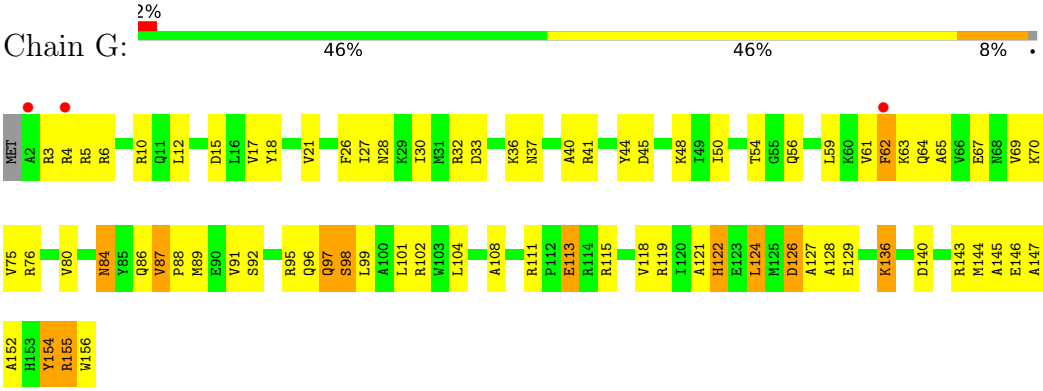
• Molecule 6: RIBOSOMAL PROTEIN S6

Chain F:



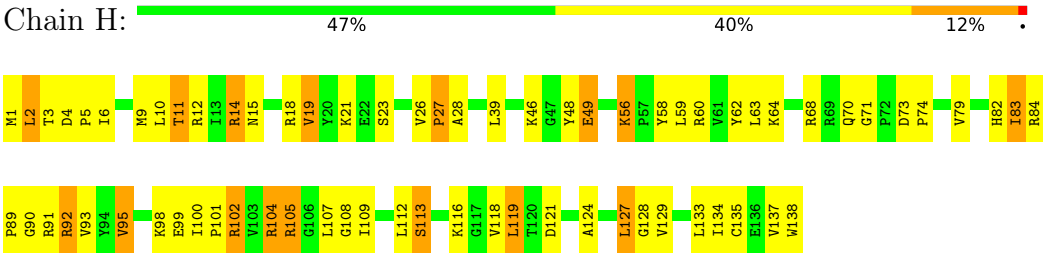
• Molecule 7: RIBOSOMAL PROTEIN S7

Chain G:



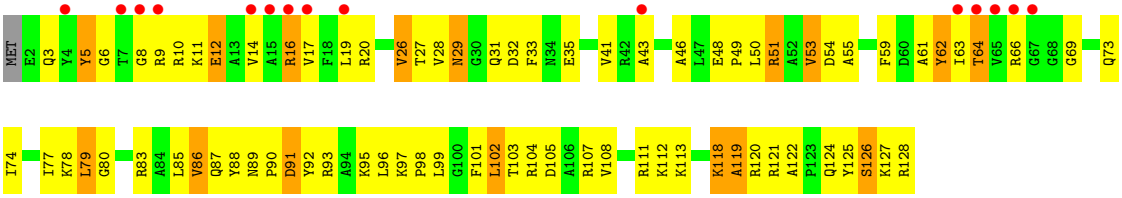
• Molecule 8: RIBOSOMAL PROTEIN S8

Chain H:



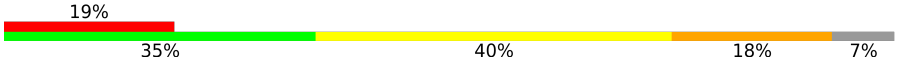
• Molecule 9: RIBOSOMAL PROTEIN S9

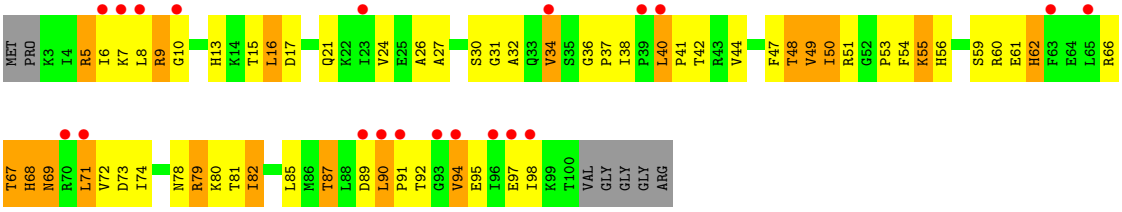
Chain I:



• Molecule 10: RIBOSOMAL PROTEIN S10

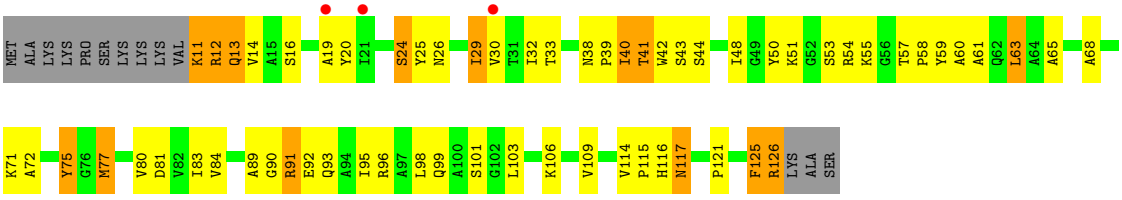
Chain J:





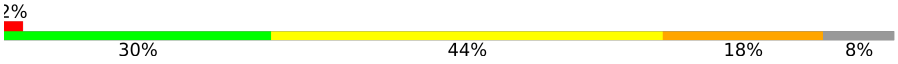
• Molecule 11: RIBOSOMAL PROTEIN S11

Chain K:



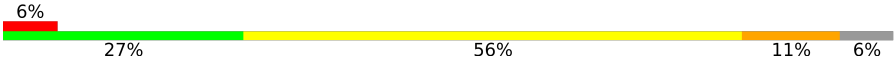
• Molecule 12: RIBOSOMAL PROTEIN S12

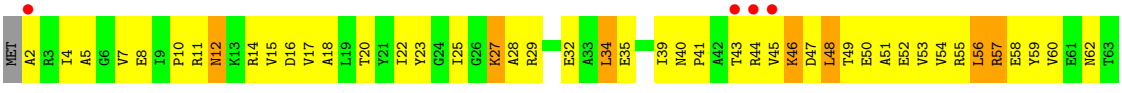
Chain L:

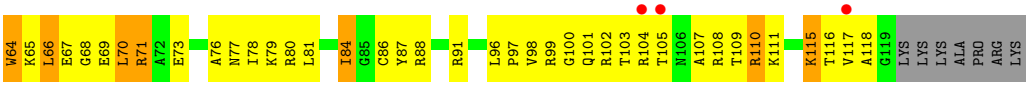


• Molecule 13: RIBOSOMAL PROTEIN S13

Chain M:

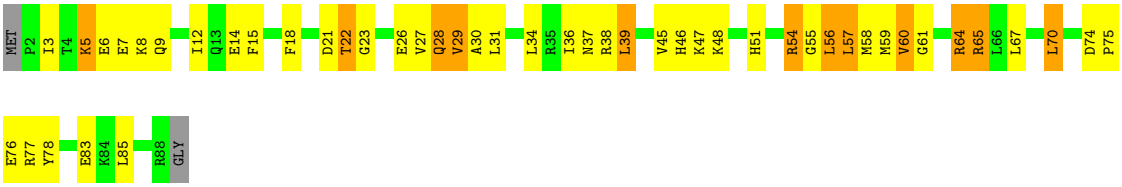




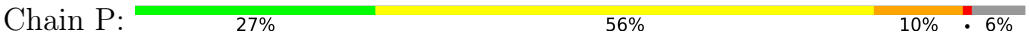


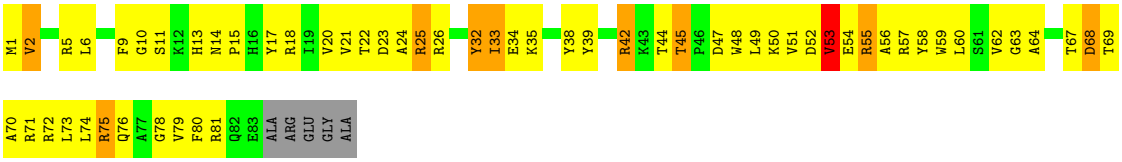
• Molecule 14: RIBOSOMAL PROTEIN S14

• Molecule 15: RIBOSOMAL PROTEIN S15

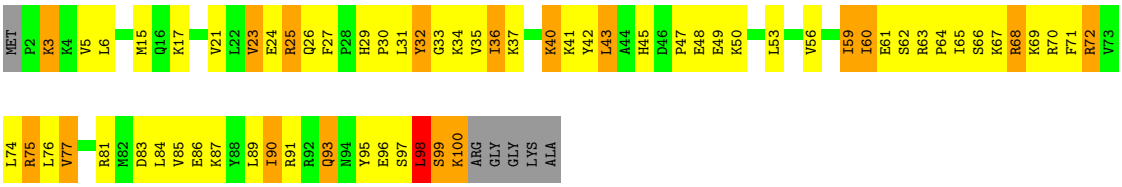


• Molecule 16: RIBOSOMAL PROTEIN S16

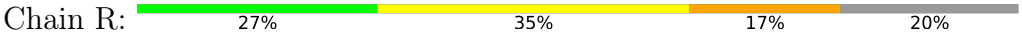


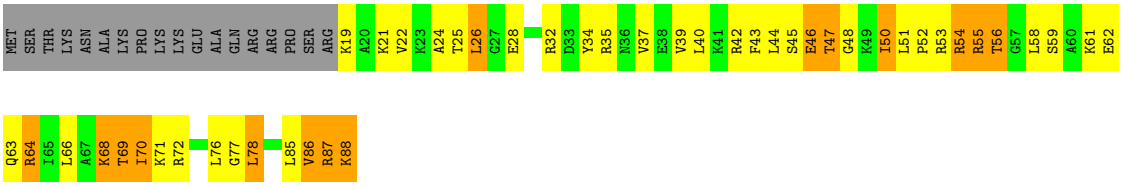


• Molecule 17: RIBOSOMAL PROTEIN S17



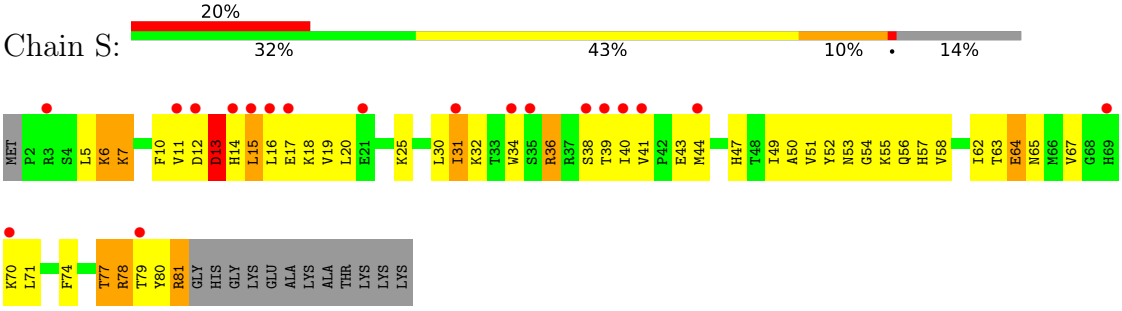
• Molecule 18: RIBOSOMAL PROTEIN S18





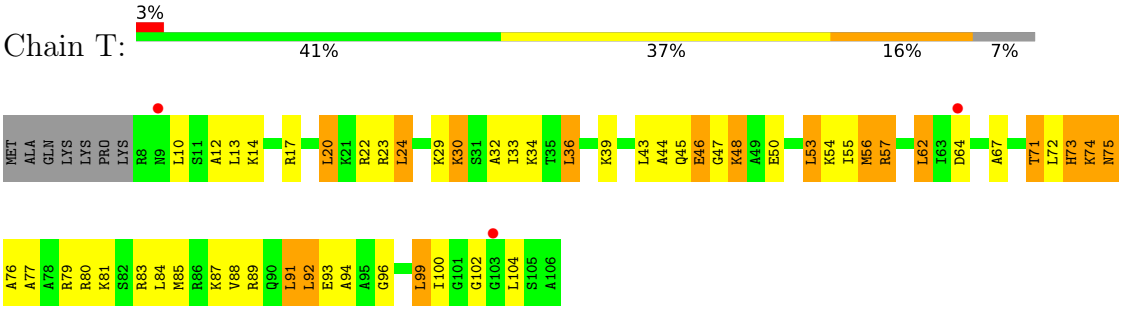
• Molecule 19: RIBOSOMAL PROTEIN S19

Chain S:



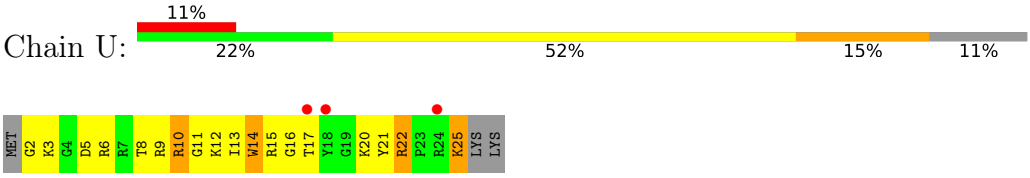
• Molecule 20: RIBOSOMAL PROTEIN S20

Chain T:



• Molecule 21: RIBOSOMAL PROTEIN THX

Chain U:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	402.45Å 402.45Å 174.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.34 – 3.64 49.57 – 3.64	Depositor EDS
% Data completeness (in resolution range)	98.9 (48.34-3.64) 98.9 (49.57-3.64)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.00 (at 3.67Å)	Xtriage
Refinement program	PHENIX dev_1119	Depositor
R, R_{free}	0.155 , 0.211 0.158 , 0.213	Depositor DCC
R_{free} test set	7893 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	120.3	Xtriage
Anisotropy	0.253	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 134.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	52307	wwPDB-VP
Average B, all atoms (Å^2)	153.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.70% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.21	178/36139 (0.5%)	2.00	1849/56396 (3.3%)
2	B	0.71	0/1935	0.91	3/2609 (0.1%)
3	C	0.58	1/1636 (0.1%)	0.84	1/2205 (0.0%)
4	D	0.75	1/1733 (0.1%)	0.89	3/2318 (0.1%)
5	E	0.99	0/1162	1.13	2/1564 (0.1%)
6	F	0.61	0/856	0.81	0/1154
7	G	0.58	0/1276	0.78	0/1709
8	H	1.07	2/1136 (0.2%)	1.15	2/1527 (0.1%)
9	I	0.57	0/1029	0.79	0/1379
10	J	0.53	0/805	0.83	1/1082 (0.1%)
11	K	0.69	0/879	0.92	1/1187 (0.1%)
12	L	0.79	0/994	0.98	0/1331
13	M	0.64	0/947	0.87	0/1270
14	N	0.55	0/501	0.77	0/664
15	O	0.79	0/740	0.96	0/987
16	P	0.84	0/716	1.01	3/963 (0.3%)
17	Q	1.02	1/836 (0.1%)	1.14	2/1117 (0.2%)
18	R	0.75	0/579	0.98	1/768 (0.1%)
19	S	0.52	0/661	0.80	0/890
20	T	0.73	0/765	0.99	2/1007 (0.2%)
21	U	0.64	0/212	0.76	0/277
All	All	1.07	183/55537 (0.3%)	1.74	1870/82404 (2.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	2
3	C	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
4	D	0	1
7	G	0	1
8	H	0	2
10	J	0	2
12	L	0	2
13	M	0	1
18	R	0	1
19	S	0	1
20	T	0	2
All	All	0	18

All (183) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	279	A	N9-C4	-13.71	1.29	1.37
1	A	279	A	N3-C4	-13.61	1.26	1.34
1	A	279	A	N7-C5	-11.36	1.32	1.39
1	A	817	C	N1-C6	-10.06	1.31	1.37
1	A	793	U	C2-N3	9.46	1.44	1.37
1	A	722	A	C5-C6	-9.32	1.32	1.41
1	A	915	A	N9-C4	-8.68	1.32	1.37
1	A	882	C	N3-C4	-8.61	1.27	1.33
1	A	729	A	N9-C4	-8.47	1.32	1.37
1	A	566	G	N7-C5	-8.30	1.34	1.39
1	A	1509	C	N3-C4	-8.22	1.28	1.33
1	A	1504	G	N7-C5	-8.21	1.34	1.39
1	A	793	U	N3-C4	8.11	1.45	1.38
1	A	574	A	C5-C4	-8.01	1.33	1.38
1	A	1502	A	C5-C6	-7.88	1.33	1.41
1	A	824	C	N1-C6	-7.80	1.32	1.37
1	A	779	C	N1-C6	-7.77	1.32	1.37
1	A	814	A	N9-C4	-7.69	1.33	1.37
1	A	1377	A	N9-C4	-7.65	1.33	1.37
1	A	860	A	N3-C4	-7.65	1.30	1.34
1	A	852	G	C6-O6	7.61	1.31	1.24
1	A	122	G	C2-N3	-7.57	1.26	1.32
4	D	12	CYS	CB-SG	7.56	1.95	1.82
1	A	1514	C	N3-C4	-7.51	1.28	1.33
1	A	882	C	N1-C6	-7.37	1.32	1.37
1	A	1514	C	N1-C6	-7.33	1.32	1.37
1	A	1077	G	N9-C8	-7.32	1.32	1.37
1	A	722	A	N7-C5	-7.30	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	329	A	N9-C4	-7.21	1.33	1.37
1	A	574	A	N7-C5	-7.21	1.34	1.39
1	A	1509	C	N1-C6	-7.18	1.32	1.37
1	A	266	G	N7-C5	-7.01	1.35	1.39
1	A	1504	G	N9-C8	-6.92	1.33	1.37
1	A	715	A	N9-C4	-6.89	1.33	1.37
1	A	1502	A	N9-C4	-6.87	1.33	1.37
1	A	228	A	N9-C4	-6.81	1.33	1.37
1	A	122	G	C5-C6	-6.74	1.35	1.42
1	A	576	G	N3-C4	-6.73	1.30	1.35
1	A	298	A	N3-C4	-6.72	1.30	1.34
1	A	569	C	N3-C4	-6.71	1.29	1.33
1	A	727	G	C6-N1	-6.70	1.34	1.39
1	A	728	A	N9-C4	-6.69	1.33	1.37
1	A	16	A	N9-C4	-6.68	1.33	1.37
1	A	787	A	N9-C4	-6.55	1.33	1.37
1	A	574	A	N9-C8	-6.52	1.32	1.37
1	A	703	G	C6-O6	6.40	1.29	1.24
1	A	1502	A	N7-C5	-6.39	1.35	1.39
1	A	828	A	N9-C4	-6.38	1.34	1.37
1	A	295	C	N3-C4	-6.35	1.29	1.33
1	A	236	G	N7-C5	-6.31	1.35	1.39
1	A	1094	G	C6-N1	-6.29	1.35	1.39
1	A	1499	A	N9-C4	-6.27	1.34	1.37
1	A	574	A	N3-C4	-6.25	1.31	1.34
1	A	568	G	C6-N1	-6.24	1.35	1.39
1	A	263	A	N9-C4	-6.23	1.34	1.37
1	A	558	G	C5-C6	-6.22	1.36	1.42
1	A	573	A	N7-C5	-6.20	1.35	1.39
1	A	119	A	N9-C4	-6.19	1.34	1.37
1	A	122	G	N3-C4	-6.19	1.31	1.35
1	A	279	A	C5-C6	-6.16	1.35	1.41
1	A	298	A	N9-C4	-6.13	1.34	1.37
1	A	1079	G	N7-C5	-6.09	1.35	1.39
1	A	329	A	C5-C6	-6.07	1.35	1.41
1	A	865	A	C5-C4	-6.07	1.34	1.38
1	A	797	C	N1-C6	-6.06	1.33	1.37
1	A	130	A	N3-C4	-6.05	1.31	1.34
8	H	135	CYS	CB-SG	-6.03	1.72	1.82
1	A	915	A	N3-C4	-6.02	1.31	1.34
1	A	876	G	C6-N1	-5.99	1.35	1.39
1	A	1064	G	N3-C4	-5.98	1.31	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1394	A	C5-C6	-5.98	1.35	1.41
1	A	646	U	C4-O4	5.98	1.28	1.23
1	A	753	A	N3-C4	-5.94	1.31	1.34
1	A	124	G	C6-N1	-5.93	1.35	1.39
1	A	1502	A	N3-C4	-5.93	1.31	1.34
1	A	1076	C	N1-C6	-5.91	1.33	1.37
1	A	246	A	C5-C4	-5.89	1.34	1.38
1	A	635	G	C6-O6	5.89	1.29	1.24
1	A	828	A	N3-C4	-5.88	1.31	1.34
1	A	938	A	N9-C4	-5.88	1.34	1.37
1	A	727	G	N7-C5	-5.87	1.35	1.39
1	A	248	C	N1-C6	-5.87	1.33	1.37
3	C	169	ALA	CA-CB	-5.86	1.40	1.52
1	A	570	G	C5-C4	-5.85	1.34	1.38
1	A	589	C	N1-C6	-5.84	1.33	1.37
1	A	703	G	C5-C6	5.84	1.48	1.42
1	A	873	A	C6-N1	-5.80	1.31	1.35
1	A	288	A	N9-C4	-5.78	1.34	1.37
1	A	909	A	N9-C4	-5.78	1.34	1.37
1	A	325	A	N9-C4	-5.77	1.34	1.37
1	A	1499	A	N3-C4	-5.75	1.31	1.34
1	A	923	A	C5-C6	-5.74	1.35	1.41
1	A	1401	G	C6-N1	-5.73	1.35	1.39
1	A	1386	G	N9-C8	-5.73	1.33	1.37
1	A	574	A	N9-C4	-5.73	1.34	1.37
1	A	1504	G	C5-C4	-5.71	1.34	1.38
1	A	569	C	N1-C6	-5.71	1.33	1.37
1	A	561	U	N1-C6	-5.71	1.32	1.38
1	A	266	G	C2-N3	5.70	1.37	1.32
1	A	873	A	C6-N6	-5.69	1.29	1.33
1	A	855	G	N3-C4	-5.67	1.31	1.35
1	A	803	G	C5-C4	-5.66	1.34	1.38
1	A	298	A	C5-C4	-5.65	1.34	1.38
1	A	1232	U	N1-C2	-5.65	1.33	1.38
1	A	836	G	C6-O6	5.64	1.29	1.24
1	A	236	G	C5-C4	-5.63	1.34	1.38
1	A	130	A	N9-C4	-5.59	1.34	1.37
1	A	828	A	N7-C5	-5.57	1.35	1.39
1	A	1507	A	N9-C4	-5.56	1.34	1.37
1	A	856	C	N1-C6	-5.56	1.33	1.37
1	A	918	A	C5-C4	-5.54	1.34	1.38
1	A	877	C	N3-C4	-5.53	1.30	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1500	A	N3-C4	-5.52	1.31	1.34
1	A	861	G	N3-C4	-5.51	1.31	1.35
1	A	803	G	N1-C2	-5.50	1.33	1.37
1	A	291	C	N1-C6	-5.48	1.33	1.37
1	A	570	G	N1-C2	-5.46	1.33	1.37
1	A	553	A	N9-C4	-5.45	1.34	1.37
1	A	722	A	N9-C4	-5.44	1.34	1.37
1	A	269	C	N3-C4	-5.44	1.30	1.33
1	A	817	C	N3-C4	-5.43	1.30	1.33
1	A	739	C	N3-C4	-5.42	1.30	1.33
1	A	1525	G	N3-C4	-5.41	1.31	1.35
1	A	482	A	N7-C5	-5.39	1.36	1.39
1	A	856	C	N1-C2	-5.38	1.34	1.40
1	A	896	C	N3-C4	-5.36	1.30	1.33
1	A	852	G	C5-C4	5.36	1.42	1.38
1	A	807	A	C6-N1	-5.36	1.31	1.35
1	A	861	G	N7-C5	-5.35	1.36	1.39
1	A	1526	G	C5-C6	-5.33	1.37	1.42
1	A	634	C	N3-C4	-5.32	1.30	1.33
1	A	109	A	N9-C4	-5.32	1.34	1.37
1	A	329	A	N7-C5	-5.32	1.36	1.39
1	A	733	A	N9-C4	-5.32	1.34	1.37
1	A	150	C	N1-C6	-5.31	1.33	1.37
1	A	1513	A	N9-C4	-5.31	1.34	1.37
1	A	814	A	N3-C4	-5.30	1.31	1.34
1	A	570	G	C6-N1	-5.29	1.35	1.39
1	A	632	A	N3-C4	-5.29	1.31	1.34
1	A	862	C	C4-N4	-5.29	1.29	1.33
1	A	882	C	C2-N3	-5.29	1.31	1.35
1	A	1080	A	N3-C4	-5.28	1.31	1.34
1	A	120	A	N9-C4	-5.27	1.34	1.37
1	A	862	C	C4-C5	-5.26	1.38	1.43
1	A	448	A	N7-C5	-5.25	1.36	1.39
1	A	308	C	N1-C6	-5.24	1.34	1.37
1	A	568	G	C5-C4	-5.23	1.34	1.38
1	A	807	A	N9-C4	-5.22	1.34	1.37
1	A	559	A	N7-C5	-5.22	1.36	1.39
17	Q	32	TYR	CD1-CE1	5.21	1.47	1.39
1	A	125	U	C2-N3	-5.19	1.34	1.37
1	A	1487	G	C6-N1	-5.19	1.35	1.39
1	A	306	G	C6-N1	5.19	1.43	1.39
1	A	881	G	N3-C4	-5.18	1.31	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	497	A	N9-C4	-5.17	1.34	1.37
1	A	861	G	C5-C6	-5.16	1.37	1.42
1	A	931	C	N1-C6	-5.15	1.34	1.37
1	A	753	A	N9-C4	-5.14	1.34	1.37
1	A	852	G	C6-N1	5.14	1.43	1.39
1	A	798	G	N3-C4	-5.13	1.31	1.35
8	H	49	GLU	CG-CD	5.13	1.59	1.51
1	A	802	A	C5-C6	-5.13	1.36	1.41
1	A	860	A	N9-C4	-5.12	1.34	1.37
1	A	855	G	C5-C4	-5.11	1.34	1.38
1	A	1066	C	N1-C6	-5.11	1.34	1.37
1	A	1078	U	C4-C5	-5.11	1.39	1.43
1	A	820	U	C4-O4	-5.11	1.19	1.23
1	A	828	A	C5-C4	-5.10	1.35	1.38
1	A	563	A	N3-C4	-5.09	1.31	1.34
1	A	1052	U	C2-N3	5.09	1.41	1.37
1	A	825	G	C5-C4	-5.08	1.34	1.38
1	A	151	A	N9-C4	-5.07	1.34	1.37
1	A	640	A	N3-C4	-5.06	1.31	1.34
1	A	655	A	C6-N6	-5.05	1.29	1.33
1	A	821	G	C5-C6	-5.05	1.37	1.42
1	A	874	G	N9-C8	-5.04	1.34	1.37
1	A	576	G	C6-N1	-5.04	1.36	1.39
1	A	564	C	N3-C4	-5.03	1.30	1.33
1	A	1064	G	N9-C4	-5.03	1.33	1.38
1	A	119	A	N3-C4	-5.02	1.31	1.34
1	A	771	G	N9-C8	-5.02	1.34	1.37
1	A	712	A	N9-C4	-5.01	1.34	1.37
1	A	1513	A	N3-C4	-5.01	1.31	1.34

All (1870) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	266	G	C6-C5-N7	-17.70	119.78	130.40
1	A	735	C	C6-N1-C2	16.27	126.81	120.30
1	A	117	G	N1-C6-O6	15.58	129.25	119.90
1	A	1516[A]	G	C8-N9-C4	-14.80	100.48	106.40
1	A	1516[B]	G	C8-N9-C4	-14.80	100.48	106.40
1	A	635	G	C5-C6-N1	-14.69	104.16	111.50
1	A	117	G	C6-C5-N7	-14.54	121.67	130.40
1	A	770	C	O5'-P-OP2	-14.03	93.08	105.70
1	A	722	A	N1-C6-N6	13.90	126.94	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	317	G	N1-C6-O6	13.37	127.92	119.90
1	A	558	G	C4-C5-N7	13.37	116.15	110.80
1	A	242	C	C6-N1-C2	13.32	125.63	120.30
1	A	793	U	C5-C6-N1	13.23	129.31	122.70
1	A	852	G	C5-C6-N1	-13.22	104.89	111.50
1	A	232	G	N9-C4-C5	-12.93	100.23	105.40
1	A	1532	U	C5-C6-N1	12.85	129.13	122.70
1	A	279	A	C2-N3-C4	-12.72	104.24	110.60
1	A	481	G	N3-C4-N9	12.71	133.62	126.00
1	A	873	A	N1-C6-N6	-12.70	110.98	118.60
1	A	266	G	N7-C8-N9	12.63	119.42	113.10
1	A	266	G	C5-N7-C8	-12.57	98.01	104.30
1	A	919	A	O5'-P-OP2	-12.55	94.40	105.70
1	A	279	A	C4-C5-C6	12.54	123.27	117.00
1	A	232	G	N1-C6-O6	12.46	127.38	119.90
1	A	774	G	N1-C6-O6	12.43	127.36	119.90
1	A	122	G	N1-C6-O6	12.42	127.35	119.90
1	A	266	G	C4-C5-N7	12.34	115.73	110.80
1	A	279	A	C6-C5-N7	-12.16	123.78	132.30
1	A	117	G	C5-C6-N1	-12.08	105.46	111.50
1	A	279	A	N7-C8-N9	12.07	119.83	113.80
1	A	366	C	N1-C2-O2	12.02	126.11	118.90
1	A	722	A	C2-N3-C4	-11.93	104.64	110.60
1	A	573	A	C8-N9-C4	-11.85	101.06	105.80
1	A	266	G	N1-C6-O6	11.81	126.98	119.90
1	A	279	A	C5-N7-C8	-11.79	98.00	103.90
1	A	117	G	C4-C5-C6	11.78	125.86	118.80
1	A	722	A	C6-C5-N7	-11.69	124.12	132.30
1	A	245	C	C5-C4-N4	-11.62	112.07	120.20
1	A	279	A	C8-N9-C4	-11.56	101.18	105.80
1	A	266	G	C4-N9-C1'	11.51	141.47	126.50
1	A	279	A	N1-C2-N3	11.48	135.04	129.30
1	A	1370	G	C8-N9-C4	-11.46	101.81	106.40
1	A	884	U	C5-C6-N1	-11.43	116.99	122.70
1	A	1502	A	C2-N3-C4	-11.41	104.89	110.60
1	A	1386	G	C8-N9-C4	11.35	110.94	106.40
1	A	835	U	C5-C4-O4	11.32	132.69	125.90
1	A	277	C	N3-C4-C5	11.28	126.41	121.90
1	A	805	C	C6-N1-C2	11.25	124.80	120.30
1	A	301	G	O5'-P-OP2	-11.23	95.59	105.70
1	A	635	G	C2-N3-C4	-11.19	106.31	111.90
1	A	277	C	C6-N1-C2	11.18	124.77	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	873	A	C5-C6-N1	11.15	123.28	117.70
1	A	1516[A]	G	N9-C4-C5	11.12	109.85	105.40
1	A	1516[B]	G	N9-C4-C5	11.12	109.85	105.40
1	A	570	G	N1-C6-O6	-11.10	113.24	119.90
1	A	948	C	C6-N1-C2	11.09	124.73	120.30
1	A	117	G	C2-N3-C4	-11.06	106.37	111.90
1	A	817	C	C5-C6-N1	-10.96	115.52	121.00
1	A	722	A	C4-C5-N7	10.92	116.16	110.70
1	A	1344	C	C6-N1-C2	10.87	124.65	120.30
1	A	703	G	C4-C5-N7	-10.84	106.46	110.80
1	A	1190	G	C6-C5-N7	-10.79	123.92	130.40
1	A	283	C	N3-C4-C5	-10.79	117.58	121.90
1	A	245	C	N3-C4-N4	10.74	125.52	118.00
1	A	1395	C	O5'-P-OP2	-10.74	96.03	105.70
1	A	1436	U	N3-C2-O2	-10.63	114.76	122.20
1	A	117	G	C8-N9-C1'	-10.63	113.19	127.00
1	A	836	G	C5-C6-N1	-10.59	106.20	111.50
1	A	825	G	C8-N9-C4	10.58	110.63	106.40
1	A	1346	A	O5'-P-OP2	-10.58	96.18	105.70
1	A	525	C	C6-N1-C2	10.57	124.53	120.30
1	A	814	A	C2-N3-C4	-10.56	105.32	110.60
1	A	875	C	C6-N1-C2	10.56	124.52	120.30
1	A	824	C	C6-N1-C2	10.55	124.52	120.30
1	A	16	A	C8-N9-C4	10.55	110.02	105.80
1	A	283	C	C6-N1-C2	-10.53	116.09	120.30
1	A	1502	A	C6-C5-N7	-10.51	124.95	132.30
1	A	1190	G	C4-N9-C1'	10.50	140.16	126.50
1	A	882	C	C5-C6-N1	-10.48	115.76	121.00
1	A	1528	U	O5'-P-OP2	-10.48	96.26	105.70
1	A	635	G	N1-C6-O6	10.47	126.18	119.90
1	A	1158	C	C6-N1-C2	-10.44	116.12	120.30
1	A	1369	C	C6-N1-C2	-10.44	116.12	120.30
1	A	875	C	C5-C6-N1	-10.42	115.79	121.00
1	A	125	U	C5-C6-N1	-10.42	117.49	122.70
1	A	558	G	C5-N7-C8	-10.40	99.10	104.30
1	A	1374	A	O5'-P-OP2	-10.39	96.35	105.70
1	A	865	A	C5-C6-N1	10.38	122.89	117.70
1	A	1502	A	C5-N7-C8	-10.33	98.74	103.90
1	A	1502	A	N1-C6-N6	10.31	124.79	118.60
1	A	731	G	N1-C6-O6	10.30	126.08	119.90
1	A	558	G	C6-C5-N7	-10.30	124.22	130.40
1	A	481	G	C5-C6-O6	-10.29	122.43	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1526	G	N1-C6-O6	10.27	126.06	119.90
1	A	15	G	N1-C6-O6	10.23	126.04	119.90
1	A	703	G	C5-C6-O6	10.23	134.74	128.60
1	A	232	G	C4-C5-N7	10.21	114.88	110.80
1	A	745	C	N3-C4-C5	10.19	125.98	121.90
1	A	481	G	N3-C4-C5	-10.18	123.51	128.60
1	A	1200	C	C2-N1-C1'	10.16	129.97	118.80
1	A	856	C	N1-C2-O2	-10.14	112.82	118.90
1	A	329	A	C2-N3-C4	-10.09	105.56	110.60
1	A	1227	A	N1-C6-N6	10.08	124.65	118.60
1	A	570	G	C2-N3-C4	10.07	116.94	111.90
1	A	568	G	O5'-P-OP2	-10.07	96.64	105.70
1	A	836	G	N1-C6-O6	10.05	125.93	119.90
1	A	283	C	C5-C6-N1	10.04	126.02	121.00
1	A	817	C	C4-C5-C6	9.85	122.32	117.40
1	A	511	C	C5-C6-N1	-9.84	116.08	121.00
1	A	117	G	C4-N9-C1'	9.82	139.27	126.50
1	A	812	C	N3-C4-C5	-9.79	117.98	121.90
1	A	774	G	C4-C5-N7	9.78	114.71	110.80
1	A	871	U	O5'-P-OP1	-9.77	96.91	105.70
1	A	144	G	N1-C6-O6	9.74	125.75	119.90
1	A	933	G	N1-C6-O6	9.73	125.74	119.90
1	A	122	G	N3-C4-C5	9.68	133.44	128.60
1	A	745	C	C6-N1-C2	9.67	124.17	120.30
1	A	1052	U	C5-C6-N1	9.66	127.53	122.70
1	A	252	U	C5-C6-N1	-9.59	117.91	122.70
1	A	600	C	C2-N3-C4	-9.53	115.13	119.90
1	A	558	G	N1-C6-O6	9.52	125.61	119.90
1	A	860	A	N1-C2-N3	9.52	134.06	129.30
1	A	317	G	C6-C5-N7	-9.51	124.70	130.40
1	A	519	C	C6-N1-C2	9.51	124.10	120.30
1	A	1530	G	C8-N9-C4	9.49	110.20	106.40
1	A	266	G	C4-C5-C6	9.48	124.48	118.80
1	A	317	G	C4-C5-N7	9.46	114.58	110.80
1	A	600	C	N3-C4-C5	9.44	125.68	121.90
1	A	853	G	C5-C6-N1	-9.42	106.79	111.50
1	A	1347	G	N3-C4-C5	-9.41	123.89	128.60
1	A	266	G	C8-N9-C1'	-9.41	114.76	127.00
1	A	774	G	C5-C6-O6	-9.41	122.95	128.60
1	A	1502	A	C4-C5-N7	9.41	115.41	110.70
1	A	366	C	N3-C2-O2	-9.39	115.33	121.90
1	A	379	C	C6-N1-C2	9.38	124.05	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1200	C	C5-C6-N1	9.37	125.69	121.00
1	A	1528	U	O5'-P-OP1	9.37	121.94	110.70
1	A	862	C	N3-C4-C5	9.37	125.65	121.90
1	A	742	G	N1-C6-O6	9.36	125.52	119.90
1	A	280	C	OP1-P-OP2	9.35	133.63	119.60
1	A	559	A	C8-N9-C4	-9.35	102.06	105.80
1	A	835	U	N1-C2-N3	9.34	120.50	114.90
1	A	314	C	C6-N1-C2	9.31	124.03	120.30
1	A	722	A	C5-N7-C8	-9.30	99.25	103.90
1	A	1490	C	C4-C5-C6	-9.27	112.76	117.40
1	A	1190	G	C8-N9-C1'	-9.27	114.95	127.00
1	A	721	G	C4-N9-C1'	9.26	138.54	126.50
1	A	389	A	N9-C4-C5	9.26	109.50	105.80
1	A	1200	C	N1-C2-O2	9.26	124.45	118.90
1	A	793	U	N1-C2-N3	-9.25	109.35	114.90
1	A	615	C	C6-N1-C2	-9.23	116.61	120.30
1	A	1227	A	C5-N7-C8	-9.20	99.30	103.90
1	A	900	A	C2-N3-C4	-9.19	106.00	110.60
1	A	1344	C	C5-C6-N1	-9.17	116.42	121.00
1	A	51	A	C8-N9-C4	-9.16	102.14	105.80
1	A	721	G	C8-N9-C1'	-9.14	115.12	127.00
1	A	816	A	C8-N9-C4	9.11	109.44	105.80
1	A	389	A	N1-C2-N3	9.08	133.84	129.30
1	A	835	U	N3-C4-C5	-9.07	109.16	114.60
1	A	1532	U	C4-C5-C6	-9.07	114.26	119.70
1	A	852	G	C2-N3-C4	-9.07	107.37	111.90
1	A	1516[A]	G	N7-C8-N9	9.06	117.63	113.10
1	A	1516[B]	G	N7-C8-N9	9.06	117.63	113.10
1	A	1383	C	C6-N1-C2	-9.05	116.68	120.30
1	A	1526	G	C5-C6-O6	-9.04	123.17	128.60
1	A	774	G	C6-C5-N7	-9.02	124.99	130.40
1	A	120	A	C2-N3-C4	-8.99	106.11	110.60
1	A	232	G	C6-C5-N7	-8.98	125.01	130.40
1	A	599	C	C6-N1-C2	8.98	123.89	120.30
1	A	793	U	N3-C4-O4	8.98	125.69	119.40
1	A	1233	G	N1-C6-O6	8.98	125.29	119.90
1	A	235	C	C6-N1-C2	8.96	123.88	120.30
1	A	239	U	O5'-P-OP1	-8.96	97.64	105.70
1	A	864	A	N1-C6-N6	-8.96	113.23	118.60
1	A	647	C	C6-N1-C2	8.96	123.88	120.30
1	A	16	A	N7-C8-N9	-8.94	109.33	113.80
1	A	579	G	C5-C6-O6	-8.93	123.25	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1347	G	P-O3'-C3'	8.92	130.40	119.70
1	A	872	A	N1-C6-N6	8.91	123.95	118.60
1	A	920	U	C5-C4-O4	8.90	131.24	125.90
1	A	945	G	C5-C6-O6	-8.89	123.27	128.60
1	A	242	C	O5'-P-OP2	-8.89	97.70	105.70
1	A	933	G	C5-C6-O6	-8.88	123.27	128.60
1	A	1347	G	N3-C4-N9	8.89	131.33	126.00
1	A	570	G	C5-C6-N1	8.86	115.93	111.50
1	A	309	G	N9-C4-C5	-8.84	101.86	105.40
1	A	1181	G	C8-N9-C4	8.84	109.94	106.40
1	A	1394	A	N1-C6-N6	8.83	123.90	118.60
1	A	481	G	C2-N3-C4	8.81	116.31	111.90
1	A	666	G	C5-C6-N1	-8.81	107.09	111.50
1	A	279	A	C5-C6-N1	-8.80	113.30	117.70
1	A	882	C	N3-C2-O2	-8.80	115.74	121.90
1	A	529	G	C6-C5-N7	-8.79	125.13	130.40
1	A	626	U	C6-N1-C2	-8.79	115.73	121.00
1	A	867	G	N3-C4-N9	8.78	131.27	126.00
1	A	637	G	C8-N9-C4	8.78	109.91	106.40
1	A	126	G	C5-C6-N1	-8.77	107.12	111.50
1	A	511	C	C6-N1-C2	8.76	123.80	120.30
1	A	654	G	N3-C2-N2	-8.76	113.77	119.90
1	A	805	C	N3-C4-C5	8.76	125.40	121.90
1	A	1483	A	C8-N9-C4	8.76	109.30	105.80
1	A	864	A	C5-C6-N6	8.74	130.69	123.70
1	A	279	A	N1-C6-N6	8.74	123.84	118.60
1	A	570	G	N3-C4-C5	-8.73	124.23	128.60
1	A	232	G	C8-N9-C4	8.73	109.89	106.40
1	A	29	G	C2-N3-C4	-8.72	107.54	111.90
1	A	600	C	C5-C6-N1	-8.72	116.64	121.00
1	A	856	C	N3-C4-C5	-8.72	118.41	121.90
1	A	1490	C	N1-C2-O2	8.72	124.13	118.90
1	A	128	G	N1-C6-O6	8.71	125.12	119.90
1	A	1504	G	O5'-P-OP1	-8.70	97.87	105.70
1	A	167	G	C8-N9-C1'	-8.67	115.72	127.00
1	A	823	G	N1-C2-N3	8.67	129.10	123.90
1	A	824	C	C5-C6-N1	-8.67	116.66	121.00
1	A	874	G	O5'-P-OP2	-8.66	97.90	105.70
1	A	588	G	O5'-P-OP2	-8.64	97.92	105.70
1	A	1448	C	C6-N1-C2	8.62	123.75	120.30
1	A	389	A	C4-C5-N7	-8.61	106.40	110.70
1	A	569	C	C5-C6-N1	-8.60	116.70	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	8	A	C8-N9-C4	-8.59	102.36	105.80
1	A	1365	G	C8-N9-C4	-8.59	102.96	106.40
1	A	817	C	C6-N1-C2	8.59	123.74	120.30
1	A	721	G	N3-C4-N9	8.59	131.15	126.00
1	A	774	G	N9-C4-C5	-8.57	101.97	105.40
1	A	110	C	N3-C2-O2	8.57	127.90	121.90
1	A	7	G	N3-C4-N9	8.56	131.14	126.00
1	A	933	G	C6-C5-N7	-8.56	125.26	130.40
1	A	309	G	C2-N3-C4	-8.56	107.62	111.90
1	A	353	A	N1-C6-N6	-8.56	113.46	118.60
1	A	1073	U	C5-C6-N1	-8.54	118.43	122.70
17	Q	98	LEU	CA-CB-CG	8.53	134.91	115.30
1	A	1227	A	C4-C5-N7	8.50	114.95	110.70
1	A	703	G	C5-C6-N1	-8.50	107.25	111.50
1	A	167	G	N3-C4-N9	8.49	131.10	126.00
1	A	131	C	C5-C6-N1	-8.49	116.75	121.00
1	A	793	U	N3-C2-O2	8.49	128.14	122.20
1	A	232	G	C5-C6-O6	-8.48	123.51	128.60
1	A	579	G	N1-C6-O6	8.47	124.98	119.90
1	A	815	A	N1-C6-N6	8.47	123.68	118.60
1	A	289	G	C5-C6-O6	-8.46	123.53	128.60
3	C	179	ARG	N-CA-C	-8.45	88.17	111.00
1	A	1529	G	O5'-P-OP1	-8.45	98.10	105.70
1	A	858	G	N1-C6-O6	8.44	124.97	119.90
1	A	867	G	C8-N9-C1'	-8.44	116.03	127.00
1	A	293	G	C5-C6-N1	-8.42	107.29	111.50
1	A	931	C	C5-C6-N1	-8.42	116.79	121.00
1	A	1531	A	N7-C8-N9	8.40	118.00	113.80
1	A	117	G	N1-C2-N3	8.40	128.94	123.90
1	A	286	G	N1-C6-O6	8.40	124.94	119.90
1	A	1501	C	C6-N1-C2	8.39	123.66	120.30
1	A	248	C	C5-C6-N1	-8.36	116.82	121.00
1	A	1414	U	N3-C2-O2	-8.35	116.36	122.20
1	A	874	G	C8-N9-C4	8.33	109.73	106.40
1	A	329	A	N1-C6-N6	8.32	123.59	118.60
1	A	228	A	C2-N3-C4	-8.32	106.44	110.60
1	A	1521	G	N1-C6-O6	-8.32	114.91	119.90
1	A	573	A	N9-C4-C5	8.31	109.12	105.80
1	A	614	A	C8-N9-C4	-8.31	102.48	105.80
1	A	1505	G	C8-N9-C4	-8.31	103.08	106.40
1	A	970	C	N1-C2-O2	8.30	123.88	118.90
1	A	835	U	C6-N1-C2	-8.29	116.03	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	260	G	C8-N9-C4	-8.28	103.09	106.40
1	A	251	G	C6-C5-N7	-8.27	125.44	130.40
1	A	659	U	C5-C6-N1	-8.27	118.57	122.70
1	A	1129	C	C6-N1-C2	-8.27	116.99	120.30
1	A	246	A	C5-C6-N1	8.26	121.83	117.70
1	A	1052	U	C6-N1-C2	-8.25	116.05	121.00
1	A	526	C	O5'-P-OP2	-8.25	98.28	105.70
1	A	814	A	N1-C2-N3	8.25	133.42	129.30
1	A	739	C	N3-C4-C5	8.24	125.19	121.90
1	A	1232	U	O5'-P-OP1	-8.23	98.29	105.70
1	A	1108	G	N3-C4-C5	-8.22	124.49	128.60
1	A	793	U	C2-N3-C4	8.22	131.93	127.00
1	A	731	G	C5-C6-O6	-8.21	123.67	128.60
1	A	317	G	C5-C6-O6	-8.21	123.67	128.60
1	A	731	G	C8-N9-C4	8.21	109.68	106.40
1	A	529	G	N1-C6-O6	8.21	124.82	119.90
1	A	276	G	C8-N9-C4	8.20	109.68	106.40
1	A	1052	U	N3-C4-O4	8.20	125.14	119.40
1	A	80	G	N3-C2-N2	-8.20	114.16	119.90
1	A	283	C	C2-N3-C4	8.18	123.99	119.90
1	A	314	C	C5-C6-N1	-8.18	116.91	121.00
1	A	354	G	O5'-P-OP1	-8.17	98.35	105.70
1	A	1490	C	N3-C4-C5	8.17	125.17	121.90
1	A	125	U	N1-C2-N3	8.16	119.80	114.90
1	A	1092	A	N1-C6-N6	8.15	123.49	118.60
1	A	936	C	C6-N1-C2	8.14	123.56	120.30
1	A	389	A	N1-C6-N6	-8.13	113.72	118.60
1	A	524	G	C5-C6-O6	-8.13	123.72	128.60
1	A	736	C	N3-C2-O2	-8.12	116.22	121.90
1	A	560	U	N1-C2-O2	8.12	128.48	122.80
1	A	328	C	N3-C4-N4	-8.11	112.32	118.00
1	A	929	G	N1-C6-O6	8.10	124.76	119.90
1	A	50	A	C8-N9-C4	8.09	109.04	105.80
1	A	733	A	C2-N3-C4	-8.09	106.56	110.60
1	A	126	G	C2-N3-C4	-8.08	107.86	111.90
1	A	285	G	C2-N3-C4	-8.06	107.87	111.90
1	A	802	A	N9-C4-C5	-8.05	102.58	105.80
1	A	269	C	C5-C6-N1	-8.04	116.98	121.00
1	A	139	G	N1-C6-O6	8.04	124.72	119.90
1	A	825	G	N7-C8-N9	-8.03	109.08	113.10
1	A	1195	C	N1-C2-O2	-8.03	114.08	118.90
1	A	938	A	C8-N9-C4	8.02	109.01	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1516[A]	G	N3-C4-N9	-8.02	121.19	126.00
1	A	1516[B]	G	N3-C4-N9	-8.02	121.19	126.00
1	A	302	G	C5-C6-O6	-8.02	123.79	128.60
1	A	8	A	N9-C4-C5	8.02	109.01	105.80
1	A	293	G	N3-C2-N2	-8.01	114.29	119.90
1	A	900	A	N1-C2-N3	8.01	133.30	129.30
1	A	266	G	C5-C6-O6	-8.00	123.80	128.60
1	A	823	G	C2-N3-C4	-8.00	107.90	111.90
1	A	289	G	N1-C6-O6	7.99	124.70	119.90
1	A	1485	U	C6-N1-C2	-7.99	116.21	121.00
1	A	122	G	C2-N3-C4	-7.97	107.91	111.90
1	A	579	G	C4-C5-N7	7.97	113.99	110.80
1	A	122	G	C5-C6-N1	-7.96	107.52	111.50
1	A	522	C	O5'-P-OP2	-7.94	98.55	105.70
1	A	167	G	N9-C4-C5	-7.94	102.22	105.40
1	A	600	C	C6-N1-C2	7.94	123.47	120.30
1	A	306	G	N3-C2-N2	-7.93	114.35	119.90
1	A	1232	U	O5'-P-OP2	7.93	120.22	110.70
1	A	266	G	O4'-C1'-N9	-7.92	101.86	108.20
1	A	366	C	C2-N1-C1'	7.92	127.51	118.80
1	A	593	G	C5-C6-N1	-7.91	107.55	111.50
1	A	882	C	C2-N3-C4	-7.91	115.94	119.90
1	A	1347	G	C8-N9-C1'	-7.91	116.72	127.00
1	A	281	G	C4-C5-N7	7.90	113.96	110.80
1	A	321	A	O5'-P-OP2	-7.90	98.59	105.70
1	A	1525	G	C2-N3-C4	-7.90	107.95	111.90
1	A	821	G	O5'-P-OP1	-7.89	98.60	105.70
1	A	1442	G	N3-C4-N9	7.88	130.73	126.00
1	A	835	U	C4-C5-C6	7.88	124.43	119.70
1	A	675	A	C2-N3-C4	-7.87	106.66	110.60
1	A	21	G	C8-N9-C4	7.87	109.55	106.40
1	A	853	G	C4-C5-C6	7.86	123.52	118.80
1	A	1153	C	C6-N1-C2	7.86	123.44	120.30
1	A	295	C	C5-C6-N1	-7.86	117.07	121.00
1	A	413	G	O4'-C1'-N9	7.84	114.47	108.20
1	A	295	C	N3-C4-C5	7.84	125.04	121.90
1	A	947	G	N9-C4-C5	-7.84	102.27	105.40
1	A	609	A	C2-N3-C4	-7.82	106.69	110.60
1	A	853	G	C6-C5-N7	-7.81	125.71	130.40
1	A	913	A	P-O3'-C3'	7.81	129.07	119.70
1	A	642	A	O5'-P-OP2	-7.81	98.67	105.70
1	A	1386	G	N7-C8-N9	-7.80	109.20	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	7	G	O4'-C1'-N9	7.80	114.44	108.20
1	A	371	G	O5'-P-OP1	-7.80	98.68	105.70
1	A	588	G	N9-C4-C5	-7.79	102.28	105.40
1	A	723	U	N1-C2-O2	7.79	128.25	122.80
1	A	1078	U	C5-C4-O4	-7.79	121.23	125.90
1	A	279	A	O4'-C1'-N9	-7.78	101.98	108.20
1	A	779	C	C5-C6-N1	-7.76	117.12	121.00
1	A	947	G	N1-C6-O6	7.76	124.56	119.90
1	A	89	C	C6-N1-C2	-7.75	117.20	120.30
1	A	624	C	C6-N1-C2	7.75	123.40	120.30
1	A	865	A	C6-N1-C2	-7.75	113.95	118.60
1	A	1395	C	C6-N1-C2	7.74	123.40	120.30
1	A	1436	U	N1-C2-O2	7.74	128.22	122.80
1	A	1483	A	N9-C4-C5	-7.73	102.71	105.80
1	A	129	U	N3-C4-C5	-7.71	109.97	114.60
1	A	529	G	C4-C5-C6	7.71	123.43	118.80
1	A	654	G	C5-C6-O6	-7.71	123.97	128.60
1	A	739	C	N3-C4-N4	-7.71	112.60	118.00
1	A	1527	C	OP2-P-O3'	7.69	122.11	105.20
1	A	281	G	C5-C6-O6	-7.69	123.99	128.60
1	A	885	G	O5'-P-OP1	-7.69	98.78	105.70
1	A	550	G	C2-N3-C4	-7.69	108.06	111.90
1	A	331	G	C5-C6-N1	-7.68	107.66	111.50
1	A	367	U	O5'-P-OP1	-7.68	98.78	105.70
1	A	760	G	C2-N3-C4	-7.68	108.06	111.90
1	A	875	C	C2-N3-C4	-7.68	116.06	119.90
1	A	947	G	N3-C4-N9	7.68	130.61	126.00
1	A	880	C	C2-N3-C4	-7.68	116.06	119.90
1	A	651	C	C6-N1-C2	7.67	123.37	120.30
1	A	859	A	N1-C6-N6	7.67	123.20	118.60
1	A	1531	A	N1-C6-N6	7.67	123.20	118.60
1	A	1532	U	C5-C4-O4	-7.67	121.30	125.90
1	A	1366	C	C6-N1-C2	-7.67	117.23	120.30
1	A	721	G	C6-C5-N7	-7.67	125.80	130.40
1	A	666	G	N1-C2-N3	7.66	128.50	123.90
1	A	1347	G	C4-N9-C1'	7.65	136.45	126.50
1	A	280	C	O5'-P-OP2	-7.65	98.81	105.70
1	A	331	G	N1-C6-O6	7.65	124.49	119.90
1	A	1417	G	C8-N9-C4	-7.64	103.34	106.40
1	A	29	G	N1-C2-N3	7.64	128.48	123.90
1	A	1403	C	C5-C4-N4	-7.63	114.86	120.20
1	A	1370	G	N7-C8-N9	7.63	116.92	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	753	A	N9-C4-C5	7.62	108.85	105.80
1	A	1158	C	N3-C2-O2	-7.59	116.59	121.90
1	A	1399	C	N1-C2-O2	-7.59	114.35	118.90
1	A	89	C	C5-C6-N1	7.59	124.79	121.00
1	A	524	G	C6-C5-N7	-7.58	125.85	130.40
1	A	858	G	C6-C5-N7	-7.58	125.85	130.40
1	A	1067	A	P-O3'-C3'	7.57	128.79	119.70
1	A	558	G	N7-C8-N9	7.57	116.89	113.10
1	A	787	A	C5-N7-C8	-7.57	100.12	103.90
1	A	735	C	C5-C6-N1	-7.56	117.22	121.00
1	A	928	G	N1-C6-O6	7.55	124.43	119.90
1	A	566	G	C6-C5-N7	-7.55	125.87	130.40
1	A	117	G	N9-C4-C5	-7.54	102.38	105.40
1	A	712	A	C2-N3-C4	-7.54	106.83	110.60
1	A	799	G	C5-C6-O6	-7.53	124.08	128.60
1	A	838	G	C8-N9-C4	7.53	109.41	106.40
1	A	1417	G	N9-C4-C5	7.53	108.41	105.40
1	A	666	G	C2-N3-C4	-7.53	108.14	111.90
1	A	722	A	N9-C4-C5	-7.53	102.79	105.80
1	A	242	C	C5-C6-N1	-7.51	117.25	121.00
1	A	723	U	C2-N1-C1'	7.51	126.71	117.70
1	A	1108	G	C8-N9-C4	-7.50	103.40	106.40
1	A	635	G	C8-N9-C4	7.49	109.39	106.40
1	A	1516[A]	G	C5-C6-O6	7.49	133.09	128.60
1	A	1516[B]	G	C5-C6-O6	7.49	133.09	128.60
1	A	392	G	C5-C6-O6	-7.48	124.11	128.60
1	A	976	G	C4-C5-N7	-7.48	107.81	110.80
1	A	316	G	N1-C6-O6	7.48	124.39	119.90
1	A	1232	U	N1-C2-O2	-7.48	117.57	122.80
1	A	295	C	C6-N1-C2	7.47	123.29	120.30
1	A	577	G	C8-N9-C4	7.47	109.39	106.40
1	A	7	G	C6-N1-C2	-7.47	120.62	125.10
1	A	1373	G	N3-C4-N9	7.47	130.48	126.00
1	A	481	G	N1-C6-O6	7.46	124.38	119.90
1	A	762	C	C5-C4-N4	-7.46	114.98	120.20
1	A	738	C	N3-C4-N4	-7.46	112.78	118.00
1	A	721	G	C4-C5-C6	7.46	123.27	118.80
1	A	228	A	C5-N7-C8	-7.45	100.17	103.90
1	A	126	G	N1-C6-O6	7.45	124.37	119.90
1	A	701	C	N1-C2-O2	7.44	123.37	118.90
1	A	1384	C	N3-C4-C5	7.44	124.88	121.90
1	A	445	G	N1-C6-O6	7.43	124.36	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	853	G	C4-N9-C1'	7.42	136.15	126.50
1	A	445	G	C6-C5-N7	-7.42	125.95	130.40
1	A	635	G	N1-C2-N3	7.42	128.35	123.90
1	A	933	G	C4-C5-N7	7.42	113.77	110.80
1	A	103	C	N3-C4-C5	-7.42	118.93	121.90
1	A	309	G	C4-C5-N7	7.42	113.77	110.80
1	A	295	C	N3-C4-N4	-7.41	112.81	118.00
1	A	246	A	C2-N3-C4	7.40	114.30	110.60
1	A	1417	G	C4-C5-N7	-7.40	107.84	110.80
1	A	327	A	C5-C6-N1	7.40	121.40	117.70
1	A	593	G	C2-N3-C4	-7.40	108.20	111.90
20	T	94	ALA	N-CA-C	-7.40	91.02	111.00
1	A	598	U	C5-C6-N1	-7.39	119.00	122.70
1	A	569	C	C2-N3-C4	-7.39	116.21	119.90
1	A	1108	G	C4-C5-C6	7.38	123.23	118.80
1	A	1149	C	C6-N1-C2	-7.38	117.35	120.30
1	A	51	A	N7-C8-N9	7.37	117.48	113.80
1	A	183	G	O5'-P-OP1	-7.37	99.07	105.70
1	A	392	G	N1-C6-O6	7.37	124.32	119.90
1	A	250	A	C5-C6-N1	-7.36	114.02	117.70
1	A	1307	U	N3-C2-O2	-7.36	117.05	122.20
1	A	309	G	N1-C2-N2	-7.34	109.59	116.20
1	A	1530	G	N3-C4-C5	7.34	132.27	128.60
1	A	481	G	C8-N9-C1'	-7.34	117.46	127.00
1	A	850	U	C5-C4-O4	7.33	130.30	125.90
1	A	550	G	N1-C2-N3	7.33	128.30	123.90
1	A	1354	C	C6-N1-C2	-7.33	117.37	120.30
1	A	125	U	C4-C5-C6	7.33	124.09	119.70
1	A	812	C	C4-C5-C6	7.32	121.06	117.40
1	A	1525	G	N1-C2-N3	7.32	128.29	123.90
1	A	389	A	C5-C6-N6	7.31	129.55	123.70
1	A	328	C	N1-C2-O2	7.31	123.28	118.90
1	A	591	U	C5-C6-N1	-7.30	119.05	122.70
1	A	293	G	C2-N3-C4	-7.29	108.25	111.90
1	A	278	G	O5'-P-OP2	-7.29	99.14	105.70
1	A	839	U	C2-N1-C1'	7.29	126.44	117.70
1	A	283	C	C2-N1-C1'	7.28	126.81	118.80
1	A	1442	G	N3-C4-C5	-7.28	124.96	128.60
1	A	746	A	N1-C2-N3	7.28	132.94	129.30
1	A	526	C	C5-C6-N1	-7.28	117.36	121.00
1	A	719	C	C6-N1-C2	7.26	123.20	120.30
1	A	92	C	N1-C2-O2	7.26	123.25	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	831	U	N1-C2-O2	-7.25	117.72	122.80
1	A	919	A	C5-C6-N1	7.25	121.32	117.70
1	A	121	C	C6-N1-C2	7.24	123.20	120.30
1	A	1442	G	C4-N9-C1'	7.24	135.91	126.50
1	A	1502	A	N7-C8-N9	7.23	117.42	113.80
1	A	597	G	O5'-P-OP1	-7.22	99.20	105.70
1	A	248	C	C4-C5-C6	7.22	121.01	117.40
1	A	739	C	C5-C6-N1	-7.21	117.40	121.00
1	A	793	U	C5-C4-O4	-7.21	121.58	125.90
1	A	947	G	C5-C6-O6	-7.21	124.28	128.60
1	A	901	A	C2-N3-C4	-7.20	107.00	110.60
1	A	1305	G	P-O3'-C3'	7.19	128.33	119.70
1	A	661	G	N1-C6-O6	7.19	124.22	119.90
1	A	89	C	C2-N1-C1'	7.19	126.70	118.80
1	A	1108	G	C6-C5-N7	-7.18	126.09	130.40
1	A	119	A	C2-N3-C4	-7.18	107.01	110.60
1	A	880	C	O5'-P-OP1	-7.17	99.24	105.70
1	A	1304	G	O5'-P-OP1	-7.17	99.25	105.70
1	A	648	A	C8-N9-C4	7.16	108.66	105.80
1	A	919	A	C8-N9-C4	7.16	108.66	105.80
1	A	106	C	C6-N1-C2	-7.15	117.44	120.30
1	A	1334	G	C8-N9-C4	7.15	109.26	106.40
1	A	813	U	C5-C4-O4	-7.15	121.61	125.90
1	A	266	G	C8-N9-C4	-7.15	103.54	106.40
1	A	867	G	C4-N9-C1'	7.15	135.79	126.50
1	A	562	C	C6-N1-C2	7.15	123.16	120.30
1	A	29	G	N1-C6-O6	7.14	124.18	119.90
1	A	1524	C	N1-C2-O2	-7.14	114.62	118.90
1	A	305	G	C2-N3-C4	-7.13	108.33	111.90
1	A	376	G	C5-C6-N1	-7.13	107.93	111.50
1	A	1103	C	C5-C6-N1	-7.13	117.43	121.00
1	A	873	A	N9-C4-C5	7.13	108.65	105.80
1	A	939	G	C5-C6-O6	-7.12	124.33	128.60
1	A	558	G	C5-C6-O6	-7.12	124.33	128.60
1	A	721	G	N3-C4-C5	-7.12	125.04	128.60
1	A	821	G	C5-C6-O6	-7.11	124.33	128.60
1	A	802	A	N1-C6-N6	7.10	122.86	118.60
1	A	851	G	N1-C6-O6	7.10	124.16	119.90
1	A	328	C	N3-C2-O2	-7.10	116.93	121.90
1	A	1092	A	C4-C5-N7	7.10	114.25	110.70
1	A	797	C	C6-N1-C2	7.09	123.14	120.30
1	A	1227	A	C6-C5-N7	-7.08	127.34	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	376	G	N1-C6-O6	7.08	124.15	119.90
1	A	1073	U	C6-N1-C2	7.08	125.25	121.00
1	A	658	G	C8-N9-C1'	-7.08	117.79	127.00
1	A	286	G	C8-N9-C4	-7.07	103.57	106.40
1	A	235	C	C5-C6-N1	-7.07	117.46	121.00
1	A	947	G	C6-C5-N7	-7.07	126.16	130.40
1	A	874	G	C8-N9-C1'	-7.06	117.82	127.00
1	A	7	G	N3-C4-C5	-7.06	125.07	128.60
1	A	645	C	C2-N1-C1'	7.06	126.57	118.80
1	A	312	C	N3-C4-C5	7.05	124.72	121.90
1	A	658	G	N9-C4-C5	-7.05	102.58	105.40
1	A	1153	C	C5-C6-N1	-7.05	117.48	121.00
1	A	252	U	C2-N3-C4	-7.04	122.77	127.00
1	A	626	U	N3-C2-O2	-7.03	117.28	122.20
1	A	580	U	N3-C4-C5	-7.03	110.38	114.60
1	A	1158	C	N1-C2-O2	7.03	123.12	118.90
1	A	1158	C	C2-N1-C1'	7.03	126.53	118.80
1	A	971	G	C8-N9-C4	7.03	109.21	106.40
1	A	1366	C	C5-C6-N1	7.02	124.51	121.00
1	A	131	C	C6-N1-C2	7.02	123.11	120.30
1	A	524	G	N1-C6-O6	7.01	124.11	119.90
1	A	877	C	C2-N3-C4	-7.01	116.39	119.90
1	A	248	C	C6-N1-C2	7.00	123.10	120.30
1	A	626	U	N1-C2-N3	7.00	119.10	114.90
4	D	12	CYS	CA-CB-SG	7.00	126.60	114.00
1	A	1200	C	C6-N1-C2	-7.00	117.50	120.30
1	A	658	G	C6-C5-N7	-6.99	126.20	130.40
1	A	822	C	C6-N1-C2	6.99	123.10	120.30
1	A	588	G	C8-N9-C4	6.99	109.19	106.40
1	A	118	U	C5-C4-O4	6.98	130.09	125.90
1	A	864	A	N9-C4-C5	6.98	108.59	105.80
1	A	723	U	C5-C6-N1	6.98	126.19	122.70
1	A	1483	A	N1-C6-N6	6.98	122.79	118.60
1	A	1394	A	C5-C6-N6	-6.98	118.12	123.70
1	A	1200	C	C6-N1-C1'	-6.97	112.43	120.80
1	A	761	G	C2-N3-C4	-6.97	108.42	111.90
1	A	769	G	O5'-P-OP2	-6.96	99.43	105.70
1	A	555	C	C6-N1-C2	-6.96	117.52	120.30
1	A	907	A	O5'-P-OP1	-6.96	99.44	105.70
1	A	945	G	C5-C6-N1	6.96	114.98	111.50
1	A	111	G	O5'-P-OP1	-6.95	99.44	105.70
1	A	939	G	N1-C6-O6	6.95	124.07	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	920	U	C6-N1-C1'	6.94	130.92	121.20
1	A	312	C	C6-N1-C2	6.94	123.08	120.30
1	A	366	C	C6-N1-C1'	-6.94	112.47	120.80
1	A	227	G	C2-N3-C4	-6.94	108.43	111.90
1	A	583	A	N1-C2-N3	6.94	132.77	129.30
1	A	882	C	C4-C5-C6	6.94	120.87	117.40
1	A	742	G	C6-C5-N7	-6.93	126.24	130.40
1	A	757	U	C5-C6-N1	-6.93	119.23	122.70
1	A	309	G	C8-N9-C4	6.93	109.17	106.40
1	A	579	G	C5-N7-C8	-6.93	100.84	104.30
1	A	1147	C	C6-N1-C2	-6.92	117.53	120.30
1	A	167	G	C4-N9-C1'	6.92	135.50	126.50
1	A	1058	G	C5-C6-O6	6.91	132.75	128.60
1	A	379	C	O5'-P-OP2	-6.91	99.48	105.70
1	A	21	G	N1-C2-N2	-6.91	109.98	116.20
1	A	122	G	C4-C5-N7	6.90	113.56	110.80
1	A	573	A	C4-C5-C6	6.90	120.45	117.00
1	A	901	A	N1-C2-N3	6.89	132.75	129.30
1	A	940	C	C6-N1-C2	6.89	123.06	120.30
1	A	285	G	N1-C6-O6	6.88	124.03	119.90
1	A	1373	G	C6-C5-N7	-6.88	126.27	130.40
1	A	62	U	N3-C4-C5	-6.88	110.47	114.60
1	A	89	C	N1-C2-O2	6.88	123.03	118.90
1	A	608	A	C2-N3-C4	-6.88	107.16	110.60
1	A	703	G	N9-C4-C5	6.87	108.15	105.40
1	A	893	C	N1-C2-O2	6.87	123.02	118.90
1	A	90	U	OP1-P-O3'	6.87	120.31	105.20
1	A	808	C	C6-N1-C2	6.86	123.04	120.30
1	A	333	G	C8-N9-C4	6.86	109.14	106.40
1	A	872	A	N9-C4-C5	-6.85	103.06	105.80
1	A	1344	C	O5'-P-OP2	-6.85	99.53	105.70
1	A	1532	U	N1-C2-N3	-6.85	110.79	114.90
1	A	667	G	N1-C6-O6	6.84	124.01	119.90
1	A	853	G	C8-N9-C1'	-6.84	118.10	127.00
1	A	238	G	C2-N3-C4	-6.84	108.48	111.90
1	A	1190	G	N7-C8-N9	6.84	116.52	113.10
1	A	1530	G	N9-C4-C5	-6.83	102.67	105.40
1	A	882	C	N3-C4-N4	-6.83	113.22	118.00
1	A	1529	G	N3-C4-C5	-6.82	125.19	128.60
1	A	1416	G	N1-C6-O6	6.82	123.99	119.90
1	A	1523	G	N1-C6-O6	6.82	123.99	119.90
1	A	1190	G	N3-C4-N9	6.80	130.08	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	286	G	C5-C6-N1	-6.79	108.10	111.50
1	A	597	G	N3-C4-C5	-6.79	125.20	128.60
1	A	1441	G	C5-C6-N1	-6.79	108.10	111.50
1	A	76	C	N1-C2-O2	-6.79	114.83	118.90
1	A	122	G	N3-C4-N9	-6.79	121.93	126.00
1	A	654	G	N3-C4-N9	-6.79	121.93	126.00
1	A	860	A	C6-N1-C2	-6.78	114.53	118.60
1	A	745	C	C5-C6-N1	-6.77	117.62	121.00
1	A	824	C	O5'-P-OP2	-6.77	99.61	105.70
1	A	903	G	N1-C2-N3	6.77	127.96	123.90
1	A	646	U	N3-C4-C5	-6.77	110.54	114.60
1	A	1515[A]	C	O5'-P-OP2	-6.77	99.61	105.70
1	A	1515[B]	C	O5'-P-OP2	-6.77	99.61	105.70
1	A	722	A	C5-C6-N6	-6.77	118.29	123.70
1	A	317	G	C2-N3-C4	-6.76	108.52	111.90
1	A	676	A	C8-N9-C4	6.76	108.50	105.80
1	A	121	C	N3-C2-O2	6.76	126.63	121.90
1	A	21	G	C8-N9-C1'	-6.75	118.22	127.00
1	A	867	G	C6-C5-N7	-6.75	126.35	130.40
1	A	1108	G	C4-N9-C1'	6.75	135.28	126.50
1	A	32	A	N1-C2-N3	6.75	132.68	129.30
1	A	318	G	N3-C2-N2	-6.75	115.17	119.90
1	A	770	C	C6-N1-C2	6.75	123.00	120.30
1	A	33	A	C5-C6-N1	6.75	121.07	117.70
1	A	1109	C	O5'-P-OP1	-6.74	99.63	105.70
1	A	827	U	C2-N3-C4	-6.74	122.95	127.00
1	A	1197	G	O5'-P-OP1	-6.74	99.63	105.70
1	A	228	A	C4-C5-N7	6.74	114.07	110.70
1	A	658	G	N3-C4-N9	6.74	130.04	126.00
1	A	1373	G	N1-C6-O6	6.74	123.94	119.90
1	A	243	A	N1-C6-N6	6.74	122.64	118.60
1	A	738	C	N3-C4-C5	6.74	124.59	121.90
1	A	284	G	N1-C6-O6	6.73	123.94	119.90
1	A	687	A	P-O3'-C3'	6.72	127.77	119.70
1	A	29	G	C8-N9-C4	6.72	109.09	106.40
1	A	5	U	P-O3'-C3'	6.72	127.76	119.70
1	A	1479	C	C6-N1-C2	-6.71	117.62	120.30
1	A	597	G	N3-C4-N9	6.71	130.03	126.00
1	A	671	G	C8-N9-C4	6.71	109.08	106.40
1	A	1403	C	N3-C4-N4	6.71	122.69	118.00
1	A	26	A	C2-N3-C4	-6.70	107.25	110.60
1	A	859	A	O5'-P-OP2	6.70	118.74	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1367	C	C5-C6-N1	6.70	124.35	121.00
1	A	745	C	C2-N3-C4	-6.70	116.55	119.90
1	A	593	G	C6-C5-N7	-6.69	126.38	130.40
1	A	116	A	C2-N3-C4	-6.69	107.25	110.60
1	A	806	C	C6-N1-C2	6.69	122.98	120.30
1	A	1112	C	C5-C6-N1	-6.69	117.66	121.00
1	A	406	G	N1-C6-O6	6.68	123.91	119.90
1	A	833	U	N3-C2-O2	-6.68	117.52	122.20
1	A	862	C	C5-C4-N4	-6.68	115.53	120.20
1	A	1181	G	N7-C8-N9	-6.67	109.76	113.10
1	A	128	G	C5-C6-O6	-6.67	124.60	128.60
1	A	277	C	C5-C6-N1	-6.67	117.67	121.00
1	A	262	A	N1-C6-N6	-6.67	114.60	118.60
1	A	753	A	N1-C2-N3	6.67	132.63	129.30
1	A	1227	A	N7-C8-N9	6.67	117.13	113.80
1	A	59	A	O5'-P-OP2	-6.66	99.70	105.70
1	A	106	C	OP2-P-O3'	6.66	119.85	105.20
1	A	289	G	C4-C5-N7	6.66	113.46	110.80
1	A	304	U	O5'-P-OP2	6.66	118.69	110.70
1	A	648	A	C6-N1-C2	-6.66	114.61	118.60
1	A	7	G	C8-N9-C1'	-6.65	118.35	127.00
1	A	945	G	C4-C5-N7	6.65	113.46	110.80
1	A	176	C	C6-N1-C2	6.65	122.96	120.30
1	A	653	A	N1-C6-N6	-6.65	114.61	118.60
1	A	835	U	N3-C2-O2	-6.65	117.55	122.20
1	A	856	C	C2-N1-C1'	-6.65	111.49	118.80
1	A	884	U	C6-N1-C2	6.65	124.99	121.00
1	A	576	G	N1-C2-N3	6.64	127.88	123.90
1	A	1505	G	P-O3'-C3'	6.64	127.67	119.70
1	A	655	A	C5-C6-N1	6.63	121.02	117.70
1	A	1512	U	N3-C4-C5	-6.63	110.62	114.60
1	A	1527	C	C2-N1-C1'	6.62	126.09	118.80
1	A	39	G	C5-C6-N1	6.62	114.81	111.50
1	A	1058	G	C4-C5-N7	-6.62	108.15	110.80
1	A	400	C	N3-C4-C5	6.61	124.54	121.90
1	A	127	G	N1-C6-O6	6.60	123.86	119.90
1	A	269	C	C2-N3-C4	-6.60	116.60	119.90
1	A	63	C	N1-C2-O2	-6.60	114.94	118.90
1	A	731	G	N3-C4-C5	6.60	131.90	128.60
1	A	654	G	C5-N7-C8	-6.59	101.00	104.30
1	A	1075	C	N3-C4-C5	6.59	124.53	121.90
1	A	746	A	C6-N1-C2	-6.58	114.65	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	789	U	C5-C4-O4	6.58	129.84	125.90
1	A	873	A	C8-N9-C4	-6.58	103.17	105.80
1	A	111	G	N3-C4-N9	-6.57	122.06	126.00
1	A	874	G	N9-C4-C5	-6.57	102.77	105.40
1	A	269	C	N3-C4-N4	-6.57	113.40	118.00
1	A	931	C	C2-N3-C4	-6.57	116.62	119.90
1	A	577	G	N1-C6-O6	6.56	123.84	119.90
1	A	770	C	C5-C6-N1	-6.56	117.72	121.00
1	A	1099	G	N3-C4-N9	-6.56	122.06	126.00
1	A	1225	A	C8-N9-C4	-6.56	103.18	105.80
1	A	230	G	C8-N9-C1'	-6.56	118.47	127.00
1	A	297	G	C6-C5-N7	-6.56	126.47	130.40
1	A	403	C	C5-C6-N1	-6.55	117.72	121.00
1	A	579	G	C6-C5-N7	-6.55	126.47	130.40
1	A	877	C	C5-C6-N1	-6.55	117.72	121.00
1	A	663	A	N1-C6-N6	-6.55	114.67	118.60
1	A	581	G	O5'-P-OP2	-6.55	99.81	105.70
1	A	62	U	C4-C5-C6	6.54	123.63	119.70
1	A	959	A	N1-C6-N6	6.54	122.53	118.60
1	A	1077	G	N1-C2-N2	-6.54	110.31	116.20
1	A	150	C	N3-C4-C5	-6.53	119.29	121.90
1	A	10	A	N1-C2-N3	6.53	132.56	129.30
1	A	10	A	C2-N3-C4	-6.53	107.34	110.60
1	A	715	A	C2-N3-C4	-6.53	107.34	110.60
1	A	742	G	C5-C6-O6	-6.53	124.69	128.60
1	A	1090	U	N3-C4-C5	-6.53	110.69	114.60
1	A	733	A	O5'-P-OP1	-6.52	99.83	105.70
1	A	839	U	N1-C2-O2	6.52	127.37	122.80
1	A	291	C	C2-N3-C4	-6.52	116.64	119.90
1	A	279	A	C4-N9-C1'	6.51	138.01	126.30
1	A	285	G	C5-C6-N1	-6.51	108.25	111.50
1	A	250	A	N1-C6-N6	6.50	122.50	118.60
1	A	129(A)	G	C4-N9-C1'	6.50	134.95	126.50
1	A	293	G	N1-C6-O6	6.50	123.80	119.90
1	A	1190	G	C4-C5-C6	6.50	122.70	118.80
1	A	129	U	C4-C5-C6	6.49	123.59	119.70
1	A	118	U	N1-C2-N3	6.49	118.79	114.90
1	A	1339	A	N1-C6-N6	-6.49	114.71	118.60
1	A	24	U	C6-N1-C2	6.49	124.89	121.00
1	A	572	A	N1-C6-N6	-6.48	114.71	118.60
1	A	29	G	C6-C5-N7	-6.48	126.51	130.40
1	A	813	U	C2-N1-C1'	6.48	125.47	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	582	U	C5-C6-N1	-6.47	119.46	122.70
1	A	1531	A	C5-C6-N1	-6.47	114.46	117.70
1	A	703	G	C5-N7-C8	6.47	107.53	104.30
1	A	1215	G	C6-C5-N7	-6.47	126.52	130.40
1	A	122	G	N3-C2-N2	-6.47	115.37	119.90
1	A	403	C	C4-C5-C6	6.47	120.63	117.40
1	A	814	A	N1-C6-N6	6.47	122.48	118.60
1	A	31	G	N1-C6-O6	-6.46	116.02	119.90
1	A	107	G	C4-C5-N7	6.46	113.39	110.80
1	A	1441	G	C4-C5-N7	-6.46	108.21	110.80
1	A	33	A	C6-N1-C2	-6.46	114.72	118.60
1	A	242	C	N3-C4-C5	6.46	124.48	121.90
1	A	1227	A	C5-C6-N6	-6.46	118.54	123.70
1	A	854	G	N1-C2-N3	6.45	127.77	123.90
1	A	251	G	N1-C6-O6	6.45	123.77	119.90
1	A	507	C	N3-C4-C5	6.45	124.48	121.90
1	A	1405	G	O5'-P-OP2	-6.45	99.89	105.70
1	A	237	C	N3-C4-C5	-6.45	119.32	121.90
1	A	588	G	C2-N3-C4	-6.45	108.68	111.90
1	A	303	A	N1-C6-N6	6.44	122.47	118.60
1	A	559	A	C6-N1-C2	-6.44	114.73	118.60
1	A	1053	G	C8-N9-C4	6.44	108.98	106.40
1	A	1419	G	C8-N9-C4	-6.44	103.82	106.40
1	A	1190	G	C4-C5-N7	6.44	113.38	110.80
1	A	580	U	C6-N1-C2	-6.43	117.14	121.00
1	A	922	G	N3-C4-C5	-6.43	125.38	128.60
1	A	965	A	C8-N9-C4	6.43	108.37	105.80
1	A	762	C	O5'-P-OP2	6.43	118.41	110.70
1	A	799	G	C4-C5-N7	6.43	113.37	110.80
1	A	1342	C	N1-C2-O2	-6.43	115.04	118.90
1	A	645	C	C5-C6-N1	6.42	124.21	121.00
1	A	1193	G	N1-C6-O6	6.42	123.75	119.90
1	A	653	A	N9-C4-C5	6.42	108.37	105.80
1	A	772	U	N1-C2-O2	-6.42	118.31	122.80
1	A	317	G	C5-N7-C8	-6.42	101.09	104.30
1	A	17	U	C2-N3-C4	-6.41	123.15	127.00
18	R	78	LEU	CA-CB-CG	-6.41	100.55	115.30
1	A	875	C	N3-C4-C5	6.41	124.46	121.90
1	A	1452	C	N1-C2-O2	6.41	122.75	118.90
1	A	333	G	OP2-P-O3'	6.41	119.29	105.20
1	A	105	G	O5'-P-OP2	-6.40	99.94	105.70
1	A	228	A	N1-C6-N6	6.40	122.44	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	880	C	N3-C4-C5	6.40	124.46	121.90
1	A	582	U	C2-N3-C4	-6.40	123.16	127.00
1	A	856	C	C4-C5-C6	6.40	120.60	117.40
1	A	873	A	C4-C5-C6	-6.40	113.80	117.00
1	A	78	G	N1-C6-O6	6.39	123.74	119.90
1	A	867	G	N9-C4-C5	-6.39	102.84	105.40
1	A	855	G	N1-C6-O6	6.39	123.73	119.90
1	A	1215	G	C4-C5-N7	6.38	113.35	110.80
1	A	388	G	N3-C4-C5	-6.38	125.41	128.60
1	A	1414	U	C6-N1-C2	-6.38	117.17	121.00
1	A	90	U	O5'-P-OP2	6.38	118.35	110.70
1	A	586	C	C5-C6-N1	-6.38	117.81	121.00
1	A	802	A	C8-N9-C4	6.38	108.35	105.80
1	A	853	G	N1-C2-N3	6.37	127.72	123.90
1	A	9	G	O5'-P-OP1	6.37	118.35	110.70
1	A	481	G	N9-C4-C5	-6.37	102.85	105.40
1	A	768	A	OP2-P-O3'	6.37	119.22	105.20
1	A	121	C	N1-C2-O2	-6.36	115.08	118.90
1	A	852	G	N1-C6-O6	6.36	123.72	119.90
1	A	281	G	N9-C4-C5	-6.36	102.86	105.40
1	A	553	A	C2-N3-C4	-6.36	107.42	110.60
1	A	524	G	C8-N9-C1'	-6.36	118.74	127.00
1	A	1167	A	C8-N9-C4	-6.36	103.26	105.80
1	A	317	G	N9-C4-C5	-6.35	102.86	105.40
1	A	529	G	C5-C6-N1	-6.35	108.32	111.50
1	A	370	C	O5'-P-OP1	-6.35	99.98	105.70
1	A	572	A	N9-C4-C5	6.35	108.34	105.80
1	A	1197	G	C4-N9-C1'	6.35	134.75	126.50
1	A	1542	U	C6-N1-C2	6.35	124.81	121.00
1	A	117	G	O5'-P-OP2	-6.34	99.99	105.70
1	A	21	G	N3-C4-N9	6.34	129.80	126.00
1	A	131	C	C2-N3-C4	-6.34	116.73	119.90
1	A	138	G	C8-N9-C4	6.34	108.94	106.40
1	A	1351	U	N3-C2-O2	-6.34	117.76	122.20
1	A	22	G	O5'-P-OP2	-6.33	100.00	105.70
1	A	329	A	C5-C6-N1	-6.33	114.53	117.70
1	A	1181	G	C4-N9-C1'	-6.33	118.27	126.50
1	A	851	G	C6-C5-N7	-6.33	126.60	130.40
1	A	310	G	N1-C6-O6	6.33	123.70	119.90
1	A	590	C	OP2-P-O3'	6.32	119.11	105.20
1	A	309	G	C6-C5-N7	-6.32	126.61	130.40
1	A	890	G	C4-C5-N7	-6.32	108.27	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	277	C	C2-N3-C4	-6.32	116.74	119.90
1	A	1322	C	C6-N1-C2	-6.32	117.77	120.30
1	A	407	G	C8-N9-C4	6.31	108.92	106.40
1	A	718	G	N1-C6-O6	6.31	123.69	119.90
1	A	1529	G	C4-N9-C1'	6.31	134.71	126.50
1	A	1350	A	C8-N9-C4	-6.31	103.28	105.80
1	A	836	G	C2-N3-C4	-6.31	108.75	111.90
1	A	814	A	C8-N9-C4	6.31	108.32	105.80
1	A	345	C	C6-N1-C2	-6.30	117.78	120.30
1	A	1301	U	P-O3'-C3'	6.30	127.26	119.70
1	A	353	A	C5-C6-N6	6.30	128.74	123.70
1	A	350	G	N7-C8-N9	6.30	116.25	113.10
1	A	21	G	N3-C2-N2	6.30	124.31	119.90
1	A	112	G	C2-N3-C4	-6.30	108.75	111.90
1	A	625	G	C5-C6-N1	6.30	114.65	111.50
1	A	803	G	OP2-P-O3'	6.30	119.05	105.20
1	A	920	U	C2-N1-C1'	-6.30	110.14	117.70
1	A	1268	A	N1-C6-N6	-6.30	114.82	118.60
1	A	730	G	N9-C4-C5	6.29	107.92	105.40
1	A	664	G	C4-C5-N7	-6.29	108.28	110.80
1	A	774	G	C2-N3-C4	-6.29	108.75	111.90
1	A	1051	C	C2-N1-C1'	6.29	125.72	118.80
1	A	734	G	N9-C4-C5	-6.29	102.89	105.40
1	A	661	G	N3-C4-C5	6.29	131.74	128.60
1	A	1442	G	C8-N9-C1'	-6.29	118.83	127.00
1	A	144	G	N3-C2-N2	-6.28	115.50	119.90
1	A	190(I)	G	C8-N9-C4	6.28	108.91	106.40
1	A	326	G	C4-C5-N7	-6.28	108.29	110.80
1	A	862	C	C6-N1-C2	6.28	122.81	120.30
1	A	395	C	C6-N1-C2	6.28	122.81	120.30
1	A	877	C	N3-C4-N4	-6.28	113.61	118.00
1	A	788	U	N3-C4-C5	-6.28	110.83	114.60
1	A	809	G	C5-C6-O6	-6.28	124.83	128.60
1	A	1452	C	C6-N1-C2	6.28	122.81	120.30
1	A	228	A	N3-C4-C5	6.28	131.19	126.80
1	A	168	G	N1-C6-O6	6.27	123.66	119.90
1	A	654	G	C5-C6-N1	6.27	114.64	111.50
1	A	615	C	C2-N1-C1'	6.27	125.69	118.80
1	A	302	G	C8-N9-C4	6.26	108.91	106.40
1	A	677	U	N1-C2-O2	-6.26	118.42	122.80
1	A	144	G	N3-C4-C5	6.26	131.73	128.60
1	A	286	G	C6-C5-N7	-6.26	126.64	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	746	A	C8-N9-C4	6.26	108.30	105.80
1	A	1512	U	N1-C2-O2	-6.25	118.42	122.80
1	A	1117	G	N3-C4-C5	6.25	131.73	128.60
1	A	80	G	N1-C2-N2	6.25	121.83	116.20
1	A	1103	C	C2-N3-C4	-6.25	116.78	119.90
1	A	1190	G	P-O3'-C3'	6.25	127.20	119.70
1	A	1306	A	C8-N9-C4	6.25	108.30	105.80
1	A	856	C	C6-N1-C1'	6.25	128.30	120.80
1	A	878	G	OP1-P-O3'	6.25	118.94	105.20
1	A	1452	C	N1-C2-N3	-6.25	114.83	119.20
1	A	1098	C	C6-N1-C2	6.25	122.80	120.30
1	A	1240	U	C5-C6-N1	-6.24	119.58	122.70
1	A	129(A)	G	C8-N9-C1'	-6.24	118.89	127.00
1	A	14	U	C6-N1-C2	-6.23	117.26	121.00
1	A	1190	G	N1-C6-O6	6.23	123.64	119.90
1	A	32	A	OP1-P-O3'	6.23	118.91	105.20
1	A	1523	G	N3-C2-N2	-6.23	115.54	119.90
1	A	962	C	N1-C2-O2	6.23	122.64	118.90
1	A	1527	C	C5-C4-N4	-6.23	115.84	120.20
1	A	400	C	C6-N1-C2	6.22	122.79	120.30
1	A	243	A	OP1-P-O3'	6.22	118.89	105.20
1	A	329	A	N3-C4-C5	6.22	131.16	126.80
1	A	130	A	C4-C5-C6	6.22	120.11	117.00
1	A	874	G	N1-C6-O6	6.22	123.63	119.90
1	A	1390	U	N3-C4-C5	-6.22	110.87	114.60
1	A	1388	C	O5'-P-OP1	6.22	118.16	110.70
1	A	283	C	N3-C4-N4	6.21	122.35	118.00
1	A	730	G	C4-C5-N7	-6.21	108.32	110.80
1	A	185	A	O5'-P-OP2	-6.21	100.12	105.70
1	A	806	C	C2-N3-C4	-6.20	116.80	119.90
1	A	560	U	N3-C2-O2	-6.20	117.86	122.20
1	A	648	A	N7-C8-N9	-6.20	110.70	113.80
1	A	940	C	C5-C6-N1	-6.20	117.90	121.00
1	A	518	C	C5-C4-N4	6.20	124.54	120.20
1	A	254	G	O5'-P-OP1	-6.20	100.12	105.70
1	A	900	A	C8-N9-C4	-6.20	103.32	105.80
1	A	1051	C	N1-C2-O2	6.19	122.62	118.90
1	A	524	G	C4-N9-C1'	6.19	134.55	126.50
1	A	599	C	C5-C6-N1	-6.19	117.90	121.00
1	A	662	G	C8-N9-C4	6.19	108.88	106.40
1	A	317	G	C5-C6-N1	-6.19	108.41	111.50
1	A	583	A	C2-N3-C4	-6.19	107.51	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1501	C	C5-C6-N1	-6.19	117.91	121.00
1	A	723	U	N3-C2-O2	-6.18	117.87	122.20
1	A	289	G	C5-N7-C8	-6.18	101.21	104.30
1	A	1403	C	C2-N1-C1'	6.18	125.60	118.80
1	A	600	C	N3-C4-N4	-6.18	113.67	118.00
1	A	874	G	N3-C4-N9	6.18	129.71	126.00
1	A	79	G	N3-C4-C5	-6.17	125.51	128.60
1	A	385	C	N3-C4-C5	6.17	124.37	121.90
1	A	106	C	O5'-P-OP1	-6.17	100.15	105.70
1	A	570	G	C8-N9-C4	-6.17	103.93	106.40
1	A	872	A	C5-C6-N6	-6.17	118.77	123.70
1	A	450	G	C8-N9-C4	6.17	108.87	106.40
1	A	1436	U	C2-N1-C1'	6.17	125.10	117.70
1	A	29	G	N9-C4-C5	-6.16	102.94	105.40
1	A	168	G	C4-C5-N7	6.16	113.27	110.80
1	A	795	C	N1-C2-O2	-6.16	115.20	118.90
1	A	558	G	O5'-P-OP1	6.16	118.09	110.70
1	A	1526	G	N3-C2-N2	-6.16	115.59	119.90
1	A	873	A	C2-N3-C4	6.16	113.68	110.60
1	A	739	C	C6-N1-C2	6.16	122.76	120.30
1	A	448	A	N7-C8-N9	6.16	116.88	113.80
1	A	1301	U	N3-C4-O4	6.16	123.71	119.40
1	A	1052	U	N3-C4-C5	-6.15	110.91	114.60
1	A	779	C	C4-C5-C6	6.15	120.48	117.40
1	A	802	A	C4-C5-N7	6.15	113.78	110.70
1	A	859	A	C6-C5-N7	-6.15	128.00	132.30
1	A	780	A	N1-C2-N3	6.15	132.37	129.30
1	A	230	G	C8-N9-C4	6.15	108.86	106.40
1	A	1509	C	C5-C6-N1	-6.15	117.93	121.00
1	A	308	C	N3-C2-O2	-6.14	117.60	121.90
1	A	448	A	C6-C5-N7	-6.14	128.00	132.30
1	A	812	C	C5-C4-N4	6.14	124.50	120.20
1	A	1399	C	N3-C4-C5	-6.14	119.44	121.90
1	A	1062	U	C5-C4-O4	6.14	129.58	125.90
1	A	232	G	C8-N9-C1'	-6.14	119.02	127.00
1	A	310	G	C5-C6-O6	-6.14	124.92	128.60
1	A	129(A)	G	N3-C4-N9	6.14	129.68	126.00
1	A	721	G	N1-C2-N2	-6.14	110.68	116.20
1	A	21	G	N9-C4-C5	-6.13	102.95	105.40
1	A	576	G	C8-N9-C1'	-6.13	119.02	127.00
1	A	168	G	C6-C5-N7	-6.13	126.72	130.40
1	A	1236	A	C5-C6-N6	-6.13	118.80	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	125	U	N3-C2-O2	-6.13	117.91	122.20
1	A	876	G	C6-N1-C2	-6.13	121.42	125.10
1	A	909	A	C6-N1-C2	-6.13	114.92	118.60
1	A	908	A	C8-N9-C4	6.13	108.25	105.80
1	A	266	G	N3-C4-N9	6.13	129.68	126.00
1	A	750	G	O5'-P-OP1	-6.13	100.19	105.70
1	A	1092	A	N9-C4-C5	-6.12	103.35	105.80
1	A	864	A	N3-C4-N9	-6.12	122.50	127.40
1	A	1499	A	C6-N1-C2	-6.12	114.93	118.60
1	A	812	C	P-O3'-C3'	6.12	127.04	119.70
1	A	780	A	C6-N1-C2	-6.12	114.93	118.60
1	A	726	C	C2-N3-C4	-6.11	116.84	119.90
1	A	167	G	C6-C5-N7	-6.11	126.73	130.40
1	A	259	G	C5-C6-N1	-6.11	108.44	111.50
1	A	1197	G	C8-N9-C1'	-6.11	119.06	127.00
1	A	280	C	C5-C6-N1	-6.11	117.94	121.00
1	A	1224	G	C8-N9-C4	6.11	108.84	106.40
1	A	1064	G	N3-C4-N9	-6.11	122.34	126.00
1	A	838	G	N9-C4-C5	-6.11	102.96	105.40
1	A	1512	U	N3-C4-O4	6.10	123.67	119.40
1	A	667	G	C6-C5-N7	-6.10	126.74	130.40
1	A	816	A	C2-N3-C4	-6.10	107.55	110.60
1	A	1478	C	C6-N1-C2	-6.10	117.86	120.30
1	A	720	C	N3-C4-C5	6.10	124.34	121.90
1	A	1397	C	C6-N1-C2	6.10	122.74	120.30
1	A	975	A	O4'-C1'-N9	-6.09	103.33	108.20
1	A	1315	U	N3-C2-O2	-6.09	117.93	122.20
1	A	1355	G	C8-N9-C4	-6.09	103.96	106.40
1	A	1477	C	C6-N1-C2	-6.09	117.86	120.30
1	A	884	U	C4-C5-C6	6.09	123.36	119.70
1	A	1232	U	N3-C2-O2	6.09	126.46	122.20
1	A	716	A	O5'-P-OP1	-6.09	100.22	105.70
1	A	1344	C	C2-N1-C1'	-6.09	112.11	118.80
1	A	130	A	N1-C2-N3	6.08	132.34	129.30
1	A	827	U	C5-C6-N1	-6.08	119.66	122.70
1	A	931	C	C6-N1-C2	6.08	122.73	120.30
1	A	916	G	C5-C6-O6	-6.08	124.95	128.60
1	A	799	G	C5-N7-C8	-6.08	101.26	104.30
1	A	300	A	C6-N1-C2	-6.08	114.95	118.60
1	A	760	G	C5-C6-N1	-6.08	108.46	111.50
1	A	316	G	C5-C6-O6	-6.07	124.96	128.60
1	A	806	C	C5-C6-N1	-6.07	117.97	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	34	C	N1-C2-O2	-6.07	115.26	118.90
1	A	373	A	N1-C2-N3	6.06	132.33	129.30
1	A	118	U	N3-C4-O4	-6.06	115.16	119.40
1	A	774	G	C5-N7-C8	-6.06	101.27	104.30
1	A	1531	A	C6-C5-N7	-6.06	128.06	132.30
1	A	331	G	C6-C5-N7	-6.05	126.77	130.40
1	A	1441	G	N3-C2-N2	-6.05	115.66	119.90
1	A	8	A	N1-C6-N6	-6.05	114.97	118.60
1	A	1514	C	C2-N3-C4	-6.05	116.88	119.90
1	A	947	G	C8-N9-C1'	-6.04	119.14	127.00
1	A	1514	C	C5-C6-N1	-6.04	117.98	121.00
1	A	1441	G	N9-C4-C5	6.04	107.82	105.40
1	A	1380	U	N3-C4-O4	-6.04	115.17	119.40
1	A	1442	G	C6-C5-N7	-6.04	126.78	130.40
1	A	593	G	N1-C6-O6	6.04	123.52	119.90
1	A	916	G	N3-C4-N9	6.04	129.62	126.00
1	A	7	G	C5-C6-O6	-6.03	124.98	128.60
1	A	729	A	C5-N7-C8	-6.03	100.88	103.90
1	A	728	A	N3-C4-N9	-6.03	122.58	127.40
1	A	309	G	O5'-P-OP2	-6.03	100.28	105.70
1	A	559	A	N7-C8-N9	6.03	116.81	113.80
1	A	1282	C	C6-N1-C2	-6.03	117.89	120.30
1	A	372	C	C4-C5-C6	6.02	120.41	117.40
1	A	820	U	O4'-C1'-N1	6.02	113.02	108.20
1	A	824	C	N1-C2-O2	-6.02	115.29	118.90
1	A	976	G	N3-C4-C5	-6.02	125.59	128.60
1	A	1234	C	C6-N1-C2	6.02	122.71	120.30
1	A	118	U	C5-C6-N1	-6.02	119.69	122.70
1	A	353	A	N9-C4-C5	6.02	108.21	105.80
1	A	614	A	N1-C2-N3	6.02	132.31	129.30
1	A	379	C	C2-N1-C1'	-6.01	112.19	118.80
1	A	945	G	C4-C5-C6	-6.01	115.19	118.80
1	A	103	C	C4-C5-C6	6.01	120.41	117.40
1	A	112	G	N3-C4-C5	6.01	131.61	128.60
1	A	888	G	C4-N9-C1'	6.01	134.32	126.50
1	A	1401	G	N1-C6-O6	-6.01	116.29	119.90
1	A	79	G	C2-N3-C4	6.01	114.90	111.90
1	A	618	C	N1-C2-N3	-6.01	114.99	119.20
1	A	1530	G	OP1-P-OP2	6.00	128.61	119.60
1	A	522	C	C5-C6-N1	-6.00	118.00	121.00
1	A	448	A	C8-N9-C4	-6.00	103.40	105.80
1	A	898	G	N1-C2-N2	-6.00	110.80	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1497	G	N3-C4-C5	-6.00	125.60	128.60
1	A	96	G	C8-N9-C4	-5.99	104.00	106.40
1	A	288	A	C2-N3-C4	-5.99	107.60	110.60
1	A	656	C	N3-C4-C5	5.99	124.30	121.90
1	A	1304	G	C5-C6-N1	-5.99	108.50	111.50
1	A	1295	G	C8-N9-C4	-5.99	104.00	106.40
1	A	329	A	C4-C5-N7	5.99	113.69	110.70
1	A	858	G	C4-C5-C6	5.99	122.39	118.80
1	A	753	A	C4-C5-N7	-5.98	107.71	110.70
1	A	802	A	C5-C6-N6	-5.98	118.91	123.70
1	A	747	C	C5-C6-N1	-5.98	118.01	121.00
1	A	605	U	N3-C4-O4	5.97	123.58	119.40
1	A	1351	U	C6-N1-C2	-5.97	117.42	121.00
1	A	481	G	C4-N9-C1'	5.96	134.25	126.50
1	A	130	A	C6-C5-N7	-5.96	128.13	132.30
1	A	238	G	C5-C6-N1	-5.96	108.52	111.50
1	A	739	C	C2-N3-C4	-5.96	116.92	119.90
1	A	1334	G	OP1-P-OP2	5.96	128.54	119.60
1	A	1373	G	C5-C6-O6	-5.96	125.02	128.60
1	A	10	A	C8-N9-C4	5.96	108.19	105.80
1	A	738	C	C5-C6-N1	-5.96	118.02	121.00
1	A	783	C	N1-C2-O2	-5.96	115.32	118.90
1	A	833	U	N3-C4-C5	-5.96	111.02	114.60
1	A	855	G	C8-N9-C4	5.96	108.78	106.40
1	A	651	C	C5-C6-N1	-5.96	118.02	121.00
1	A	1346	A	N1-C6-N6	-5.95	115.03	118.60
1	A	562	C	N1-C2-O2	5.95	122.47	118.90
1	A	886	G	N1-C6-O6	5.95	123.47	119.90
1	A	188	C	C6-N1-C2	5.95	122.68	120.30
1	A	1380	U	P-O3'-C3'	5.95	126.83	119.70
1	A	835	U	C6-N1-C1'	5.94	129.52	121.20
1	A	529	G	C8-N9-C1'	-5.94	119.28	127.00
1	A	337	C	C5-C6-N1	-5.94	118.03	121.00
1	A	389	A	C8-N9-C4	-5.94	103.42	105.80
1	A	747	C	C6-N1-C2	5.94	122.67	120.30
1	A	1077	G	N3-C2-N2	5.94	124.06	119.90
1	A	1268	A	N9-C4-C5	5.94	108.17	105.80
1	A	793	U	C4-C5-C6	-5.93	116.14	119.70
1	A	922	G	C4-N9-C1'	5.93	134.21	126.50
1	A	117	G	N3-C4-N9	5.93	129.56	126.00
1	A	727	G	N3-C2-N2	5.93	124.05	119.90
1	A	1307	U	N1-C2-O2	5.93	126.95	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	853	G	N1-C6-O6	5.93	123.46	119.90
1	A	1502	A	N1-C2-N3	5.93	132.26	129.30
1	A	15	G	C5-C6-N1	-5.92	108.54	111.50
1	A	386	C	C2-N1-C1'	5.92	125.32	118.80
1	A	1100	C	OP2-P-O3'	5.92	118.23	105.20
1	A	923	A	C4-C5-N7	5.92	113.66	110.70
1	A	167	G	C8-N9-C4	5.92	108.77	106.40
1	A	617	G	C8-N9-C4	5.92	108.77	106.40
1	A	403	C	C2-N3-C4	-5.92	116.94	119.90
1	A	1345	U	O5'-P-OP1	-5.92	100.38	105.70
1	A	1531	A	C5-N7-C8	-5.92	100.94	103.90
1	A	640	A	C4-C5-C6	5.92	119.96	117.00
1	A	1394	A	C6-C5-N7	-5.92	128.16	132.30
16	P	26	ARG	NE-CZ-NH1	-5.92	117.34	120.30
1	A	298	A	C6-N1-C2	-5.91	115.05	118.60
1	A	481	G	C6-C5-N7	-5.91	126.85	130.40
1	A	893	C	N3-C2-O2	-5.91	117.76	121.90
1	A	560	U	C2-N1-C1'	5.91	124.79	117.70
1	A	655	A	N7-C8-N9	-5.91	110.85	113.80
1	A	1330	U	C5-C4-O4	-5.91	122.36	125.90
1	A	830	G	C5-C6-O6	5.90	132.14	128.60
1	A	981	U	C6-N1-C2	-5.90	117.46	121.00
1	A	1263	C	C6-N1-C2	5.90	122.66	120.30
1	A	122	G	C6-C5-N7	-5.90	126.86	130.40
1	A	285	G	N3-C2-N2	-5.90	115.77	119.90
1	A	334	C	C6-N1-C2	5.90	122.66	120.30
1	A	1108	G	N7-C8-N9	5.90	116.05	113.10
1	A	1186	G	N1-C6-O6	5.89	123.44	119.90
5	E	12	LEU	CA-CB-CG	5.89	128.86	115.30
8	H	85	ARG	NE-CZ-NH1	-5.89	117.36	120.30
1	A	827	U	N3-C2-O2	-5.89	118.08	122.20
1	A	859	A	C5-C6-N6	-5.89	118.99	123.70
1	A	80	G	C8-N9-C4	-5.88	104.05	106.40
1	A	115	G	C5-C6-N1	5.88	114.44	111.50
1	A	250	A	C8-N9-C4	5.88	108.15	105.80
1	A	727	G	N1-C2-N2	-5.88	110.91	116.20
1	A	1279	A	N7-C8-N9	5.88	116.74	113.80
1	A	112	G	C5-C6-N1	-5.87	108.56	111.50
1	A	456	C	C6-N1-C2	5.87	122.65	120.30
1	A	658	G	N1-C6-O6	5.87	123.42	119.90
1	A	720	C	C6-N1-C2	5.87	122.65	120.30
17	Q	99	SER	N-CA-C	5.87	126.84	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	14	U	N3-C4-C5	-5.87	111.08	114.60
1	A	924	C	OP2-P-O3'	5.86	118.10	105.20
1	A	1527	C	C6-N1-C2	-5.86	117.95	120.30
1	A	1112	C	C2-N3-C4	-5.86	116.97	119.90
1	A	585	G	O5'-P-OP2	-5.86	100.43	105.70
1	A	1197	G	N3-C4-N9	5.86	129.51	126.00
1	A	1501	C	N3-C4-C5	5.86	124.24	121.90
1	A	190(D)	U	C6-N1-C2	5.85	124.51	121.00
1	A	722	A	C5-C6-N1	-5.85	114.77	117.70
1	A	190(G)	G	C5-C6-N1	-5.85	108.57	111.50
1	A	108	G	C8-N9-C4	-5.85	104.06	106.40
1	A	1515[A]	C	O5'-P-OP1	5.85	117.72	110.70
1	A	1515[B]	C	O5'-P-OP1	5.85	117.72	110.70
1	A	1302	U	OP2-P-O3'	5.85	118.07	105.20
1	A	389	A	C4-C5-C6	5.84	119.92	117.00
1	A	618	C	C6-N1-C2	5.84	122.64	120.30
1	A	884	U	O5'-P-OP1	-5.84	100.44	105.70
1	A	232	G	N3-C4-N9	5.84	129.50	126.00
1	A	779	C	C2-N3-C4	-5.84	116.98	119.90
1	A	888	G	C8-N9-C1'	-5.84	119.41	127.00
1	A	260	G	N9-C4-C5	5.84	107.74	105.40
1	A	948	C	N3-C4-C5	5.84	124.24	121.90
1	A	872	A	OP2-P-O3'	5.83	118.04	105.20
1	A	872	A	C2-N3-C4	-5.83	107.68	110.60
1	A	326	G	C5-C6-N1	-5.83	108.58	111.50
1	A	626	U	O5'-P-OP1	-5.83	100.45	105.70
1	A	919	A	C4-C5-C6	-5.83	114.08	117.00
1	A	1305	G	C8-N9-C4	-5.83	104.07	106.40
1	A	852	G	N3-C4-C5	5.83	131.51	128.60
1	A	921	U	N3-C4-C5	-5.82	111.11	114.60
1	A	168	G	C5-C6-O6	-5.82	125.11	128.60
1	A	1279	A	C8-N9-C4	-5.82	103.47	105.80
1	A	1502	A	OP1-P-O3'	5.82	118.01	105.20
1	A	48	C	N1-C2-O2	-5.82	115.41	118.90
1	A	808	C	N3-C4-C5	5.82	124.23	121.90
1	A	1139	G	P-O3'-C3'	5.82	126.68	119.70
1	A	461	C	N1-C2-O2	5.81	122.39	118.90
1	A	1072	G	OP2-P-O3'	5.81	117.99	105.20
1	A	125	U	C2-N3-C4	-5.81	123.51	127.00
1	A	830	G	N1-C6-O6	-5.81	116.41	119.90
1	A	250	A	C2-N3-C4	-5.81	107.69	110.60
1	A	665	A	C5-C6-N1	5.81	120.61	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	350	G	C8-N9-C4	-5.81	104.08	106.40
1	A	821	G	C4-C5-N7	5.81	113.12	110.80
1	A	23	C	C4-C5-C6	5.80	120.30	117.40
1	A	833	U	C5-C4-O4	5.80	129.38	125.90
1	A	1237	C	C4-C5-C6	5.80	120.30	117.40
1	A	129(A)	G	C6-C5-N7	-5.80	126.92	130.40
1	A	173	U	N3-C2-O2	-5.80	118.14	122.20
1	A	570	G	C6-N1-C2	-5.80	121.62	125.10
1	A	635	G	C4-C5-C6	5.80	122.28	118.80
1	A	637	G	N7-C8-N9	-5.80	110.20	113.10
1	A	648	A	N1-C2-N3	5.80	132.20	129.30
1	A	122	G	C5-C6-O6	-5.80	125.12	128.60
1	A	293	G	N1-C2-N3	5.80	127.38	123.90
1	A	306	G	C5-C6-N1	-5.80	108.60	111.50
1	A	416	G	C6-C5-N7	-5.80	126.92	130.40
1	A	572	A	C5-C6-N1	5.80	120.60	117.70
1	A	1447	G	C4-C5-N7	5.80	113.12	110.80
1	A	876	G	C5-C6-N1	5.79	114.40	111.50
1	A	309	G	N1-C2-N3	5.79	127.38	123.90
1	A	484	G	C8-N9-C1'	-5.79	119.47	127.00
1	A	328	C	N3-C4-C5	5.79	124.22	121.90
1	A	733	A	N1-C2-N3	5.79	132.19	129.30
1	A	412	A	C8-N9-C4	5.79	108.11	105.80
1	A	511	C	C2-N1-C1'	-5.79	112.44	118.80
1	A	947	G	C8-N9-C4	5.79	108.71	106.40
1	A	1502	A	C5-C6-N1	-5.79	114.81	117.70
1	A	251	G	N3-C4-N9	5.78	129.47	126.00
1	A	569	C	C4-C5-C6	5.78	120.29	117.40
1	A	697	U	OP2-P-O3'	5.78	117.92	105.20
1	A	932	C	N3-C4-C5	5.78	124.21	121.90
1	A	888	G	C4-C5-C6	5.78	122.27	118.80
1	A	1531	A	C8-N9-C4	-5.78	103.49	105.80
1	A	190(G)	G	C6-C5-N7	-5.78	126.94	130.40
1	A	262	A	C5-C6-N6	5.78	128.32	123.70
1	A	659	U	N1-C2-N3	5.78	118.37	114.90
1	A	667	G	C8-N9-C1'	-5.78	119.49	127.00
1	A	658	G	N1-C2-N3	5.77	127.36	123.90
1	A	1470	G	N7-C8-N9	-5.77	110.21	113.10
1	A	731	G	N9-C4-C5	-5.77	103.09	105.40
1	A	477	G	C5-C6-N1	-5.77	108.61	111.50
1	A	573	A	N7-C8-N9	5.77	116.69	113.80
1	A	605	U	N3-C4-C5	-5.77	111.14	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	115	G	P-O3'-C3'	5.77	126.62	119.70
1	A	1319	A	N1-C6-N6	5.77	122.06	118.60
1	A	170	U	N1-C2-O2	-5.76	118.77	122.80
1	A	1200	C	C4-C5-C6	-5.76	114.52	117.40
1	A	733	A	OP1-P-OP2	5.76	128.24	119.60
1	A	1277	C	C6-N1-C2	-5.76	118.00	120.30
1	A	1527	C	OP1-P-O3'	-5.76	92.53	105.20
1	A	333	G	N1-C6-O6	5.75	123.35	119.90
1	A	1300	G	OP2-P-O3'	5.75	117.85	105.20
1	A	364	A	C4-C5-C6	5.75	119.88	117.00
1	A	745	C	N3-C4-N4	-5.75	113.97	118.00
1	A	1092	A	O4'-C1'-N9	-5.75	103.60	108.20
1	A	511	C	C2-N3-C4	-5.75	117.03	119.90
1	A	235	C	N3-C4-N4	-5.75	113.98	118.00
1	A	1092	A	C5-C6-N6	-5.75	119.10	123.70
1	A	605	U	C4-C5-C6	5.74	123.14	119.70
1	A	1217	C	C6-N1-C2	-5.73	118.01	120.30
1	A	934	C	N3-C4-C5	5.73	124.19	121.90
1	A	1211	U	C2-N1-C1'	5.73	124.58	117.70
1	A	1401	G	N3-C4-C5	-5.73	125.73	128.60
1	A	333	G	N3-C2-N2	-5.73	115.89	119.90
1	A	815	A	C8-N9-C4	5.73	108.09	105.80
1	A	1235	U	N1-C2-N3	5.73	118.34	114.90
1	A	770	C	N3-C4-C5	5.73	124.19	121.90
1	A	237	C	N1-C2-N3	5.72	123.21	119.20
1	A	640	A	N1-C6-N6	5.72	122.03	118.60
1	A	654	G	N1-C2-N2	5.72	121.35	116.20
16	P	58	TYR	CB-CA-C	-5.72	98.95	110.40
1	A	109	A	C2-N3-C4	-5.72	107.74	110.60
1	A	580	U	N1-C2-N3	5.72	118.33	114.90
1	A	1276	G	N1-C6-O6	5.72	123.33	119.90
1	A	529	G	C4-N9-C1'	5.71	133.93	126.50
1	A	976	G	O4'-C1'-N9	5.71	112.77	108.20
1	A	379	C	C5-C6-N1	-5.71	118.14	121.00
1	A	1383	C	C5-C6-N1	5.71	123.86	121.00
1	A	1490	C	C5-C6-N1	5.71	123.86	121.00
1	A	124	G	N1-C2-N2	-5.70	111.07	116.20
1	A	792	A	N1-C6-N6	5.70	122.02	118.60
1	A	1529	G	C4-C5-C6	5.70	122.22	118.80
1	A	386	C	C6-N1-C1'	-5.70	113.96	120.80
1	A	193	C	C6-N1-C2	5.70	122.58	120.30
1	A	827	U	N1-C2-N3	5.70	118.32	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	186	C	N3-C2-O2	-5.70	117.91	121.90
1	A	277	C	N3-C4-N4	-5.70	114.01	118.00
1	A	365	U	N3-C4-O4	5.70	123.39	119.40
1	A	1233	G	C5-C6-N1	-5.70	108.65	111.50
1	A	576	G	C4-N9-C1'	5.69	133.90	126.50
1	A	1441	G	N3-C4-N9	-5.69	122.58	126.00
1	A	35	G	N1-C6-O6	5.69	123.32	119.90
1	A	240	C	N1-C2-O2	-5.69	115.48	118.90
1	A	428	G	P-O3'-C3'	5.69	126.53	119.70
1	A	1508	G	C5-C6-N1	5.69	114.34	111.50
1	A	444	C	N3-C4-C5	5.69	124.17	121.90
1	A	1108	G	N3-C4-N9	5.68	129.41	126.00
1	A	392	G	C6-C5-N7	-5.68	126.99	130.40
1	A	1149	C	C2-N1-C1'	5.68	125.05	118.80
1	A	583	A	C6-N1-C2	-5.68	115.19	118.60
1	A	577	G	C2-N3-C4	-5.68	109.06	111.90
1	A	787	A	N7-C8-N9	5.68	116.64	113.80
1	A	1068	G	O5'-P-OP1	-5.67	100.59	105.70
1	A	1336	C	C2-N1-C1'	5.67	125.04	118.80
1	A	1367	C	C6-N1-C2	-5.67	118.03	120.30
1	A	816	A	N7-C8-N9	-5.66	110.97	113.80
1	A	329	A	C6-C5-N7	-5.66	128.34	132.30
1	A	832	C	C5-C4-N4	-5.66	116.24	120.20
1	A	17	U	C5-C6-N1	-5.66	119.87	122.70
1	A	654	G	C8-N9-C1'	5.66	134.35	127.00
1	A	742	G	N3-C2-N2	-5.65	115.94	119.90
1	A	1394	A	N9-C4-C5	-5.65	103.54	105.80
1	A	475	G	C5-C6-N1	-5.65	108.67	111.50
1	A	820	U	C2-N1-C1'	-5.65	110.92	117.70
1	A	93	G	OP1-P-O3'	5.65	117.62	105.20
1	A	448	A	C5-N7-C8	-5.64	101.08	103.90
1	A	620	C	OP1-P-O3'	5.64	117.62	105.20
1	A	1074	G	C5-C6-N1	-5.64	108.68	111.50
1	A	144	G	C5-C6-O6	-5.64	125.22	128.60
1	A	655	A	C8-N9-C4	5.64	108.06	105.80
1	A	1347	G	OP2-P-O3'	5.64	117.61	105.20
1	A	1373	G	C8-N9-C1'	-5.64	119.67	127.00
1	A	1092	A	C5-N7-C8	-5.64	101.08	103.90
1	A	1246	C	C2-N1-C1'	-5.64	112.60	118.80
1	A	27	G	C4-C5-N7	5.64	113.06	110.80
1	A	139	G	C5-C6-O6	-5.64	125.22	128.60
1	A	805	C	C5-C4-N4	-5.64	116.25	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	574	A	N7-C8-N9	-5.63	110.98	113.80
1	A	1350	A	C5-N7-C8	-5.63	101.08	103.90
1	A	898	G	C5-C6-O6	5.63	131.98	128.60
1	A	909	A	C5-C6-N6	-5.63	119.19	123.70
1	A	1433	A	C8-N9-C4	-5.63	103.55	105.80
1	A	827	U	OP2-P-O3'	5.63	117.58	105.20
1	A	659	U	C2-N3-C4	-5.62	123.62	127.00
1	A	568	G	N1-C6-O6	-5.62	116.53	119.90
1	A	365	U	C6-N1-C1'	-5.62	113.33	121.20
1	A	1232	U	N3-C4-O4	5.62	123.33	119.40
1	A	21	G	N7-C8-N9	-5.62	110.29	113.10
1	A	703	G	C4-C5-C6	5.62	122.17	118.80
1	A	793	U	OP2-P-O3'	5.62	117.56	105.20
1	A	507	C	C5-C4-N4	-5.62	116.27	120.20
1	A	912	C	C5-C4-N4	-5.62	116.27	120.20
1	A	1469	G	N1-C6-O6	5.62	123.27	119.90
1	A	318	G	N1-C6-O6	5.62	123.27	119.90
1	A	1305	G	C5-C6-N1	-5.62	108.69	111.50
1	A	324	G	C5-C6-N1	-5.61	108.69	111.50
1	A	791	G	N1-C6-O6	5.61	123.27	119.90
1	A	806	C	N3-C4-C5	5.61	124.15	121.90
1	A	927	G	C5-C6-N1	-5.61	108.69	111.50
1	A	1074	G	C2-N3-C4	-5.61	109.09	111.90
1	A	1093	A	P-O3'-C3'	5.61	126.43	119.70
1	A	260	G	N7-C8-N9	5.61	115.90	113.10
1	A	424	G	N1-C6-O6	5.61	123.27	119.90
1	A	945	G	N1-C2-N2	5.61	121.25	116.20
1	A	566	G	N1-C6-O6	5.61	123.27	119.90
1	A	731	G	C2-N3-C4	-5.61	109.10	111.90
1	A	1447	G	C6-C5-N7	-5.61	127.03	130.40
1	A	861	G	C6-C5-N7	-5.61	127.04	130.40
1	A	911	U	C5-C6-N1	-5.61	119.90	122.70
1	A	286	G	N7-C8-N9	5.60	115.90	113.10
1	A	695	A	C5-N7-C8	-5.60	101.10	103.90
1	A	744	C	C6-N1-C2	5.60	122.54	120.30
1	A	852	G	N1-C2-N3	5.60	127.26	123.90
1	A	948	C	C5-C6-N1	-5.60	118.20	121.00
1	A	121	C	O5'-P-OP2	-5.60	100.66	105.70
1	A	350	G	C5-N7-C8	-5.60	101.50	104.30
1	A	27	G	C5-C6-O6	-5.59	125.24	128.60
1	A	658	G	C5-C6-O6	-5.59	125.24	128.60
1	A	19	C	C2-N3-C4	-5.59	117.11	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	754	C	C2-N3-C4	-5.59	117.11	119.90
1	A	116	A	C5-C6-N1	-5.58	114.91	117.70
1	A	246	A	C6-N1-C2	-5.58	115.25	118.60
1	A	1526	G	C4-C5-N7	5.58	113.03	110.80
1	A	121	C	O5'-P-OP1	5.58	117.40	110.70
1	A	576	G	C6-N1-C2	-5.58	121.75	125.10
1	A	522	C	C2-N1-C1'	-5.58	112.66	118.80
1	A	637	G	N9-C4-C5	-5.58	103.17	105.40
1	A	921	U	C6-N1-C2	-5.58	117.65	121.00
1	A	326	G	C5-C6-O6	5.58	131.94	128.60
1	A	129	U	N1-C2-O2	-5.57	118.90	122.80
1	A	795	C	N3-C2-O2	5.57	125.80	121.90
1	A	799	G	C6-C5-N7	-5.57	127.06	130.40
1	A	259	G	C2-N3-C4	-5.56	109.12	111.90
1	A	248	C	C2-N3-C4	-5.56	117.12	119.90
1	A	832	C	N3-C2-O2	-5.56	118.01	121.90
1	A	839	U	C6-N1-C1'	-5.56	113.42	121.20
1	A	301	G	OP1-P-OP2	5.56	127.94	119.60
1	A	5	U	OP2-P-O3'	5.56	117.42	105.20
1	A	475	G	N1-C2-N3	5.56	127.23	123.90
4	D	196	LEU	CA-CB-CG	-5.56	102.52	115.30
1	A	571	U	N3-C4-C5	5.56	117.93	114.60
1	A	949	A	C8-N9-C4	5.56	108.02	105.80
1	A	110	C	N1-C2-O2	-5.55	115.57	118.90
1	A	119	A	N1-C2-N3	5.55	132.08	129.30
1	A	725	G	C5-C6-O6	-5.55	125.27	128.60
1	A	586	C	C4-C5-C6	5.55	120.18	117.40
1	A	189	G	N3-C4-C5	-5.55	125.82	128.60
1	A	357	G	C8-N9-C4	5.55	108.62	106.40
1	A	482	A	N7-C8-N9	5.55	116.58	113.80
1	A	575	G	OP1-P-OP2	5.55	127.93	119.60
1	A	1187	G	C4-N9-C1'	5.55	133.72	126.50
1	A	308	C	N1-C2-O2	5.55	122.23	118.90
1	A	712	A	N1-C6-N6	5.55	121.93	118.60
1	A	1448	C	N3-C4-C5	5.55	124.12	121.90
1	A	132	C	N3-C2-O2	-5.55	118.02	121.90
1	A	505	G	N1-C6-O6	-5.55	116.57	119.90
1	A	1149	C	C5-C6-N1	5.55	123.77	121.00
1	A	138	G	N7-C8-N9	-5.54	110.33	113.10
1	A	874	G	OP1-P-OP2	5.54	127.91	119.60
1	A	16	A	O5'-P-OP1	5.54	117.34	110.70
1	A	353	A	C4-C5-N7	-5.53	107.93	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	576	G	C4-C5-N7	-5.53	108.59	110.80
1	A	716	A	C5-C6-N6	-5.53	119.27	123.70
1	A	852	G	C6-N1-C2	5.53	128.42	125.10
1	A	237	C	C6-N1-C2	-5.53	118.09	120.30
1	A	117	G	C5-C6-O6	-5.53	125.28	128.60
1	A	279	A	N9-C4-C5	5.53	108.01	105.80
1	A	731	G	N3-C2-N2	-5.53	116.03	119.90
1	A	655	A	N1-C6-N6	-5.53	115.28	118.60
1	A	1200	C	O5'-P-OP2	5.53	117.33	110.70
1	A	823	G	C5-C6-O6	-5.52	125.29	128.60
1	A	560	U	C6-N1-C1'	-5.52	113.47	121.20
1	A	658	G	C4-N9-C1'	5.52	133.68	126.50
1	A	896	C	C2-N3-C4	-5.52	117.14	119.90
1	A	1514	C	C4-C5-C6	5.52	120.16	117.40
1	A	1305	G	N7-C8-N9	5.52	115.86	113.10
1	A	1287	A	C5-C6-N6	5.51	128.11	123.70
1	A	558	G	C8-N9-C4	-5.51	104.19	106.40
1	A	1542	U	C5-C6-N1	-5.51	119.94	122.70
1	A	76	C	C2-N1-C1'	-5.51	112.74	118.80
1	A	787	A	C2-N3-C4	-5.51	107.84	110.60
1	A	1416	G	N3-C2-N2	-5.51	116.04	119.90
1	A	524	G	C4-C5-N7	5.51	113.00	110.80
1	A	445	G	N7-C8-N9	5.51	115.85	113.10
1	A	771	G	C8-N9-C1'	-5.51	119.84	127.00
1	A	877	C	N1-C2-O2	-5.51	115.60	118.90
1	A	280	C	N3-C4-N4	-5.50	114.15	118.00
1	A	863	U	N3-C4-C5	-5.50	111.30	114.60
1	A	823	G	N1-C6-O6	5.50	123.20	119.90
1	A	1079	G	C8-N9-C4	-5.50	104.20	106.40
1	A	1403	C	C6-N1-C1'	-5.50	114.20	120.80
1	A	872	A	C6-C5-N7	-5.50	128.45	132.30
1	A	614	A	C6-N1-C2	-5.50	115.30	118.60
1	A	1336	C	P-O3'-C3'	-5.50	113.11	119.70
1	A	599	C	C2-N3-C4	-5.49	117.16	119.90
1	A	895	G	C8-N9-C4	-5.49	104.20	106.40
1	A	1242	C	C2-N1-C1'	5.49	124.84	118.80
1	A	297	G	OP1-P-OP2	-5.49	111.37	119.60
1	A	300	A	C5-C6-N1	5.49	120.44	117.70
1	A	1078	U	C5-C6-N1	5.49	125.44	122.70
1	A	1341	U	C2-N1-C1'	-5.49	111.11	117.70
1	A	821	G	C6-C5-N7	-5.49	127.11	130.40
1	A	111	G	N9-C4-C5	5.49	107.59	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	475	G	C2-N3-C4	-5.48	109.16	111.90
1	A	1526	G	C6-C5-N7	-5.48	127.11	130.40
1	A	592	G	C5-C6-N1	-5.48	108.76	111.50
1	A	892	A	N1-C2-N3	5.48	132.04	129.30
1	A	720	C	N1-C2-O2	5.47	122.19	118.90
1	A	736	C	C2-N3-C4	-5.47	117.16	119.90
1	A	894	G	N1-C6-O6	5.47	123.19	119.90
10	J	40	LEU	CA-CB-CG	5.47	127.89	115.30
1	A	104	G	N1-C6-O6	5.47	123.18	119.90
1	A	1167	A	N7-C8-N9	5.47	116.54	113.80
1	A	1336	C	C6-N1-C1'	-5.47	114.24	120.80
1	A	1318	A	C8-N9-C4	5.47	107.99	105.80
1	A	635	G	N3-C4-C5	5.47	131.33	128.60
2	B	61	LEU	CA-CB-CG	5.46	127.87	115.30
1	A	124	G	N1-C2-N3	5.46	127.18	123.90
1	A	579	G	C2-N3-C4	-5.46	109.17	111.90
1	A	653	A	OP2-P-O3'	5.46	117.22	105.20
1	A	657	G	C8-N9-C4	5.46	108.58	106.40
1	A	805	C	N1-C2-N3	-5.46	115.38	119.20
1	A	854	G	C8-N9-C1'	-5.46	119.90	127.00
1	A	245	C	C2-N1-C1'	5.46	124.81	118.80
1	A	250	A	N9-C4-C5	-5.46	103.62	105.80
1	A	1336	C	N1-C2-O2	5.46	122.17	118.90
1	A	1049	U	P-O3'-C3'	5.46	126.25	119.70
1	A	235	C	C2-N1-C1'	-5.45	112.80	118.80
1	A	1431	C	N1-C2-O2	-5.45	115.63	118.90
1	A	645	C	C6-N1-C2	-5.45	118.12	120.30
1	A	667	G	C8-N9-C4	5.45	108.58	106.40
1	A	819	A	OP2-P-O3'	5.45	117.19	105.20
1	A	202	U	N3-C2-O2	5.45	126.01	122.20
1	A	251	G	C8-N9-C1'	-5.45	119.92	127.00
1	A	276	G	N7-C8-N9	-5.45	110.38	113.10
1	A	342	C	N3-C4-C5	-5.45	119.72	121.90
1	A	1395	C	OP2-P-O3'	5.45	117.19	105.20
1	A	1414	U	C5-C4-O4	5.45	129.17	125.90
1	A	70	G	N3-C4-N9	-5.45	122.73	126.00
1	A	295	C	C2-N3-C4	-5.45	117.18	119.90
1	A	722	A	C4-C5-C6	5.44	119.72	117.00
1	A	770	C	C2-N3-C4	-5.44	117.18	119.90
1	A	570	G	C4-N9-C1'	5.44	133.57	126.50
1	A	867	G	N3-C4-C5	-5.44	125.88	128.60
1	A	562	C	C5-C6-N1	-5.44	118.28	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1416	G	OP2-P-O3'	5.44	117.17	105.20
1	A	823	G	OP2-P-O3'	5.44	117.16	105.20
1	A	18	C	C6-N1-C2	5.43	122.47	120.30
1	A	413	G	C8-N9-C4	-5.43	104.23	106.40
1	A	577	G	N9-C4-C5	-5.43	103.23	105.40
1	A	765	G	C5-C6-N1	-5.43	108.78	111.50
11	K	125	PHE	N-CA-C	5.43	125.66	111.00
1	A	303	A	C5-C6-N6	-5.43	119.36	123.70
1	A	747	C	C2-N3-C4	-5.43	117.19	119.90
1	A	63	C	N3-C2-O2	5.42	125.70	121.90
1	A	126	G	N3-C2-N2	-5.42	116.10	119.90
1	A	876	G	N3-C4-C5	-5.42	125.89	128.60
1	A	181	G	C4-N9-C1'	5.42	133.55	126.50
1	A	554	C	C6-N1-C2	5.42	122.47	120.30
1	A	584	G	OP2-P-O3'	5.42	117.13	105.20
1	A	59	A	N1-C6-N6	-5.42	115.35	118.60
1	A	482	A	C4-C5-C6	5.42	119.71	117.00
1	A	483	C	C4-C5-C6	5.42	120.11	117.40
1	A	938	A	N7-C8-N9	-5.42	111.09	113.80
1	A	1394	A	C4-C5-N7	5.42	113.41	110.70
1	A	1063	C	N3-C4-C5	5.42	124.07	121.90
1	A	1469	G	C5-C6-O6	-5.42	125.35	128.60
1	A	644	G	C5-C6-O6	-5.41	125.35	128.60
1	A	934	C	C6-N1-C2	5.41	122.46	120.30
1	A	867	G	C5-C6-O6	-5.41	125.36	128.60
1	A	1055	A	C5-C6-N1	5.41	120.40	117.70
1	A	70	G	C5-C6-N1	-5.40	108.80	111.50
1	A	181	G	N3-C4-N9	5.40	129.24	126.00
1	A	972	C	O5'-P-OP2	-5.40	100.84	105.70
1	A	1347	G	N1-C2-N2	-5.40	111.34	116.20
1	A	840	C	N1-C2-O2	5.40	122.14	118.90
1	A	872	A	C4-C5-N7	5.40	113.40	110.70
1	A	522	C	N1-C2-O2	-5.40	115.66	118.90
1	A	605	U	N1-C2-N3	5.40	118.14	114.90
1	A	799	G	N1-C6-O6	5.39	123.14	119.90
1	A	920	U	N1-C2-O2	-5.39	119.03	122.80
1	A	1078	U	N3-C4-O4	5.39	123.17	119.40
1	A	9	G	O5'-P-OP2	-5.39	100.85	105.70
1	A	617	G	N7-C8-N9	-5.39	110.41	113.10
1	A	170	U	N1-C2-N3	5.39	118.13	114.90
1	A	824	C	C2-N3-C4	-5.39	117.21	119.90
1	A	941	G	C5-N7-C8	-5.39	101.61	104.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1414	U	N1-C2-O2	5.39	126.57	122.80
1	A	146	G	N3-C2-N2	-5.38	116.13	119.90
1	A	564	C	OP2-P-O3'	5.38	117.04	105.20
1	A	851	G	C5-C6-O6	-5.38	125.37	128.60
1	A	1527	C	N3-C2-O2	-5.38	118.13	121.90
1	A	771	G	N3-C4-N9	5.38	129.23	126.00
1	A	1238	A	N9-C4-C5	5.38	107.95	105.80
1	A	614	A	N7-C8-N9	5.38	116.49	113.80
1	A	716	A	N9-C4-C5	-5.38	103.65	105.80
1	A	1182	G	P-O3'-C3'	5.38	126.15	119.70
1	A	1310	G	N3-C4-C5	-5.37	125.91	128.60
1	A	484	G	C4-N9-C1'	5.37	133.48	126.50
1	A	12	U	O5'-P-OP2	-5.37	100.87	105.70
1	A	1543	C	N1-C2-O2	5.37	122.12	118.90
1	A	365	U	C2-N1-C1'	5.37	124.14	117.70
1	A	623	C	C6-N1-C2	5.37	122.45	120.30
1	A	831	U	N3-C2-O2	5.37	125.96	122.20
1	A	1078	U	C2-N1-C1'	5.36	124.13	117.70
1	A	1373	G	N9-C4-C5	-5.36	103.26	105.40
1	A	518	C	P-O3'-C3'	5.36	126.13	119.70
1	A	1200	C	C5-C4-N4	-5.36	116.45	120.20
1	A	1211	U	N1-C2-O2	5.36	126.55	122.80
1	A	576	G	N3-C4-C5	-5.35	125.92	128.60
1	A	266	G	N9-C4-C5	-5.35	103.26	105.40
1	A	394	G	C4-C5-N7	-5.35	108.66	110.80
1	A	890	G	C5-C6-N1	-5.35	108.83	111.50
1	A	47	C	C5-C4-N4	-5.35	116.46	120.20
1	A	484	G	N1-C2-N2	-5.35	111.39	116.20
1	A	771	G	C6-C5-N7	-5.35	127.19	130.40
1	A	1153	C	N3-C4-N4	-5.35	114.26	118.00
1	A	1512	U	C4-C5-C6	5.35	122.91	119.70
1	A	445	G	C8-N9-C4	-5.35	104.26	106.40
1	A	1350	A	N7-C8-N9	5.35	116.47	113.80
1	A	712	A	C8-N9-C4	5.34	107.94	105.80
1	A	885	G	OP1-P-OP2	5.34	127.62	119.60
1	A	919	A	N7-C8-N9	-5.34	111.13	113.80
1	A	390	C	O5'-P-OP2	-5.34	100.89	105.70
1	A	1283	G	C8-N9-C4	-5.34	104.26	106.40
1	A	909	A	C5-C6-N1	5.34	120.37	117.70
1	A	284	G	C2-N3-C4	-5.34	109.23	111.90
1	A	615	C	C5-C6-N1	5.34	123.67	121.00
1	A	9	G	C2-N3-C4	-5.34	109.23	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	451	A	C8-N9-C4	5.34	107.94	105.80
1	A	130	A	N1-C6-N6	5.33	121.80	118.60
1	A	190	C	C5-C6-N1	-5.33	118.33	121.00
1	A	66	G	C8-N9-C4	-5.33	104.27	106.40
1	A	661	G	C2-N3-C4	-5.33	109.24	111.90
1	A	782	A	C2-N3-C4	-5.33	107.94	110.60
1	A	251	G	C4-C5-C6	5.32	121.99	118.80
1	A	1469	G	N3-C2-N2	-5.32	116.17	119.90
1	A	145	G	N1-C6-O6	5.32	123.09	119.90
1	A	291	C	C4-C5-C6	5.32	120.06	117.40
1	A	485	G	C8-N9-C4	5.32	108.53	106.40
1	A	581	G	C2-N3-C4	-5.32	109.24	111.90
1	A	723	U	C6-N1-C2	-5.32	117.81	121.00
1	A	224	C	C5-C6-N1	-5.32	118.34	121.00
1	A	524	G	N3-C4-N9	5.32	129.19	126.00
1	A	920	U	N3-C4-C5	-5.32	111.41	114.60
1	A	923	A	N9-C4-C5	-5.32	103.67	105.80
1	A	1200	C	N3-C2-O2	-5.32	118.18	121.90
1	A	643	C	N3-C4-C5	5.32	124.03	121.90
1	A	448	A	N1-C6-N6	5.31	121.79	118.60
1	A	645	C	N3-C4-N4	5.31	121.72	118.00
1	A	686	U	C4-C5-C6	5.31	122.89	119.70
1	A	48	C	N3-C2-O2	5.31	125.62	121.90
1	A	126	G	N1-C2-N3	5.31	127.09	123.90
1	A	144	G	N1-C2-N2	5.31	120.98	116.20
1	A	251	G	C4-N9-C1'	5.31	133.40	126.50
1	A	642	A	C6-N1-C2	-5.31	115.42	118.60
1	A	127	G	C5-C6-O6	-5.31	125.42	128.60
1	A	15	G	C5-C6-O6	-5.30	125.42	128.60
1	A	50	A	N9-C4-C5	-5.30	103.68	105.80
1	A	320	C	C5-C6-N1	-5.30	118.35	121.00
1	A	864	A	OP2-P-O3'	5.30	116.87	105.20
1	A	863	U	C5-C4-O4	5.30	129.08	125.90
1	A	1130	A	C8-N9-C4	-5.30	103.68	105.80
1	A	79	G	C8-N9-C4	-5.30	104.28	106.40
1	A	484	G	N3-C4-N9	5.30	129.18	126.00
1	A	32	A	C4-C5-C6	5.30	119.65	117.00
1	A	322	C	N3-C4-C5	5.30	124.02	121.90
1	A	328	C	C2-N1-C1'	5.30	124.63	118.80
1	A	1436	U	C6-N1-C2	-5.30	117.82	121.00
1	A	1485	U	C2-N1-C1'	5.30	124.06	117.70
1	A	831	U	O5'-P-OP2	5.29	117.05	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	881	G	N1-C2-N3	5.29	127.08	123.90
1	A	929	G	C2-N3-C4	-5.29	109.25	111.90
1	A	1158	C	C5-C4-N4	5.29	123.91	120.20
1	A	1470	G	C4-C5-N7	-5.29	108.68	110.80
1	A	1529	G	C8-N9-C1'	-5.29	120.12	127.00
1	A	1190	G	N1-C2-N2	-5.29	111.44	116.20
1	A	1447	G	N1-C6-O6	5.29	123.08	119.90
1	A	746	A	O5'-P-OP1	5.29	117.05	110.70
1	A	943	U	O5'-P-OP2	-5.29	100.94	105.70
1	A	1502	A	C4-C5-C6	5.29	119.64	117.00
20	T	62	LEU	CB-CG-CD1	-5.29	102.01	111.00
1	A	48	C	C2-N1-C1'	-5.29	112.99	118.80
1	A	729	A	OP2-P-O3'	5.29	116.83	105.20
1	A	43	C	C5-C6-N1	-5.28	118.36	121.00
1	A	330	C	OP2-P-O3'	5.28	116.82	105.20
1	A	1485	U	C5-C6-N1	5.28	125.34	122.70
1	A	817	C	O4'-C1'-N1	-5.27	103.98	108.20
1	A	167	G	N1-C2-N2	-5.27	111.46	116.20
1	A	239	U	OP1-P-OP2	5.27	127.51	119.60
1	A	47	C	C6-N1-C1'	-5.27	114.48	120.80
1	A	580	U	C5-C4-O4	5.27	129.06	125.90
1	A	634	C	N3-C2-O2	-5.27	118.21	121.90
1	A	1370	G	N1-C6-O6	-5.27	116.74	119.90
1	A	767	A	O5'-P-OP2	-5.27	100.96	105.70
1	A	232	G	C6-N1-C2	5.26	128.26	125.10
1	A	735	C	N1-C2-N3	-5.26	115.52	119.20
1	A	753	A	C5-C6-N6	5.26	127.91	123.70
1	A	365	U	C5-C4-O4	-5.26	122.74	125.90
1	A	617	G	C5-N7-C8	5.26	106.93	104.30
1	A	1053	G	N7-C8-N9	-5.26	110.47	113.10
1	A	1342	C	N3-C2-O2	5.26	125.58	121.90
1	A	238	G	N1-C6-O6	5.26	123.05	119.90
1	A	402	G	C5-C6-O6	-5.26	125.45	128.60
1	A	879	C	N3-C4-C5	5.26	124.00	121.90
1	A	1236	A	OP2-P-O3'	5.26	116.77	105.20
1	A	1341	U	C6-N1-C2	5.25	124.15	121.00
1	A	873	A	C6-C5-N7	5.25	135.98	132.30
1	A	1447	G	C5-N7-C8	-5.25	101.67	104.30
1	A	393	A	C8-N9-C4	5.25	107.90	105.80
1	A	862	C	N3-C2-O2	5.25	125.57	121.90
1	A	176	C	OP1-P-OP2	5.25	127.47	119.60
1	A	313	A	C8-N9-C4	5.25	107.90	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	589	C	C5-C6-N1	-5.25	118.38	121.00
1	A	646	U	C5-C4-O4	5.25	129.05	125.90
1	A	736	C	N1-C2-O2	5.25	122.05	118.90
2	B	68	ILE	CB-CA-C	-5.25	101.11	111.60
1	A	1099	G	N3-C4-C5	5.25	131.22	128.60
1	A	941	G	C4-C5-N7	5.24	112.90	110.80
1	A	1341	U	C5-C6-N1	-5.24	120.08	122.70
1	A	770	C	O5'-P-OP1	5.24	116.98	110.70
1	A	970	C	N3-C2-O2	-5.24	118.24	121.90
1	A	788	U	N3-C4-O4	5.23	123.06	119.40
1	A	934	C	C2-N1-C1'	-5.23	113.04	118.80
1	A	742	G	C4-C5-C6	5.23	121.94	118.80
1	A	1526	G	C5-N7-C8	-5.23	101.68	104.30
1	A	243	A	O4'-C1'-N9	5.23	112.38	108.20
1	A	302	G	N9-C4-C5	-5.23	103.31	105.40
1	A	47	C	C6-N1-C2	5.23	122.39	120.30
1	A	252	U	N1-C2-N3	5.23	118.04	114.90
1	A	1361(A)	C	C5-C6-N1	5.23	123.61	121.00
1	A	70	G	N3-C4-C5	5.23	131.21	128.60
1	A	808	C	OP2-P-O3'	5.23	116.70	105.20
1	A	939	G	C6-C5-N7	-5.23	127.26	130.40
1	A	360	A	C5-N7-C8	-5.22	101.29	103.90
1	A	557	G	O5'-P-OP1	5.22	116.97	110.70
1	A	853	G	N1-C2-N2	-5.22	111.50	116.20
1	A	1509	C	C4-C5-C6	5.22	120.01	117.40
1	A	7	G	C4-C5-C6	5.22	121.93	118.80
1	A	190(B)	C	C5-C6-N1	5.22	123.61	121.00
1	A	555	C	C2-N1-C1'	5.22	124.54	118.80
1	A	792	A	P-O3'-C3'	5.22	125.96	119.70
1	A	860	A	C4-C5-C6	5.22	119.61	117.00
1	A	881	G	C6-N1-C2	-5.22	121.97	125.10
1	A	167	G	N1-C6-O6	5.22	123.03	119.90
1	A	1527	C	N3-C4-N4	5.22	121.65	118.00
1	A	323	U	C5-C6-N1	-5.21	120.09	122.70
1	A	644	G	C5-C6-N1	5.21	114.11	111.50
1	A	1365	G	N3-C4-C5	-5.21	125.99	128.60
1	A	1389	C	O5'-P-OP1	5.21	116.95	110.70
1	A	190(G)	G	N1-C6-O6	5.21	123.03	119.90
1	A	971	G	N7-C8-N9	-5.21	110.50	113.10
1	A	181	G	C6-C5-N7	-5.21	127.28	130.40
1	A	771	G	C8-N9-C4	5.21	108.48	106.40
1	A	1085	U	O5'-P-OP2	-5.21	101.01	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1508	G	O5'-P-OP2	5.21	116.95	110.70
1	A	460	A	N3-C4-C5	-5.21	123.16	126.80
1	A	1461	G	C8-N9-C4	5.20	108.48	106.40
1	A	518	C	N3-C4-N4	-5.20	114.36	118.00
1	A	793	U	OP1-P-OP2	-5.20	111.80	119.60
1	A	1317	C	C6-N1-C2	5.20	122.38	120.30
1	A	460	A	C6-N1-C2	-5.20	115.48	118.60
1	A	771	G	N9-C4-C5	-5.20	103.32	105.40
1	A	942	G	O5'-P-OP1	5.20	116.94	110.70
1	A	604	G	C8-N9-C4	5.20	108.48	106.40
1	A	833	U	C4-C5-C6	5.20	122.82	119.70
1	A	1355	G	N3-C4-C5	-5.20	126.00	128.60
1	A	1416	G	C5-C6-N1	-5.20	108.90	111.50
1	A	77	G	N3-C4-N9	5.20	129.12	126.00
1	A	1055	A	C2-N3-C4	5.20	113.20	110.60
1	A	851	G	C4-N9-C1'	5.19	133.25	126.50
1	A	874	G	N1-C2-N3	5.19	127.02	123.90
1	A	923	A	N1-C6-N6	5.19	121.72	118.60
1	A	1058	G	N1-C6-O6	-5.19	116.78	119.90
1	A	221	C	N3-C4-N4	-5.19	114.37	118.00
1	A	604	G	N7-C8-N9	-5.19	110.50	113.10
1	A	302	G	C5-C6-N1	5.19	114.09	111.50
1	A	874	G	C5-C6-O6	-5.19	125.49	128.60
1	A	1399	C	C6-N1-C2	-5.19	118.22	120.30
1	A	962	C	OP2-P-O3'	5.18	116.61	105.20
1	A	1064	G	N3-C2-N2	-5.18	116.27	119.90
1	A	1212	U	O4'-C1'-N1	5.18	112.35	108.20
1	A	1497	G	N3-C4-N9	5.18	129.11	126.00
1	A	314	C	O5'-P-OP2	-5.18	101.04	105.70
1	A	1532	U	N3-C2-O2	5.18	125.83	122.20
1	A	841	U	C5-C6-N1	5.18	125.29	122.70
1	A	721	G	N1-C2-N3	5.18	127.01	123.90
1	A	907	A	N7-C8-N9	-5.18	111.21	113.80
1	A	522	C	C6-N1-C2	5.17	122.37	120.30
1	A	599	C	C5-C4-N4	-5.17	116.58	120.20
1	A	1516[A]	G	N1-C6-O6	-5.17	116.80	119.90
1	A	1516[B]	G	N1-C6-O6	-5.17	116.80	119.90
1	A	759	A	OP2-P-O3'	5.17	116.58	105.20
1	A	818	G	C8-N9-C4	-5.17	104.33	106.40
1	A	991	U	P-O3'-C3'	5.17	125.91	119.70
2	B	213	LEU	CA-CB-CG	5.17	127.19	115.30
1	A	43	C	C6-N1-C2	5.17	122.37	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	120	A	O4'-C1'-N9	-5.17	104.06	108.20
1	A	922	G	N3-C4-N9	5.17	129.10	126.00
1	A	1414	U	C2-N1-C1'	5.17	123.90	117.70
1	A	391	G	N3-C4-N9	5.17	129.10	126.00
1	A	910	C	C6-N1-C2	5.17	122.37	120.30
1	A	1081	G	O5'-P-OP2	-5.17	101.05	105.70
1	A	7	G	C6-C5-N7	-5.16	127.30	130.40
1	A	193	C	O5'-P-OP1	5.16	116.89	110.70
1	A	306	G	N1-C2-N2	5.16	120.84	116.20
1	A	500	G	C4-C5-N7	5.16	112.86	110.80
1	A	735	C	C2-N1-C1'	-5.16	113.12	118.80
1	A	969	A	N1-C6-N6	5.16	121.70	118.60
4	D	94	LEU	CA-CB-CG	-5.16	103.43	115.30
1	A	278	G	OP1-P-OP2	5.16	127.34	119.60
1	A	666	G	C4-C5-C6	5.16	121.89	118.80
1	A	836	G	C6-C5-N7	-5.16	127.31	130.40
1	A	646	U	C2-N3-C4	5.15	130.09	127.00
1	A	1341	U	N3-C2-O2	5.15	125.81	122.20
1	A	230	G	N1-C2-N2	-5.15	111.56	116.20
1	A	738	C	C2-N3-C4	-5.15	117.33	119.90
1	A	826	C	C6-N1-C2	5.15	122.36	120.30
1	A	509	A	C3'-C2'-C1'	-5.15	97.38	101.50
1	A	964	A	C8-N9-C4	-5.15	103.74	105.80
1	A	331	G	C4-C5-C6	5.14	121.89	118.80
1	A	485	G	N7-C8-N9	-5.14	110.53	113.10
1	A	1294	G	N3-C4-N9	-5.14	122.91	126.00
1	A	667	G	N9-C4-C5	-5.14	103.34	105.40
1	A	856	C	N1-C2-N3	5.14	122.80	119.20
1	A	1390	U	C4-C5-C6	5.14	122.78	119.70
1	A	154	C	C6-N1-C2	5.14	122.36	120.30
1	A	833	U	O4'-C1'-N1	5.14	112.31	108.20
1	A	858	G	C2-N3-C4	-5.14	109.33	111.90
1	A	1280	A	O5'-P-OP1	-5.14	101.07	105.70
1	A	370	C	OP2-P-O3'	5.14	116.51	105.20
1	A	681	C	C6-N1-C2	5.14	122.36	120.30
1	A	1385	G	C8-N9-C4	5.14	108.45	106.40
1	A	871	U	OP1-P-OP2	5.14	127.31	119.60
1	A	364	A	N1-C2-N3	5.14	131.87	129.30
1	A	836	G	O4'-C1'-N9	-5.14	104.09	108.20
1	A	246	A	OP1-P-O3'	5.13	116.50	105.20
1	A	653	A	C8-N9-C4	-5.13	103.75	105.80
1	A	734	G	C4-C5-N7	5.13	112.85	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	26	A	C8-N9-C4	5.13	107.85	105.80
1	A	858	G	C4-N9-C1'	5.13	133.17	126.50
1	A	595	G	C5-C6-N1	-5.13	108.94	111.50
1	A	491	G	N1-C6-O6	5.12	122.97	119.90
1	A	254	G	C2-N3-C4	-5.12	109.34	111.90
1	A	930	C	C2-N3-C4	-5.12	117.34	119.90
1	A	632	A	N1-C2-N3	5.12	131.86	129.30
1	A	484	G	P-O3'-C3'	5.12	125.84	119.70
1	A	1215	G	N1-C6-O6	5.12	122.97	119.90
1	A	394	G	C5-C6-O6	5.12	131.67	128.60
1	A	22	G	P-O3'-C3'	5.12	125.84	119.70
1	A	304	U	N3-C4-O4	-5.12	115.82	119.40
1	A	1135	U	C2-N1-C1'	5.12	123.84	117.70
1	A	945	G	C5-N7-C8	-5.11	101.74	104.30
1	A	1528	U	C6-N1-C1'	-5.11	114.05	121.20
1	A	59	A	C5-C6-N1	5.11	120.25	117.70
1	A	131	C	C4-C5-C6	5.11	119.95	117.40
1	A	1383	C	N3-C4-C5	-5.11	119.86	121.90
1	A	975	A	C5-C6-N1	-5.11	115.15	117.70
1	A	1530	G	C2-N3-C4	-5.11	109.35	111.90
16	P	60	LEU	CA-CB-CG	-5.11	103.56	115.30
1	A	698	G	C4-N9-C1'	5.10	133.13	126.50
1	A	732	C	N3-C4-C5	5.10	123.94	121.90
1	A	757	U	C2-N1-C1'	-5.10	111.58	117.70
1	A	975	A	N1-C6-N6	5.10	121.66	118.60
1	A	976	G	C5-C6-O6	5.10	131.66	128.60
1	A	28	G	C2-N3-C4	-5.10	109.35	111.90
1	A	482	A	C8-N9-C4	-5.10	103.76	105.80
1	A	658	G	N1-C2-N2	-5.10	111.61	116.20
1	A	1065	U	P-O3'-C3'	5.10	125.82	119.70
1	A	1373	G	C4-N9-C1'	5.10	133.13	126.50
1	A	1425	U	O4'-C1'-N1	5.10	112.28	108.20
1	A	668	G	C8-N9-C4	5.10	108.44	106.40
1	A	777	A	C6-N1-C2	-5.10	115.54	118.60
1	A	78	G	OP1-P-O3'	5.09	116.41	105.20
1	A	247	G	O5'-P-OP1	5.09	116.81	110.70
1	A	281	G	N1-C6-O6	5.09	122.96	119.90
1	A	1215	G	C5-N7-C8	-5.09	101.75	104.30
1	A	1380	U	C5-C4-O4	5.09	128.96	125.90
1	A	107	G	C6-C5-N7	-5.09	127.35	130.40
1	A	485	G	C4-C5-N7	-5.09	108.76	110.80
1	A	395	C	C5-C6-N1	-5.09	118.45	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	817	C	OP1-P-O3'	5.09	116.39	105.20
1	A	68	G	C4-N9-C1'	-5.09	119.89	126.50
1	A	932	C	C2-N3-C4	-5.09	117.36	119.90
1	A	1342	C	N3-C4-N4	5.09	121.56	118.00
1	A	606	G	C5-C6-N1	-5.09	108.96	111.50
1	A	1153	C	N3-C4-C5	5.09	123.93	121.90
1	A	21	G	C5-N7-C8	5.08	106.84	104.30
1	A	551	U	C5-C4-O4	-5.08	122.85	125.90
1	A	384	G	C8-N9-C4	5.08	108.43	106.40
1	A	1243	C	C2-N1-C1'	-5.08	113.22	118.80
1	A	902	G	O5'-P-OP2	-5.08	101.13	105.70
1	A	807	A	N1-C6-N6	-5.08	115.55	118.60
1	A	576	G	C4-C5-C6	5.07	121.84	118.80
1	A	1333	A	C6-N1-C2	-5.07	115.56	118.60
1	A	697	U	C5-C6-N1	-5.07	120.16	122.70
1	A	1161	C	C6-N1-C2	5.07	122.33	120.30
1	A	789	U	N1-C2-N3	5.07	117.94	114.90
1	A	1414	U	OP1-P-O3'	5.07	116.35	105.20
1	A	1417	G	N3-C2-N2	-5.07	116.35	119.90
1	A	189	G	N3-C4-N9	5.07	129.04	126.00
1	A	305	G	N3-C4-C5	5.07	131.13	128.60
1	A	807	A	N7-C8-N9	-5.07	111.27	113.80
1	A	869	G	O5'-P-OP1	-5.06	101.14	105.70
1	A	181	G	P-O3'-C3'	5.06	125.77	119.70
1	A	267	C	N3-C4-C5	5.06	123.92	121.90
1	A	529	G	N3-C4-N9	5.06	129.04	126.00
1	A	1092	A	C6-C5-N7	-5.06	128.76	132.30
1	A	762	C	N3-C4-N4	5.06	121.54	118.00
1	A	240	C	N3-C4-C5	5.06	123.92	121.90
1	A	448	A	C4-C5-N7	5.06	113.23	110.70
5	E	41	VAL	CB-CA-C	-5.06	101.79	111.40
1	A	21	G	OP2-P-O3'	5.06	116.33	105.20
1	A	183	G	C6-C5-N7	-5.06	127.36	130.40
1	A	959	A	C5-C6-N6	-5.06	119.65	123.70
1	A	787	A	C8-N9-C4	-5.05	103.78	105.80
1	A	559	A	P-O3'-C3'	5.05	125.76	119.70
1	A	882	C	N1-C2-O2	5.05	121.93	118.90
1	A	992	U	P-O3'-C3'	5.05	125.76	119.70
1	A	26	A	C5-C6-N6	5.05	127.74	123.70
1	A	647	C	N1-C2-O2	5.05	121.93	118.90
1	A	596	C	OP1-P-O3'	5.05	116.31	105.20
1	A	622	A	C4-C5-N7	5.05	113.22	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	728	A	C2-N3-C4	-5.05	108.08	110.60
1	A	259	G	N1-C2-N3	5.05	126.93	123.90
1	A	135	C	N3-C2-O2	5.05	125.43	121.90
1	A	823	G	C6-N1-C2	-5.04	122.07	125.10
1	A	1383	C	C2-N1-C1'	5.04	124.35	118.80
1	A	640	A	C6-C5-N7	-5.04	128.77	132.30
1	A	289	G	C6-C5-N7	-5.04	127.38	130.40
1	A	724	G	N9-C1'-C2'	-5.04	106.46	112.00
1	A	1190	G	C5-N7-C8	-5.04	101.78	104.30
1	A	389	A	C5-N7-C8	5.04	106.42	103.90
1	A	898	G	N1-C2-N3	5.03	126.92	123.90
1	A	1129	C	O4'-C1'-N1	5.03	112.22	108.20
1	A	1200	C	OP1-P-OP2	-5.03	112.05	119.60
1	A	590	C	C4-C5-C6	5.03	119.91	117.40
1	A	702	A	OP1-P-OP2	-5.03	112.06	119.60
1	A	908	A	C4-C5-C6	-5.03	114.49	117.00
1	A	122	G	O5'-P-OP1	-5.03	101.17	105.70
1	A	644	G	C4-C5-N7	5.03	112.81	110.80
1	A	887	G	O5'-P-OP1	5.03	116.73	110.70
1	A	1074	G	C6-C5-N7	-5.03	127.39	130.40
1	A	1334	G	C8-N9-C1'	-5.03	120.47	127.00
1	A	50	A	N7-C8-N9	-5.02	111.29	113.80
1	A	588	G	N1-C6-O6	5.02	122.91	119.90
1	A	1197	G	N3-C4-C5	-5.02	126.09	128.60
1	A	32	A	OP2-P-O3'	-5.02	94.15	105.20
1	A	676	A	N7-C8-N9	-5.02	111.29	113.80
1	A	25	C	C4-C5-C6	5.02	119.91	117.40
1	A	309	G	C5-C6-O6	-5.02	125.59	128.60
1	A	919	A	N1-C2-N3	-5.02	126.79	129.30
1	A	1188	A	O5'-P-OP1	-5.02	101.18	105.70
1	A	1243	C	C6-N1-C1'	5.02	126.82	120.80
1	A	15	G	N3-C2-N2	-5.02	116.39	119.90
1	A	500	G	N3-C4-C5	5.02	131.11	128.60
1	A	1084	G	N1-C2-N3	5.02	126.91	123.90
1	A	190(B)	C	N3-C4-N4	5.01	121.51	118.00
1	A	1310	G	N3-C4-N9	5.01	129.01	126.00
1	A	773	G	C5-C6-O6	-5.01	125.59	128.60
1	A	932	C	N3-C2-O2	-5.01	118.39	121.90
1	A	128	G	C4-C5-N7	5.01	112.80	110.80
1	A	599	C	N3-C4-C5	5.01	123.90	121.90
1	A	648	A	C5-C6-N1	5.01	120.20	117.70
1	A	695	A	N7-C8-N9	5.01	116.31	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1246	C	N3-C2-O2	5.01	125.41	121.90
1	A	389	A	C6-N1-C2	-5.01	115.60	118.60
1	A	832	C	C2-N3-C4	-5.01	117.40	119.90
1	A	1190	G	C5-C6-N1	-5.01	109.00	111.50
1	A	1343	G	N3-C4-C5	5.01	131.10	128.60
8	H	105	ARG	NE-CZ-NH1	5.01	122.80	120.30
1	A	664	G	O5'-P-OP2	-5.00	101.19	105.70
1	A	1077	G	C8-N9-C4	5.00	108.40	106.40
1	A	169	C	N1-C2-O2	5.00	121.90	118.90
1	A	1515[A]	C	C6-N1-C2	-5.00	118.30	120.30
1	A	1515[B]	C	C6-N1-C2	-5.00	118.30	120.30
1	A	294	U	C5-C4-O4	-5.00	122.90	125.90
1	A	1530	G	O5'-P-OP2	-5.00	101.20	105.70

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	20	GLU	Peptide
2	B	8	LYS	Peptide
3	C	166	GLU	Peptide
3	C	3	ASN	Peptide
3	C	89	GLU	Peptide
4	D	3	ARG	Peptide
7	G	154	TYR	Peptide
8	H	27	PRO	Peptide
8	H	90	GLY	Peptide
10	J	50	ILE	Peptide
10	J	90	LEU	Peptide
12	L	25	PRO	Peptide
12	L	90	VAL	Peptide
13	M	62	ASN	Peptide
18	R	86	VAL	Peptide
19	S	13	ASP	Peptide
20	T	48	LYS	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	32644	0	16503	1058	0
2	B	1900	0	1950	123	0
3	C	1612	0	1676	115	0
4	D	1703	0	1763	132	0
5	E	1146	0	1207	66	0
6	F	843	0	857	38	0
7	G	1257	0	1296	78	0
8	H	1116	0	1177	70	0
9	I	1010	0	1037	78	0
10	J	792	0	835	59	0
11	K	864	0	881	51	0
12	L	977	0	1060	78	0
13	M	937	0	995	72	0
14	N	492	0	529	37	0
15	O	729	0	768	38	0
16	P	700	0	720	45	0
17	Q	823	0	891	59	0
18	R	574	0	644	50	0
19	S	647	0	673	42	0
20	T	763	0	861	44	0
21	U	208	0	221	22	0
22	A	276	0	0	0	0
22	B	3	0	0	0	0
22	C	2	0	0	0	0
22	D	3	0	0	0	0
22	E	1	0	0	0	0
22	F	1	0	0	0	0
22	H	1	0	0	0	0
22	I	1	0	0	0	0
22	J	1	0	0	0	0
22	N	1	0	0	0	0
22	P	2	0	0	0	0
22	Q	1	0	0	0	0
23	D	1	0	0	0	0
23	N	1	0	0	0	0
24	A	266	0	0	7	0
24	E	3	0	0	0	0
24	K	1	0	0	0	0
24	L	1	0	0	0	0
24	Q	2	0	0	0	0
24	T	2	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	52307	0	36544	2147	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 25.

All (2147) 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)
6:F:14:LEU:HD13	6:F:18:GLN:HB3	1.36	1.05
4:D:3:ARG:HH11	4:D:71:SER:H	1.13	0.94
1:A:1240:U:OP1	7:G:119:ARG:NH2	2.01	0.93
1:A:1399:C:H4'	1:A:1400:5MC:H5"	1.51	0.93
1:A:992:U:H3	1:A:1044:A:H62	1.09	0.92
19:S:41:VAL:HG22	19:S:44:MET:HG3	1.53	0.90
1:A:664:G:H22	1:A:741:G:H1	1.20	0.89
14:N:53:LEU:HD12	14:N:56:VAL:HG21	1.55	0.89
1:A:413:G:H8	1:A:428:G:H21	1.20	0.89
18:R:50:ILE:HD11	18:R:70:ILE:HG21	1.55	0.88
1:A:1348:U:H4'	9:I:120:ARG:HD2	1.54	0.88
1:A:912:C:OP1	12:L:46:LYS:NZ	2.07	0.88
1:A:1195:C:H3'	1:A:1196:U:H5"	1.54	0.88
18:R:37:VAL:O	18:R:40:LEU:N	2.07	0.87
9:I:50:LEU:HB3	9:I:55:ALA:HB3	1.56	0.87
2:B:15:VAL:HG11	2:B:213:LEU:HD23	1.55	0.86
1:A:76:C:H42	1:A:95:U:H3	1.23	0.86
5:E:144:THR:O	5:E:148:VAL:HG23	1.75	0.86
1:A:130:A:H5'	17:Q:63:ARG:HE	1.40	0.85
1:A:584:G:OP2	17:Q:87:LYS:NZ	2.09	0.85
17:Q:66:SER:O	17:Q:70:ARG:NH1	2.07	0.85
12:L:27:LEU:O	12:L:29:GLY:N	2.09	0.85
1:A:1413:A:H2'	1:A:1414:U:H6	1.41	0.85
1:A:263:A:OP2	20:T:79:ARG:NH1	2.10	0.84
1:A:1349:A:OP1	9:I:118:LYS:NZ	2.10	0.84
1:A:839:U:H5'	1:A:840:C:H5	1.43	0.83
1:A:130:A:OP2	1:A:190(E):U:O2'	1.96	0.83
1:A:132:C:O2	1:A:230:G:N2	2.11	0.83
4:D:103:ASN:OD1	4:D:114:ARG:NH2	2.10	0.83
1:A:1051:C:N4	1:A:1207:2MG:O6	2.11	0.83
3:C:11:ARG:HG3	3:C:178:LEU:HD11	1.59	0.83
5:E:121:LYS:HG2	5:E:123:LEU:HD23	1.61	0.82
15:O:70:LEU:HD13	15:O:78:TYR:HA	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:91:LEU:HD21	3:C:99:VAL:HG22	1.62	0.82
18:R:55:ARG:HB3	18:R:55:ARG:HH11	1.43	0.81
9:I:86:VAL:HG21	9:I:93:ARG:HG3	1.61	0.81
1:A:79:G:N1	1:A:80:G:N7	2.28	0.81
1:A:1406:U:O2'	1:A:1517[B]:G:N2	2.14	0.80
6:F:8:ILE:HB	6:F:61:LEU:HD12	1.63	0.80
4:D:187:ARG:NE	4:D:188:LEU:H	1.79	0.80
1:A:1034:G:H2'	1:A:1035:A:H8	1.46	0.80
1:A:1009:G:H1	1:A:1020:U:H3	1.30	0.80
1:A:35:G:O2'	12:L:118:SER:O	2.00	0.80
3:C:12:LEU:HD11	14:N:51:GLY:HA2	1.63	0.79
21:U:10:ARG:HH11	21:U:10:ARG:HB2	1.47	0.79
15:O:6:GLU:OE1	15:O:6:GLU:N	2.12	0.79
1:A:262:A:H5'	20:T:74:LYS:HD3	1.66	0.78
14:N:57:ARG:HB3	14:N:57:ARG:HH11	1.48	0.78
1:A:409:G:H1	1:A:433:C:H42	1.31	0.78
7:G:71:PRO:O	7:G:96:GLN:NE2	2.16	0.78
12:L:24:VAL:HG13	12:L:98:TYR:HE2	1.47	0.78
1:A:547:A:OP2	4:D:2:GLY:N	2.15	0.78
1:A:1497:G:H2'	1:A:1498:UR3:H5'	1.66	0.78
7:G:87:VAL:HG11	7:G:154:TYR:HB2	1.64	0.78
8:H:87:SER:HA	8:H:93:VAL:HG13	1.66	0.78
1:A:1279:A:OP1	10:J:7:LYS:NZ	2.17	0.78
3:C:139:GLN:O	3:C:143:GLU:N	2.16	0.78
13:M:96:LEU:O	13:M:110:ARG:NH1	2.17	0.78
1:A:1124:G:N2	1:A:1126:U:O4	2.16	0.77
20:T:83:ARG:NH2	24:T:202:HOH:O	2.16	0.77
13:M:68:GLY:HA2	13:M:71:ARG:HD2	1.66	0.77
1:A:1376:U:OP1	7:G:98:SER:OG	2.03	0.77
10:J:50:ILE:HA	10:J:60:ARG:HB3	1.65	0.77
14:N:40:CYS:O	14:N:44:LEU:N	2.14	0.77
1:A:95:U:H2'	1:A:96:G:H8	1.50	0.77
1:A:279:A:OP2	17:Q:95:TYR:OH	2.02	0.77
13:M:49:THR:HB	13:M:52:GLU:H	1.48	0.77
1:A:1422:G:H2'	1:A:1423:G:H8	1.49	0.77
1:A:1263:C:N4	1:A:1272:G:O6	2.17	0.76
1:A:1009:G:N2	1:A:1010:G:N3	2.33	0.76
7:G:86:GLN:HB2	7:G:148:ASN:HD22	1.51	0.76
1:A:103:C:OP1	20:T:17:ARG:NH1	2.19	0.76
1:A:1168:A:H2'	1:A:1169:A:C8	2.19	0.76
1:A:1347:G:H3'	9:I:108:VAL:O	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:150:LYS:HA	3:C:169:ALA:CB	2.16	0.76
12:L:25:PRO:C	12:L:27:LEU:H	1.87	0.76
1:A:1347:G:N2	1:A:1373:G:H2'	2.00	0.75
5:E:11:ILE:HB	5:E:31:LEU:HB3	1.66	0.75
16:P:9:PHE:CD1	16:P:18:ARG:HG3	2.22	0.75
1:A:1416:G:N2	1:A:1484:C:O2	2.19	0.75
2:B:103:THR:HA	2:B:180:LEU:HD11	1.68	0.75
4:D:22:LYS:HB2	4:D:26:CYS:SG	2.26	0.75
4:D:25:ARG:HG3	4:D:30:LYS:HD3	1.67	0.75
5:E:84:PHE:HB3	5:E:134:ALA:HB2	1.69	0.75
11:K:57:THR:HG23	11:K:60:ALA:H	1.50	0.75
1:A:953:G:N7	13:M:104:ARG:NH2	2.35	0.75
1:A:1367:C:O5'	9:I:112:LYS:NZ	2.20	0.75
3:C:20:SER:HB3	3:C:57:ILE:HB	1.69	0.74
4:D:50:ARG:NH1	4:D:51:PRO:O	2.19	0.74
2:B:21:ARG:HH11	2:B:22:LYS:HB3	1.52	0.74
4:D:154:ASN:O	4:D:159:ARG:NH2	2.19	0.74
1:A:959:A:O2'	1:A:984:C:O2'	2.04	0.74
1:A:1004:A:H5"	1:A:1025:U:C2	2.22	0.74
1:A:1368:G:H5"	9:I:112:LYS:HB3	1.69	0.74
1:A:1491:G:N2	1:A:1492:A:N7	2.35	0.74
14:N:26:ARG:HD2	14:N:47:LEU:HD21	1.69	0.74
1:A:1413:A:H2	1:A:1487:G:H22	1.35	0.74
21:U:10:ARG:HB2	21:U:10:ARG:NH1	2.03	0.74
1:A:1049:U:O2'	14:N:3:ARG:NH1	2.19	0.74
2:B:24:TRP:CZ3	2:B:26:PRO:HA	2.23	0.74
1:A:384:G:H2'	1:A:385:C:C6	2.23	0.74
1:A:736:C:H2'	1:A:737:A:C8	2.23	0.74
3:C:84:ILE:HG23	3:C:88:ARG:HH12	1.51	0.74
1:A:1125:U:O4	10:J:5:ARG:NH2	2.21	0.73
1:A:1255:G:N2	1:A:1259:C:O2	2.19	0.73
3:C:88:ARG:HH21	3:C:101:LEU:HB2	1.54	0.73
1:A:989:C:N3	1:A:1216:G:N2	2.35	0.73
2:B:17:PHE:HD1	2:B:18:GLY:H	1.37	0.73
3:C:150:LYS:HB2	3:C:201:TYR:HB2	1.71	0.73
10:J:61:GLU:OE2	14:N:58:LYS:NZ	2.20	0.73
1:A:1063:C:H2'	1:A:1064:G:C8	2.24	0.73
14:N:8:GLU:HA	14:N:11:LYS:HD3	1.70	0.73
1:A:95:U:H2'	1:A:96:G:C8	2.24	0.72
1:A:986:A:H1'	19:S:55:LYS:HA	1.71	0.72
11:K:48:ILE:HD12	11:K:63:LEU:HB2	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:83:ASP:OD1	17:Q:84:LEU:N	2.22	0.72
1:A:235:C:N4	24:A:1986:HOH:O	2.22	0.72
4:D:63:LYS:NZ	4:D:197:PRO:O	2.20	0.72
1:A:1305:G:N2	1:A:1331:G:H1'	2.05	0.72
18:R:51:LEU:HD22	18:R:55:ARG:HH12	1.55	0.72
18:R:88:LYS:OXT	18:R:88:LYS:NZ	2.20	0.72
3:C:150:LYS:HA	3:C:169:ALA:HB2	1.69	0.72
1:A:436:C:H2'	1:A:437:U:H6	1.53	0.71
1:A:1291:G:OP1	7:G:37:ASN:ND2	2.23	0.71
1:A:1435:G:H2'	1:A:1436:U:H6	1.55	0.71
2:B:47:THR:OG1	2:B:202:PRO:O	2.06	0.71
18:R:55:ARG:HB3	18:R:55:ARG:NH1	2.05	0.71
1:A:1195:C:H3'	1:A:1196:U:C5'	2.20	0.71
2:B:97:TRP:HZ2	2:B:102:LEU:HD13	1.54	0.71
20:T:100:ILE:HG22	20:T:102:GLY:H	1.55	0.71
1:A:1316:G:N1	1:A:1319:A:OP2	2.23	0.71
1:A:149:A:H2'	1:A:150:C:H6	1.54	0.71
1:A:1175:G:H2'	1:A:1176:A:C8	2.26	0.71
1:A:677:U:H3	1:A:713:G:H22	1.37	0.71
3:C:88:ARG:HG3	3:C:91:LEU:HD22	1.72	0.71
1:A:144:G:H1	1:A:178:C:H42	1.35	0.70
9:I:91:ASP:N	9:I:91:ASP:OD1	2.22	0.70
12:L:113:ARG:HH11	12:L:116:SER:H	1.37	0.70
1:A:1435:G:H2'	1:A:1436:U:C6	2.26	0.70
1:A:1190:G:H5'	3:C:4:LYS:H	1.57	0.70
2:B:16:HIS:HB3	2:B:210:SER:HB3	1.73	0.70
1:A:1497:G:C2'	1:A:1498:UR3:H5'	2.22	0.70
1:A:144:G:N2	1:A:178:C:N3	2.39	0.70
1:A:1298:C:H4'	1:A:1299:A:H5"	1.72	0.70
13:M:11:ARG:HG3	13:M:12:ASN:HB2	1.74	0.70
13:M:49:THR:HG22	13:M:51:ALA:H	1.56	0.70
1:A:839:U:H5'	1:A:840:C:C5	2.26	0.70
11:K:72:ALA:HB1	11:K:77:MET:HG3	1.73	0.70
1:A:854:G:H3'	1:A:871:U:O4	1.92	0.70
1:A:1030(A):G:N2	1:A:1030(D):A:OP2	2.24	0.70
3:C:17:ASP:O	3:C:54:ARG:NH2	2.20	0.70
3:C:147:LYS:HD3	3:C:205:GLY:H	1.56	0.70
8:H:6:ILE:HB	8:H:85:ARG:NH1	2.07	0.70
9:I:48:GLU:OE1	9:I:51:ARG:NH2	2.25	0.70
19:S:18:LYS:HD2	19:S:31:ILE:HG13	1.73	0.70
6:F:50:TYR:CE1	18:R:77:GLY:HA2	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:39:LEU:HD13	15:O:56:LEU:HG	1.73	0.69
12:L:27:LEU:C	12:L:29:GLY:H	1.93	0.69
16:P:67:THR:HG22	16:P:69:THR:H	1.57	0.69
5:E:17:ALA:HA	5:E:26:PHE:HB3	1.74	0.69
5:E:80:ILE:HG22	8:H:104:ARG:HH21	1.56	0.69
16:P:22:THR:HA	16:P:33:ILE:HG12	1.75	0.69
1:A:501:C:H2'	1:A:502:G:C8	2.26	0.69
1:A:1391:U:H2'	1:A:1392:G:C8	2.27	0.69
1:A:343:U:O2'	1:A:346:G:O6	2.06	0.69
7:G:65:ALA:HB1	7:G:127:ALA:HB3	1.73	0.69
1:A:279:A:H5"	1:A:281:G:O4'	1.92	0.69
1:A:419:C:H42	1:A:424:G:H1	1.41	0.69
1:A:1055:A:N7	1:A:1200:C:N4	2.41	0.69
1:A:344:A:H5'	1:A:345:C:C5	2.28	0.69
20:T:45:GLN:HA	20:T:91:LEU:HD12	1.74	0.69
1:A:258:G:H2'	1:A:259:G:H8	1.57	0.69
1:A:324:G:OP1	20:T:22:ARG:NH1	2.26	0.69
2:B:21:ARG:HA	2:B:39:ILE:HG23	1.75	0.68
1:A:1367:C:H5'	10:J:60:ARG:HH11	1.57	0.68
11:K:90:GLY:HA2	11:K:93:GLN:HB2	1.74	0.68
17:Q:81:ARG:HB3	17:Q:84:LEU:HD12	1.75	0.68
18:R:58:LEU:HD22	18:R:62:GLU:HB3	1.73	0.68
1:A:966:M2G:H3'	1:A:967:5MC:HM51	1.76	0.68
8:H:2:LEU:HD23	8:H:3:THR:H	1.57	0.68
20:T:39:LYS:HG2	20:T:55:ILE:HD13	1.73	0.68
1:A:79:G:C2	1:A:80:G:N7	2.61	0.68
1:A:986:A:N3	19:S:52:TYR:OH	2.24	0.68
1:A:986:A:O2'	19:S:55:LYS:O	2.12	0.68
1:A:1012:U:H2'	1:A:1013:G:C8	2.28	0.68
1:A:1244:C:H42	1:A:1293:G:H1	1.40	0.68
16:P:21:VAL:HG12	16:P:33:ILE:HG13	1.75	0.68
1:A:1125:U:OP2	1:A:1145:C:N4	2.27	0.68
1:A:1100:C:OP2	2:B:96:ARG:NH1	2.27	0.68
1:A:1290:G:H2'	1:A:1291:G:C8	2.28	0.68
2:B:102:LEU:HD23	2:B:182:ILE:HD12	1.75	0.68
1:A:646:U:H2'	1:A:647:C:C6	2.28	0.68
1:A:1220:G:N2	19:S:54:GLY:O	2.23	0.68
5:E:15:ARG:HG3	5:E:28:PHE:CE2	2.29	0.68
10:J:79:ARG:O	10:J:82:ILE:N	2.27	0.68
14:N:29:ARG:NH1	14:N:40:CYS:SG	2.67	0.68
1:A:1123:A:H4'	10:J:37:PRO:HD2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:206:PHE:HD2	4:D:207:TYR:CD2	2.12	0.67
13:M:10:PRO:HB2	13:M:18:ALA:HB1	1.75	0.67
13:M:76:ALA:HA	13:M:79:LYS:HG3	1.75	0.67
1:A:1226:C:OP2	13:M:91:ARG:NH2	2.27	0.67
7:G:115:ARG:HB3	7:G:118:VAL:HG23	1.75	0.67
4:D:25:ARG:HA	4:D:28:SER:HB2	1.76	0.67
5:E:80:ILE:HG22	8:H:104:ARG:NH2	2.08	0.67
1:A:1047:G:H5"	14:N:4:LYS:HD2	1.76	0.67
1:A:1261:A:H1'	1:A:1283:G:H5"	1.77	0.67
5:E:65:ASN:ND2	5:E:65:ASN:O	2.28	0.67
15:O:15:PHE:CD2	15:O:30:ALA:HB2	2.30	0.67
1:A:1228:C:H5'	13:M:115:LYS:O	1.95	0.67
1:A:1309:G:OP2	13:M:99:ARG:NH1	2.27	0.67
4:D:173:TRP:HB2	4:D:187:ARG:O	1.94	0.66
5:E:18:ARG:HG2	5:E:19:MET:N	2.09	0.66
1:A:517:G:N1	1:A:533:A:OP2	2.18	0.66
1:A:793:U:H4'	1:A:794:A:OP2	1.94	0.66
1:A:1249:C:O2'	9:I:73:GLN:NE2	2.29	0.66
1:A:1257:U:H4'	1:A:1258:G:O5'	1.95	0.66
14:N:24:CYS:HB3	14:N:29:ARG:HB3	1.76	0.66
3:C:24:ALA:HB3	3:C:29:TYR:CD1	2.29	0.66
11:K:40:ILE:HG22	11:K:41:THR:HG22	1.77	0.66
1:A:101:A:H2'	1:A:102:G:H8	1.60	0.66
1:A:627:G:H2'	1:A:628:G:H8	1.61	0.66
1:A:1426:C:H2'	1:A:1427:U:C6	2.31	0.66
1:A:1515[B]:C:H42	1:A:1520[B]:G:H1	1.41	0.66
6:F:47:ARG:HA	6:F:57:GLN:HG2	1.78	0.66
8:H:28:ALA:HB2	8:H:59:LEU:HG	1.78	0.66
1:A:1316:G:H4'	14:N:18:VAL:HG11	1.77	0.66
11:K:80:VAL:HG21	11:K:103:LEU:HD13	1.77	0.66
12:L:33:ARG:O	12:L:85:ILE:HG22	1.96	0.66
17:Q:62:SER:HB3	17:Q:72:ARG:HD3	1.78	0.66
1:A:1517[A]:G:H2'	1:A:1518[A]:MA6:H8	1.76	0.66
1:A:1034:G:H2'	1:A:1035:A:C8	2.29	0.66
20:T:100:ILE:HG22	20:T:102:GLY:N	2.10	0.66
11:K:41:THR:OG1	11:K:42:TRP:N	2.27	0.65
1:A:1124:G:H5'	10:J:36:GLY:HA3	1.78	0.65
1:A:1349:A:P	9:I:118:LYS:HZ1	2.20	0.65
3:C:130:VAL:HG12	3:C:134:ILE:HD11	1.78	0.65
1:A:1347:G:C8	9:I:107:ARG:HB3	2.31	0.65
1:A:1418:A:H2'	1:A:1419:G:O4'	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1387:G:O2'	24:A:2055:HOH:O	2.15	0.65
2:B:107:THR:O	2:B:110:GLN:HB2	1.95	0.65
8:H:95:VAL:HG12	8:H:99:GLU:HB2	1.77	0.65
9:I:112:LYS:HA	9:I:119:ALA:HB2	1.77	0.65
1:A:964:A:O2'	10:J:55:LYS:NZ	2.24	0.65
1:A:966:M2G:HM13	1:A:967:5MC:H1'	1.78	0.65
1:A:1020:U:H2'	1:A:1021:G:C8	2.32	0.65
1:A:1179:A:H2'	1:A:1180:A:O4'	1.96	0.65
1:A:831:U:H2'	1:A:832:C:H6	1.61	0.65
1:A:1060:C:OP1	14:N:45:ARG:NH2	2.30	0.65
9:I:43:ALA:HA	9:I:74:ILE:HD12	1.78	0.65
17:Q:59:ILE:HG23	17:Q:71:PHE:HD1	1.61	0.65
3:C:52:LEU:HD11	3:C:68:VAL:HG22	1.79	0.65
1:A:1181:G:O2'	1:A:1182:G:O5'	2.14	0.65
3:C:154:SER:OG	3:C:155:GLY:N	2.28	0.65
2:B:189:ASP:O	2:B:192:SER:OG	2.15	0.65
4:D:149:ALA:O	4:D:152:SER:N	2.31	0.64
13:M:117:VAL:HG12	13:M:118:ALA:H	1.62	0.64
1:A:1014:A:H5'	19:S:14:HIS:CD2	2.32	0.64
5:E:122:GLU:OE1	5:E:131:ILE:HG13	1.96	0.64
2:B:17:PHE:HD1	2:B:18:GLY:N	1.95	0.64
5:E:116:THR:OG1	5:E:117:ASP:OD2	2.15	0.64
1:A:793:U:H5"	24:A:2162:HOH:O	1.98	0.64
1:A:1128:C:O2'	1:A:1130:A:N7	2.30	0.64
2:B:18:GLY:O	2:B:204:ASN:ND2	2.31	0.64
2:B:44:LEU:HA	2:B:47:THR:HB	1.79	0.64
1:A:833:U:H2'	1:A:834:C:C6	2.32	0.64
1:A:967:5MC:H5"	1:A:968:A:H2'	1.78	0.64
1:A:75:G:C2	1:A:96:G:C2	2.86	0.64
1:A:668:G:H1	1:A:738:C:H42	1.45	0.64
1:A:1070:U:H2'	1:A:1071:C:H6	1.61	0.64
1:A:1402:4OC:HM42	1:A:1500:A:H61	1.61	0.64
8:H:4:ASP:OD1	8:H:85:ARG:NH1	2.31	0.64
1:A:1443:G:H4'	1:A:1446:A:H5'	1.80	0.64
20:T:10:LEU:HD13	20:T:12:ALA:H	1.62	0.64
21:U:10:ARG:HG3	21:U:13:ILE:HD11	1.79	0.64
1:A:1425:U:H2'	1:A:1426:C:H6	1.63	0.64
1:A:1020:U:H2'	1:A:1021:G:H8	1.63	0.63
2:B:118:LEU:HB2	2:B:142:LEU:HD23	1.80	0.63
1:A:427:U:OP1	4:D:13:ARG:NH2	2.31	0.63
1:A:89:C:H2'	1:A:90:U:C6	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:97:LYS:HA	9:I:102:LEU:HD11	1.79	0.63
1:A:1402:4OC:H2'	1:A:1403:C:O4'	1.98	0.63
7:G:108:ALA:O	7:G:119:ARG:HB3	1.98	0.63
10:J:51:ARG:CZ	10:J:61:GLU:HB3	2.28	0.63
16:P:20:VAL:HG11	16:P:32:TYR:CD1	2.34	0.63
21:U:17:THR:O	21:U:22:ARG:NH1	2.32	0.63
1:A:89:C:H2'	1:A:90:U:H6	1.64	0.63
2:B:18:GLY:HA3	2:B:41:ILE:HA	1.80	0.63
1:A:1103:C:H5'	2:B:98:LEU:HD13	1.79	0.63
3:C:131:ARG:HH22	3:C:157:ILE:HG21	1.63	0.63
7:G:84:ASN:N	7:G:84:ASN:OD1	2.31	0.63
1:A:991:U:O4	1:A:1215:G:N1	2.31	0.63
13:M:97:PRO:HG3	13:M:110:ARG:HB3	1.81	0.63
1:A:560:U:H5'	1:A:566:G:C2	2.34	0.62
1:A:1152:A:H5"	10:J:13:HIS:CD2	2.34	0.62
1:A:1202:G:H1'	14:N:42:ILE:HD12	1.81	0.62
13:M:97:PRO:HA	13:M:110:ARG:HD3	1.81	0.62
1:A:258:G:H2'	1:A:259:G:C8	2.33	0.62
2:B:21:ARG:NH1	2:B:22:LYS:HB3	2.13	0.62
2:B:114:ARG:HH11	2:B:118:LEU:HD21	1.64	0.62
7:G:87:VAL:HG12	7:G:88:PRO:HD2	1.82	0.62
8:H:2:LEU:HD23	8:H:3:THR:N	2.14	0.62
1:A:350:G:H5"	1:A:350:G:H8	1.64	0.62
1:A:436:C:H2'	1:A:437:U:C6	2.34	0.62
1:A:955:U:H1'	1:A:1227:A:H61	1.65	0.62
1:A:989:C:H42	1:A:1216:G:H1	1.47	0.62
1:A:1003:G:H1	1:A:1038:C:H42	1.46	0.62
1:A:1141:C:H2'	1:A:1142:G:C8	2.34	0.62
1:A:1425:U:H3	1:A:1475:G:H1	1.44	0.62
12:L:25:PRO:HA	12:L:27:LEU:H	1.64	0.62
1:A:1532:U:H2'	1:A:1533:C:H5"	1.81	0.62
1:A:966:M2G:H2'	1:A:967:5MC:H6	1.63	0.62
1:A:1327:C:OP2	21:U:12:LYS:NZ	2.32	0.62
2:B:16:HIS:CB	2:B:210:SER:HB3	2.30	0.62
2:B:23:ARG:NH1	2:B:23:ARG:HA	2.14	0.62
4:D:111:ALA:HB2	4:D:120:LEU:HD12	1.82	0.62
1:A:875:C:O2'	8:H:14:ARG:NH1	2.33	0.62
4:D:187:ARG:HE	4:D:188:LEU:H	1.45	0.62
9:I:64:THR:OG1	9:I:66:ARG:NH1	2.32	0.62
13:M:4:ILE:HG23	13:M:57:ARG:HA	1.80	0.62
13:M:55:ARG:O	13:M:58:GLU:HB2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:21:VAL:HG21	16:P:59:TRP:CD1	2.35	0.62
17:Q:90:ILE:HD13	17:Q:93:GLN:HB3	1.82	0.62
1:A:538:G:H5"	12:L:114:LYS:HB2	1.82	0.62
9:I:5:TYR:HD1	9:I:6:GLY:N	1.97	0.62
1:A:1139:G:O2'	1:A:1140:C:OP2	2.15	0.62
1:A:828:A:H5"	1:A:859:A:C2	2.35	0.62
1:A:992:U:H3	1:A:1044:A:N6	1.90	0.62
2:B:21:ARG:HB2	2:B:38:GLY:O	2.00	0.62
2:B:166:ASP:HB2	2:B:205:ASP:OD2	2.00	0.62
13:M:5:ALA:HB3	13:M:8:GLU:HG3	1.80	0.62
4:D:25:ARG:NH1	4:D:30:LYS:HB2	2.15	0.62
1:A:31:G:N2	1:A:48:C:OP1	2.32	0.61
1:A:1234:C:H1'	1:A:1364:U:O2	2.00	0.61
1:A:1422:G:H2'	1:A:1423:G:C8	2.34	0.61
1:A:1498:UR3:O4'	1:A:1519[A]:MA6:H2	2.00	0.61
4:D:150:GLU:HA	4:D:153:ARG:HB2	1.82	0.61
10:J:38:ILE:HD11	10:J:71:LEU:HB2	1.80	0.61
13:M:34:LEU:HD21	13:M:41:PRO:HA	1.81	0.61
19:S:77:THR:HG22	19:S:78:ARG:HG2	1.82	0.61
1:A:401:C:O2'	1:A:621:A:N3	2.29	0.61
1:A:1510:U:H2'	1:A:1511:G:C8	2.34	0.61
3:C:21:ARG:HH22	3:C:56:ASP:HB3	1.65	0.61
1:A:9:G:OP2	5:E:121:LYS:NZ	2.31	0.61
10:J:50:ILE:H	14:N:41:ARG:HD2	1.65	0.61
4:D:13:ARG:NH1	4:D:36:ARG:HE	1.97	0.61
5:E:82:VAL:HG21	5:E:138:ALA:HA	1.82	0.61
1:A:143:A:O3'	1:A:144:G:H8	1.83	0.61
1:A:835:U:OP1	18:R:64:ARG:NH2	2.33	0.61
1:A:872:A:O2'	1:A:873:A:H5"	2.00	0.61
4:D:70:ILE:HD11	4:D:100:ARG:NE	2.15	0.61
1:A:673:G:H2'	1:A:674:G:C8	2.35	0.61
1:A:1404:5MC:H1'	1:A:1499:A:C2	2.36	0.61
12:L:25:PRO:C	12:L:27:LEU:N	2.54	0.61
14:N:27:CYS:SG	14:N:29:ARG:HB2	2.41	0.61
17:Q:43:LEU:HG	17:Q:68:ARG:HH12	1.66	0.61
20:T:46:GLU:HG2	20:T:48:LYS:HE3	1.83	0.61
1:A:1356:G:H2'	1:A:1357:A:C8	2.36	0.61
20:T:46:GLU:HB3	20:T:48:LYS:HG3	1.83	0.61
1:A:256:U:H2'	1:A:257:G:C8	2.36	0.61
4:D:142:PRO:HA	4:D:185:PHE:HD2	1.66	0.61
16:P:23:ASP:OD1	16:P:24:ALA:N	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:150:GLU:N	4:D:150:GLU:OE2	2.31	0.61
7:G:70:LYS:O	7:G:72:ARG:NH1	2.34	0.61
11:K:16:SER:HB2	11:K:106:LYS:HZ3	1.66	0.61
4:D:24:GLU:HG3	4:D:112:VAL:HG11	1.83	0.60
7:G:149:ARG:NH1	7:G:149:ARG:O	2.34	0.60
1:A:633:G:H2'	1:A:634:C:C6	2.36	0.60
2:B:127:ILE:O	2:B:135:GLN:NE2	2.33	0.60
3:C:91:LEU:HD23	3:C:92:ALA:N	2.15	0.60
12:L:24:VAL:HG13	12:L:98:TYR:CE2	2.33	0.60
18:R:53:ARG:HG2	18:R:63:GLN:OE1	2.00	0.60
20:T:89:ARG:HH21	20:T:104:LEU:HB3	1.67	0.60
1:A:377:G:N2	1:A:386:C:O2	2.32	0.60
1:A:1441:G:H4'	1:A:1442:G:C5	2.37	0.60
7:G:144:MET:O	7:G:147:ALA:HB3	2.01	0.60
10:J:89:ASP:HB3	10:J:91:PRO:HD3	1.83	0.60
17:Q:59:ILE:HG23	17:Q:71:PHE:CD1	2.37	0.60
2:B:91:PRO:HG3	2:B:155:LEU:HD21	1.84	0.60
13:M:16:ASP:N	13:M:16:ASP:OD1	2.33	0.60
1:A:444:C:H2'	1:A:445:G:C8	2.36	0.60
11:K:121:PRO:HG2	11:K:126:ARG:HG2	1.82	0.60
1:A:103:C:O2'	1:A:172:A:N1	2.25	0.60
1:A:1371:G:H2'	1:A:1372:U:H6	1.66	0.60
1:A:1413:A:H2'	1:A:1414:U:C6	2.31	0.60
12:L:24:VAL:HG12	12:L:26:ALA:H	1.66	0.60
16:P:17:TYR:HB2	16:P:39:TYR:HB3	1.82	0.60
1:A:45:U:H2'	1:A:46:G:C8	2.37	0.60
1:A:190(J):U:H2'	1:A:190(K):G:C8	2.37	0.60
1:A:793:U:H3'	1:A:794:A:H5"	1.84	0.60
1:A:1229:A:OP1	13:M:116:THR:OG1	2.14	0.60
1:A:1367:C:H5'	10:J:60:ARG:NH1	2.17	0.60
2:B:219:VAL:O	2:B:223:ILE:HG13	2.02	0.60
3:C:22:TRP:CH2	3:C:33:LEU:HD13	2.37	0.60
3:C:86:VAL:HG12	3:C:87:LEU:HG	1.82	0.60
10:J:7:LYS:HB3	10:J:97:GLU:HB2	1.82	0.60
13:M:67:GLU:O	13:M:71:ARG:HG3	2.00	0.60
1:A:1130:A:H4'	9:I:3:GLN:HE22	1.66	0.60
1:A:1211:U:H5'	1:A:1212:U:OP1	2.02	0.60
1:A:1255:G:O2'	1:A:1258:G:H1'	2.02	0.60
1:A:1366:C:H2'	1:A:1367:C:H6	1.67	0.60
10:J:55:LYS:HD2	10:J:56:HIS:H	1.67	0.60
1:A:1323:G:H2'	1:A:1324:A:C8	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:A:C6	1:A:263:A:C6	2.90	0.59
1:A:626:U:H2'	1:A:627:G:H8	1.68	0.59
1:A:665:A:N3	1:A:732:C:H2'	2.17	0.59
2:B:97:TRP:HH2	2:B:176:GLU:CD	2.06	0.59
3:C:24:ALA:HB3	3:C:29:TYR:HD1	1.67	0.59
4:D:155:LEU:HD13	4:D:156:GLU:N	2.17	0.59
12:L:124:LYS:HD2	12:L:125:PRO:HD2	1.84	0.59
1:A:56:U:H2'	1:A:57:G:C8	2.37	0.59
1:A:202:U:H3'	1:A:203:U:C5'	2.32	0.59
1:A:1260:C:OP1	1:A:1284:C:O2'	2.20	0.59
1:A:1425:U:H2'	1:A:1426:C:C6	2.38	0.59
4:D:3:ARG:HH11	4:D:71:SER:N	1.94	0.59
1:A:204:U:H5'	1:A:216:G:N9	2.17	0.59
1:A:580:U:H2'	1:A:581:G:O4'	2.02	0.59
1:A:1511:G:H2'	1:A:1512:U:O4'	2.03	0.59
2:B:131:PRO:O	2:B:134:GLU:HB3	2.02	0.59
2:B:178:ARG:O	8:H:71:GLY:HA2	2.02	0.59
2:B:98:LEU:HB2	2:B:101:MET:HG3	1.83	0.59
4:D:187:ARG:HH21	4:D:188:LEU:HB2	1.65	0.59
5:E:98:THR:HB	5:E:117:ASP:HB3	1.82	0.59
12:L:19:ARG:HA	12:L:20:LYS:NZ	2.17	0.59
13:M:51:ALA:HA	13:M:54:VAL:HG12	1.83	0.59
15:O:70:LEU:HD13	15:O:78:TYR:CA	2.32	0.59
16:P:15:PRO:HD2	16:P:42:ARG:HD3	1.83	0.59
1:A:792:A:H5"	1:A:793:U:C5	2.38	0.59
1:A:1424:C:H2'	1:A:1425:U:H6	1.67	0.59
4:D:187:ARG:HE	4:D:188:LEU:N	2.00	0.59
7:G:40:ALA:HB3	9:I:41:VAL:HG21	1.85	0.59
12:L:27:LEU:HD23	12:L:28:LYS:HG2	1.84	0.59
1:A:297:G:N2	1:A:300:A:OP2	2.34	0.59
1:A:358:U:H2'	1:A:359:U:H6	1.68	0.59
1:A:790:A:H2'	1:A:791:G:C8	2.37	0.59
1:A:1058:G:H2'	1:A:1059:C:O4'	2.02	0.59
1:A:1111:A:H61	3:C:177:THR:HA	1.68	0.59
4:D:107:ARG:HH21	4:D:194:LEU:HD11	1.66	0.59
1:A:794:A:C5	1:A:795:C:C4	2.90	0.59
1:A:1064:G:H1'	1:A:1190:G:H21	1.67	0.59
4:D:108:LEU:HD11	4:D:183:GLY:HA3	1.84	0.59
21:U:5:ASP:O	21:U:11:GLY:HA3	2.02	0.59
5:E:86:ALA:HB3	5:E:125:SER:HB3	1.84	0.59
6:F:62:TRP:CH2	6:F:64:GLN:HB2	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:121:ALA:O	7:G:124:LEU:HD12	2.03	0.59
1:A:56:U:H2'	1:A:57:G:H8	1.68	0.59
1:A:836:G:OP1	18:R:61:LYS:NZ	2.27	0.59
1:A:881:G:P	12:L:12:ARG:HH22	2.26	0.59
1:A:1222:G:OP1	19:S:77:THR:HG21	2.02	0.59
1:A:1339:A:H5"	1:A:1340:A:OP2	2.03	0.59
9:I:64:THR:HG1	9:I:66:ARG:HH12	1.51	0.59
1:A:953:G:H5'	1:A:965:A:H61	1.68	0.59
1:A:1055:A:O2'	3:C:156:ARG:NH2	2.36	0.59
2:B:7:VAL:N	2:B:8:LYS:HZ3	2.01	0.59
7:G:17:VAL:HG12	7:G:18:TYR:CD1	2.38	0.59
12:L:25:PRO:CA	12:L:27:LEU:H	2.15	0.59
16:P:53:VAL:O	16:P:56:ALA:N	2.35	0.59
1:A:539:A:H2'	1:A:540:G:C8	2.38	0.58
1:A:865:A:H2'	1:A:866:C:C6	2.38	0.58
1:A:1003:G:H2'	1:A:1003(A):G:H5"	1.84	0.58
1:A:1064:G:N2	1:A:1190:G:H2'	2.17	0.58
3:C:130:VAL:HG23	3:C:131:ARG:NH1	2.17	0.58
5:E:101:ILE:O	5:E:120:THR:HB	2.02	0.58
17:Q:40:LYS:HE2	17:Q:42:TYR:CZ	2.37	0.58
1:A:401:C:H2'	1:A:402:G:C8	2.38	0.58
1:A:551:U:H2'	1:A:552:U:C6	2.38	0.58
1:A:939:G:H5"	7:G:102:ARG:NH1	2.19	0.58
1:A:382:A:H2'	1:A:383:A:C8	2.38	0.58
1:A:411:A:N9	1:A:413:G:H1'	2.18	0.58
1:A:627:G:H2'	1:A:628:G:C8	2.37	0.58
1:A:895:G:H2'	1:A:896:C:C6	2.38	0.58
1:A:1440:C:H2'	1:A:1441:G:O4'	2.03	0.58
8:H:10:LEU:HD13	8:H:83:ILE:HD13	1.86	0.58
8:H:14:ARG:HE	8:H:83:ILE:HG22	1.69	0.58
7:G:86:GLN:HB2	7:G:148:ASN:ND2	2.19	0.58
8:H:82:HIS:NE2	8:H:84:ARG:HD3	2.18	0.58
11:K:117:ASN:OD1	11:K:117:ASN:N	2.36	0.58
12:L:41:ARG:HG2	12:L:42:THR:H	1.68	0.58
13:M:16:ASP:HB3	13:M:34:LEU:HD23	1.85	0.58
1:A:1287:A:H2'	1:A:1288:A:C8	2.38	0.58
1:A:1366:C:H2'	1:A:1367:C:C6	2.39	0.58
9:I:48:GLU:N	9:I:49:PRO:HD2	2.17	0.58
21:U:13:ILE:O	21:U:16:GLY:N	2.25	0.58
1:A:380:G:N2	1:A:382:A:H3'	2.18	0.58
1:A:403:C:OP2	4:D:74:GLN:NE2	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1152:A:OP1	10:J:68:HIS:ND1	2.35	0.58
1:A:1475:G:H2'	1:A:1476:G:C8	2.39	0.58
9:I:88:TYR:HD2	9:I:89:ASN:HB2	1.69	0.58
11:K:84:VAL:HG11	11:K:91:ARG:HD3	1.85	0.58
1:A:149:A:H2'	1:A:150:C:C6	2.38	0.58
1:A:390:C:H2'	1:A:391:G:C8	2.39	0.58
1:A:973:G:H3'	1:A:974:A:H5"	1.86	0.58
4:D:187:ARG:NH2	4:D:188:LEU:HB2	2.18	0.58
8:H:83:ILE:HG12	8:H:137:VAL:HG22	1.86	0.58
1:A:359:U:H2'	1:A:360:A:C8	2.39	0.58
7:G:69:VAL:HG11	7:G:104:LEU:HD21	1.86	0.58
1:A:79:G:C2	1:A:80:G:C8	2.92	0.58
1:A:202:U:H3'	1:A:203:U:H5'	1.83	0.58
1:A:827:U:H5"	1:A:828:A:OP2	2.04	0.58
1:A:1373:G:H5"	7:G:36:LYS:HD2	1.85	0.58
6:F:94:GLN:HB3	18:R:32:ARG:HD3	1.84	0.58
8:H:116:LYS:HD2	8:H:129:VAL:HG11	1.85	0.58
17:Q:29:HIS:CE1	17:Q:32:TYR:H	2.22	0.58
21:U:10:ARG:HA	21:U:13:ILE:HG12	1.85	0.58
1:A:36:C:N4	24:A:2134:HOH:O	2.37	0.57
1:A:540:G:H2'	1:A:541:G:O4'	2.03	0.57
1:A:1131:G:H2'	1:A:1132:C:C6	2.39	0.57
3:C:150:LYS:CB	3:C:201:TYR:HB2	2.34	0.57
9:I:86:VAL:HG22	9:I:90:PRO:HA	1.86	0.57
18:R:87:ARG:HB2	18:R:87:ARG:HH11	1.68	0.57
1:A:1104:G:O5'	2:B:111:ARG:HD2	2.04	0.57
1:A:1243:C:OP1	21:U:10:ARG:NH1	2.37	0.57
1:A:1296:C:H4'	1:A:1302:U:C5	2.39	0.57
17:Q:97:SER:OG	17:Q:98:LEU:HD23	2.03	0.57
1:A:269:C:H2'	1:A:270:A:C8	2.38	0.57
1:A:90:U:O2'	1:A:91:C:O5'	2.19	0.57
1:A:673:G:H5"	6:F:87:ARG:NH1	2.19	0.57
1:A:1143:G:H2'	1:A:1144:G:C8	2.39	0.57
7:G:17:VAL:HB	7:G:44:TYR:OH	2.04	0.57
10:J:7:LYS:HZ3	10:J:9:ARG:HH21	1.53	0.57
3:C:134:ILE:HG23	3:C:151:VAL:HB	1.85	0.57
7:G:27:ILE:HD13	7:G:40:ALA:HA	1.86	0.57
9:I:9:ARG:HD3	9:I:14:VAL:HG22	1.87	0.57
10:J:49:VAL:HG23	10:J:62:HIS:HA	1.86	0.57
16:P:6:LEU:HD11	16:P:73:LEU:HD12	1.86	0.57
1:A:667:G:H4'	15:O:51:HIS:CE1	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1092:A:N3	1:A:1183:A:N6	2.51	0.57
1:A:1150:U:H4'	10:J:41:PRO:HG3	1.87	0.57
1:A:142:G:H2'	1:A:143:A:H8	1.70	0.57
1:A:895:G:H2'	1:A:896:C:H6	1.69	0.57
2:B:19:HIS:ND1	2:B:189:ASP:OD2	2.36	0.57
3:C:26:LYS:HG2	3:C:27:LYS:HG3	1.85	0.57
15:O:29:VAL:HG11	15:O:67:LEU:HD21	1.87	0.57
1:A:243:A:H4'	1:A:244:U:H5"	1.87	0.57
1:A:300:A:H8	1:A:300:A:O5'	1.87	0.57
1:A:401:C:H2'	1:A:402:G:H8	1.70	0.57
1:A:1181:G:C2	1:A:1182:G:N2	2.72	0.57
4:D:104:VAL:HG11	4:D:146:ILE:HG13	1.87	0.57
18:R:59:SER:H	18:R:62:GLU:HB2	1.69	0.57
1:A:1090:U:H2'	1:A:1091:U:H6	1.70	0.57
13:M:65:LYS:O	13:M:70:LEU:HG	2.05	0.57
1:A:141:A:H1'	1:A:182:U:O2	2.05	0.56
1:A:620:C:H2'	1:A:621:A:C8	2.39	0.56
1:A:298:A:N6	24:A:2052:HOH:O	2.01	0.56
1:A:960:U:H1'	1:A:1223:C:H5'	1.87	0.56
1:A:1007:C:H42	1:A:1022:G:H1	1.53	0.56
1:A:1474:G:H2'	1:A:1475:G:C8	2.40	0.56
2:B:15:VAL:HG13	2:B:209:ARG:HG3	1.86	0.56
4:D:11:LEU:HD13	4:D:66:ARG:HD3	1.87	0.56
1:A:551:U:H2'	1:A:552:U:H6	1.70	0.56
4:D:9:CYS:O	4:D:12:CYS:HB2	2.03	0.56
7:G:111:ARG:HD3	7:G:113:GLU:HG3	1.87	0.56
11:K:121:PRO:HB2	11:K:125:PHE:HB2	1.87	0.56
16:P:74:LEU:O	16:P:79:VAL:HG23	2.05	0.56
18:R:50:ILE:HD11	18:R:70:ILE:CG2	2.32	0.56
19:S:11:VAL:HA	19:S:38:SER:HB3	1.87	0.56
1:A:686:U:HO2'	1:A:687:A:H8	1.53	0.56
1:A:827:U:O2'	8:H:19:VAL:HG11	2.06	0.56
10:J:87:THR:HA	10:J:89:ASP:OD2	2.05	0.56
11:K:33:THR:HA	11:K:39:PRO:HA	1.88	0.56
1:A:344:A:H4'	1:A:345:C:OP2	2.05	0.56
4:D:175:SER:N	4:D:186:LEU:HD21	2.21	0.56
1:A:89:C:H2'	1:A:90:U:O4'	2.06	0.56
1:A:998:G:N2	1:A:1043:C:O2	2.24	0.56
1:A:1274:G:H2'	1:A:1275:A:H8	1.70	0.56
7:G:151:TYR:O	7:G:155:ARG:NH2	2.38	0.56
20:T:20:LEU:O	20:T:23:ARG:HB3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:877:C:O2	8:H:3:THR:HG21	2.05	0.56
4:D:61:LYS:HA	4:D:203:VAL:HG13	1.87	0.56
1:A:407:G:OP1	4:D:115:ARG:NH2	2.39	0.56
1:A:1200:C:O2	1:A:1205:U:N3	2.25	0.56
2:B:91:PRO:HG3	2:B:155:LEU:CD2	2.35	0.56
3:C:88:ARG:HA	3:C:91:LEU:HB3	1.88	0.56
13:M:52:GLU:HG2	13:M:55:ARG:NH2	2.21	0.56
19:S:55:LYS:NZ	19:S:56:GLN:HB2	2.21	0.56
1:A:795:C:H5"	1:A:796:C:OP2	2.06	0.56
1:A:981:U:H2'	1:A:982:U:H5	1.71	0.56
4:D:206:PHE:HD2	4:D:207:TYR:CE2	2.24	0.56
17:Q:27:PHE:CZ	17:Q:36:ILE:HD11	2.41	0.56
17:Q:63:ARG:HG2	17:Q:64:PRO:HD2	1.88	0.56
18:R:22:VAL:HG23	18:R:56:THR:HA	1.87	0.56
18:R:34:TYR:CE1	18:R:35:ARG:HG3	2.40	0.56
1:A:103:C:P	20:T:17:ARG:HH12	2.28	0.56
1:A:908:A:C2	1:A:909:A:C4	2.94	0.56
1:A:1329:A:P	13:M:28:ALA:HB3	2.46	0.56
2:B:118:LEU:HD11	2:B:141:GLU:OE1	2.05	0.56
6:F:2:ARG:HE	6:F:69:GLU:HG2	1.71	0.56
13:M:56:LEU:O	13:M:60:VAL:HG23	2.05	0.56
1:A:528:C:H41	12:L:49:ASN:ND2	2.04	0.55
1:A:659:U:OP2	15:O:8:LYS:HE2	2.06	0.55
1:A:902:G:H2'	1:A:903:G:H8	1.71	0.55
16:P:68:ASP:OD1	16:P:68:ASP:N	2.39	0.55
20:T:54:LYS:HA	20:T:57:ARG:HD3	1.88	0.55
1:A:179:A:H2'	1:A:180:U:C6	2.41	0.55
1:A:390:C:H2'	1:A:391:G:H8	1.71	0.55
1:A:419:C:N4	1:A:424:G:H1	2.04	0.55
1:A:1199:U:H5"	1:A:1200:C:OP2	2.06	0.55
6:F:27:GLN:O	6:F:31:GLU:HG3	2.06	0.55
7:G:92:SER:HB3	7:G:95:ARG:H	1.70	0.55
8:H:86:ILE:HG22	8:H:87:SER:N	2.21	0.55
12:L:83:VAL:HG21	12:L:100:ILE:HG13	1.87	0.55
16:P:71:ARG:HG3	16:P:80:PHE:HE1	1.71	0.55
21:U:9:ARG:HG3	21:U:22:ARG:HG2	1.88	0.55
1:A:626:U:H2'	1:A:627:G:C8	2.42	0.55
1:A:1497:G:O2'	1:A:1518[A]:MA6:H92	2.06	0.55
7:G:26:PHE:CD1	7:G:101:LEU:HD22	2.42	0.55
7:G:80:VAL:HG11	7:G:154:TYR:HE1	1.71	0.55
13:M:91:ARG:HB3	13:M:98:VAL:HG12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:8:GLU:HA	14:N:11:LYS:HB2	1.89	0.55
1:A:939:G:H1	1:A:1344:C:H42	1.55	0.55
1:A:978:A:H8	1:A:978:A:OP1	1.89	0.55
3:C:41:GLY:O	3:C:45:LYS:HB2	2.06	0.55
11:K:98:LEU:HA	11:K:101:SER:HB3	1.87	0.55
12:L:47:LYS:H	12:L:47:LYS:HD2	1.71	0.55
21:U:14:TRP:CZ3	21:U:15:ARG:HG3	2.42	0.55
1:A:235:C:H5'	17:Q:70:ARG:HG2	1.88	0.55
4:D:31:CYS:C	4:D:33:MET:H	2.10	0.55
12:L:41:ARG:HH21	12:L:43:VAL:HG13	1.71	0.55
13:M:25:ILE:HG12	13:M:66:LEU:HD13	1.88	0.55
15:O:55:GLY:HA2	15:O:58:MET:HE2	1.88	0.55
20:T:89:ARG:HE	20:T:104:LEU:HD13	1.71	0.55
1:A:21:G:H2'	1:A:22:G:C8	2.41	0.55
1:A:445:G:H1	1:A:489:C:H42	1.54	0.55
1:A:647:C:H2'	1:A:648:A:H8	1.71	0.55
1:A:666:G:H5'	1:A:726:C:H1'	1.89	0.55
3:C:58:GLU:H	3:C:65:ALA:HB3	1.72	0.55
3:C:179:ARG:HD2	3:C:206:GLU:HG2	1.89	0.55
8:H:87:SER:CA	8:H:93:VAL:HG13	2.36	0.55
10:J:10:GLY:HA3	10:J:16:LEU:HD21	1.89	0.55
11:K:32:ILE:O	11:K:40:ILE:N	2.36	0.55
1:A:1228:C:H4'	13:M:116:THR:HA	1.88	0.55
1:A:1415:G:H3'	1:A:1416:G:H8	1.71	0.55
3:C:131:ARG:HA	3:C:134:ILE:HD12	1.89	0.55
4:D:57:ARG:HG3	4:D:202:LEU:HD12	1.89	0.55
1:A:77:G:C6	1:A:93:G:N1	2.75	0.55
1:A:337:C:H2'	1:A:338:A:H8	1.71	0.55
1:A:481:G:O2'	1:A:482:A:H8	1.90	0.55
4:D:107:ARG:HH21	4:D:194:LEU:CD1	2.20	0.55
16:P:6:LEU:HD23	16:P:17:TYR:CD1	2.42	0.55
1:A:765:G:C6	1:A:812:C:C2	2.95	0.55
12:L:27:LEU:HG	12:L:28:LYS:H	1.72	0.55
20:T:50:GLU:HB3	20:T:99:LEU:HB2	1.89	0.55
1:A:40:C:H2'	1:A:41:G:C8	2.42	0.55
1:A:106:C:O2	1:A:379:C:H4'	2.07	0.55
1:A:792:A:H1'	1:A:793:U:OP2	2.07	0.55
1:A:1241:G:H2'	1:A:1242:C:H6	1.72	0.55
1:A:1351:U:H4'	7:G:33:ASP:OD2	2.07	0.55
1:A:1487:G:H2'	1:A:1488:G:O4'	2.07	0.55
10:J:51:ARG:HG3	10:J:59:SER:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1442:G:N7	1:A:1446:A:N6	2.55	0.54
2:B:88:ALA:HB2	2:B:219:VAL:HG13	1.89	0.54
7:G:61:VAL:HG22	7:G:128:ALA:HB1	1.90	0.54
1:A:1259:C:H42	1:A:1276:G:H1	1.53	0.54
1:A:1484:C:H2'	1:A:1485:U:O4'	2.06	0.54
2:B:21:ARG:NH1	2:B:22:LYS:O	2.40	0.54
3:C:130:VAL:HG11	3:C:153:VAL:HG21	1.88	0.54
4:D:101:LEU:O	4:D:105:VAL:HG23	2.07	0.54
1:A:7:G:H5'	1:A:298:A:H5'	1.89	0.54
1:A:17:U:H2'	1:A:18:C:C6	2.42	0.54
1:A:373:A:H2'	1:A:374:A:H8	1.73	0.54
1:A:1006:C:H2'	1:A:1007:C:C6	2.43	0.54
1:A:1539:C:H2'	1:A:1540:PSU:O4'	2.07	0.54
14:N:23:ARG:HD3	14:N:29:ARG:O	2.07	0.54
16:P:20:VAL:HG12	16:P:35:LYS:HA	1.88	0.54
1:A:129(A):G:H1'	1:A:190(E):U:H2'	1.90	0.54
1:A:1238:A:OP1	1:A:1336:C:N4	2.39	0.54
3:C:149:ALA:O	3:C:169:ALA:HB1	2.07	0.54
1:A:509:A:C8	1:A:509:A:H3'	2.42	0.54
1:A:859:A:H2'	1:A:860:A:O4'	2.08	0.54
1:A:1191:A:OP1	3:C:4:LYS:NZ	2.29	0.54
1:A:1414:U:H2'	1:A:1415:G:C8	2.42	0.54
7:G:26:PHE:HA	7:G:101:LEU:HD13	1.88	0.54
12:L:59:ARG:CZ	12:L:65:GLU:HG2	2.38	0.54
1:A:579:G:O3'	15:O:54:ARG:NH2	2.41	0.54
1:A:1147:C:H2'	1:A:1148:U:C6	2.43	0.54
8:H:6:ILE:HB	8:H:85:ARG:HH12	1.71	0.54
12:L:34:ARG:HB2	12:L:105:TYR:HE1	1.73	0.54
16:P:67:THR:HB	16:P:70:ALA:H	1.72	0.54
1:A:345:C:OP2	1:A:345:C:H6	1.91	0.54
5:E:118:ILE:HG12	5:E:119:LEU:N	2.22	0.54
8:H:86:ILE:HG21	8:H:133:LEU:HD22	1.89	0.54
14:N:37:PHE:C	14:N:39:LEU:H	2.09	0.54
18:R:53:ARG:NH1	18:R:59:SER:HA	2.22	0.54
1:A:731:G:OP1	1:A:766:A:H1'	2.08	0.54
1:A:831:U:H2'	1:A:832:C:C6	2.42	0.54
1:A:949:A:C2	1:A:1233:G:N3	2.76	0.54
1:A:1329:A:O2'	1:A:1330:U:H5'	2.08	0.54
2:B:16:HIS:HB2	2:B:204:ASN:HB2	1.90	0.54
12:L:86:ARG:HH11	12:L:86:ARG:HG2	1.73	0.54
20:T:44:ALA:HB1	20:T:91:LEU:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:C:OP2	20:T:14:LYS:HD2	2.08	0.54
1:A:270:A:H2'	1:A:271:C:C6	2.43	0.54
1:A:376:G:C4	1:A:389:A:C2	2.96	0.54
1:A:1391:U:H2'	1:A:1392:G:H8	1.73	0.54
1:A:1414:U:H5"	1:A:1415:G:OP2	2.08	0.54
15:O:26:GLU:OE2	15:O:77:ARG:NH1	2.41	0.54
16:P:67:THR:HG22	16:P:68:ASP:N	2.23	0.54
1:A:946:A:H2'	1:A:947:G:C8	2.43	0.54
1:A:1051:C:H3'	1:A:1052:U:C6	2.43	0.54
1:A:1058:G:C2	1:A:1059:C:H1'	2.43	0.54
1:A:1059:C:H2'	1:A:1060:C:C6	2.43	0.54
1:A:1113:C:H42	1:A:1187:G:H1	1.54	0.54
1:A:1147:C:O2	9:I:16:ARG:NH2	2.40	0.54
3:C:136:GLN:O	3:C:140:ARG:HG3	2.08	0.54
1:A:1354:C:H2'	1:A:1355:G:H8	1.72	0.53
1:A:1426:C:H2'	1:A:1427:U:H6	1.72	0.53
1:A:1502:A:H2	1:A:1505:G:H1	1.56	0.53
2:B:21:ARG:HD2	2:B:22:LYS:H	1.72	0.53
4:D:57:ARG:CG	4:D:202:LEU:HD12	2.38	0.53
16:P:57:ARG:HG3	16:P:79:VAL:HG12	1.88	0.53
1:A:204:U:H5'	1:A:216:G:C8	2.43	0.53
1:A:587:G:H3'	24:A:1962:HOH:O	2.09	0.53
2:B:87:ARG:HH21	2:B:233:SER:HA	1.73	0.53
12:L:67:THR:HB	12:L:96:VAL:HG13	1.90	0.53
16:P:53:VAL:O	16:P:55:ARG:N	2.42	0.53
1:A:373:A:H1'	1:A:481:G:N3	2.23	0.53
1:A:1222:G:N2	1:A:1223:C:O2	2.41	0.53
1:A:1493:A:H2'	1:A:1494:G:H8	1.73	0.53
3:C:202:ILE:HG22	3:C:204:LEU:HD23	1.91	0.53
21:U:13:ILE:HG22	21:U:22:ARG:CZ	2.39	0.53
21:U:13:ILE:HG22	21:U:22:ARG:NH2	2.23	0.53
1:A:858:G:C6	1:A:869:G:C8	2.97	0.53
1:A:1392:G:H21	1:A:1502:A:H8	1.56	0.53
8:H:49:GLU:HG2	8:H:62:TYR:HE2	1.72	0.53
10:J:54:PHE:O	10:J:55:LYS:HG3	2.08	0.53
17:Q:60:ILE:O	17:Q:62:SER:OG	2.24	0.53
1:A:383:A:C6	1:A:384:G:H1'	2.44	0.53
1:A:1328:C:OP1	21:U:20:LYS:NZ	2.36	0.53
1:A:1346:A:OP1	9:I:120:ARG:NH1	2.41	0.53
9:I:118:LYS:O	9:I:120:ARG:N	2.34	0.53
1:A:174:C:H2'	1:A:175:C:H6	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:U:H4'	1:A:216:G:O5'	2.07	0.53
1:A:679:C:H2'	1:A:680:C:H6	1.74	0.53
1:A:828:A:H2'	1:A:829:G:O4'	2.09	0.53
1:A:853:G:C2	1:A:854:G:C8	2.97	0.53
1:A:1009:G:H21	1:A:1010:G:H1'	1.73	0.53
1:A:1053:G:O2'	1:A:1199:U:H5	1.91	0.53
1:A:1225:A:H3'	13:M:103:THR:OG1	2.09	0.53
2:B:172:ILE:H	2:B:172:ILE:HD12	1.74	0.53
1:A:236:G:H2'	1:A:237:C:O4'	2.08	0.53
2:B:23:ARG:HA	2:B:23:ARG:CZ	2.38	0.53
5:E:5:ASP:OD2	5:E:6:PHE:HB2	2.08	0.53
1:A:426:G:OP1	4:D:38:TYR:OH	2.20	0.53
1:A:1318:A:H4'	19:S:10:PHE:CE2	2.44	0.53
1:A:1474:G:H2'	1:A:1475:G:H8	1.71	0.53
4:D:78:LEU:O	4:D:81:GLU:HB3	2.08	0.53
7:G:113:GLU:O	7:G:119:ARG:HD3	2.08	0.53
7:G:146:GLU:OE2	7:G:149:ARG:HG3	2.09	0.53
8:H:112:LEU:N	8:H:112:LEU:HD23	2.23	0.53
9:I:78:LYS:HD2	9:I:101:PHE:CE2	2.44	0.53
1:A:88:A:H2'	1:A:89:C:O4'	2.08	0.53
1:A:115:G:H1'	1:A:116:A:N7	2.23	0.53
1:A:152:A:N6	1:A:170:U:C2	2.77	0.53
1:A:184:G:H2'	1:A:185:A:H8	1.74	0.53
1:A:190(C):C:H2'	1:A:190(D):U:O4'	2.09	0.53
1:A:517:G:H5'	1:A:519:C:C2	2.43	0.53
1:A:1053:G:HO2'	1:A:1199:U:H5	1.57	0.53
16:P:34:GLU:OE2	16:P:55:ARG:HD2	2.08	0.53
17:Q:62:SER:CB	17:Q:72:ARG:HD3	2.38	0.53
1:A:679:C:H2'	1:A:680:C:C6	2.43	0.53
1:A:1118:C:H1'	1:A:1179:A:C4	2.43	0.53
13:M:40:ASN:HD22	13:M:43:THR:HG23	1.73	0.53
1:A:342:C:H2'	1:A:343:U:O4'	2.09	0.52
1:A:802:A:H8	1:A:802:A:O5'	1.93	0.52
1:A:1006:C:OP1	1:A:1037:C:O2'	2.26	0.52
1:A:1070:U:H2'	1:A:1071:C:C6	2.43	0.52
1:A:1389:C:H2'	1:A:1390:U:O4'	2.09	0.52
1:A:1465:C:H2'	1:A:1466:C:O4'	2.09	0.52
6:F:11:ASN:ND2	6:F:13:ASN:OD1	2.41	0.52
7:G:73:MET:HB2	7:G:89:MET:O	2.09	0.52
9:I:90:PRO:O	9:I:93:ARG:HB2	2.07	0.52
12:L:69:TYR:HE2	12:L:71:PRO:HA	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:86:ARG:N	12:L:99:HIS:O	2.41	0.52
1:A:192:U:H2'	1:A:193:C:C6	2.44	0.52
1:A:399:G:H2'	1:A:400:C:H6	1.74	0.52
4:D:20:TYR:HA	4:D:26:CYS:SG	2.49	0.52
11:K:12:ARG:HB3	11:K:14:VAL:HG13	1.91	0.52
11:K:50:TYR:CD2	11:K:54:ARG:HB3	2.45	0.52
16:P:13:HIS:O	16:P:42:ARG:NH1	2.43	0.52
20:T:64:ASP:O	20:T:67:ALA:HB3	2.09	0.52
1:A:77:G:N2	1:A:78:G:N3	2.57	0.52
1:A:241:C:H4'	12:L:19:ARG:NH2	2.24	0.52
1:A:1049:U:H4'	1:A:1050:G:O5'	2.09	0.52
1:A:1226:C:OP2	13:M:103:THR:HG21	2.08	0.52
1:A:1417:G:O2'	1:A:1483:A:N6	2.38	0.52
1:A:1499:A:H1'	1:A:1520[A]:G:H5'	1.91	0.52
1:A:1216:G:H2'	1:A:1217:C:C6	2.44	0.52
4:D:180:GLY:C	4:D:182:LYS:H	2.12	0.52
10:J:26:ALA:HB3	10:J:85:LEU:HD11	1.92	0.52
17:Q:3:LYS:HB3	17:Q:60:ILE:HD11	1.90	0.52
1:A:643:C:C2'	1:A:644:G:H5'	2.38	0.52
1:A:851:G:H8	1:A:851:G:H5"	1.74	0.52
1:A:1026:G:O6	1:A:1036:G:N1	2.38	0.52
5:E:43:LEU:HD11	5:E:132:ALA:HB1	1.92	0.52
13:M:101:GLN:OE1	13:M:101:GLN:N	2.43	0.52
16:P:22:THR:HA	16:P:33:ILE:CG1	2.40	0.52
19:S:5:LEU:HD22	19:S:70:LYS:NZ	2.24	0.52
1:A:80:G:H2'	1:A:81:U:H5'	1.91	0.52
1:A:474:G:H5"	16:P:81:ARG:HG2	1.92	0.52
1:A:922:G:C2	1:A:1396:A:C6	2.98	0.52
1:A:1437:C:H2'	1:A:1438:G:H8	1.75	0.52
2:B:19:HIS:CE1	2:B:206:ASP:H	2.27	0.52
2:B:104:ASN:OD1	2:B:107:THR:OG1	2.27	0.52
2:B:187:LEU:HD12	2:B:205:ASP:HA	1.92	0.52
7:G:18:TYR:CD2	7:G:59:LEU:HD13	2.44	0.52
1:A:268:C:H2'	1:A:269:C:H6	1.74	0.52
1:A:299:G:C6	1:A:300:A:C6	2.98	0.52
1:A:448:A:P	1:A:485:G:H22	2.32	0.52
1:A:836:G:H5"	1:A:836:G:H8	1.74	0.52
6:F:36:ARG:NH1	6:F:38:GLU:OE1	2.43	0.52
12:L:7:ILE:O	12:L:10:LEU:N	2.42	0.52
17:Q:89:LEU:O	17:Q:93:GLN:HB2	2.09	0.52
1:A:191:G:O2'	20:T:102:GLY:O	2.13	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1150:U:O4	1:A:1151:A:N6	2.41	0.52
1:A:1514:C:H2'	1:A:1515[A]:C:O4'	2.09	0.52
3:C:18:TRP:HZ2	14:N:56:VAL:O	1.93	0.52
5:E:81:GLU:HG3	5:E:90:VAL:HG22	1.92	0.52
6:F:2:ARG:O	6:F:66:GLU:HA	2.09	0.52
14:N:53:LEU:HD23	14:N:53:LEU:H	1.75	0.52
1:A:115:G:O2'	1:A:116:A:OP2	2.26	0.52
1:A:217:C:H2'	1:A:218:C:H6	1.75	0.52
1:A:707:C:H2'	1:A:708:C:C6	2.45	0.52
1:A:1006:C:H42	1:A:1024:G:N2	2.07	0.52
3:C:36:ASP:O	3:C:40:ARG:HG2	2.09	0.52
5:E:82:VAL:HB	5:E:89:ILE:HG22	1.91	0.52
10:J:48:THR:OG1	10:J:62:HIS:ND1	2.42	0.52
1:A:349:A:H2'	1:A:350:G:H5"	1.92	0.52
1:A:692:U:OP2	11:K:26:ASN:ND2	2.42	0.52
1:A:1417:G:C2'	1:A:1483:A:H61	2.23	0.52
3:C:108:ASN:HB3	3:C:111:LEU:HB2	1.92	0.52
13:M:4:ILE:HD12	13:M:57:ARG:HB2	1.91	0.52
1:A:77:G:C2	1:A:78:G:C4	2.98	0.51
1:A:383:A:C5	1:A:384:G:H1'	2.44	0.51
1:A:1498:UR3:C4'	1:A:1519[A]:MA6:H2	2.39	0.51
1:A:1509:C:H42	1:A:1526:G:H1	1.57	0.51
5:E:80:ILE:HD11	5:E:138:ALA:HB1	1.92	0.51
11:K:29:ILE:HG12	11:K:30:VAL:N	2.24	0.51
13:M:39:ILE:HG13	13:M:55:ARG:HH21	1.75	0.51
16:P:6:LEU:HD23	16:P:17:TYR:CG	2.44	0.51
1:A:131:C:H2'	1:A:132:C:C6	2.45	0.51
1:A:229:U:O2'	1:A:230:G:H5'	2.10	0.51
1:A:869:G:N7	24:A:2102:HOH:O	2.34	0.51
3:C:129:ALA:HB1	3:C:131:ARG:HH11	1.75	0.51
17:Q:66:SER:H	17:Q:69:LYS:HB2	1.76	0.51
1:A:16:A:O2'	1:A:17:U:H5'	2.10	0.51
1:A:932:C:H4'	7:G:4:ARG:HH21	1.74	0.51
1:A:981:U:H2'	1:A:982:U:C5	2.45	0.51
1:A:1382:C:H2'	1:A:1383:C:H6	1.76	0.51
3:C:40:ARG:HB3	3:C:44:GLU:OE2	2.11	0.51
4:D:93:PHE:CE1	4:D:97:LEU:HD11	2.46	0.51
1:A:112:G:O2'	1:A:113:G:H5'	2.10	0.51
1:A:232:G:H1'	1:A:262:A:N1	2.26	0.51
1:A:358:U:H2'	1:A:359:U:C6	2.45	0.51
1:A:579:G:H2'	1:A:580:U:C6	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:933:G:N2	1:A:1384:C:O2	2.38	0.51
1:A:1030(D):A:C8	1:A:1031:G:H1'	2.45	0.51
1:A:1415:G:H3'	1:A:1416:G:C8	2.46	0.51
4:D:201:GLN:O	4:D:205:GLU:HB2	2.11	0.51
8:H:27:PRO:HB3	8:H:58:TYR:CE2	2.45	0.51
9:I:105:ASP:OD1	9:I:107:ARG:HG3	2.10	0.51
17:Q:93:GLN:NE2	17:Q:96:GLU:OE2	2.41	0.51
19:S:11:VAL:HG21	19:S:16:LEU:HD13	1.93	0.51
1:A:97:G:H2'	1:A:98:U:O4'	2.11	0.51
1:A:512:U:H2'	1:A:513:C:C6	2.46	0.51
1:A:1190:G:OP1	3:C:4:LYS:HA	2.10	0.51
1:A:1228:C:H2'	1:A:1229:A:H8	1.76	0.51
1:A:1504:G:H4'	1:A:1505:G:H5'	1.91	0.51
3:C:38:ARG:CZ	3:C:38:ARG:HB2	2.40	0.51
6:F:67:MET:HB2	6:F:68:PRO:HD2	1.93	0.51
11:K:43:SER:HB3	11:K:68:ALA:HB2	1.92	0.51
11:K:92:GLU:HB3	11:K:96:ARG:HH22	1.73	0.51
12:L:36:VAL:HG12	12:L:82:VAL:HB	1.92	0.51
1:A:966:M2G:HM22	1:A:967:5MC:C2	2.45	0.51
2:B:127:ILE:HG22	2:B:135:GLN:HG2	1.92	0.51
5:E:86:ALA:CB	5:E:125:SER:HB3	2.41	0.51
11:K:33:THR:HG22	11:K:39:PRO:HA	1.92	0.51
11:K:60:ALA:HA	11:K:63:LEU:HD12	1.92	0.51
1:A:853:G:C2'	1:A:854:G:H5'	2.41	0.51
3:C:58:GLU:HB3	10:J:92:THR:HG23	1.92	0.51
9:I:27:THR:HG22	9:I:62:TYR:HA	1.93	0.51
18:R:46:GLU:H	18:R:46:GLU:CD	2.14	0.51
18:R:87:ARG:O	18:R:88:LYS:HB2	2.11	0.51
1:A:21:G:C2	1:A:22:G:C6	2.99	0.51
1:A:99:C:H2'	1:A:101:A:C8	2.45	0.51
1:A:603:U:H3	1:A:635:G:H1	1.59	0.51
1:A:1355:G:H1	1:A:1367:C:H42	1.58	0.51
9:I:69:GLY:O	9:I:73:GLN:HG3	2.10	0.51
12:L:66:VAL:HG11	12:L:98:TYR:HE1	1.76	0.51
1:A:463:A:H2'	1:A:474:G:O4'	2.11	0.51
1:A:496:A:C2	1:A:497:A:C5	2.99	0.51
1:A:1505:G:C8	1:A:1505:G:H3'	2.46	0.51
15:O:3:ILE:HA	15:O:7:GLU:OE1	2.11	0.51
1:A:184:G:H2'	1:A:185:A:C8	2.46	0.51
1:A:757:U:H2'	1:A:758:G:O4'	2.11	0.51
1:A:909:A:H2'	1:A:910:C:O4'	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:966:M2G:H2'	1:A:967:5MC:C6	2.44	0.51
5:E:90:VAL:C	5:E:91:LEU:HD23	2.31	0.51
8:H:11:THR:O	8:H:14:ARG:N	2.43	0.51
1:A:135:C:O2	16:P:1:MET:HB2	2.12	0.50
1:A:144:G:H1	1:A:178:C:N4	2.07	0.50
1:A:372:C:H4'	1:A:373:A:O5'	2.11	0.50
1:A:502:G:P	12:L:118:SER:HG	2.34	0.50
1:A:782:A:OP1	1:A:1521:G:N2	2.41	0.50
1:A:1346:A:O2'	1:A:1347:G:OP2	2.28	0.50
1:A:1347:G:H21	1:A:1373:G:H2'	1.71	0.50
1:A:1516[A]:G:H2'	1:A:1518[A]:MA6:OP2	2.11	0.50
1:A:283:C:C2	1:A:284:G:C8	2.99	0.50
1:A:976:G:OP2	1:A:1358:U:O2'	2.18	0.50
1:A:1057:G:N2	1:A:1203:C:O2	2.43	0.50
1:A:1112:C:H1'	3:C:179:ARG:NH1	2.26	0.50
1:A:1328:C:H2'	1:A:1329:A:C8	2.47	0.50
13:M:86:CYS:SG	13:M:87:TYR:N	2.85	0.50
1:A:79:G:C4	1:A:91:C:O2	2.64	0.50
1:A:164:U:H2'	1:A:165:C:C6	2.46	0.50
1:A:521:G:OP1	12:L:54:LYS:HE2	2.11	0.50
1:A:647:C:H2'	1:A:648:A:C8	2.46	0.50
1:A:1338:G:H2'	1:A:1339:A:C8	2.46	0.50
1:A:1489:G:H2'	1:A:1490:C:C6	2.46	0.50
2:B:181:PHE:CE2	8:H:70:GLN:HB3	2.47	0.50
20:T:45:GLN:HA	20:T:91:LEU:CD1	2.40	0.50
1:A:256:U:H2'	1:A:257:G:H8	1.77	0.50
1:A:385:C:H2'	1:A:386:C:H6	1.77	0.50
1:A:1074:G:C6	1:A:1075:C:C4	3.00	0.50
1:A:1172:C:H2'	1:A:1173:G:H8	1.76	0.50
1:A:1221:G:H4'	19:S:53:ASN:O	2.10	0.50
3:C:139:GLN:O	3:C:142:MET:N	2.45	0.50
8:H:46:LYS:HD3	8:H:64:LYS:HG3	1.93	0.50
12:L:76:ASN:OD1	12:L:77:LEU:HD23	2.12	0.50
19:S:40:ILE:HB	19:S:67:VAL:O	2.12	0.50
1:A:1007:C:N3	1:A:1022:G:N2	2.59	0.50
2:B:7:VAL:HG11	2:B:221:LEU:HD23	1.94	0.50
2:B:40:HIS:HB2	2:B:190:THR:HG21	1.92	0.50
4:D:187:ARG:NH2	4:D:188:LEU:HD12	2.26	0.50
5:E:75:THR:HB	5:E:117:ASP:O	2.11	0.50
6:F:4:TYR:CZ	6:F:72:VAL:HG21	2.46	0.50
7:G:111:ARG:HD3	7:G:113:GLU:CG	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:933:G:OP2	7:G:3:ARG:HB3	2.12	0.50
1:A:1190:G:O2'	1:A:1191:A:O5'	2.29	0.50
3:C:106:VAL:HG11	3:C:115:LEU:HD11	1.94	0.50
3:C:121:ALA:O	3:C:125:GLU:HG3	2.12	0.50
12:L:33:ARG:O	12:L:84:LEU:HD12	2.12	0.50
12:L:39:VAL:HG12	12:L:41:ARG:HB2	1.93	0.50
16:P:10:GLY:HA3	16:P:14:ASN:O	2.11	0.50
17:Q:5:VAL:O	17:Q:6:LEU:HD23	2.11	0.50
1:A:644:G:C5	1:A:645:C:C5	3.00	0.50
2:B:114:ARG:HD2	2:B:118:LEU:HG	1.93	0.50
6:F:14:LEU:HD22	6:F:18:GLN:OE1	2.12	0.50
1:A:285:G:C2	1:A:286:G:C8	3.00	0.50
1:A:994:A:O2'	14:N:11:LYS:HG2	2.12	0.50
1:A:1057:G:H2'	1:A:1058:G:O4'	2.11	0.50
1:A:1442:G:C5	1:A:1446:A:C6	3.00	0.50
2:B:114:ARG:NH1	2:B:118:LEU:HD21	2.25	0.50
3:C:19:GLU:HB2	14:N:52:GLN:HA	1.94	0.50
5:E:79:GLU:HB3	5:E:92:LYS:HA	1.92	0.50
10:J:21:GLN:HA	10:J:24:VAL:HG12	1.93	0.50
12:L:8:ASN:HB2	17:Q:34:LYS:HZ3	1.76	0.50
1:A:92:C:H2'	1:A:92:C:O2	2.11	0.50
1:A:397:A:H5'	1:A:398:C:OP1	2.12	0.50
5:E:76:ILE:HD11	5:E:118:ILE:HD12	1.94	0.50
6:F:91:VAL:HG11	18:R:72:ARG:HH12	1.77	0.50
8:H:4:ASP:OD2	8:H:85:ARG:NH1	2.45	0.50
14:N:22:THR:HB	14:N:33:VAL:HB	1.93	0.50
1:A:250:A:H4'	1:A:251:G:O5'	2.11	0.49
1:A:1441:G:H21	1:A:1460:A:H62	1.59	0.49
1:A:1516[A]:G:N1	1:A:1519[A]:MA6:OP2	2.39	0.49
3:C:180:ALA:HB1	3:C:182:ILE:HG13	1.94	0.49
1:A:645:C:H2'	1:A:645:C:O2	2.12	0.49
9:I:8:GLY:HA3	9:I:79:LEU:HB3	1.94	0.49
10:J:66:ARG:NH1	10:J:66:ARG:HB3	2.27	0.49
14:N:48:ALA:HB2	14:N:53:LEU:HD11	1.94	0.49
1:A:76:C:N4	1:A:93:G:H1	2.09	0.49
1:A:266:G:H5"	1:A:266:G:H8	1.76	0.49
1:A:299:G:H2'	1:A:300:A:C8	2.47	0.49
1:A:474:G:H2'	1:A:475:G:O4'	2.12	0.49
1:A:665:A:C2	1:A:732:C:C2	3.00	0.49
1:A:779:C:H2'	1:A:780:A:O4'	2.12	0.49
1:A:838:G:C3'	1:A:839:U:H5"	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1402:4OC:HM42	1:A:1500:A:N6	2.26	0.49
4:D:3:ARG:NH1	4:D:71:SER:H	1.95	0.49
7:G:18:TYR:CD2	7:G:59:LEU:HD22	2.47	0.49
1:A:78:G:N1	1:A:92:C:N4	2.60	0.49
1:A:112:G:C2'	1:A:113:G:H5'	2.43	0.49
1:A:391:G:C6	1:A:392:G:C5	2.99	0.49
1:A:788:U:H2'	1:A:789:U:C6	2.47	0.49
3:C:7:PRO:HG2	3:C:184:TYR:CD1	2.47	0.49
3:C:127:ARG:HG2	3:C:193:TYR:OH	2.13	0.49
4:D:15:GLU:HB3	4:D:63:LYS:HG3	1.95	0.49
4:D:206:PHE:CD2	4:D:207:TYR:CE2	3.00	0.49
5:E:71:LEU:HD21	5:E:113:ALA:O	2.13	0.49
12:L:46:LYS:N	12:L:92:ASP:O	2.43	0.49
13:M:52:GLU:HG2	13:M:55:ARG:HH22	1.76	0.49
1:A:1032:G:H2'	1:A:1033:G:C8	2.47	0.49
1:A:1228:C:H2'	1:A:1229:A:C8	2.48	0.49
3:C:42:LEU:HD23	3:C:43:LEU:HD22	1.94	0.49
11:K:58:PRO:O	11:K:61:ALA:HB3	2.12	0.49
13:M:34:LEU:CD2	13:M:41:PRO:HA	2.42	0.49
1:A:142:G:H2'	1:A:143:A:C8	2.48	0.49
1:A:330:C:H2'	1:A:331:G:H5'	1.93	0.49
1:A:459:G:H1'	1:A:463:A:H61	1.78	0.49
1:A:475:G:H2'	1:A:476:G:O4'	2.13	0.49
1:A:836:G:C6	1:A:851:G:C6	3.00	0.49
1:A:1142:G:H2'	1:A:1143:G:O4'	2.11	0.49
1:A:1520[B]:G:H2'	1:A:1521:G:H8	1.76	0.49
7:G:122:HIS:O	7:G:126:ASP:HB2	2.12	0.49
12:L:55:VAL:CG2	12:L:67:THR:HG22	2.42	0.49
17:Q:68:ARG:HB3	17:Q:68:ARG:HH11	1.76	0.49
21:U:14:TRP:HZ3	21:U:15:ARG:HG3	1.78	0.49
1:A:279:A:H5'	1:A:279:A:H8	1.78	0.49
1:A:316:G:H2'	1:A:317:G:H8	1.76	0.49
1:A:825:G:H21	8:H:11:THR:HG21	1.77	0.49
1:A:1382:C:H2'	1:A:1383:C:C6	2.48	0.49
1:A:1407:5MC:O2'	1:A:1408:A:H5'	2.13	0.49
4:D:111:ALA:HA	4:D:161:ASN:HD22	1.78	0.49
5:E:105:VAL:HG23	5:E:106:PRO:HD3	1.94	0.49
8:H:85:ARG:NE	8:H:87:SER:O	2.46	0.49
15:O:36:ILE:CD1	15:O:60:VAL:HG23	2.43	0.49
18:R:59:SER:N	18:R:62:GLU:OE1	2.45	0.49
1:A:714:G:H2'	1:A:715:A:C8	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:811:C:O2'	1:A:901:A:N1	2.40	0.49
2:B:189:ASP:HB3	2:B:203:GLY:O	2.13	0.49
12:L:58:VAL:O	12:L:65:GLU:HA	2.11	0.49
13:M:17:VAL:O	13:M:20:THR:HG22	2.13	0.49
13:M:91:ARG:HH22	13:M:103:THR:HG21	1.77	0.49
16:P:52:ASP:O	16:P:55:ARG:HB2	2.13	0.49
1:A:966:M2G:CM1	1:A:967:5MC:H1'	2.43	0.49
2:B:17:PHE:CD1	2:B:18:GLY:N	2.74	0.49
3:C:123:GLN:O	3:C:128:PHE:HD1	1.96	0.49
1:A:253:U:H2'	1:A:254:G:C8	2.48	0.49
1:A:381:C:H2'	1:A:382:A:O4'	2.12	0.49
1:A:866:C:C2	1:A:867:G:H1'	2.48	0.49
1:A:1501:C:N4	1:A:1504:G:C2	2.81	0.49
4:D:21:LEU:HD23	4:D:115:ARG:HD2	1.94	0.49
7:G:62:PHE:C	7:G:62:PHE:CD2	2.86	0.49
18:R:25:THR:OG1	18:R:42:ARG:NH2	2.46	0.49
1:A:129:U:O3'	1:A:129(A):G:H3'	2.12	0.48
1:A:1063:C:H2'	1:A:1064:G:H8	1.75	0.48
1:A:1223:C:OP1	19:S:78:ARG:NH2	2.45	0.48
1:A:1306:A:H2'	1:A:1307:U:O4'	2.12	0.48
1:A:1348:U:OP2	1:A:1373:G:N2	2.43	0.48
6:F:14:LEU:CD1	6:F:18:GLN:HB3	2.27	0.48
12:L:22:SER:C	12:L:24:VAL:H	2.16	0.48
12:L:30:ALA:HB1	12:L:31:PRO:HD2	1.94	0.48
20:T:29:LYS:O	20:T:32:ALA:HB3	2.13	0.48
20:T:71:THR:O	20:T:72:LEU:HD23	2.12	0.48
1:A:109:A:C6	1:A:326:G:C6	3.01	0.48
1:A:451:A:N6	1:A:481:G:C4	2.81	0.48
1:A:737:A:H2'	1:A:738:C:C6	2.47	0.48
1:A:737:A:H1'	6:F:73:ASN:OD1	2.14	0.48
1:A:750:G:H1'	15:O:23:GLY:H	1.77	0.48
1:A:854:G:N2	1:A:855:G:C4	2.81	0.48
1:A:1188:A:O2'	14:N:58:LYS:HE2	2.14	0.48
2:B:68:ILE:HD12	2:B:222:ILE:HD11	1.95	0.48
2:B:185:ILE:HA	2:B:199:TYR:O	2.13	0.48
5:E:99:GLY:H	5:E:117:ASP:CG	2.17	0.48
6:F:1:MET:HB3	6:F:66:GLU:HG2	1.95	0.48
11:K:59:TYR:CE2	11:K:63:LEU:HD11	2.48	0.48
19:S:32:LYS:HB3	19:S:34:TRP:CZ3	2.47	0.48
20:T:92:LEU:O	20:T:96:GLY:HA3	2.13	0.48
1:A:960:U:H2'	1:A:1225:A:H62	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1336:C:H6	1:A:1336:C:H5"	1.78	0.48
1:A:1420:C:H2'	1:A:1421:G:H8	1.79	0.48
1:A:1484:C:H2'	1:A:1485:U:C1'	2.42	0.48
5:E:84:PHE:CB	5:E:134:ALA:HB2	2.42	0.48
7:G:136:LYS:HE3	7:G:140:ASP:OD2	2.12	0.48
8:H:56:LYS:HD3	8:H:56:LYS:N	2.27	0.48
1:A:435:C:H2'	1:A:436:C:C6	2.48	0.48
1:A:918:A:H2'	1:A:919:A:C8	2.49	0.48
1:A:981:U:H5'	14:N:21:TYR:CE1	2.49	0.48
1:A:1228:C:O3'	13:M:116:THR:HG23	2.14	0.48
1:A:1290:G:O2'	1:A:1291:G:H5'	2.13	0.48
3:C:46:GLU:HG2	3:C:83:ARG:HH21	1.78	0.48
15:O:9:GLN:HA	15:O:12:ILE:HD12	1.95	0.48
17:Q:53:LEU:HD21	17:Q:85:VAL:HG11	1.94	0.48
1:A:411:A:C8	1:A:413:G:H1'	2.48	0.48
1:A:645:C:H5"	1:A:646:U:OP2	2.13	0.48
1:A:960:U:H4'	1:A:961:U:C5'	2.43	0.48
1:A:1260:C:O5'	1:A:1284:C:H4'	2.13	0.48
2:B:106:LYS:O	2:B:110:GLN:HG3	2.14	0.48
8:H:82:HIS:ND1	8:H:138:TRP:CE2	2.75	0.48
17:Q:24:GLU:OE2	17:Q:37:LYS:HD2	2.13	0.48
1:A:253:U:H2'	1:A:254:G:H8	1.77	0.48
1:A:509:A:H5'	4:D:54:TYR:HD2	1.78	0.48
1:A:512:U:H2'	1:A:513:C:H6	1.76	0.48
1:A:643:C:H2'	1:A:644:G:H5'	1.95	0.48
1:A:1011:G:H2'	1:A:1011:G:N3	2.28	0.48
1:A:1152:A:H5"	10:J:13:HIS:CG	2.48	0.48
1:A:1392:G:N2	1:A:1502:A:H8	2.11	0.48
2:B:178:ARG:NH2	8:H:68:ARG:HH22	2.11	0.48
4:D:174:LEU:O	4:D:186:LEU:HD11	2.13	0.48
16:P:2:VAL:O	16:P:64:ALA:HA	2.14	0.48
20:T:77:ALA:O	20:T:81:LYS:HG3	2.13	0.48
1:A:865:A:H2'	1:A:866:C:H6	1.77	0.48
1:A:1305:G:H22	1:A:1331:G:H1'	1.75	0.48
1:A:1406:U:HO2'	1:A:1517[B]:G:N2	2.12	0.48
1:A:1505:G:H3'	1:A:1505:G:H8	1.79	0.48
2:B:12:GLU:HG2	2:B:15:VAL:HB	1.96	0.48
3:C:148:GLY:HA3	3:C:172:ARG:O	2.14	0.48
4:D:20:TYR:HB3	4:D:26:CYS:HB3	1.96	0.48
4:D:196:LEU:HD23	4:D:196:LEU:HA	1.60	0.48
5:E:149:GLU:O	5:E:153:LYS:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:12:ILE:HG12	15:O:31:LEU:HD11	1.95	0.48
18:R:22:VAL:HG13	18:R:42:ARG:NH1	2.28	0.48
19:S:55:LYS:HZ3	19:S:56:GLN:HB2	1.77	0.48
1:A:502:G:C2	1:A:503:C:C2	3.01	0.48
1:A:781:A:H2'	1:A:782:A:H5'	1.95	0.48
1:A:1005:A:H2	1:A:1026:G:H1'	1.78	0.48
1:A:1047:G:C2'	1:A:1048:G:H5'	2.44	0.48
1:A:1086:U:H3	1:A:1099:G:H22	1.60	0.48
1:A:1244:C:H5"	1:A:1245:A:OP2	2.14	0.48
1:A:1297:C:O2'	1:A:1298:C:OP2	2.30	0.48
4:D:170:VAL:HG13	4:D:174:LEU:HD12	1.95	0.48
5:E:11:ILE:HG22	5:E:12:LEU:N	2.29	0.48
15:O:36:ILE:HD12	15:O:60:VAL:HG23	1.95	0.48
20:T:84:LEU:HA	20:T:87:LYS:HZ2	1.79	0.48
1:A:1094:G:O2'	1:A:1108:G:N2	2.47	0.48
1:A:1157:A:H4'	1:A:1158:C:O5'	2.14	0.48
1:A:1296:C:H4'	1:A:1302:U:H5	1.77	0.48
3:C:81:GLY:O	3:C:84:ILE:HB	2.14	0.48
3:C:156:ARG:HG2	3:C:160:ALA:O	2.14	0.48
4:D:158:ILE:HA	4:D:158:ILE:HD13	1.64	0.48
7:G:154:TYR:H	7:G:155:ARG:HH21	1.61	0.48
10:J:6:ILE:HD12	10:J:98:ILE:HG12	1.95	0.48
1:A:77:G:C4	1:A:93:G:N2	2.82	0.48
1:A:78:G:C2	1:A:92:C:C4	3.01	0.48
1:A:179:A:H2'	1:A:180:U:H6	1.79	0.48
1:A:190(F):G:H4'	1:A:190(G):G:OP2	2.14	0.48
1:A:216:G:C2	1:A:217:C:C4	3.01	0.48
1:A:268:C:H2'	1:A:269:C:C6	2.48	0.48
1:A:337:C:H2'	1:A:338:A:C8	2.48	0.48
1:A:434:U:H2'	1:A:435:C:C6	2.49	0.48
1:A:581:G:O3'	15:O:64:ARG:NH2	2.47	0.48
1:A:642:A:H2'	1:A:643:C:O4'	2.14	0.48
1:A:1004:A:H5"	1:A:1025:U:N3	2.27	0.48
1:A:1077:G:N2	1:A:1080:A:OP2	2.45	0.48
1:A:1101:A:H4'	1:A:1102:A:O5'	2.14	0.48
1:A:1355:G:H2'	1:A:1356:G:H8	1.78	0.48
1:A:1416:G:N2	1:A:1484:C:C2	2.82	0.48
1:A:1488:G:H2'	1:A:1489:G:C8	2.48	0.48
9:I:28:VAL:HG12	9:I:29:ASN:HB2	1.95	0.48
20:T:89:ARG:NH2	20:T:104:LEU:HB3	2.28	0.48
1:A:691:G:H2'	1:A:692:U:C6	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1451:A:H5”	1:A:1452:C:H5	1.78	0.47
2:B:21:ARG:CG	2:B:22:LYS:H	2.26	0.47
3:C:98:ASN:OD1	3:C:98:ASN:N	2.47	0.47
7:G:113:GLU:H	7:G:113:GLU:HG2	1.40	0.47
1:A:161:A:H2’	1:A:162:A:C8	2.49	0.47
1:A:376:G:N3	1:A:389:A:C2	2.82	0.47
1:A:518:C:C5	1:A:529:G:N7	2.82	0.47
1:A:620:C:C2	4:D:135:LEU:HD13	2.49	0.47
3:C:131:ARG:O	3:C:135:LYS:HG2	2.13	0.47
8:H:1:MET:HG2	8:H:2:LEU:N	2.29	0.47
8:H:48:TYR:HA	8:H:60:ARG:O	2.15	0.47
9:I:26:VAL:HG12	9:I:61:ALA:HB3	1.94	0.47
14:N:14:PRO:HB2	14:N:16:PHE:O	2.14	0.47
17:Q:3:LYS:HD3	17:Q:61:GLU:O	2.14	0.47
1:A:76:C:H2’	1:A:77:G:H8	1.78	0.47
1:A:830:G:C6	1:A:831:U:C4	3.02	0.47
1:A:858:G:C6	1:A:869:G:N7	2.82	0.47
3:C:138:VAL:HG13	3:C:149:ALA:HB3	1.96	0.47
4:D:141:ARG:HB2	4:D:141:ARG:NH1	2.29	0.47
8:H:26:VAL:HG23	8:H:27:PRO:HD2	1.95	0.47
13:M:2:ALA:O	13:M:10:PRO:HD2	2.15	0.47
14:N:37:PHE:HB3	14:N:39:LEU:HD12	1.95	0.47
1:A:60:A:H4’	1:A:61:G:O5’	2.15	0.47
1:A:404:U:H2’	1:A:405:U:H6	1.78	0.47
1:A:618:C:N3	1:A:622:A:N6	2.62	0.47
1:A:826:C:H5’	8:H:12:ARG:NH1	2.29	0.47
1:A:1144:G:H21	1:A:1146:A:H62	1.63	0.47
1:A:1184:G:H2’	1:A:1185:G:H8	1.79	0.47
2:B:178:ARG:NH2	8:H:74:PRO:HG3	2.29	0.47
3:C:10:PHE:CD2	3:C:178:LEU:HD12	2.49	0.47
4:D:111:ALA:HB1	4:D:116:GLN:HG2	1.97	0.47
7:G:59:LEU:HD11	7:G:63:LYS:HE3	1.96	0.47
4:D:24:GLU:O	4:D:25:ARG:HB3	2.14	0.47
9:I:9:ARG:HG3	9:I:14:VAL:HG13	1.95	0.47
11:K:29:ILE:HB	11:K:44:SER:CB	2.45	0.47
20:T:64:ASP:OD2	20:T:81:LYS:NZ	2.44	0.47
1:A:176:C:O2’	1:A:177:C:H5’	2.15	0.47
1:A:820:U:H4’	1:A:821:G:OP2	2.15	0.47
1:A:866:C:N3	1:A:867:G:H1’	2.30	0.47
1:A:1130:A:H8	1:A:1130:A:OP2	1.98	0.47
2:B:167:PRO:HG2	2:B:192:SER:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:3:ARG:HD2	4:D:71:SER:N	2.30	0.47
5:E:48:ALA:HB2	5:E:57:LYS:HE2	1.97	0.47
6:F:98:LEU:HD13	18:R:28:GLU:HG3	1.96	0.47
20:T:50:GLU:H	20:T:99:LEU:HD12	1.80	0.47
1:A:19:C:H5"	5:E:86:ALA:HB2	1.97	0.47
1:A:376:G:H5"	16:P:5:ARG:HD2	1.96	0.47
1:A:399:G:H2'	1:A:400:C:C6	2.49	0.47
1:A:860:A:N6	1:A:861:G:C2	2.83	0.47
1:A:935:A:O2'	1:A:1383:C:O2	2.33	0.47
1:A:943:U:H1'	9:I:124:GLN:HE22	1.79	0.47
1:A:978:A:C6	1:A:1318:A:C6	3.02	0.47
1:A:1112:C:H42	3:C:178:LEU:H	1.62	0.47
1:A:1201:A:H4'	1:A:1202:G:H5"	1.96	0.47
1:A:1243:C:H2'	1:A:1244:C:H6	1.80	0.47
1:A:1406:U:H2'	1:A:1407:5MC:C6	2.49	0.47
1:A:1415:G:C6	1:A:1416:G:C6	3.03	0.47
1:A:1481:U:H2'	1:A:1482:G:O4'	2.15	0.47
2:B:175:ARG:HH11	2:B:175:ARG:HG3	1.79	0.47
2:B:189:ASP:CG	2:B:205:ASP:HB3	2.35	0.47
3:C:22:TRP:HB3	3:C:59:ARG:HB2	1.95	0.47
4:D:92:VAL:O	4:D:96:LEU:HD13	2.13	0.47
7:G:18:TYR:HD2	7:G:59:LEU:HD13	1.79	0.47
7:G:62:PHE:C	7:G:62:PHE:HD2	2.18	0.47
8:H:95:VAL:HG12	8:H:99:GLU:CB	2.45	0.47
8:H:107:LEU:HD23	8:H:107:LEU:N	2.30	0.47
9:I:17:VAL:HG21	9:I:80:GLY:HA3	1.96	0.47
9:I:112:LYS:HG3	9:I:118:LYS:HA	1.97	0.47
10:J:32:ALA:O	10:J:34:VAL:HG23	2.15	0.47
13:M:32:GLU:HG2	13:M:64:TRP:HZ2	1.80	0.47
16:P:38:TYR:HE2	16:P:50:LYS:HE2	1.78	0.47
16:P:75:ARG:C	16:P:78:GLY:H	2.18	0.47
17:Q:29:HIS:HB2	17:Q:36:ILE:HD12	1.97	0.47
18:R:44:LEU:HD13	18:R:48:GLY:O	2.15	0.47
19:S:13:ASP:O	19:S:17:GLU:HG3	2.15	0.47
19:S:25:LYS:HE2	19:S:25:LYS:HB3	1.67	0.47
19:S:74:PHE:CD1	19:S:74:PHE:N	2.82	0.47
1:A:78:G:C6	1:A:79:G:C8	3.02	0.47
1:A:280:C:C4	17:Q:91:ARG:NH1	2.83	0.47
1:A:860:A:H2'	1:A:861:G:O4'	2.15	0.47
1:A:1301:U:O2'	1:A:1302:U:H3'	2.14	0.47
1:A:1419:G:C6	1:A:1420:C:C4	3.03	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1491:G:H5”	12:L:47:LYS:HE3	1.96	0.47
2:B:8:LYS:HE2	2:B:8:LYS:HB2	1.70	0.47
3:C:43:LEU:HD13	3:C:47:LEU:HD13	1.97	0.47
4:D:157:LEU:O	4:D:160:GLN:HB3	2.15	0.47
8:H:118:VAL:C	8:H:119:LEU:HD23	2.34	0.47
18:R:43:PHE:HB3	18:R:66:LEU:HD21	1.97	0.47
1:A:102:G:H2’	1:A:103:C:H6	1.79	0.47
1:A:352:C:H6	1:A:352:C:H5”	1.80	0.47
1:A:1069:C:O2’	1:A:1192:C:H1’	2.15	0.47
1:A:1112:C:O2	3:C:179:ARG:HG3	2.15	0.47
8:H:119:LEU:HD12	8:H:124:ALA:HA	1.97	0.47
9:I:49:PRO:HD3	9:I:101:PHE:CE2	2.50	0.47
9:I:53:VAL:HB	9:I:92:TYR:CZ	2.50	0.47
19:S:32:LYS:HB3	19:S:34:TRP:HZ3	1.79	0.47
1:A:6:G:H2’	5:E:119:LEU:HD11	1.97	0.47
1:A:303:A:H2’	1:A:304:U:O4’	2.15	0.47
1:A:443:C:H42	1:A:491:G:H1	1.63	0.47
1:A:501:C:H2’	1:A:502:G:H8	1.74	0.47
1:A:520:A:H61	1:A:529:G:H1’	1.79	0.47
1:A:953:G:C5’	1:A:965:A:H61	2.27	0.47
1:A:1250:A:C6	1:A:1251:A:N1	2.83	0.47
3:C:43:LEU:HD12	3:C:47:LEU:HD22	1.96	0.47
12:L:87:GLY:H	12:L:99:HIS:H	1.62	0.47
18:R:21:LYS:O	18:R:24:ALA:HB3	2.15	0.47
1:A:325:A:H2’	1:A:326:G:O4’	2.15	0.46
1:A:858:G:H3’	1:A:869:G:O6	2.15	0.46
1:A:1255:G:H2’	1:A:1279:A:N6	2.29	0.46
2:B:21:ARG:CD	2:B:22:LYS:H	2.28	0.46
4:D:70:ILE:HD11	4:D:100:ARG:CZ	2.45	0.46
9:I:85:LEU:O	9:I:88:TYR:HB3	2.14	0.46
17:Q:65:ILE:HG21	17:Q:69:LYS:HZ3	1.80	0.46
1:A:284:G:H2’	1:A:285:G:C8	2.50	0.46
1:A:485:G:O2’	1:A:486:U:P	2.73	0.46
1:A:511:C:O2	4:D:43:HIS:NE2	2.46	0.46
1:A:602:A:H2’	1:A:603:U:O4’	2.15	0.46
1:A:1032:G:H2’	1:A:1033:G:H8	1.79	0.46
1:A:1078:U:H5”	1:A:1079:G:OP2	2.16	0.46
1:A:1130:A:OP2	1:A:1130:A:C8	2.68	0.46
2:B:31:TYR:CD2	2:B:31:TYR:N	2.83	0.46
4:D:187:ARG:NE	4:D:188:LEU:N	2.54	0.46
6:F:25:ILE:HD12	6:F:28:ARG:NH1	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:75:LEU:O	6:F:79:LEU:HD13	2.16	0.46
9:I:97:LYS:HB2	9:I:98:PRO:HD3	1.97	0.46
12:L:35:GLY:HA3	12:L:60:LEU:HD13	1.97	0.46
17:Q:65:ILE:HB	17:Q:69:LYS:HB2	1.96	0.46
1:A:110:C:H2'	1:A:111:G:O4'	2.15	0.46
1:A:284:G:H2'	1:A:285:G:H8	1.81	0.46
1:A:357:G:C2	1:A:358:U:C5	3.03	0.46
1:A:1195:C:C4	1:A:1197:G:C8	3.03	0.46
1:A:1347:G:H1'	1:A:1348:U:H5	1.79	0.46
1:A:1381:U:C1'	7:G:156:TRP:HH2	2.28	0.46
1:A:1399:C:C2	1:A:1502:A:N6	2.84	0.46
2:B:170:GLU:OE2	2:B:170:GLU:HA	2.14	0.46
3:C:167:TRP:CG	3:C:168:ALA:N	2.84	0.46
4:D:59:ARG:HE	4:D:59:ARG:HB3	1.66	0.46
6:F:69:GLU:OE1	6:F:69:GLU:N	2.47	0.46
17:Q:29:HIS:HE1	17:Q:31:LEU:HB3	1.80	0.46
18:R:37:VAL:O	18:R:39:VAL:N	2.48	0.46
18:R:43:PHE:C	18:R:51:LEU:HD12	2.35	0.46
1:A:442:C:H2'	1:A:443:C:C6	2.51	0.46
1:A:951:G:OP2	13:M:102:ARG:NH2	2.37	0.46
1:A:1250:A:C6	1:A:1251:A:C6	3.04	0.46
1:A:1327:C:H2'	1:A:1328:C:C6	2.50	0.46
1:A:1330:U:H2'	1:A:1331:G:H5'	1.96	0.46
2:B:223:ILE:HB	2:B:230:VAL:HG22	1.98	0.46
7:G:152:ALA:O	7:G:155:ARG:NE	2.48	0.46
8:H:104:ARG:HD2	8:H:138:TRP:CD2	2.50	0.46
8:H:127:LEU:HA	8:H:127:LEU:HD13	1.66	0.46
9:I:97:LYS:HE3	9:I:97:LYS:HB3	1.76	0.46
11:K:19:ALA:HB2	11:K:80:VAL:HG11	1.97	0.46
13:M:99:ARG:HB2	13:M:101:GLN:NE2	2.30	0.46
1:A:166:G:C6	1:A:167:G:C6	3.03	0.46
1:A:279:A:H5'	1:A:279:A:C8	2.50	0.46
1:A:437:U:H1'	4:D:119:GLN:NE2	2.31	0.46
1:A:451:A:O5'	1:A:451:A:H8	1.99	0.46
1:A:707:C:H2'	1:A:708:C:H6	1.80	0.46
1:A:924:C:H5'	1:A:1399:C:OP2	2.16	0.46
1:A:1241:G:C4	1:A:1242:C:C5	3.03	0.46
1:A:1355:G:H2'	1:A:1356:G:C8	2.50	0.46
2:B:18:GLY:HA2	2:B:42:ILE:HD12	1.98	0.46
4:D:59:ARG:HA	4:D:62:GLN:HB2	1.96	0.46
7:G:40:ALA:CB	9:I:41:VAL:HG21	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:12:ILE:C	15:O:14:GLU:N	2.68	0.46
17:Q:90:ILE:HA	17:Q:93:GLN:HB2	1.98	0.46
1:A:142:G:N3	1:A:196:A:H2	2.13	0.46
1:A:247:G:OP2	17:Q:100:LYS:HD2	2.16	0.46
1:A:375:U:H2'	1:A:376:G:O4'	2.16	0.46
1:A:437:U:H5'	4:D:155:LEU:HD11	1.98	0.46
1:A:513:C:H2'	1:A:514:C:C6	2.50	0.46
1:A:691:G:H2'	1:A:692:U:H6	1.80	0.46
1:A:837:G:H1	1:A:849:C:H42	1.62	0.46
1:A:1006:C:N3	1:A:1007:C:N4	2.63	0.46
1:A:1063:C:H3'	1:A:1064:G:H2'	1.98	0.46
1:A:1196:U:H3'	1:A:1197:G:H5'	1.96	0.46
4:D:79:PHE:HA	4:D:93:PHE:CE2	2.51	0.46
4:D:148:VAL:HG12	4:D:153:ARG:NH1	2.30	0.46
7:G:44:TYR:O	7:G:48:LYS:HD3	2.15	0.46
8:H:124:ALA:O	8:H:128:GLY:N	2.39	0.46
10:J:15:THR:HG22	10:J:94:VAL:HG13	1.97	0.46
16:P:51:VAL:HG12	16:P:53:VAL:N	2.31	0.46
16:P:78:GLY:C	16:P:80:PHE:N	2.69	0.46
1:A:132:C:O2'	1:A:133:U:H5'	2.16	0.46
1:A:1095:U:H2'	1:A:1096:C:O4'	2.15	0.46
1:A:1130:A:OP1	1:A:1131:G:H8	1.98	0.46
1:A:1218:C:H2'	1:A:1219:U:C6	2.51	0.46
1:A:1402:4OC:O2	1:A:1500:A:N1	2.49	0.46
1:A:1493:A:O2'	1:A:1494:G:O4'	2.30	0.46
2:B:131:PRO:HB3	2:B:133:LYS:NZ	2.31	0.46
3:C:174:PRO:HB2	3:C:177:THR:OG1	2.16	0.46
9:I:125:TYR:CD2	9:I:125:TYR:N	2.84	0.46
11:K:13:GLN:OE1	11:K:13:GLN:N	2.49	0.46
12:L:5:PRO:HG2	12:L:10:LEU:HD21	1.97	0.46
17:Q:56:VAL:O	17:Q:77:VAL:HG23	2.16	0.46
1:A:22:G:H2'	1:A:23:C:C6	2.50	0.46
1:A:56:U:O2'	1:A:57:G:H5'	2.15	0.46
1:A:183:G:HO2'	1:A:224:C:HO2'	1.63	0.46
1:A:243:A:C2	1:A:245:C:H2'	2.51	0.46
1:A:413:G:H8	1:A:428:G:N2	1.99	0.46
1:A:571:U:H5"	1:A:572:A:OP2	2.16	0.46
1:A:663:A:H2'	1:A:664:G:O4'	2.16	0.46
1:A:939:G:H5"	7:G:102:ARG:HH12	1.80	0.46
1:A:977:A:O3'	1:A:980:C:N4	2.48	0.46
1:A:1163:C:H2'	1:A:1164:G:C8	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1418:A:H3'	1:A:1418:A:OP2	2.16	0.46
2:B:122:PHE:HE2	2:B:139:LYS:HD2	1.81	0.46
4:D:43:HIS:HB3	4:D:46:LYS:HD2	1.98	0.46
4:D:118:ARG:O	4:D:122:ARG:HB2	2.16	0.46
8:H:64:LYS:HB3	8:H:79:VAL:HG21	1.96	0.46
9:I:46:ALA:HB1	9:I:77:ILE:CG2	2.46	0.46
10:J:17:ASP:O	10:J:21:GLN:HB2	2.16	0.46
10:J:42:THR:HG23	10:J:67:THR:O	2.15	0.46
10:J:48:THR:HA	10:J:62:HIS:HB3	1.97	0.46
19:S:16:LEU:O	19:S:20:LEU:HG	2.15	0.46
1:A:53:A:N6	1:A:54:C:C4	2.84	0.46
1:A:229:U:H2'	1:A:230:G:H8	1.81	0.46
1:A:544:G:C5	1:A:545:C:C5	3.04	0.46
1:A:695:A:H61	1:A:797:C:H1'	1.80	0.46
1:A:1007:C:N4	1:A:1022:G:H1	2.14	0.46
1:A:1053:G:H4'	1:A:1054:C:H5'	1.98	0.46
1:A:1201:A:H4'	1:A:1202:G:O5'	2.15	0.46
1:A:1232:U:P	9:I:126:SER:HB2	2.56	0.46
1:A:1385:G:H2'	1:A:1386:G:O4'	2.15	0.46
1:A:1416:G:H3'	1:A:1417:G:H8	1.81	0.46
3:C:8:ILE:O	3:C:12:LEU:N	2.49	0.46
5:E:109:ILE:HG22	5:E:110:LEU:N	2.31	0.46
5:E:151:LEU:HD22	5:E:151:LEU:O	2.16	0.46
10:J:51:ARG:NE	10:J:61:GLU:HB3	2.30	0.46
11:K:20:TYR:CE2	11:K:83:ILE:HD13	2.50	0.46
11:K:40:ILE:CG2	11:K:41:THR:HG22	2.43	0.46
11:K:51:LYS:HD3	11:K:51:LYS:HA	1.57	0.46
13:M:81:LEU:HA	13:M:84:ILE:HD11	1.97	0.46
16:P:23:ASP:OD1	16:P:25:ARG:HG3	2.16	0.46
17:Q:40:LYS:HG2	17:Q:42:TYR:CE1	2.51	0.46
19:S:56:GLN:HG2	19:S:57:HIS:H	1.81	0.46
1:A:222:U:H2'	1:A:223:U:C6	2.50	0.46
1:A:392:G:H2'	1:A:393:A:C8	2.51	0.46
1:A:902:G:H2'	1:A:903:G:C8	2.50	0.46
1:A:1240:U:N3	7:G:32:ARG:HD2	2.31	0.46
1:A:1258:G:H2'	1:A:1259:C:C6	2.51	0.46
2:B:223:ILE:O	2:B:227:GLY:N	2.45	0.46
3:C:21:ARG:NH2	3:C:56:ASP:HB3	2.30	0.46
9:I:16:ARG:HB2	9:I:64:THR:HG23	1.97	0.46
18:R:55:ARG:O	18:R:55:ARG:HD2	2.15	0.46
1:A:113:G:H2'	1:A:114:U:C6	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:620:C:N1	4:D:135:LEU:HD13	2.31	0.45
1:A:633:G:H2'	1:A:634:C:H6	1.81	0.45
1:A:689:C:O2'	1:A:705:U:O2'	2.25	0.45
2:B:21:ARG:HD2	2:B:22:LYS:N	2.31	0.45
2:B:30:ARG:HG3	2:B:31:TYR:CD2	2.51	0.45
4:D:108:LEU:CD1	4:D:183:GLY:HA3	2.46	0.45
6:F:82:ARG:HD2	6:F:82:ARG:HA	1.77	0.45
8:H:86:ILE:HG22	8:H:133:LEU:O	2.16	0.45
9:I:32:ASP:OD1	9:I:33:PHE:N	2.49	0.45
15:O:37:ASN:O	15:O:38:ARG:C	2.55	0.45
18:R:32:ARG:C	18:R:69:THR:HG21	2.37	0.45
18:R:53:ARG:HH11	18:R:59:SER:HA	1.80	0.45
1:A:659:U:OP1	15:O:8:LYS:HD3	2.15	0.45
1:A:1067:A:H4'	1:A:1068:G:O5'	2.16	0.45
1:A:1201:A:H4'	1:A:1202:G:C5'	2.46	0.45
1:A:1437:C:H2'	1:A:1438:G:C8	2.51	0.45
3:C:22:TRP:CE3	3:C:32:LEU:HD23	2.50	0.45
20:T:20:LEU:O	20:T:24:LEU:HD13	2.16	0.45
1:A:802:A:H2'	1:A:803:G:O4'	2.16	0.45
1:A:1009:G:N2	1:A:1010:G:H1'	2.31	0.45
1:A:1329:A:C5'	13:M:29:ARG:HD2	2.46	0.45
1:A:1332:A:H2'	1:A:1333:A:C8	2.52	0.45
1:A:1395:C:O2'	1:A:1396:A:H5'	2.15	0.45
2:B:9:GLU:OE2	2:B:12:GLU:N	2.49	0.45
2:B:30:ARG:HD2	2:B:31:TYR:CE2	2.51	0.45
3:C:62:ASP:O	3:C:97:LYS:HD2	2.15	0.45
4:D:18:LYS:HD3	4:D:20:TYR:HE2	1.81	0.45
5:E:68:GLU:O	5:E:68:GLU:HG3	2.16	0.45
7:G:156:TRP:CD1	7:G:156:TRP:O	2.70	0.45
8:H:11:THR:O	8:H:12:ARG:C	2.53	0.45
11:K:16:SER:HB2	11:K:106:LYS:NZ	2.31	0.45
1:A:858:G:O6	1:A:869:G:C8	2.69	0.45
1:A:1179:A:O3'	9:I:103:THR:HG23	2.16	0.45
1:A:1375:A:OP1	7:G:12:LEU:HD21	2.16	0.45
2:B:193:ASP:O	2:B:196:LEU:HD12	2.17	0.45
4:D:112:VAL:HG23	4:D:116:GLN:OE1	2.17	0.45
5:E:135:THR:O	5:E:138:ALA:HB3	2.17	0.45
10:J:66:ARG:HB3	10:J:66:ARG:HH11	1.82	0.45
20:T:14:LYS:HB2	20:T:17:ARG:NH2	2.32	0.45
1:A:299:G:H8	1:A:299:G:O5'	2.00	0.45
1:A:413:G:H2'	1:A:428:G:N2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:500:G:C6	1:A:546:G:C2	3.04	0.45
1:A:600:C:N3	1:A:638:G:N2	2.62	0.45
2:B:80:ILE:HG22	2:B:215:LEU:HD12	1.98	0.45
2:B:130:ARG:NH1	2:B:134:GLU:OE1	2.50	0.45
3:C:22:TRP:CH2	3:C:32:LEU:HB3	2.52	0.45
7:G:113:GLU:HG3	7:G:119:ARG:HA	1.99	0.45
9:I:78:LYS:HD2	9:I:101:PHE:HE2	1.81	0.45
1:A:192:U:H2'	1:A:193:C:H6	1.81	0.45
1:A:452:A:O4'	16:P:72:ARG:NH1	2.50	0.45
1:A:514:C:H2'	1:A:515:G:C8	2.51	0.45
1:A:1068:G:OP2	1:A:1094:G:H8	1.99	0.45
1:A:1253:G:O2'	1:A:1356:G:H4'	2.16	0.45
2:B:117:GLU:O	2:B:120:ALA:HB3	2.17	0.45
2:B:187:LEU:HD22	2:B:187:LEU:HA	1.46	0.45
4:D:43:HIS:HA	4:D:46:LYS:HE3	1.99	0.45
4:D:194:LEU:HA	4:D:194:LEU:HD13	1.55	0.45
13:M:40:ASN:ND2	13:M:43:THR:HG23	2.31	0.45
13:M:78:ILE:HD13	13:M:78:ILE:HA	1.64	0.45
15:O:46:HIS:C	15:O:48:LYS:H	2.18	0.45
15:O:55:GLY:O	15:O:59:MET:HG3	2.17	0.45
1:A:340:U:H2'	1:A:341:C:H6	1.81	0.45
1:A:554:C:H2'	1:A:555:C:C6	2.51	0.45
1:A:1015:A:C5	1:A:1016:A:C5	3.05	0.45
1:A:1027:C:H42	1:A:1035:A:N6	2.15	0.45
1:A:1041:A:H2'	1:A:1042:G:O4'	2.17	0.45
3:C:10:PHE:HD2	3:C:10:PHE:O	2.00	0.45
4:D:83:SER:HA	4:D:89:THR:HG23	1.98	0.45
4:D:126:ILE:HD13	4:D:126:ILE:HA	1.66	0.45
4:D:186:LEU:H	4:D:186:LEU:HG	1.46	0.45
8:H:113:SER:HB3	8:H:134:ILE:HD11	1.98	0.45
11:K:84:VAL:HG21	11:K:95:ILE:HD11	1.98	0.45
17:Q:21:VAL:O	17:Q:41:LYS:HA	2.17	0.45
1:A:35:G:H2'	1:A:36:C:C6	2.52	0.45
1:A:1141:C:H2'	1:A:1142:G:H8	1.80	0.45
2:B:80:ILE:HD13	2:B:212:GLN:HG2	1.99	0.45
2:B:118:LEU:CB	2:B:142:LEU:HD23	2.46	0.45
3:C:31:HIS:HA	3:C:34:LEU:HB2	1.99	0.45
3:C:151:VAL:H	3:C:169:ALA:HB2	1.82	0.45
3:C:155:GLY:HA2	3:C:164:ARG:O	2.16	0.45
4:D:63:LYS:O	4:D:67:ILE:HG12	2.16	0.45
6:F:48:LEU:HD13	6:F:52:ILE:HG13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:59:LEU:O	7:G:62:PHE:HB3	2.16	0.45
8:H:15:ASN:N	8:H:15:ASN:OD1	2.50	0.45
10:J:48:THR:HG1	10:J:62:HIS:HD1	1.63	0.45
19:S:40:ILE:HD13	19:S:62:ILE:HD11	1.98	0.45
20:T:56:MET:HG3	20:T:88:VAL:HG21	1.97	0.45
1:A:538:G:P	12:L:115:LYS:HB2	2.57	0.45
1:A:935:A:H2'	1:A:936:C:O4'	2.17	0.45
1:A:1098:C:H2'	1:A:1099:G:O4'	2.17	0.45
4:D:176:LEU:HD12	4:D:177:ASP:N	2.31	0.45
8:H:100:ILE:HA	8:H:101:PRO:HD2	1.37	0.45
9:I:3:GLN:HG3	9:I:20:ARG:HG2	1.99	0.45
10:J:36:GLY:HA2	10:J:37:PRO:HD3	1.75	0.45
1:A:35:G:C6	1:A:36:C:N4	2.84	0.45
1:A:429:U:H1'	1:A:430:A:H5"	1.99	0.45
1:A:510:A:H5"	1:A:511:C:OP2	2.17	0.45
1:A:735:C:H2'	1:A:736:C:H6	1.81	0.45
1:A:901:A:N7	1:A:902:G:H1'	2.32	0.45
1:A:953:G:C6	1:A:954:G:C4	3.05	0.45
1:A:953:G:H2'	1:A:954:G:O4'	2.16	0.45
1:A:1492:A:H2'	1:A:1492:A:N3	2.32	0.45
2:B:178:ARG:HH21	8:H:68:ARG:HH22	1.63	0.45
3:C:83:ARG:HG2	3:C:87:LEU:HD12	1.98	0.45
3:C:173:VAL:HG12	3:C:175:LEU:HD21	1.99	0.45
5:E:35:GLY:HA3	5:E:112:LEU:HB3	1.98	0.45
8:H:49:GLU:O	8:H:59:LEU:HA	2.17	0.45
12:L:19:ARG:HA	12:L:20:LYS:HZ1	1.82	0.45
13:M:48:LEU:HB3	13:M:53:VAL:HG23	1.99	0.45
19:S:18:LYS:HZ1	19:S:32:LYS:H	1.65	0.45
1:A:200:G:C6	1:A:201:C:C4	3.05	0.44
1:A:217:C:H2'	1:A:218:C:C6	2.52	0.44
1:A:474:G:C2	1:A:475:G:C4	3.05	0.44
1:A:877:C:O2'	8:H:3:THR:HG23	2.17	0.44
1:A:888:G:H5"	1:A:889:A:O5'	2.16	0.44
1:A:1128:C:N4	1:A:1139:G:N3	2.66	0.44
7:G:73:MET:HA	7:G:91:VAL:HG23	1.98	0.44
12:L:76:ASN:ND2	12:L:108:ALA:H	2.15	0.44
14:N:3:ARG:HB2	14:N:6:LEU:HB2	1.99	0.44
14:N:29:ARG:NH1	14:N:42:ILE:HG13	2.32	0.44
17:Q:59:ILE:HA	17:Q:59:ILE:HD12	1.69	0.44
18:R:43:PHE:HD2	18:R:56:THR:HG22	1.83	0.44
1:A:254:G:OP1	17:Q:67:LYS:O	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:A:OP1	1:A:280:C:O2'	2.27	0.44
1:A:532:A:H2'	1:A:533:A:OP1	2.17	0.44
1:A:1347:G:O6	9:I:10:ARG:NH2	2.50	0.44
10:J:7:LYS:HG2	10:J:9:ARG:HG2	1.98	0.44
1:A:600:C:N4	1:A:638:G:H1	2.16	0.44
1:A:840:C:H5'	1:A:848:C:O2	2.17	0.44
1:A:1347:G:N2	1:A:1374:A:OP2	2.28	0.44
1:A:1424:C:H2'	1:A:1425:U:C6	2.48	0.44
2:B:134:GLU:O	2:B:137:ARG:HG2	2.18	0.44
2:B:220:ASP:HA	2:B:230:VAL:HG21	1.99	0.44
4:D:148:VAL:HB	4:D:181:MET:HB3	2.00	0.44
4:D:155:LEU:HD13	4:D:156:GLU:H	1.80	0.44
5:E:61:TYR:O	5:E:64:ARG:O	2.35	0.44
8:H:10:LEU:N	8:H:10:LEU:HD23	2.31	0.44
11:K:40:ILE:HG13	11:K:75:TYR:CD1	2.52	0.44
19:S:5:LEU:HD22	19:S:70:LYS:HZ1	1.82	0.44
19:S:15:LEU:HD12	19:S:16:LEU:H	1.83	0.44
1:A:76:C:N4	1:A:93:G:N1	2.66	0.44
1:A:76:C:N4	1:A:95:U:H3	2.04	0.44
1:A:656:C:O2'	15:O:28:GLN:NE2	2.51	0.44
1:A:1000:U:C4	1:A:1042:G:C6	3.06	0.44
1:A:1255:G:O2'	1:A:1258:G:O2'	2.35	0.44
1:A:1349:A:OP1	9:I:120:ARG:HB2	2.18	0.44
3:C:23:TYR:CD1	10:J:10:GLY:HA2	2.52	0.44
4:D:207:TYR:CD2	4:D:207:TYR:N	2.84	0.44
5:E:64:ARG:H	5:E:64:ARG:HG2	1.66	0.44
12:L:51:ALA:O	12:L:52:LEU:HD23	2.17	0.44
13:M:22:ILE:HD12	13:M:25:ILE:HG13	2.00	0.44
14:N:24:CYS:CB	14:N:40:CYS:HB3	2.47	0.44
15:O:14:GLU:HB3	15:O:15:PHE:HD1	1.82	0.44
1:A:409:G:OP1	4:D:24:GLU:O	2.35	0.44
1:A:736:C:H2'	1:A:737:A:H8	1.78	0.44
1:A:778:G:H2'	1:A:779:C:O4'	2.17	0.44
1:A:923:A:OP1	5:E:21:ALA:HB2	2.17	0.44
1:A:1221:G:C4	1:A:1222:G:C8	3.05	0.44
1:A:1310:G:H5'	13:M:77:ASN:HD21	1.81	0.44
1:A:1328:C:H2'	1:A:1329:A:H8	1.81	0.44
1:A:1343:G:H4'	9:I:122:ALA:HB3	1.99	0.44
1:A:1486:G:C6	1:A:1487:G:C6	3.06	0.44
2:B:95:GLN:HG2	2:B:148:TYR:HD2	1.82	0.44
4:D:15:GLU:HB3	4:D:63:LYS:CG	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:102:ARG:HG3	8:H:102:ARG:O	2.18	0.44
12:L:6:THR:OG1	12:L:9:GLN:HG3	2.17	0.44
13:M:20:THR:O	13:M:20:THR:OG1	2.33	0.44
16:P:11:SER:N	16:P:14:ASN:O	2.49	0.44
1:A:178:C:H2'	1:A:179:A:H5'	1.99	0.44
1:A:374:A:N3	1:A:374:A:H2'	2.33	0.44
1:A:500:G:C5	1:A:546:G:N2	2.86	0.44
1:A:537:G:H2'	1:A:538:G:C8	2.52	0.44
1:A:613:C:OP1	4:D:84:LYS:HE3	2.17	0.44
1:A:813:U:OP2	1:A:813:U:H6	2.00	0.44
1:A:1245:A:N1	1:A:1293:G:C2	2.85	0.44
7:G:145:ALA:C	7:G:147:ALA:H	2.21	0.44
10:J:31:GLY:HA3	10:J:81:THR:OG1	2.17	0.44
12:L:46:LYS:HG2	12:L:94:TRP:CE2	2.53	0.44
13:M:45:VAL:O	13:M:48:LEU:HD23	2.18	0.44
17:Q:75:ARG:HH11	17:Q:75:ARG:HB2	1.83	0.44
18:R:26:LEU:HD12	18:R:26:LEU:HA	1.56	0.44
20:T:29:LYS:O	20:T:33:ILE:HG12	2.18	0.44
1:A:581:G:O6	1:A:758:G:C8	2.71	0.44
1:A:619:U:C4	4:D:135:LEU:HD21	2.53	0.44
1:A:620:C:H2'	1:A:621:A:O4'	2.17	0.44
1:A:903:G:O2'	1:A:904:C:H5'	2.18	0.44
1:A:916:G:H2'	1:A:917:G:H8	1.83	0.44
1:A:939:G:C6	1:A:940:C:N4	2.85	0.44
1:A:1035:A:C6	1:A:1036:G:C6	3.05	0.44
2:B:154:LEU:HA	2:B:154:LEU:HD13	1.56	0.44
7:G:136:LYS:HB3	7:G:136:LYS:HE2	1.58	0.44
12:L:38:THR:HB	12:L:39:VAL:H	1.62	0.44
18:R:45:SER:OG	18:R:47:THR:O	2.31	0.44
21:U:5:ASP:HB3	21:U:8:THR:OG1	2.18	0.44
1:A:402:G:H4'	1:A:620:C:O2	2.18	0.44
1:A:614:A:H2'	1:A:615:C:H6	1.83	0.44
1:A:642:A:H2'	1:A:643:C:C6	2.53	0.44
1:A:664:G:OP1	18:R:64:ARG:HD2	2.17	0.44
4:D:111:ALA:HB3	4:D:117:ALA:HB2	1.99	0.44
17:Q:6:LEU:HB3	17:Q:23:VAL:HG11	1.99	0.44
1:A:113:G:H2'	1:A:114:U:H6	1.83	0.44
1:A:392:G:H2'	1:A:393:A:H8	1.83	0.44
1:A:447:G:H2'	1:A:485:G:N2	2.33	0.44
1:A:960:U:O5'	1:A:961:U:H5"	2.18	0.44
1:A:1058:G:H22	10:J:53:PRO:HG3	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1064:G:OP1	1:A:1386:G:H4'	2.17	0.44
1:A:1162:C:H2'	1:A:1163:C:C6	2.53	0.44
2:B:60:ASP:O	2:B:64:ARG:HG3	2.18	0.44
3:C:39:ILE:HG21	3:C:57:ILE:CD1	2.48	0.44
5:E:78:HIS:CD2	8:H:104:ARG:HG2	2.53	0.44
9:I:31:GLN:HG2	9:I:35:GLU:HB3	1.99	0.44
12:L:19:ARG:HA	12:L:20:LYS:HZ2	1.82	0.44
16:P:45:THR:O	16:P:48:TRP:HD1	2.01	0.44
19:S:64:GLU:HG3	19:S:65:ASN:H	1.82	0.44
1:A:384:G:C6	1:A:385:C:N4	2.86	0.43
1:A:819:A:H4'	1:A:820:U:OP2	2.18	0.43
1:A:1232:U:O5'	1:A:1232:U:H6	2.01	0.43
1:A:1442:G:C5	1:A:1446:A:N6	2.86	0.43
2:B:7:VAL:HG11	2:B:221:LEU:CD2	2.48	0.43
2:B:87:ARG:HD2	2:B:219:VAL:HG11	1.99	0.43
2:B:150:SER:OG	2:B:151:GLY:N	2.50	0.43
5:E:37:ARG:O	5:E:114:GLY:HA3	2.18	0.43
8:H:83:ILE:HG22	8:H:83:ILE:O	2.18	0.43
14:N:37:PHE:C	14:N:39:LEU:N	2.72	0.43
15:O:57:LEU:HD12	15:O:57:LEU:HA	1.74	0.43
15:O:85:LEU:HD23	15:O:85:LEU:HA	1.61	0.43
18:R:42:ARG:NH1	18:R:42:ARG:HB3	2.33	0.43
1:A:353:A:H5'	1:A:353:A:H8	1.83	0.43
1:A:514:C:H2'	1:A:515:G:H8	1.83	0.43
1:A:922:G:N3	1:A:1398:A:H2	2.16	0.43
1:A:1018:C:H2'	1:A:1019:C:O4'	2.18	0.43
1:A:1035:A:H2'	1:A:1036:G:C8	2.53	0.43
1:A:1519[A]:MA6:H3'	1:A:1520[A]:G:C5'	2.49	0.43
2:B:50:GLU:O	2:B:53:ARG:HG3	2.17	0.43
5:E:112:LEU:C	5:E:114:GLY:H	2.18	0.43
12:L:58:VAL:HG12	12:L:59:ARG:N	2.33	0.43
13:M:100:GLY:N	13:M:101:GLN:OE1	2.51	0.43
1:A:78:G:N2	1:A:92:C:C5	2.87	0.43
1:A:484:G:O5'	1:A:484:G:H8	1.99	0.43
1:A:542:G:OP1	4:D:10:ARG:NH2	2.51	0.43
1:A:671:G:H5'	6:F:77:ARG:HH21	1.81	0.43
1:A:736:C:OP2	18:R:68:LYS:HE3	2.19	0.43
1:A:1158:C:H42	1:A:1181:G:H1	1.67	0.43
1:A:1264:C:H2'	1:A:1265:G:C8	2.53	0.43
1:A:1349:A:C2	1:A:1374:A:C4	3.06	0.43
2:B:172:ILE:H	2:B:172:ILE:CD1	2.28	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:187:LEU:HD22	2:B:201:ILE:O	2.18	0.43
3:C:3:ASN:HB3	3:C:4:LYS:HG3	2.00	0.43
4:D:207:TYR:N	4:D:207:TYR:HD2	2.16	0.43
11:K:72:ALA:O	11:K:75:TYR:N	2.43	0.43
13:M:107:ALA:HB3	13:M:111:LYS:HE3	2.00	0.43
17:Q:26:GLN:HG2	17:Q:37:LYS:HB2	2.00	0.43
19:S:6:LYS:HE2	19:S:6:LYS:HB2	1.52	0.43
20:T:73:HIS:O	20:T:76:ALA:HB3	2.19	0.43
1:A:313:A:H2'	1:A:314:C:C6	2.53	0.43
1:A:378:G:H2'	1:A:379:C:C6	2.54	0.43
1:A:866:C:H2'	1:A:867:G:O4'	2.18	0.43
1:A:1050:G:O6	1:A:1208:C:N4	2.50	0.43
1:A:1240:U:C2	7:G:32:ARG:HD2	2.52	0.43
1:A:1354:C:H2'	1:A:1355:G:C8	2.51	0.43
2:B:180:LEU:O	2:B:181:PHE:HB2	2.18	0.43
3:C:88:ARG:NH2	3:C:101:LEU:HB2	2.29	0.43
4:D:170:VAL:CG1	4:D:174:LEU:HB2	2.48	0.43
5:E:137:GLU:HA	5:E:140:ARG:HH11	1.81	0.43
9:I:62:TYR:HD1	9:I:63:ILE:N	2.17	0.43
11:K:20:TYR:CZ	11:K:83:ILE:HD13	2.52	0.43
12:L:42:THR:HG21	12:L:52:LEU:HB3	1.99	0.43
1:A:429:U:H4'	1:A:430:A:O5'	2.17	0.43
1:A:502:G:H2'	1:A:503:C:O4'	2.19	0.43
1:A:675:A:H1'	11:K:116:HIS:CD2	2.53	0.43
1:A:782:A:H2'	1:A:783:C:O4'	2.18	0.43
1:A:925:G:C2	1:A:927:G:C8	3.06	0.43
1:A:1073:U:O2	2:B:104:ASN:ND2	2.51	0.43
1:A:1203:C:H2'	1:A:1204:A:O4'	2.18	0.43
1:A:1212:U:H4'	1:A:1213:A:C8	2.54	0.43
1:A:1328:C:OP1	21:U:21:TYR:OH	2.35	0.43
1:A:1412:C:H42	1:A:1488:G:H1	1.66	0.43
2:B:16:HIS:ND1	2:B:17:PHE:O	2.51	0.43
2:B:113:HIS:HD1	2:B:113:HIS:H	1.65	0.43
2:B:215:LEU:HD23	2:B:215:LEU:HA	1.79	0.43
2:B:238:LEU:HD22	2:B:238:LEU:HA	1.83	0.43
3:C:47:LEU:HD21	3:C:76:VAL:HG23	1.98	0.43
4:D:100:ARG:HH12	4:D:137:SER:HB3	1.83	0.43
9:I:5:TYR:CD1	9:I:6:GLY:N	2.83	0.43
9:I:73:GLN:O	9:I:77:ILE:HG12	2.18	0.43
12:L:27:LEU:C	12:L:29:GLY:N	2.60	0.43
18:R:51:LEU:HB2	18:R:56:THR:HG23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:78:LEU:HA	18:R:78:LEU:HD23	1.58	0.43
1:A:1065:U:H5"	1:A:1190:G:N2	2.33	0.43
1:A:1189:C:P	10:J:51:ARG:HH22	2.41	0.43
4:D:196:LEU:HA	4:D:197:PRO:HD3	1.69	0.43
9:I:27:THR:HG23	9:I:63:ILE:H	1.83	0.43
11:K:30:VAL:HG21	11:K:65:ALA:HA	2.00	0.43
12:L:113:ARG:O	12:L:113:ARG:HG3	2.17	0.43
1:A:11:G:C5	1:A:12:U:C5	3.07	0.43
1:A:95:U:O2'	1:A:96:G:H5'	2.17	0.43
1:A:731:G:O2'	1:A:732:C:H5'	2.18	0.43
1:A:894:G:C6	1:A:895:G:C5	3.06	0.43
1:A:968:A:C8	1:A:1062:U:H4'	2.54	0.43
1:A:1130:A:OP1	1:A:1131:G:C8	2.71	0.43
1:A:1236:A:OP1	21:U:3:LYS:HG3	2.19	0.43
1:A:1494:G:H2'	1:A:1495:U:H5'	2.01	0.43
1:A:1526:G:H2'	1:A:1527:C:H6	1.83	0.43
2:B:11:LEU:O	2:B:11:LEU:HD23	2.18	0.43
4:D:154:ASN:C	4:D:159:ARG:HH21	2.20	0.43
5:E:69:VAL:HG21	5:E:113:ALA:HB1	2.00	0.43
5:E:142:LEU:HA	5:E:142:LEU:HD23	1.61	0.43
10:J:7:LYS:HA	10:J:71:LEU:HD12	1.99	0.43
10:J:27:ALA:HA	10:J:81:THR:CG2	2.47	0.43
20:T:81:LYS:O	20:T:85:MET:HG3	2.18	0.43
1:A:767:A:H2'	1:A:768:A:O4'	2.18	0.43
2:B:73:THR:HG23	2:B:95:GLN:O	2.19	0.43
4:D:88:VAL:O	4:D:92:VAL:HG23	2.18	0.43
6:F:95:GLU:O	6:F:97:PHE:N	2.52	0.43
7:G:26:PHE:O	7:G:30:ILE:HG13	2.19	0.43
9:I:8:GLY:HA2	9:I:79:LEU:CD1	2.48	0.43
9:I:99:LEU:HB3	9:I:101:PHE:CD1	2.54	0.43
17:Q:15:MET:HE3	17:Q:15:MET:HB2	1.83	0.43
21:U:25:LYS:HA	21:U:25:LYS:HE3	2.00	0.43
1:A:193:C:H2'	1:A:194:C:H6	1.84	0.43
1:A:501:C:O3'	12:L:118:SER:OG	2.36	0.43
1:A:927:G:H1	1:A:1390:U:H3	1.64	0.43
1:A:1032:G:C2	1:A:1033:G:C4	3.07	0.43
1:A:1092:A:H8	1:A:1092:A:O5'	2.01	0.43
1:A:1147:C:H4'	9:I:5:TYR:HE2	1.83	0.43
1:A:1228:C:OP1	13:M:115:LYS:HG2	2.18	0.43
1:A:1269:A:N1	1:A:1312:G:O2'	2.49	0.43
1:A:1477:C:H2'	1:A:1478:C:C6	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:28:ALA:CB	8:H:59:LEU:HG	2.46	0.43
8:H:89:PRO:HA	8:H:92:ARG:NH1	2.34	0.43
11:K:40:ILE:HG23	11:K:75:TYR:HD1	1.84	0.43
12:L:113:ARG:HD3	12:L:115:LYS:H	1.83	0.43
19:S:7:LYS:HE3	19:S:7:LYS:HB3	1.91	0.43
20:T:36:LEU:HD22	20:T:36:LEU:HA	1.81	0.43
1:A:243:A:H2	1:A:245:C:H2'	1.84	0.43
1:A:586:C:O3'	8:H:89:PRO:HB2	2.19	0.43
1:A:728:A:H2'	1:A:729:A:O4'	2.19	0.43
1:A:827:U:H2'	1:A:859:A:N1	2.34	0.43
1:A:836:G:H5"	1:A:836:G:C8	2.53	0.43
1:A:893:C:H2'	1:A:894:G:C8	2.54	0.43
1:A:1026:G:C8	1:A:1027:C:C6	3.07	0.43
1:A:1283:G:H2'	1:A:1284:C:H6	1.83	0.43
1:A:1517[A]:G:H2'	1:A:1518[A]:MA6:C8	2.46	0.43
4:D:4:TYR:CE2	4:D:11:LEU:HD11	2.53	0.43
4:D:117:ALA:O	4:D:121:VAL:HG23	2.19	0.43
5:E:11:ILE:HG21	5:E:31:LEU:HD12	2.01	0.43
6:F:11:ASN:OD1	6:F:14:LEU:HD23	2.18	0.43
6:F:53:ALA:C	6:F:55:ASP:H	2.22	0.43
12:L:71:PRO:O	12:L:102:ARG:HD3	2.19	0.43
17:Q:29:HIS:CG	17:Q:30:PRO:HD2	2.54	0.43
1:A:407:G:O6	1:A:408:A:N6	2.51	0.42
1:A:409:G:H1	1:A:433:C:N4	2.09	0.42
1:A:414:A:OP2	1:A:428:G:N2	2.21	0.42
1:A:451:A:N7	1:A:481:G:N1	2.67	0.42
1:A:481:G:O2'	1:A:482:A:C8	2.71	0.42
1:A:1329:A:H5'	13:M:29:ARG:HD2	2.00	0.42
1:A:1368:G:H5'	9:I:112:LYS:O	2.19	0.42
1:A:1416:G:H2'	1:A:1417:G:O4'	2.19	0.42
2:B:24:TRP:CG	2:B:25:ASN:N	2.86	0.42
2:B:44:LEU:HD12	2:B:44:LEU:H	1.83	0.42
4:D:60:GLU:OE1	4:D:60:GLU:HA	2.17	0.42
7:G:80:VAL:HG11	7:G:154:TYR:CE1	2.51	0.42
11:K:24:SER:OG	11:K:25:TYR:N	2.52	0.42
1:A:328:C:H4'	1:A:329:A:H5'	2.00	0.42
1:A:448:A:OP2	1:A:485:G:N2	2.44	0.42
1:A:815:A:N6	1:A:1509:C:H1'	2.34	0.42
1:A:824:C:H2'	1:A:825:G:C8	2.54	0.42
1:A:939:G:H2'	1:A:940:C:C6	2.54	0.42
1:A:1236:A:O5'	21:U:2:GLY:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1357:A:C5	1:A:1358:U:C4	3.07	0.42
3:C:126:ARG:HA	3:C:126:ARG:HD3	1.82	0.42
4:D:3:ARG:HD2	4:D:71:SER:H	1.85	0.42
5:E:12:LEU:HD13	5:E:31:LEU:HB2	2.00	0.42
5:E:80:ILE:CD1	5:E:138:ALA:HB1	2.49	0.42
7:G:151:TYR:N	7:G:151:TYR:CD1	2.85	0.42
8:H:39:LEU:HD23	8:H:39:LEU:HA	1.64	0.42
10:J:40:LEU:HD12	10:J:69:ASN:HB2	2.01	0.42
17:Q:29:HIS:O	17:Q:33:GLY:HA2	2.19	0.42
19:S:19:VAL:HG23	19:S:47:HIS:CE1	2.54	0.42
20:T:75:ASN:OD1	20:T:75:ASN:N	2.51	0.42
1:A:634:C:O2'	1:A:635:G:H5'	2.19	0.42
1:A:839:U:O2	1:A:839:U:H2'	2.18	0.42
1:A:1010:G:H2'	1:A:1011:G:H5"	2.01	0.42
1:A:1315:U:H2'	1:A:1316:G:O4'	2.19	0.42
2:B:88:ALA:HB1	2:B:90:MET:HG2	2.01	0.42
3:C:77:ILE:CG2	3:C:81:GLY:HA2	2.49	0.42
3:C:199:LYS:HB3	3:C:201:TYR:HE1	1.83	0.42
4:D:57:ARG:NH2	5:E:107:ARG:HD3	2.34	0.42
6:F:25:ILE:HD12	6:F:25:ILE:HA	1.88	0.42
8:H:1:MET:HG2	8:H:2:LEU:O	2.18	0.42
10:J:30:SER:OG	10:J:81:THR:HG23	2.18	0.42
11:K:109:VAL:HA	18:R:85:LEU:O	2.19	0.42
1:A:439:A:C4	1:A:497:A:C2	3.07	0.42
1:A:691:G:O2'	1:A:797:C:H4'	2.19	0.42
1:A:768:A:C5	1:A:769:G:C8	3.07	0.42
1:A:942:G:H21	9:I:124:GLN:NE2	2.18	0.42
1:A:1256:A:H4'	1:A:1257:U:O5'	2.18	0.42
1:A:1320:C:H42	19:S:36:ARG:HD3	1.84	0.42
1:A:1355:G:H1	1:A:1367:C:N4	2.17	0.42
1:A:1498:UR3:H1'	1:A:1499:A:N7	2.34	0.42
3:C:39:ILE:HG21	3:C:57:ILE:HD12	2.01	0.42
11:K:58:PRO:HD3	11:K:89:ALA:HB1	2.01	0.42
12:L:77:LEU:HD21	12:L:107:ALA:HA	2.02	0.42
12:L:89:ARG:HG2	12:L:97:ARG:HA	2.01	0.42
15:O:65:ARG:HE	15:O:65:ARG:HB2	1.35	0.42
17:Q:90:ILE:O	17:Q:91:ARG:C	2.58	0.42
1:A:8:A:H5'	5:E:101:ILE:HG22	2.02	0.42
1:A:355:C:C4	1:A:356:A:N7	2.87	0.42
1:A:444:C:H2'	1:A:445:G:H8	1.82	0.42
1:A:663:A:H61	1:A:742:G:H1	1.65	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:806:C:O2'	1:A:807:A:H5'	2.20	0.42
1:A:1314:C:O2'	1:A:1315:U:H5'	2.19	0.42
1:A:1332:A:H2'	1:A:1333:A:H8	1.83	0.42
1:A:1478:C:H2'	1:A:1479:C:C6	2.54	0.42
1:A:1515[B]:C:N4	1:A:1520[B]:G:H1	2.12	0.42
2:B:23:ARG:HA	2:B:23:ARG:HH11	1.85	0.42
2:B:82:ARG:HG3	2:B:92:TYR:CE1	2.55	0.42
2:B:87:ARG:NH1	2:B:219:VAL:HB	2.35	0.42
4:D:150:GLU:OE1	4:D:151:LYS:HG2	2.18	0.42
5:E:144:THR:HG22	5:E:145:LYS:N	2.34	0.42
7:G:54:THR:C	7:G:56:GLN:H	2.22	0.42
12:L:46:LYS:HG3	12:L:92:ASP:O	2.20	0.42
16:P:38:TYR:O	16:P:49:LEU:HD12	2.20	0.42
17:Q:62:SER:OG	17:Q:72:ARG:HG2	2.19	0.42
19:S:49:ILE:HG22	19:S:51:VAL:HG22	2.02	0.42
1:A:49:U:O2'	1:A:50:A:H2'	2.20	0.42
1:A:77:G:N2	1:A:78:G:C4	2.87	0.42
1:A:259:G:O2'	1:A:260:G:H5'	2.20	0.42
1:A:350:G:H8	1:A:350:G:C5'	2.31	0.42
1:A:695:A:H2'	1:A:696:A:C8	2.54	0.42
1:A:781:A:C4	1:A:802:A:C2	3.07	0.42
1:A:1064:G:H22	1:A:1190:G:H2'	1.83	0.42
1:A:1198:G:H2'	1:A:1199:U:C6	2.55	0.42
1:A:1279:A:H4'	1:A:1280:A:OP1	2.19	0.42
1:A:1300:G:H5"	1:A:1335:C:N4	2.34	0.42
1:A:1367:C:N3	1:A:1368:G:C8	2.88	0.42
1:A:1520[B]:G:H2'	1:A:1521:G:C8	2.53	0.42
2:B:87:ARG:HH11	2:B:219:VAL:HB	1.83	0.42
3:C:52:LEU:HD11	3:C:68:VAL:CG2	2.47	0.42
4:D:202:LEU:HA	4:D:202:LEU:HD13	1.37	0.42
9:I:127:LYS:O	9:I:128:ARG:C	2.57	0.42
10:J:47:PHE:O	10:J:62:HIS:HB2	2.20	0.42
12:L:34:ARG:HB2	12:L:105:TYR:CE1	2.54	0.42
12:L:60:LEU:HB2	12:L:64:TYR:O	2.19	0.42
15:O:46:HIS:C	15:O:48:LYS:N	2.73	0.42
1:A:78:G:N2	1:A:92:C:C4	2.88	0.42
1:A:442:C:H2'	1:A:443:C:H6	1.84	0.42
1:A:824:C:H2'	1:A:825:G:H8	1.84	0.42
1:A:1003:G:H22	1:A:1004:A:H1'	1.85	0.42
1:A:1130:A:H5"	9:I:20:ARG:HH21	1.84	0.42
1:A:1266:G:N2	1:A:1269:A:OP2	2.42	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1518[A]:MA6:H93	1:A:1519[A]:MA6:N6	2.35	0.42
3:C:150:LYS:HE3	3:C:173:VAL:HB	2.02	0.42
6:F:33:TYR:HD2	6:F:71:ARG:HD2	1.84	0.42
10:J:49:VAL:HG23	10:J:61:GLU:O	2.20	0.42
11:K:53:SER:O	11:K:55:LYS:N	2.52	0.42
12:L:22:SER:C	12:L:24:VAL:N	2.73	0.42
14:N:12:ARG:HB3	14:N:13:THR:H	1.65	0.42
17:Q:17:LYS:N	17:Q:49:GLU:OE2	2.42	0.42
20:T:87:LYS:O	20:T:91:LEU:HB2	2.19	0.42
21:U:10:ARG:HG3	21:U:13:ILE:CD1	2.45	0.42
1:A:162:A:H1'	1:A:348:G:O2'	2.20	0.42
1:A:243:A:C2	1:A:246:A:C8	3.08	0.42
1:A:544:G:C6	1:A:545:C:C4	3.08	0.42
1:A:856:C:H2'	1:A:857:C:H6	1.85	0.42
1:A:1258:G:OP2	1:A:1258:G:H8	2.02	0.42
1:A:1421:G:H2'	1:A:1422:G:O4'	2.20	0.42
6:F:33:TYR:HA	6:F:71:ARG:CZ	2.50	0.42
8:H:9:MET:HG3	8:H:26:VAL:HG21	2.02	0.42
8:H:70:GLN:OE1	8:H:70:GLN:HA	2.20	0.42
16:P:75:ARG:HE	16:P:80:PHE:HD1	1.66	0.42
18:R:76:LEU:HA	18:R:76:LEU:HD23	1.57	0.42
19:S:80:TYR:CZ	19:S:81:ARG:HB3	2.55	0.42
1:A:359:U:H2'	1:A:360:A:H8	1.81	0.42
1:A:411:A:C4	1:A:413:G:H1'	2.55	0.42
1:A:442:C:H42	1:A:492:G:H1	1.67	0.42
1:A:475:G:C2	1:A:476:G:C5	3.08	0.42
1:A:500:G:C6	1:A:501:C:C4	3.08	0.42
1:A:642:A:H2'	1:A:643:C:H6	1.85	0.42
1:A:781:A:C5	1:A:802:A:C2	3.08	0.42
1:A:794:A:H2'	1:A:795:C:O4'	2.19	0.42
1:A:903:G:H2'	1:A:904:C:H6	1.84	0.42
1:A:1502:A:C2	1:A:1504:G:C2	3.08	0.42
1:A:1530:G:H2'	1:A:1531:A:C8	2.54	0.42
2:B:43:ASP:OD1	2:B:46:LYS:HG3	2.20	0.42
5:E:81:GLU:HG2	5:E:88:LYS:HE2	2.02	0.42
10:J:50:ILE:HA	10:J:60:ARG:CB	2.43	0.42
12:L:53:ARG:HH11	12:L:93:LEU:HD21	1.85	0.42
18:R:47:THR:HG22	18:R:48:GLY:H	1.85	0.42
1:A:179:A:O2'	1:A:180:U:H5'	2.20	0.42
1:A:293:G:H1	1:A:304:U:H3	1.68	0.42
1:A:411:A:N7	1:A:413:G:C4	2.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:477:G:N2	1:A:478:A:C5	2.88	0.42
1:A:881:G:H2'	1:A:882:C:O4'	2.20	0.42
1:A:1435:G:H8	1:A:1435:G:O5'	2.03	0.42
1:A:1474:G:N1	1:A:1475:G:O6	2.53	0.42
1:A:1486:G:H2'	1:A:1487:G:C1'	2.49	0.42
1:A:1493:A:HO2'	1:A:1494:G:H8	1.67	0.42
3:C:131:ARG:O	3:C:134:ILE:HB	2.19	0.42
4:D:36:ARG:N	4:D:37:PRO:HD3	2.35	0.42
7:G:62:PHE:CD2	7:G:63:LYS:HD3	2.55	0.42
13:M:71:ARG:HB3	13:M:71:ARG:HH11	1.85	0.42
13:M:81:LEU:HD11	13:M:88:ARG:NH2	2.34	0.42
14:N:54:PRO:C	14:N:56:VAL:H	2.24	0.42
15:O:5:LYS:O	15:O:8:LYS:N	2.53	0.42
15:O:22:THR:O	15:O:27:VAL:HG11	2.20	0.42
1:A:66:G:N3	1:A:66:G:H2'	2.35	0.41
1:A:102:G:H2'	1:A:103:C:C6	2.55	0.41
1:A:1003:G:N2	1:A:1038:C:N3	2.67	0.41
1:A:1199:U:O5'	1:A:1199:U:H6	2.02	0.41
1:A:1375:A:P	7:G:28:ASN:HD22	2.43	0.41
1:A:1493:A:C2'	1:A:1494:G:H8	2.32	0.41
4:D:116:GLN:NE2	4:D:157:LEU:HD11	2.34	0.41
6:F:25:ILE:HD12	6:F:28:ARG:HH11	1.85	0.41
6:F:91:VAL:HG12	6:F:92:LYS:O	2.19	0.41
7:G:140:ASP:HA	7:G:143:ARG:HB2	2.02	0.41
13:M:88:ARG:HA	13:M:91:ARG:HB2	2.02	0.41
18:R:58:LEU:HA	18:R:58:LEU:HD23	1.83	0.41
19:S:5:LEU:O	19:S:6:LYS:NZ	2.43	0.41
19:S:31:ILE:O	19:S:50:ALA:HB3	2.20	0.41
21:U:13:ILE:HG13	21:U:14:TRP:N	2.35	0.41
1:A:342:C:O5'	1:A:342:C:H6	2.03	0.41
1:A:901:A:C5	1:A:902:G:H1'	2.55	0.41
1:A:1177:G:OP2	1:A:1177:G:H8	2.04	0.41
1:A:1277:C:O2'	1:A:1279:A:H8	2.03	0.41
2:B:142:LEU:O	2:B:146:GLN:HB2	2.20	0.41
3:C:51:GLY:O	3:C:71:ALA:N	2.39	0.41
3:C:112:SER:HB3	3:C:115:LEU:CD1	2.50	0.41
3:C:187:ALA:HB3	3:C:198:VAL:HB	2.02	0.41
4:D:150:GLU:N	4:D:150:GLU:CD	2.74	0.41
4:D:163:GLU:HG3	4:D:166:LYS:CE	2.50	0.41
5:E:57:LYS:O	5:E:61:TYR:HD2	2.03	0.41
7:G:76:ARG:O	7:G:87:VAL:HG23	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:48:GLU:HB3	9:I:101:PHE:CZ	2.54	0.41
11:K:40:ILE:HG23	11:K:75:TYR:CD1	2.55	0.41
12:L:65:GLU:N	12:L:65:GLU:OE1	2.53	0.41
13:M:27:LYS:HD3	13:M:27:LYS:HA	1.94	0.41
17:Q:83:ASP:O	17:Q:86:GLU:HB2	2.20	0.41
1:A:77:G:H1	1:A:92:C:H42	1.69	0.41
1:A:78:G:C2	1:A:79:G:H1'	2.56	0.41
1:A:120:A:H2'	1:A:122:G:N7	2.35	0.41
1:A:130:A:H1'	1:A:263:A:O2'	2.19	0.41
1:A:567:G:H2'	1:A:568:G:O4'	2.20	0.41
1:A:674:G:H5'	6:F:50:TYR:CE2	2.55	0.41
1:A:686:U:O2'	1:A:687:A:H8	2.03	0.41
1:A:892:A:C2	1:A:907:A:C4	3.08	0.41
1:A:1097:C:H2'	1:A:1098:C:C6	2.55	0.41
2:B:53:ARG:HE	2:B:53:ARG:HB2	1.73	0.41
2:B:85:ALA:HB3	2:B:92:TYR:HB3	2.01	0.41
3:C:110:ASN:O	3:C:141:VAL:HG22	2.20	0.41
7:G:17:VAL:HG12	7:G:18:TYR:N	2.34	0.41
7:G:145:ALA:O	7:G:146:GLU:HB2	2.19	0.41
11:K:43:SER:OG	11:K:44:SER:N	2.53	0.41
19:S:63:THR:OG1	19:S:65:ASN:OD1	2.37	0.41
1:A:79:G:N1	1:A:80:G:C5	2.87	0.41
1:A:664:G:OP1	18:R:64:ARG:NH1	2.43	0.41
1:A:1346:A:C5	7:G:10:ARG:CZ	3.03	0.41
3:C:43:LEU:HA	3:C:47:LEU:HD13	2.03	0.41
3:C:179:ARG:NE	3:C:206:GLU:OE1	2.53	0.41
4:D:25:ARG:HG2	4:D:25:ARG:O	2.20	0.41
6:F:80:ARG:CD	6:F:88:VAL:HB	2.51	0.41
7:G:12:LEU:HD23	7:G:12:LEU:HA	1.90	0.41
7:G:97:GLN:HA	7:G:97:GLN:HE21	1.84	0.41
9:I:11:LYS:O	9:I:12:GLU:HB3	2.20	0.41
10:J:38:ILE:HD11	10:J:71:LEU:CB	2.47	0.41
10:J:40:LEU:HB2	10:J:69:ASN:O	2.20	0.41
16:P:17:TYR:HD1	16:P:39:TYR:HD2	1.67	0.41
20:T:44:ALA:O	20:T:47:GLY:N	2.46	0.41
1:A:216:G:H2'	1:A:217:C:H6	1.84	0.41
1:A:356:A:O2'	1:A:367:U:O2'	2.37	0.41
1:A:407:G:C6	1:A:408:A:C6	3.09	0.41
1:A:600:C:H42	1:A:638:G:H1	1.67	0.41
1:A:632:A:H2'	1:A:633:G:H5'	2.01	0.41
1:A:797:C:O2'	1:A:798:G:H5'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:893:C:H2'	1:A:894:G:H8	1.86	0.41
1:A:1130:A:P	1:A:1130:A:H3'	2.61	0.41
4:D:145:GLU:OE1	4:D:182:LYS:HG2	2.20	0.41
8:H:108:GLY:HA3	8:H:138:TRP:HB3	2.02	0.41
11:K:11:LYS:HE2	11:K:11:LYS:HB2	1.64	0.41
13:M:47:ASP:OD2	13:M:47:ASP:N	2.53	0.41
1:A:7:G:H5'	1:A:298:A:O4'	2.20	0.41
1:A:60:A:P	1:A:331:G:H22	2.43	0.41
1:A:137:C:O4'	16:P:63:GLY:HA3	2.20	0.41
1:A:277:C:OP1	17:Q:68:ARG:NH2	2.54	0.41
1:A:278:G:C6	17:Q:95:TYR:CD2	3.09	0.41
1:A:900:A:H2'	1:A:901:A:O4'	2.21	0.41
1:A:945:G:C2	1:A:1337:G:C2	3.09	0.41
1:A:945:G:N3	1:A:945:G:H2'	2.35	0.41
1:A:1124:G:N7	1:A:1145:C:H6	2.18	0.41
1:A:1175:G:H2'	1:A:1176:A:H8	1.81	0.41
1:A:1261:A:H5"	1:A:1262:C:OP2	2.21	0.41
1:A:1530:G:H4'	1:A:1530:G:OP1	2.20	0.41
3:C:6:HIS:CD2	3:C:8:ILE:H	2.37	0.41
3:C:178:LEU:HA	3:C:178:LEU:HD23	1.84	0.41
4:D:3:ARG:HH12	4:D:70:ILE:HG13	1.86	0.41
4:D:187:ARG:HD2	4:D:187:ARG:HA	1.41	0.41
5:E:32:VAL:HB	5:E:58:ALA:HB1	2.02	0.41
7:G:15:ASP:OD2	7:G:44:TYR:OH	2.39	0.41
10:J:8:LEU:HD11	10:J:72:VAL:HG23	2.02	0.41
10:J:68:HIS:CD2	10:J:68:HIS:N	2.88	0.41
12:L:100:ILE:HD12	12:L:100:ILE:HA	1.92	0.41
15:O:22:THR:OG1	15:O:23:GLY:N	2.53	0.41
17:Q:45:HIS:H	17:Q:72:ARG:HA	1.86	0.41
1:A:92:C:O2	1:A:93:G:C8	2.74	0.41
1:A:602:A:C2	1:A:603:U:C2	3.08	0.41
1:A:833:U:H2'	1:A:834:C:H6	1.79	0.41
1:A:997:U:H3	1:A:1044:A:H2	1.67	0.41
1:A:1148:U:H2'	1:A:1149:C:O4'	2.21	0.41
1:A:1299:A:N3	1:A:1299:A:H2'	2.35	0.41
1:A:1417:G:H8	1:A:1417:G:OP2	2.04	0.41
1:A:1502:A:H2'	1:A:1504:G:N7	2.35	0.41
5:E:127:ASN:HA	5:E:128:PRO:HD3	1.76	0.41
9:I:112:LYS:HG2	9:I:113:LYS:N	2.35	0.41
11:K:40:ILE:HD12	11:K:40:ILE:HA	1.78	0.41
13:M:15:VAL:HG21	13:M:48:LEU:HD21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:65:LYS:C	13:M:66:LEU:HD23	2.40	0.41
14:N:14:PRO:O	14:N:15:LYS:HB3	2.21	0.41
15:O:18:PHE:CE1	15:O:21:ASP:HB2	2.56	0.41
15:O:30:ALA:HA	15:O:85:LEU:HD11	2.01	0.41
15:O:36:ILE:HA	15:O:59:MET:CE	2.50	0.41
17:Q:47:PRO:HD2	17:Q:48:GLU:H	1.85	0.41
18:R:40:LEU:HD23	18:R:40:LEU:HA	1.57	0.41
1:A:340:U:H2'	1:A:341:C:C6	2.56	0.41
1:A:456:C:N3	1:A:477:G:C2	2.88	0.41
1:A:632:A:C2'	1:A:633:G:H5'	2.50	0.41
1:A:784:C:C2	1:A:799:G:N2	2.89	0.41
1:A:925:G:O4'	1:A:1502:A:C5	2.74	0.41
1:A:1054:C:OP1	1:A:1197:G:OP1	2.39	0.41
1:A:1110:A:H8	1:A:1110:A:O5'	2.04	0.41
1:A:1111:A:N1	3:C:177:THR:HB	2.35	0.41
1:A:1297:C:HO2'	1:A:1298:C:P	2.43	0.41
1:A:1422:G:C2	1:A:1423:G:N7	2.88	0.41
4:D:17:VAL:HG11	4:D:63:LYS:HE2	2.02	0.41
4:D:18:LYS:HG3	4:D:33:MET:HG3	2.03	0.41
8:H:102:ARG:HH11	8:H:105:ARG:HD3	1.86	0.41
10:J:85:LEU:HD13	10:J:85:LEU:HA	1.73	0.41
18:R:22:VAL:O	18:R:25:THR:N	2.50	0.41
1:A:74:C:H2'	1:A:75:G:O4'	2.20	0.41
1:A:77:G:O2'	1:A:78:G:H5'	2.20	0.41
1:A:204:U:H5'	1:A:216:G:C4	2.55	0.41
1:A:251:G:H4'	1:A:252:U:O5'	2.21	0.41
1:A:474:G:H4'	16:P:81:ARG:NH2	2.36	0.41
1:A:539:A:H2'	1:A:540:G:H8	1.82	0.41
1:A:644:G:C6	1:A:645:C:C5	3.08	0.41
1:A:687:A:H4'	1:A:688:G:O5'	2.21	0.41
1:A:803:G:C6	1:A:804:U:C4	3.09	0.41
1:A:851:G:H5"	1:A:851:G:C8	2.56	0.41
1:A:942:G:N2	1:A:943:U:C2	2.89	0.41
1:A:1019:C:H2'	1:A:1020:U:C6	2.56	0.41
1:A:1128:C:O2	1:A:1143:G:N2	2.47	0.41
1:A:1292:U:H2'	1:A:1293:G:C8	2.55	0.41
1:A:1340:A:H2'	1:A:1341:U:O4'	2.21	0.41
1:A:1369:C:H2'	1:A:1370:G:O4'	2.21	0.41
2:B:180:LEU:HB2	2:B:182:ILE:HG13	2.03	0.41
2:B:191:ASP:OD1	2:B:192:SER:N	2.53	0.41
2:B:240:GLN:OE1	2:B:240:GLN:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:179:ARG:O	3:C:181:ASN:N	2.54	0.41
4:D:121:VAL:HG11	4:D:136:PRO:HA	2.01	0.41
5:E:80:ILE:HG21	5:E:80:ILE:HD13	1.65	0.41
9:I:8:GLY:CA	9:I:79:LEU:HB3	2.51	0.41
11:K:68:ALA:O	11:K:71:LYS:HB2	2.21	0.41
12:L:57:LYS:HD3	12:L:67:THR:HG23	2.02	0.41
13:M:46:LYS:HE2	13:M:47:ASP:OD2	2.21	0.41
15:O:12:ILE:CG1	15:O:31:LEU:HD11	2.51	0.41
19:S:80:TYR:CG	19:S:81:ARG:N	2.89	0.41
1:A:37:U:H2'	1:A:38:G:O4'	2.20	0.41
1:A:132:C:H2'	1:A:133:U:H6	1.85	0.41
1:A:238:G:OP1	17:Q:25:ARG:NH2	2.54	0.41
1:A:456:C:H2'	1:A:457:C:C6	2.57	0.41
1:A:730:G:N2	1:A:765:G:H5"	2.36	0.41
1:A:1149:C:O2'	1:A:1280:A:N1	2.50	0.41
1:A:1320:C:N3	19:S:36:ARG:HD3	2.35	0.41
1:A:1367:C:H3'	9:I:112:LYS:HZ2	1.86	0.41
1:A:1372:U:H2'	1:A:1373:G:O4'	2.20	0.41
3:C:5:ILE:HD13	3:C:10:PHE:HB2	2.03	0.41
3:C:61:ALA:C	3:C:63:ASN:H	2.24	0.41
4:D:14:ARG:HA	4:D:14:ARG:HD3	1.97	0.41
5:E:90:VAL:O	5:E:120:THR:HA	2.21	0.41
6:F:11:ASN:HB2	6:F:86:ARG:NE	2.36	0.41
9:I:103:THR:HG22	9:I:104:ARG:O	2.21	0.41
12:L:28:LYS:C	12:L:30:ALA:H	2.24	0.41
15:O:60:VAL:HG12	15:O:61:GLY:N	2.36	0.41
1:A:391:G:C6	1:A:392:G:N7	2.89	0.40
1:A:524:G:H2'	1:A:525:C:C6	2.56	0.40
1:A:619:U:N3	4:D:135:LEU:HD21	2.36	0.40
1:A:886:G:H1	1:A:911:U:H3	1.69	0.40
1:A:1281:U:H6	1:A:1281:U:H2'	1.67	0.40
1:A:1417:G:OP2	1:A:1417:G:C8	2.74	0.40
3:C:16:ARG:NH1	3:C:183:ASP:OD2	2.54	0.40
4:D:65:ARG:NH1	4:D:72:GLU:HB2	2.36	0.40
5:E:31:LEU:HD23	5:E:31:LEU:HA	1.61	0.40
7:G:99:LEU:HD23	7:G:99:LEU:HA	1.48	0.40
11:K:24:SER:OG	11:K:26:ASN:N	2.54	0.40
12:L:46:LYS:HG2	12:L:94:TRP:CZ2	2.56	0.40
13:M:22:ILE:HB	13:M:25:ILE:HB	2.02	0.40
13:M:44:ARG:HB3	13:M:46:LYS:HD3	2.03	0.40
13:M:64:TRP:HE3	13:M:66:LEU:HD21	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:46:GLU:O	14:N:49:HIS:HB2	2.21	0.40
17:Q:72:ARG:HG2	17:Q:72:ARG:H	1.70	0.40
18:R:52:PRO:HB2	18:R:54:ARG:HG3	2.03	0.40
1:A:22:G:H2'	1:A:23:C:H6	1.86	0.40
1:A:78:G:N2	1:A:79:G:H1'	2.36	0.40
1:A:629:G:H2'	1:A:630:G:H8	1.85	0.40
1:A:853:G:C4	1:A:854:G:C8	3.09	0.40
1:A:880:C:O5'	1:A:880:C:H6	2.04	0.40
1:A:951:G:C5	1:A:952:U:C5	3.09	0.40
1:A:1061:G:C6	1:A:1062:U:N3	2.89	0.40
1:A:1250:A:C5	1:A:1251:A:C6	3.09	0.40
1:A:1368:G:H2'	1:A:1369:C:H5'	2.03	0.40
1:A:1505:G:H4'	1:A:1506:U:H5"	2.02	0.40
3:C:202:ILE:CG2	3:C:204:LEU:HD23	2.51	0.40
5:E:131:ILE:HA	5:E:131:ILE:HD13	1.50	0.40
8:H:73:ASP:N	8:H:74:PRO:HD3	2.37	0.40
9:I:32:ASP:CG	9:I:33:PHE:H	2.24	0.40
10:J:7:LYS:HE2	10:J:9:ARG:HE	1.86	0.40
11:K:38:ASN:HA	11:K:39:PRO:HD3	1.77	0.40
17:Q:63:ARG:HA	17:Q:64:PRO:HD3	1.82	0.40
18:R:70:ILE:HG22	18:R:71:LYS:N	2.35	0.40
20:T:53:LEU:HD22	20:T:53:LEU:HA	1.78	0.40
20:T:84:LEU:HA	20:T:87:LYS:NZ	2.36	0.40
1:A:1290:G:H2'	1:A:1291:G:H8	1.79	0.40
3:C:5:ILE:CD1	3:C:10:PHE:HB2	2.50	0.40
3:C:34:LEU:HD22	3:C:38:ARG:HH22	1.87	0.40
3:C:150:LYS:HG3	3:C:173:VAL:HG21	2.04	0.40
4:D:191:ARG:HA	4:D:191:ARG:HD2	1.79	0.40
7:G:36:LYS:HZ3	7:G:36:LYS:HG3	1.46	0.40
8:H:4:ASP:OD1	8:H:4:ASP:C	2.59	0.40
9:I:79:LEU:HD13	9:I:83:ARG:HD2	2.03	0.40
13:M:81:LEU:HA	13:M:81:LEU:HD23	1.92	0.40
15:O:74:ASP:HA	15:O:75:PRO:HD2	1.83	0.40
1:A:200:G:C5	1:A:201:C:C5	3.09	0.40
1:A:316:G:OP2	1:A:351:G:O2'	2.40	0.40
1:A:627:G:O2'	1:A:628:G:H5'	2.21	0.40
1:A:794:A:H2'	1:A:795:C:C6	2.56	0.40
1:A:1071:C:O2'	1:A:1072:G:H5'	2.21	0.40
1:A:1473:A:H2'	1:A:1474:G:C8	2.56	0.40
2:B:19:HIS:HE1	2:B:206:ASP:H	1.68	0.40
3:C:130:VAL:HG23	3:C:131:ARG:CZ	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:71:SER:HB3	4:D:74:GLN:HG3	2.03	0.40
4:D:118:ARG:HH21	4:D:118:ARG:HD2	1.74	0.40
5:E:137:GLU:HG3	5:E:137:GLU:O	2.21	0.40
7:G:18:TYR:CE2	7:G:59:LEU:HB2	2.57	0.40
9:I:125:TYR:O	9:I:125:TYR:CG	2.74	0.40
11:K:115:PRO:C	11:K:117:ASN:H	2.23	0.40
16:P:74:LEU:HD23	16:P:74:LEU:HA	1.70	0.40
1:A:363:A:OP1	12:L:61:THR:OG1	2.31	0.40
1:A:841:U:H5'	1:A:848:C:O4'	2.21	0.40
2:B:119:GLU:H	2:B:119:GLU:HG2	1.67	0.40
2:B:155:LEU:HD23	2:B:155:LEU:HA	1.87	0.40
3:C:150:LYS:HA	3:C:169:ALA:HB1	1.99	0.40
4:D:10:ARG:HG2	4:D:11:LEU:HD23	2.04	0.40
4:D:15:GLU:CD	4:D:59:ARG:HH21	2.25	0.40
4:D:105:VAL:HG13	4:D:110:PHE:HD2	1.85	0.40
6:F:45:LEU:HD22	6:F:46:ARG:N	2.36	0.40
9:I:19:LEU:HD21	9:I:59:PHE:CG	2.56	0.40
12:L:102:ARG:HE	12:L:102:ARG:HB3	1.56	0.40
13:M:65:LYS:H	13:M:65:LYS:HG2	1.52	0.40
16:P:51:VAL:HG12	16:P:52:ASP:C	2.42	0.40
17:Q:48:GLU:HG3	17:Q:50:LYS:HB2	2.02	0.40
19:S:30:LEU:HB3	19:S:31:ILE:H	1.65	0.40
20:T:30:LYS:O	20:T:34:LYS:HG2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	232/256 (91%)	211 (91%)	18 (8%)	3 (1%)	12	48
3	C	204/239 (85%)	170 (83%)	32 (16%)	2 (1%)	15	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	206/209 (99%)	189 (92%)	17 (8%)	0	100	100
5	E	148/162 (91%)	135 (91%)	12 (8%)	1 (1%)	22	61
6	F	99/101 (98%)	90 (91%)	9 (9%)	0	100	100
7	G	153/156 (98%)	138 (90%)	15 (10%)	0	100	100
8	H	136/138 (99%)	126 (93%)	10 (7%)	0	100	100
9	I	125/128 (98%)	112 (90%)	12 (10%)	1 (1%)	19	58
10	J	96/105 (91%)	79 (82%)	16 (17%)	1 (1%)	15	54
11	K	114/129 (88%)	100 (88%)	14 (12%)	0	100	100
12	L	122/135 (90%)	109 (89%)	12 (10%)	1 (1%)	19	58
13	M	116/126 (92%)	104 (90%)	9 (8%)	3 (3%)	5	34
14	N	58/61 (95%)	47 (81%)	11 (19%)	0	100	100
15	O	85/89 (96%)	71 (84%)	14 (16%)	0	100	100
16	P	81/88 (92%)	73 (90%)	7 (9%)	1 (1%)	13	50
17	Q	97/105 (92%)	89 (92%)	8 (8%)	0	100	100
18	R	68/88 (77%)	58 (85%)	10 (15%)	0	100	100
19	S	78/93 (84%)	68 (87%)	8 (10%)	2 (3%)	5	34
20	T	97/106 (92%)	88 (91%)	7 (7%)	2 (2%)	7	39
21	U	22/27 (82%)	20 (91%)	2 (9%)	0	100	100
All	All	2337/2541 (92%)	2077 (89%)	243 (10%)	17 (1%)	22	61

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	21	ARG
9	I	119	ALA
12	L	28	LYS
3	C	180	ALA
19	S	31	ILE
20	T	73	HIS
2	B	95	GLN
13	M	23	TYR
19	S	13	ASP
3	C	62	ASP
5	E	70	PRO
20	T	99	LEU
10	J	34	VAL

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Mol	Chain	Res	Type
13	M	84	ILE
2	B	229	VAL
13	M	7	VAL
16	P	53	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%)	148 (73%)	54 (27%)	0 3
3	C	160/188 (85%)	113 (71%)	47 (29%)	0 2
4	D	180/181 (99%)	139 (77%)	41 (23%)	1 5
5	E	115/123 (94%)	80 (70%)	35 (30%)	0 2
6	F	90/90 (100%)	68 (76%)	22 (24%)	0 4
7	G	126/127 (99%)	104 (82%)	22 (18%)	2 12
8	H	119/119 (100%)	95 (80%)	24 (20%)	1 8
9	I	98/99 (99%)	77 (79%)	21 (21%)	1 6
10	J	87/92 (95%)	65 (75%)	22 (25%)	0 4
11	K	88/99 (89%)	72 (82%)	16 (18%)	1 10
12	L	104/111 (94%)	74 (71%)	30 (29%)	0 2
13	M	94/101 (93%)	71 (76%)	23 (24%)	0 4
14	N	49/50 (98%)	42 (86%)	7 (14%)	3 21
15	O	79/80 (99%)	62 (78%)	17 (22%)	1 6
16	P	72/74 (97%)	57 (79%)	15 (21%)	1 7
17	Q	94/97 (97%)	74 (79%)	20 (21%)	1 7
18	R	61/77 (79%)	46 (75%)	15 (25%)	0 4
19	S	71/80 (89%)	57 (80%)	14 (20%)	1 8
20	T	76/82 (93%)	59 (78%)	17 (22%)	1 6
21	U	19/22 (86%)	14 (74%)	5 (26%)	0 4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1984/2112 (94%)	1517 (76%)	467 (24%)	1 5

All (467) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	7	VAL
2	B	8	LYS
2	B	9	GLU
2	B	10	LEU
2	B	12	GLU
2	B	17	PHE
2	B	21	ARG
2	B	23	ARG
2	B	44	LEU
2	B	47	THR
2	B	51	LEU
2	B	53	ARG
2	B	63	MET
2	B	69	LEU
2	B	75	LYS
2	B	87	ARG
2	B	98	LEU
2	B	101	MET
2	B	107	THR
2	B	108	ILE
2	B	111	ARG
2	B	114	ARG
2	B	115	LEU
2	B	119	GLU
2	B	121	LEU
2	B	126	GLU
2	B	127	ILE
2	B	128	GLU
2	B	133	LYS
2	B	144	ARG
2	B	146	GLN
2	B	147	LYS
2	B	157	ARG
2	B	163	PHE
2	B	164	VAL
2	B	165	VAL
2	B	170	GLU

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Mol	Chain	Res	Type
2	B	172	ILE
2	B	175	ARG
2	B	178	ARG
2	B	187	LEU
2	B	190	THR
2	B	196	LEU
2	B	200	ILE
2	B	204	ASN
2	B	205	ASP
2	B	206	ASP
2	B	208	ILE
2	B	212	GLN
2	B	213	LEU
2	B	221	LEU
2	B	231	GLU
2	B	238	LEU
2	B	239	VAL
3	C	10	PHE
3	C	11	ARG
3	C	12	LEU
3	C	14	ILE
3	C	16	ARG
3	C	17	ASP
3	C	18	TRP
3	C	20	SER
3	C	21	ARG
3	C	26	LYS
3	C	29	TYR
3	C	33	LEU
3	C	37	GLN
3	C	38	ARG
3	C	42	LEU
3	C	45	LYS
3	C	54	ARG
3	C	58	GLU
3	C	62	ASP
3	C	68	VAL
3	C	70	VAL
3	C	75	VAL
3	C	76	VAL
3	C	91	LEU
3	C	94	LEU

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Mol	Chain	Res	Type
3	C	95	THR
3	C	98	ASN
3	C	103	VAL
3	C	104	GLN
3	C	107	GLN
3	C	111	LEU
3	C	116	VAL
3	C	130	VAL
3	C	131	ARG
3	C	139	GLN
3	C	152	ILE
3	C	154	SER
3	C	166	GLU
3	C	167	TRP
3	C	172	ARG
3	C	190	ARG
3	C	191	THR
3	C	192	THR
3	C	193	TYR
3	C	195	VAL
3	C	196	LEU
3	C	204	LEU
4	D	3	ARG
4	D	8	VAL
4	D	9	CYS
4	D	10	ARG
4	D	19	LEU
4	D	25	ARG
4	D	26	CYS
4	D	30	LYS
4	D	34	GLU
4	D	35	ARG
4	D	47	ARG
4	D	50	ARG
4	D	58	LEU
4	D	59	ARG
4	D	61	LYS
4	D	89	THR
4	D	108	LEU
4	D	112	VAL
4	D	118	ARG
4	D	122	ARG

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Mol	Chain	Res	Type
4	D	127	THR
4	D	131	ARG
4	D	132	ARG
4	D	134	ASP
4	D	135	LEU
4	D	141	ARG
4	D	142	PRO
4	D	145	GLU
4	D	148	VAL
4	D	152	SER
4	D	155	LEU
4	D	159	ARG
4	D	162	LEU
4	D	174	LEU
4	D	181	MET
4	D	186	LEU
4	D	187	ARG
4	D	192	GLU
4	D	194	LEU
4	D	202	LEU
4	D	203	VAL
5	E	6	PHE
5	E	12	LEU
5	E	14	ARG
5	E	18	ARG
5	E	19	MET
5	E	25	ARG
5	E	26	PHE
5	E	31	LEU
5	E	32	VAL
5	E	38	GLN
5	E	41	VAL
5	E	43	LEU
5	E	45	PHE
5	E	47	LYS
5	E	53	LEU
5	E	55	VAL
5	E	60	TYR
5	E	64	ARG
5	E	68	GLU
5	E	71	LEU
5	E	75	THR

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Mol	Chain	Res	Type
5	E	78	HIS
5	E	79	GLU
5	E	81	GLU
5	E	87	SER
5	E	100	VAL
5	E	105	VAL
5	E	116	THR
5	E	118	ILE
5	E	120	THR
5	E	123	LEU
5	E	125	SER
5	E	131	ILE
5	E	151	LEU
5	E	152	ARG
6	F	7	ASN
6	F	9	VAL
6	F	10	LEU
6	F	14	LEU
6	F	15	ASP
6	F	19	LEU
6	F	21	LEU
6	F	24	GLU
6	F	25	ILE
6	F	30	LEU
6	F	32	ASN
6	F	37	VAL
6	F	40	VAL
6	F	43	LEU
6	F	61	LEU
6	F	69	GLU
6	F	70	ASP
6	F	80	ARG
6	F	83	ASP
6	F	86	ARG
6	F	91	VAL
6	F	92	LYS
7	G	5	ARG
7	G	6	ARG
7	G	21	VAL
7	G	41	ARG
7	G	45	ASP
7	G	50	ILE

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Mol	Chain	Res	Type
7	G	62	PHE
7	G	64	GLN
7	G	67	GLU
7	G	74	GLU
7	G	75	VAL
7	G	84	ASN
7	G	87	VAL
7	G	97	GLN
7	G	98	SER
7	G	113	GLU
7	G	122	HIS
7	G	124	LEU
7	G	126	ASP
7	G	129	GLU
7	G	136	LYS
7	G	155	ARG
8	H	2	LEU
8	H	5	PRO
8	H	11	THR
8	H	14	ARG
8	H	18	ARG
8	H	19	VAL
8	H	21	LYS
8	H	23	SER
8	H	56	LYS
8	H	63	LEU
8	H	83	ILE
8	H	85	ARG
8	H	86	ILE
8	H	91	ARG
8	H	92	ARG
8	H	95	VAL
8	H	98	LYS
8	H	102	ARG
8	H	104	ARG
8	H	109	ILE
8	H	113	SER
8	H	119	LEU
8	H	121	ASP
8	H	127	LEU
9	I	5	TYR
9	I	12	GLU

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Mol	Chain	Res	Type
9	I	16	ARG
9	I	26	VAL
9	I	29	ASN
9	I	51	ARG
9	I	53	VAL
9	I	54	ASP
9	I	62	TYR
9	I	64	THR
9	I	79	LEU
9	I	86	VAL
9	I	87	GLN
9	I	91	ASP
9	I	95	LYS
9	I	96	LEU
9	I	102	LEU
9	I	111	ARG
9	I	118	LYS
9	I	121	ARG
9	I	126	SER
10	J	5	ARG
10	J	9	ARG
10	J	16	LEU
10	J	44	VAL
10	J	48	THR
10	J	49	VAL
10	J	55	LYS
10	J	62	HIS
10	J	67	THR
10	J	68	HIS
10	J	69	ASN
10	J	71	LEU
10	J	73	ASP
10	J	74	ILE
10	J	78	ASN
10	J	79	ARG
10	J	80	LYS
10	J	82	ILE
10	J	87	THR
10	J	90	LEU
10	J	94	VAL
10	J	95	GLU
11	K	11	LYS

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Mol	Chain	Res	Type
11	K	12	ARG
11	K	13	GLN
11	K	24	SER
11	K	29	ILE
11	K	40	ILE
11	K	41	THR
11	K	63	LEU
11	K	75	TYR
11	K	77	MET
11	K	81	ASP
11	K	91	ARG
11	K	99	GLN
11	K	114	VAL
11	K	117	ASN
11	K	126	ARG
12	L	6	THR
12	L	7	ILE
12	L	10	LEU
12	L	18	VAL
12	L	20	LYS
12	L	33	ARG
12	L	41	ARG
12	L	42	THR
12	L	43	VAL
12	L	44	THR
12	L	54	LYS
12	L	55	VAL
12	L	59	ARG
12	L	61	THR
12	L	62	SER
12	L	64	TYR
12	L	66	VAL
12	L	67	THR
12	L	75	HIS
12	L	79	GLU
12	L	82	VAL
12	L	90	VAL
12	L	96	VAL
12	L	97	ARG
12	L	100	ILE
12	L	111	LYS
12	L	113	ARG

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Mol	Chain	Res	Type
12	L	116	SER
12	L	122	THR
12	L	126	LYS
13	M	12	ASN
13	M	14	ARG
13	M	27	LYS
13	M	34	LEU
13	M	35	GLU
13	M	46	LYS
13	M	48	LEU
13	M	50	GLU
13	M	56	LEU
13	M	57	ARG
13	M	59	TYR
13	M	64	TRP
13	M	66	LEU
13	M	69	GLU
13	M	70	LEU
13	M	71	ARG
13	M	73	GLU
13	M	80	ARG
13	M	105	THR
13	M	108	ARG
13	M	109	THR
13	M	110	ARG
13	M	115	LYS
14	N	22	THR
14	N	24	CYS
14	N	25	VAL
14	N	26	ARG
14	N	46	GLU
14	N	53	LEU
14	N	57	ARG
15	O	5	LYS
15	O	22	THR
15	O	28	GLN
15	O	29	VAL
15	O	34	LEU
15	O	39	LEU
15	O	45	VAL
15	O	47	LYS
15	O	54	ARG

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Mol	Chain	Res	Type
15	O	56	LEU
15	O	57	LEU
15	O	60	VAL
15	O	64	ARG
15	O	65	ARG
15	O	70	LEU
15	O	76	GLU
15	O	83	GLU
16	P	2	VAL
16	P	25	ARG
16	P	32	TYR
16	P	33	ILE
16	P	42	ARG
16	P	44	THR
16	P	45	THR
16	P	47	ASP
16	P	53	VAL
16	P	54	GLU
16	P	55	ARG
16	P	62	VAL
16	P	68	ASP
16	P	75	ARG
16	P	76	GLN
17	Q	3	LYS
17	Q	23	VAL
17	Q	25	ARG
17	Q	35	VAL
17	Q	36	ILE
17	Q	40	LYS
17	Q	43	LEU
17	Q	59	ILE
17	Q	60	ILE
17	Q	68	ARG
17	Q	72	ARG
17	Q	74	LEU
17	Q	75	ARG
17	Q	76	LEU
17	Q	77	VAL
17	Q	90	ILE
17	Q	93	GLN
17	Q	98	LEU
17	Q	99	SER

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Mol	Chain	Res	Type
17	Q	100	LYS
18	R	19	LYS
18	R	26	LEU
18	R	46	GLU
18	R	47	THR
18	R	50	ILE
18	R	54	ARG
18	R	55	ARG
18	R	56	THR
18	R	64	ARG
18	R	68	LYS
18	R	69	THR
18	R	70	ILE
18	R	86	VAL
18	R	87	ARG
18	R	88	LYS
19	S	6	LYS
19	S	7	LYS
19	S	12	ASP
19	S	15	LEU
19	S	36	ARG
19	S	39	THR
19	S	43	GLU
19	S	58	VAL
19	S	64	GLU
19	S	71	LEU
19	S	77	THR
19	S	78	ARG
19	S	79	THR
19	S	81	ARG
20	T	13	LEU
20	T	20	LEU
20	T	24	LEU
20	T	30	LYS
20	T	36	LEU
20	T	43	LEU
20	T	46	GLU
20	T	53	LEU
20	T	56	MET
20	T	57	ARG
20	T	62	LEU
20	T	71	THR

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Mol	Chain	Res	Type
20	T	74	LYS
20	T	75	ASN
20	T	80	ARG
20	T	91	LEU
20	T	92	LEU
21	U	6	ARG
21	U	10	ARG
21	U	14	TRP
21	U	22	ARG
21	U	25	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	6	HIS
4	D	62	GLN
4	D	119	GLN
5	E	65	ASN
7	G	148	ASN
9	I	73	GLN
9	I	124	GLN
11	K	116	HIS
12	L	49	ASN
15	O	28	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1504/1522 (98%)	377 (25%)	59 (3%)

All (377) 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	32	A
1	A	39	G
1	A	47	C

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Mol	Chain	Res	Type
1	A	48	C
1	A	51	A
1	A	54	C
1	A	67	C
1	A	74	C
1	A	80	G
1	A	81	U
1	A	82	U
1	A	92	C
1	A	93	G
1	A	98	U
1	A	108	G
1	A	109	A
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	145	G
1	A	151	A
1	A	159	G
1	A	160	A
1	A	163	C
1	A	182	U
1	A	183	G
1	A	188	C
1	A	190(D)	U
1	A	195	A
1	A	197	A
1	A	202	U
1	A	203	U
1	A	204	U
1	A	216	G
1	A	226	G
1	A	231	G
1	A	243	A
1	A	244	U
1	A	247	G
1	A	251	G
1	A	252	U
1	A	266	G

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Mol	Chain	Res	Type
1	A	267	C
1	A	289	G
1	A	299	G
1	A	301	G
1	A	321	A
1	A	328	C
1	A	332	G
1	A	344	A
1	A	345	C
1	A	346	G
1	A	347	G
1	A	350	G
1	A	351	G
1	A	352	C
1	A	353	A
1	A	354	G
1	A	367	U
1	A	369	C
1	A	373	A
1	A	374	A
1	A	382	A
1	A	384	G
1	A	387	U
1	A	388	G
1	A	390	C
1	A	391	G
1	A	392	G
1	A	397	A
1	A	398	C
1	A	406	G
1	A	412	A
1	A	413	G
1	A	419	C
1	A	422	C
1	A	424	G
1	A	429	U
1	A	430	A
1	A	439	A
1	A	452	A
1	A	453	A
1	A	460	A
1	A	461	C

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Mol	Chain	Res	Type
1	A	475	G
1	A	476	G
1	A	478	A
1	A	479	C
1	A	481	G
1	A	485	G
1	A	486	U
1	A	497	A
1	A	498	U
1	A	499	A
1	A	509	A
1	A	510	A
1	A	511	C
1	A	518	C
1	A	519	C
1	A	521	G
1	A	527	7MG
1	A	531	U
1	A	532	A
1	A	533	A
1	A	534	U
1	A	538	G
1	A	547	A
1	A	549	C
1	A	558	G
1	A	559	A
1	A	560	U
1	A	562	C
1	A	563	A
1	A	564	C
1	A	568	G
1	A	572	A
1	A	573	A
1	A	576	G
1	A	577	G
1	A	579	G
1	A	588	G
1	A	596	C
1	A	620	C
1	A	624	C
1	A	644	G
1	A	645	C

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Mol	Chain	Res	Type
1	A	646	U
1	A	653	A
1	A	665	A
1	A	670	G
1	A	671	G
1	A	686	U
1	A	687	A
1	A	688	G
1	A	695	A
1	A	701	C
1	A	702	A
1	A	721	G
1	A	722	A
1	A	723	U
1	A	724	G
1	A	728	A
1	A	731	G
1	A	733	A
1	A	734	G
1	A	737	A
1	A	741	G
1	A	749	C
1	A	752	G
1	A	755	G
1	A	777	A
1	A	780	A
1	A	781	A
1	A	782	A
1	A	783	C
1	A	785	G
1	A	792	A
1	A	793	U
1	A	794	A
1	A	799	G
1	A	812	C
1	A	813	U
1	A	814	A
1	A	817	C
1	A	818	G
1	A	826	C
1	A	827	U
1	A	828	A

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Mol	Chain	Res	Type
1	A	829	G
1	A	838	G
1	A	839	U
1	A	840	C
1	A	841	U
1	A	848	C
1	A	859	A
1	A	870	U
1	A	872	A
1	A	873	A
1	A	888	G
1	A	889	A
1	A	902	G
1	A	914	A
1	A	916	G
1	A	922	G
1	A	926	G
1	A	927	G
1	A	934	C
1	A	935	A
1	A	936	C
1	A	937	A
1	A	940	C
1	A	941	G
1	A	950	U
1	A	956	U
1	A	961	U
1	A	962	C
1	A	964	A
1	A	966	M2G
1	A	967	5MC
1	A	968	A
1	A	969	A
1	A	971	G
1	A	972	C
1	A	974	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	978	A
1	A	984	C
1	A	985	C

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Mol	Chain	Res	Type
1	A	986	A
1	A	991	U
1	A	992	U
1	A	993	G
1	A	994	A
1	A	1003(A)	G
1	A	1004	A
1	A	1005	A
1	A	1011	G
1	A	1012	U
1	A	1023	G
1	A	1024	G
1	A	1025	U
1	A	1028	C
1	A	1030(B)	C
1	A	1030(C)	G
1	A	1031	G
1	A	1042	G
1	A	1043	C
1	A	1045	C
1	A	1046	A
1	A	1048	G
1	A	1050	G
1	A	1053	G
1	A	1054	C
1	A	1055	A
1	A	1060	C
1	A	1064	G
1	A	1065	U
1	A	1066	C
1	A	1068	G
1	A	1078	U
1	A	1085	U
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1103	C
1	A	1104	G
1	A	1125	U
1	A	1126	U
1	A	1127	G
1	A	1129	C

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Mol	Chain	Res	Type
1	A	1130	A
1	A	1131	G
1	A	1137	C
1	A	1138	G
1	A	1139	G
1	A	1140	C
1	A	1142	G
1	A	1146	A
1	A	1152	A
1	A	1157	A
1	A	1159	U
1	A	1160	G
1	A	1164	G
1	A	1171	G
1	A	1177	G
1	A	1182	G
1	A	1183	A
1	A	1190	G
1	A	1191	A
1	A	1196	U
1	A	1197	G
1	A	1198	G
1	A	1200	C
1	A	1201	A
1	A	1202	G
1	A	1206	G
1	A	1211	U
1	A	1212	U
1	A	1213	A
1	A	1214	C
1	A	1216	G
1	A	1222	G
1	A	1224	G
1	A	1225	A
1	A	1226	C
1	A	1227	A
1	A	1228	C
1	A	1238	A
1	A	1241	G
1	A	1243	C
1	A	1244	C
1	A	1252	A

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Mol	Chain	Res	Type
1	A	1253	G
1	A	1256	A
1	A	1257	U
1	A	1258	G
1	A	1260	C
1	A	1261	A
1	A	1270	C
1	A	1278	U
1	A	1280	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	1303	C
1	A	1304	G
1	A	1306	A
1	A	1310	G
1	A	1317	C
1	A	1320	C
1	A	1322	C
1	A	1323	G
1	A	1336	C
1	A	1339	A
1	A	1346	A
1	A	1347	G
1	A	1348	U
1	A	1353	G
1	A	1359	C
1	A	1360	A
1	A	1363	A
1	A	1370	G
1	A	1379	G
1	A	1381	U
1	A	1390	U
1	A	1398	A
1	A	1399	C
1	A	1400	5MC
1	A	1406	U
1	A	1411	C

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Mol	Chain	Res	Type
1	A	1414	U
1	A	1417	G
1	A	1418	A
1	A	1421	G
1	A	1424	C
1	A	1437	C
1	A	1442	G
1	A	1443	G
1	A	1446	A
1	A	1447	G
1	A	1451	A
1	A	1453	G
1	A	1473	A
1	A	1474	G
1	A	1475	G
1	A	1477	C
1	A	1480	G
1	A	1485	U
1	A	1486	G
1	A	1487	G
1	A	1490	C
1	A	1492	A
1	A	1493	A
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	1529	G
1	A	1530	G
1	A	1531	A
1	A	1533	C

All (59) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	5	U
1	A	91	C
1	A	115	G
1	A	129(A)	G

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Mol	Chain	Res	Type
1	A	181	G
1	A	243	A
1	A	250	A
1	A	251	G
1	A	350	G
1	A	372	C
1	A	428	G
1	A	429	U
1	A	484	G
1	A	485	G
1	A	509	A
1	A	510	A
1	A	518	C
1	A	532	A
1	A	559	A
1	A	575	G
1	A	587	G
1	A	686	U
1	A	687	A
1	A	701	C
1	A	733	A
1	A	748	C
1	A	792	A
1	A	812	C
1	A	828	A
1	A	840	C
1	A	870	U
1	A	913	A
1	A	960	U
1	A	991	U
1	A	992	U
1	A	993	G
1	A	1049	U
1	A	1065	U
1	A	1067	A
1	A	1129	C
1	A	1139	G
1	A	1145	C
1	A	1181	G
1	A	1182	G
1	A	1190	G
1	A	1201	A

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Mol	Chain	Res	Type
1	A	1225	A
1	A	1256	A
1	A	1257	U
1	A	1279	A
1	A	1300	G
1	A	1301	U
1	A	1305	G
1	A	1335	C
1	A	1347	G
1	A	1380	U
1	A	1496	C
1	A	1504	G
1	A	1505	G

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

16 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	4OC	A	1402	1	20,23,24	1.15	2 (10%)	26,32,35	0.90	2 (7%)
1	MA6	A	1518[A]	1	19,26,27	1.08	2 (10%)	18,38,41	0.73	0
1	5MC	A	1400	1	18,22,23	1.31	2 (11%)	26,32,35	1.00	0
1	2MG	A	1207	1	18,26,27	1.83	3 (16%)	16,38,41	1.42	2 (12%)
1	7MG	A	527	22,1	22,26,27	4.67	7 (31%)	29,39,42	2.37	9 (31%)
1	5MC	A	1404	1	18,22,23	0.94	1 (5%)	26,32,35	1.60	5 (19%)
1	PSU	A	1541	1	18,21,22	1.04	1 (5%)	22,30,33	1.71	4 (18%)
1	PSU	A	1540	1	18,21,22	1.16	1 (5%)	22,30,33	1.70	4 (18%)
1	MA6	A	1518[B]	1	19,26,27	1.32	3 (15%)	18,38,41	1.12	2 (11%)
1	5MC	A	1407	1	18,22,23	1.11	2 (11%)	26,32,35	1.39	4 (15%)
1	5MC	A	967	1	18,22,23	1.01	1 (5%)	26,32,35	0.82	0
1	MA6	A	1519[A]	1	19,26,27	0.86	1 (5%)	18,38,41	0.75	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	MA6	A	1519[B]	1	19,26,27	1.31	4 (21%)	18,38,41	0.55	0
1	UR3	A	1498	22,1	19,22,23	1.09	2 (10%)	26,32,35	1.33	2 (7%)
1	M2G	A	966	1	20,27,28	0.85	1 (5%)	22,40,43	1.53	3 (13%)
1	PSU	A	516	1	18,21,22	1.30	2 (11%)	22,30,33	1.86	5 (22%)

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	4OC	A	1402	1	-	2/9/29/30	0/2/2/2
1	MA6	A	1518[A]	1	-	0/7/29/30	0/3/3/3
1	5MC	A	1400	1	-	2/7/25/26	0/2/2/2
1	2MG	A	1207	1	-	4/5/27/28	0/3/3/3
1	7MG	A	527	22,1	-	2/7/37/38	0/3/3/3
1	5MC	A	1404	1	-	1/7/25/26	0/2/2/2
1	PSU	A	1541	1	-	1/7/25/26	0/2/2/2
1	PSU	A	1540	1	-	2/7/25/26	0/2/2/2
1	MA6	A	1518[B]	1	-	2/7/29/30	0/3/3/3
1	5MC	A	1407	1	-	0/7/25/26	0/2/2/2
1	5MC	A	967	1	-	4/7/25/26	0/2/2/2
1	MA6	A	1519[A]	1	-	5/7/29/30	0/3/3/3
1	MA6	A	1519[B]	1	-	3/7/29/30	0/3/3/3
1	UR3	A	1498	22,1	-	2/7/25/26	0/2/2/2
1	M2G	A	966	1	-	2/7/29/30	0/3/3/3
1	PSU	A	516	1	-	0/7/25/26	0/2/2/2

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	527	7MG	C8-N9	-19.08	1.35	1.46
1	A	527	7MG	C5-N7	8.70	1.45	1.35
1	A	1207	2MG	C6-N1	4.55	1.44	1.37
1	A	516	PSU	C6-C5	4.41	1.40	1.35
1	A	1540	PSU	C6-C5	3.91	1.39	1.35
1	A	1400	5MC	C6-C5	3.72	1.40	1.34
1	A	1207	2MG	C2-N2	3.70	1.41	1.33
1	A	527	7MG	C2-N2	3.66	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1541	PSU	C6-C5	3.56	1.39	1.35
1	A	1207	2MG	C2-N1	3.48	1.42	1.36
1	A	1518[B]	MA6	C6-N1	2.91	1.37	1.33
1	A	1519[B]	MA6	C2-N3	2.80	1.36	1.32
1	A	1498	UR3	C4-N3	-2.74	1.34	1.40
1	A	1498	UR3	C6-N1	-2.69	1.31	1.38
1	A	967	5MC	C2-N3	2.67	1.41	1.36
1	A	1402	4OC	C2-N1	2.65	1.45	1.40
1	A	1407	5MC	C2-N1	2.64	1.45	1.40
1	A	1400	5MC	C2-N3	2.61	1.41	1.36
1	A	1519[B]	MA6	C4-N3	2.59	1.39	1.35
1	A	527	7MG	O6-C6	-2.55	1.18	1.23
1	A	1402	4OC	O2-C2	-2.54	1.19	1.23
1	A	1519[A]	MA6	C2-N1	2.53	1.38	1.33
1	A	1518[B]	MA6	C4-N3	2.50	1.39	1.35
1	A	1519[B]	MA6	C2-N1	2.46	1.38	1.33
1	A	1519[B]	MA6	C6-N1	2.44	1.36	1.33
1	A	527	7MG	C4-N3	2.40	1.40	1.34
1	A	1518[A]	MA6	C6-N1	2.34	1.36	1.33
1	A	1407	5MC	C6-N1	-2.24	1.34	1.38
1	A	1518[B]	MA6	C2-N1	2.24	1.38	1.33
1	A	516	PSU	C2-N1	2.23	1.39	1.36
1	A	1404	5MC	C2-N1	2.21	1.44	1.40
1	A	527	7MG	C2-N1	-2.15	1.32	1.37
1	A	1518[A]	MA6	C4-N3	2.10	1.38	1.35
1	A	527	7MG	C6-N1	-2.04	1.35	1.38
1	A	966	M2G	C5-C6	-2.03	1.43	1.47

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	527	7MG	C5-C6-N1	6.07	121.68	110.99
1	A	516	PSU	N1-C2-N3	5.02	120.82	115.13
1	A	527	7MG	C6-C5-N7	4.87	139.56	131.91
1	A	527	7MG	C2-N3-C4	4.82	120.89	112.30
1	A	516	PSU	C4-N3-C2	-4.55	119.78	126.34
1	A	1540	PSU	C4-N3-C2	-4.50	119.85	126.34
1	A	1541	PSU	C4-N3-C2	-4.38	120.03	126.34
1	A	1541	PSU	N1-C2-N3	4.37	120.08	115.13
1	A	966	M2G	O6-C6-N1	-4.35	115.51	120.65
1	A	1540	PSU	N1-C2-N3	4.34	120.05	115.13
1	A	1404	5MC	N4-C4-N3	-4.12	110.95	118.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1207	2MG	O6-C6-N1	-4.11	115.80	120.65
1	A	966	M2G	O6-C6-C5	3.99	132.16	124.37
1	A	527	7MG	C5-C4-N3	-3.81	120.87	128.13
1	A	1407	5MC	N4-C4-N3	-3.79	111.57	118.48
1	A	527	7MG	C6-C5-C4	-3.74	114.91	122.62
1	A	527	7MG	N9-C4-N3	3.42	130.58	125.47
1	A	1207	2MG	O6-C6-C5	3.20	130.62	124.37
1	A	1498	UR3	C6-N1-C2	-3.13	118.99	121.79
1	A	527	7MG	C2-N1-C6	-3.06	119.52	125.10
1	A	966	M2G	N1-C2-N2	-2.97	115.50	118.04
1	A	1541	PSU	O2-C2-N1	-2.93	119.57	122.79
1	A	1404	5MC	C5-C4-N3	2.91	124.82	121.67
1	A	1498	UR3	O3'-C3'-C2'	2.90	121.21	111.82
1	A	1404	5MC	C5-C6-N1	-2.85	120.41	123.34
1	A	1518[B]	MA6	N1-C6-N6	-2.84	114.06	117.06
1	A	1404	5MC	C4-N3-C2	-2.70	117.04	120.69
1	A	516	PSU	C6-N1-C2	-2.69	119.94	122.68
1	A	516	PSU	O2-C2-N3	-2.59	116.93	121.82
1	A	1407	5MC	C5-C6-N1	-2.53	120.73	123.34
1	A	1540	PSU	O2-C2-N1	-2.45	120.10	122.79
1	A	527	7MG	N9-C8-N7	2.42	106.84	103.38
1	A	1518[B]	MA6	C1'-N9-C4	-2.32	122.56	126.64
1	A	1402	4OC	C2'-C1'-N1	-2.31	109.75	114.22
1	A	1404	5MC	C1'-N1-C6	-2.27	117.35	121.12
1	A	527	7MG	O6-C6-C5	-2.27	121.98	127.54
1	A	1540	PSU	C6-N1-C2	-2.24	120.39	122.68
1	A	1541	PSU	C6-N1-C2	-2.23	120.40	122.68
1	A	516	PSU	O4'-C1'-C2'	2.20	108.25	105.14
1	A	1407	5MC	C5-C4-N3	2.19	124.04	121.67
1	A	1407	5MC	C4-N3-C2	-2.04	117.93	120.69
1	A	1519[A]	MA6	N3-C2-N1	2.01	131.83	128.68
1	A	1402	4OC	C5-C4-N4	-2.01	118.51	122.61

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	527	7MG	O4'-C4'-C5'-O5'
1	A	527	7MG	C3'-C4'-C5'-O5'
1	A	967	5MC	O4'-C4'-C5'-O5'
1	A	967	5MC	C3'-C4'-C5'-O5'
1	A	1207	2MG	N1-C2-N2-CM2

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Mol	Chain	Res	Type	Atoms
1	A	1207	2MG	N3-C2-N2-CM2
1	A	1400	5MC	O4'-C4'-C5'-O5'
1	A	1400	5MC	C3'-C4'-C5'-O5'
1	A	1402	4OC	O4'-C4'-C5'-O5'
1	A	1402	4OC	C3'-C4'-C5'-O5'
1	A	1519[A]	MA6	O4'-C4'-C5'-O5'
1	A	1519[A]	MA6	C3'-C4'-C5'-O5'
1	A	1519[A]	MA6	C5-C6-N6-C9
1	A	1519[B]	MA6	C5-C6-N6-C9
1	A	1519[B]	MA6	N1-C6-N6-C9
1	A	1540	PSU	O4'-C4'-C5'-O5'
1	A	1540	PSU	C3'-C4'-C5'-O5'
1	A	966	M2G	C3'-C4'-C5'-O5'
1	A	1207	2MG	C3'-C4'-C5'-O5'
1	A	1498	UR3	O4'-C4'-C5'-O5'
1	A	966	M2G	O4'-C4'-C5'-O5'
1	A	1518[B]	MA6	O4'-C4'-C5'-O5'
1	A	1207	2MG	O4'-C4'-C5'-O5'
1	A	1498	UR3	C3'-C4'-C5'-O5'
1	A	1519[A]	MA6	C5-C6-N6-C10
1	A	1519[B]	MA6	C5-C6-N6-C10
1	A	967	5MC	C2'-C1'-N1-C6
1	A	967	5MC	C2'-C1'-N1-C2
1	A	1404	5MC	O4'-C4'-C5'-O5'
1	A	1541	PSU	O4'-C1'-C5-C6
1	A	1518[B]	MA6	C3'-C4'-C5'-O5'
1	A	1519[A]	MA6	N1-C6-N6-C9

There are no ring outliers.

11 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1402	4OC	4	0
1	A	1518[A]	MA6	5	0
1	A	1400	5MC	1	0
1	A	1207	2MG	1	0
1	A	1404	5MC	1	0
1	A	1540	PSU	1	0
1	A	1407	5MC	2	0
1	A	967	5MC	7	0
1	A	1519[A]	MA6	5	0
1	A	1498	UR3	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	966	M2G	6	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 295 ligands modelled in this entry, 295 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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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^2)	Q<0.9
1	A	1498/1522 (98%)	-0.20	28 (1%) 66 52	74, 136, 280, 374	0
2	B	234/256 (91%)	-0.20	2 (0%) 84 73	104, 156, 254, 272	0
3	C	206/239 (86%)	0.01	15 (7%) 15 9	171, 215, 243, 274	0
4	D	208/209 (99%)	-0.23	5 (2%) 59 43	86, 137, 190, 243	0
5	E	150/162 (92%)	-0.36	0 100 100	70, 106, 151, 203	0
6	F	101/101 (100%)	-0.41	1 (0%) 82 71	117, 157, 185, 213	0
7	G	155/156 (99%)	-0.06	3 (1%) 66 52	136, 185, 233, 255	0
8	H	138/138 (100%)	-0.53	0 100 100	71, 98, 135, 168	0
9	I	127/128 (99%)	0.41	15 (11%) 4 3	139, 201, 245, 269	0
10	J	98/105 (93%)	0.69	20 (20%) 1 0	150, 241, 295, 344	0
11	K	116/129 (89%)	-0.14	3 (2%) 56 40	100, 131, 170, 192	0
12	L	124/135 (91%)	-0.07	3 (2%) 59 43	82, 134, 167, 216	0
13	M	118/126 (93%)	0.17	7 (5%) 22 13	125, 162, 214, 232	0
14	N	60/61 (98%)	0.10	3 (5%) 28 18	179, 215, 270, 292	0
15	O	87/89 (97%)	-0.41	0 100 100	84, 119, 159, 179	0
16	P	83/88 (94%)	-0.09	0 100 100	95, 134, 164, 208	0
17	Q	99/105 (94%)	-0.30	0 100 100	75, 110, 148, 162	0
18	R	70/88 (79%)	-0.56	0 100 100	95, 135, 187, 215	0
19	S	80/93 (86%)	0.88	19 (23%) 0 0	176, 219, 255, 273	0
20	T	99/106 (93%)	-0.18	3 (3%) 50 34	106, 136, 194, 226	0
21	U	24/27 (88%)	0.52	3 (12%) 3 3	131, 183, 201, 209	0
All	All	3875/4063 (95%)	-0.13	130 (3%) 45 31	70, 146, 250, 374	0

All (130) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1003(A)	G	7.6
19	S	38	SER	7.4
1	A	993	G	7.1
1	A	1006	C	7.1
3	C	66	VAL	5.3
1	A	1018	C	5.0
1	A	1017	G	4.9
1	A	995	C	4.7
1	A	994	A	4.6
13	M	2	ALA	4.6
9	I	15	ALA	4.6
1	A	1005	A	4.4
14	N	3	ARG	4.3
19	S	12	ASP	4.2
1	A	1037	C	4.2
9	I	65	VAL	4.2
10	J	10	GLY	4.1
10	J	90	LEU	4.0
14	N	5	ALA	4.0
9	I	8	GLY	3.9
19	S	41	VAL	3.8
21	U	18	TYR	3.8
19	S	39	THR	3.8
13	M	43	THR	3.8
9	I	66	ARG	3.7
3	C	65	ALA	3.7
9	I	9	ARG	3.5
1	A	1024	G	3.5
10	J	89	ASP	3.5
19	S	35	SER	3.5
1	A	1224	G	3.5
3	C	67	THR	3.5
7	G	2	ALA	3.4
10	J	71	LEU	3.3
1	A	1019	C	3.3
10	J	93	GLY	3.2
1	A	1539	C	3.2
19	S	40	ILE	3.2
1	A	990	C	3.1
3	C	68	VAL	3.1
10	J	97	GLU	3.1
9	I	64	THR	3.1
1	A	1007	C	3.0

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Mol	Chain	Res	Type	RSRZ
10	J	94	VAL	3.0
19	S	31	ILE	3.0
1	A	1023	G	3.0
1	A	1036	G	3.0
1	A	81	U	3.0
9	I	67	GLY	3.0
9	I	14	VAL	3.0
1	A	1004	A	3.0
21	U	24	ARG	2.9
1	A	1129	C	2.9
4	D	40	PRO	2.9
1	A	1025	U	2.9
3	C	201	TYR	2.9
9	I	43	ALA	2.8
21	U	17	THR	2.8
9	I	63	ILE	2.8
13	M	105	THR	2.8
12	L	114	LYS	2.8
1	A	1002	G	2.8
13	M	117	VAL	2.8
10	J	96	ILE	2.7
3	C	189	ALA	2.7
4	D	42	GLN	2.7
7	G	62	PHE	2.7
10	J	91	PRO	2.6
13	M	104	ARG	2.6
10	J	34	VAL	2.6
9	I	17	VAL	2.6
4	D	125	HIS	2.6
4	D	35	ARG	2.6
10	J	7	LYS	2.6
1	A	1032	G	2.6
2	B	212	GLN	2.6
3	C	102	ASN	2.6
13	M	45	VAL	2.5
2	B	203	GLY	2.5
1	A	1038	C	2.5
10	J	98	ILE	2.5
1	A	1542	U	2.5
3	C	196	LEU	2.5
9	I	19	LEU	2.5
9	I	16	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
11	K	19	ALA	2.4
10	J	65	LEU	2.4
9	I	4	TYR	2.4
7	G	4	ARG	2.4
10	J	40	LEU	2.4
19	S	16	LEU	2.4
3	C	104	GLN	2.4
19	S	14	HIS	2.4
11	K	21	ILE	2.4
20	T	103	GLY	2.4
9	I	7	THR	2.3
10	J	6	ILE	2.3
19	S	69	HIS	2.3
20	T	64	ASP	2.3
19	S	21	GLU	2.3
11	K	30	VAL	2.3
10	J	63	PHE	2.3
10	J	70	ARG	2.3
3	C	193	TYR	2.2
19	S	70	LYS	2.2
19	S	17	GLU	2.2
1	A	1026	G	2.2
3	C	195	VAL	2.2
1	A	1276	G	2.2
3	C	103	VAL	2.2
19	S	34	TRP	2.1
3	C	56	ASP	2.1
19	S	11	VAL	2.1
3	C	69	HIS	2.1
4	D	13	ARG	2.1
1	A	706	A	2.1
20	T	9	ASN	2.1
14	N	4	LYS	2.0
19	S	79	THR	2.0
19	S	15	LEU	2.0
10	J	23	ILE	2.0
10	J	8	LEU	2.0
19	S	3	ARG	2.0
6	F	63	TYR	2.0
12	L	113	ARG	2.0
19	S	44	MET	2.0
10	J	39	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
12	L	72	GLY	2.0
3	C	57	ILE	2.0
13	M	44	ARG	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^{th} 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^2)	Q<0.9
1	PSU	A	1540	20/21	0.66	0.71	296,308,331,333	0
1	PSU	A	1541	20/21	0.85	0.65	285,299,307,307	0
1	4OC	A	1402	22/23	0.92	0.23	108,116,134,137	0
1	MA6	A	1518[B]	24/25	0.93	0.22	111,120,133,136	24
1	7MG	A	527	24/25	0.93	0.22	103,120,142,145	0
1	MA6	A	1518[A]	24/25	0.93	0.22	107,118,124,124	24
1	2MG	A	1207	24/25	0.94	0.16	195,204,278,284	0
1	PSU	A	516	20/21	0.95	0.10	133,147,164,166	0
1	MA6	A	1519[A]	24/25	0.95	0.28	100,107,112,116	24
1	MA6	A	1519[B]	24/25	0.95	0.28	102,107,118,119	24
1	5MC	A	1407	21/22	0.95	0.12	136,163,172,178	0
1	5MC	A	1400	21/22	0.95	0.19	103,123,130,131	0
1	5MC	A	1404	21/22	0.96	0.16	99,108,151,155	0
1	M2G	A	966	25/26	0.96	0.15	136,150,159,160	0
1	UR3	A	1498	21/22	0.96	0.29	105,120,144,147	0
1	5MC	A	967	21/22	0.97	0.13	125,144,150,153	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^{th} 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^2)	Q<0.9
22	MG	A	1838	1/1	0.20	0.87	121,121,121,121	0
22	MG	A	1847	1/1	0.30	0.90	127,127,127,127	0
22	MG	A	1858	1/1	0.34	0.63	125,125,125,125	0
22	MG	A	1766	1/1	0.37	1.26	100,100,100,100	0
22	MG	A	1776	1/1	0.44	0.15	110,110,110,110	0
22	MG	A	1642	1/1	0.46	0.15	88,88,88,88	0
22	MG	A	1810	1/1	0.47	0.39	102,102,102,102	0
22	MG	A	1731	1/1	0.49	0.38	107,107,107,107	0
22	MG	A	1716	1/1	0.53	0.40	137,137,137,137	0
22	MG	P	102	1/1	0.53	0.45	124,124,124,124	0
22	MG	A	1849	1/1	0.55	0.28	126,126,126,126	0
22	MG	A	1704	1/1	0.56	0.44	126,126,126,126	0
22	MG	A	1753	1/1	0.56	0.37	109,109,109,109	0
22	MG	A	1826	1/1	0.59	0.76	134,134,134,134	0
22	MG	A	1751	1/1	0.59	0.93	143,143,143,143	0
22	MG	A	1829	1/1	0.60	0.37	463,463,463,463	0
22	MG	A	1682	1/1	0.61	0.32	82,82,82,82	0
22	MG	A	1781	1/1	0.61	0.64	130,130,130,130	0
22	MG	A	1842	1/1	0.62	1.15	119,119,119,119	0
22	MG	A	1822	1/1	0.63	0.22	116,116,116,116	0
22	MG	A	1777	1/1	0.65	1.28	144,144,144,144	0
22	MG	A	1794	1/1	0.66	0.91	132,132,132,132	0
22	MG	A	1811	1/1	0.68	0.25	147,147,147,147	0
22	MG	A	1830	1/1	0.68	0.66	91,91,91,91	0
22	MG	A	1601	1/1	0.69	0.43	132,132,132,132	0
22	MG	A	1833	1/1	0.70	0.26	122,122,122,122	0
22	MG	A	1845	1/1	0.70	0.92	110,110,110,110	0
22	MG	A	1763	1/1	0.70	0.29	137,137,137,137	0
22	MG	A	1770	1/1	0.71	0.97	99,99,99,99	0
22	MG	A	1672	1/1	0.71	0.14	139,139,139,139	0
22	MG	A	1735	1/1	0.71	0.51	81,81,81,81	0
22	MG	A	1866	1/1	0.71	0.49	124,124,124,124	0
22	MG	A	1846	1/1	0.71	0.21	142,142,142,142	0
22	MG	A	1749	1/1	0.72	0.41	121,121,121,121	0
22	MG	A	1809	1/1	0.72	0.37	109,109,109,109	0
22	MG	H	201	1/1	0.72	0.64	118,118,118,118	0
22	MG	A	1782	1/1	0.72	0.55	118,118,118,118	0
22	MG	A	1839	1/1	0.73	0.58	133,133,133,133	0
22	MG	A	1625	1/1	0.73	0.31	122,122,122,122	0
22	MG	A	1796	1/1	0.74	0.56	92,92,92,92	0
22	MG	A	1853	1/1	0.74	0.41	116,116,116,116	0
22	MG	A	1665	1/1	0.75	0.31	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	MG	C	301	1/1	0.75	0.44	133,133,133,133	0
22	MG	A	1660	1/1	0.75	0.14	113,113,113,113	0
22	MG	A	1769	1/1	0.75	0.41	118,118,118,118	0
22	MG	A	1857	1/1	0.76	0.54	133,133,133,133	0
22	MG	A	1662	1/1	0.76	0.37	78,78,78,78	0
22	MG	A	1715	1/1	0.77	0.52	137,137,137,137	0
22	MG	A	1808	1/1	0.77	0.11	163,163,163,163	0
22	MG	A	1720	1/1	0.77	0.77	98,98,98,98	0
22	MG	A	1872	1/1	0.78	0.13	407,407,407,407	0
22	MG	A	1703	1/1	0.79	0.39	153,153,153,153	0
22	MG	A	1834	1/1	0.79	0.35	118,118,118,118	0
22	MG	A	1835	1/1	0.79	0.55	98,98,98,98	0
22	MG	A	1683	1/1	0.79	0.65	98,98,98,98	0
22	MG	A	1761	1/1	0.79	0.34	107,107,107,107	0
22	MG	A	1780	1/1	0.79	0.50	61,61,61,61	0
22	MG	A	1868	1/1	0.80	0.36	99,99,99,99	0
22	MG	A	1854	1/1	0.80	0.45	137,137,137,137	0
22	MG	A	1787	1/1	0.80	0.12	141,141,141,141	0
22	MG	A	1824	1/1	0.80	0.20	133,133,133,133	0
22	MG	A	1841	1/1	0.80	0.78	118,118,118,118	0
22	MG	Q	201	1/1	0.80	0.21	126,126,126,126	0
22	MG	A	1843	1/1	0.81	0.80	106,106,106,106	0
22	MG	A	1832	1/1	0.82	0.77	89,89,89,89	0
22	MG	A	1729	1/1	0.83	0.32	85,85,85,85	0
22	MG	A	1622	1/1	0.83	0.23	148,148,148,148	0
22	MG	A	1865	1/1	0.84	0.21	134,134,134,134	0
22	MG	A	1759	1/1	0.84	0.26	107,107,107,107	0
22	MG	A	1684	1/1	0.84	0.33	127,127,127,127	0
22	MG	A	1736	1/1	0.84	0.22	114,114,114,114	0
22	MG	A	1679	1/1	0.84	0.47	146,146,146,146	0
22	MG	A	1605	1/1	0.84	0.80	85,85,85,85	0
22	MG	A	1783	1/1	0.84	0.41	129,129,129,129	0
22	MG	A	1677	1/1	0.84	0.14	299,299,299,299	0
22	MG	A	1711	1/1	0.85	0.33	149,149,149,149	0
22	MG	A	1851	1/1	0.85	0.28	132,132,132,132	0
22	MG	A	1633	1/1	0.85	1.02	100,100,100,100	0
22	MG	A	1798	1/1	0.85	0.20	148,148,148,148	0
22	MG	A	1836	1/1	0.85	0.42	120,120,120,120	0
22	MG	A	1815	1/1	0.85	0.46	115,115,115,115	0
22	MG	A	1687	1/1	0.85	0.25	117,117,117,117	0
22	MG	A	1856	1/1	0.86	0.28	127,127,127,127	0
22	MG	A	1850	1/1	0.86	0.36	125,125,125,125	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	MG	A	1791	1/1	0.86	0.46	99,99,99,99	0
22	MG	A	1821	1/1	0.86	0.34	96,96,96,96	0
22	MG	P	101	1/1	0.86	0.22	115,115,115,115	0
22	MG	A	1745	1/1	0.86	0.18	107,107,107,107	0
22	MG	A	1867	1/1	0.86	0.55	118,118,118,118	0
22	MG	A	1629	1/1	0.87	0.52	121,121,121,121	0
22	MG	A	1767	1/1	0.87	0.23	107,107,107,107	0
22	MG	A	1797	1/1	0.87	0.54	116,116,116,116	0
22	MG	A	1712	1/1	0.87	0.34	149,149,149,149	0
22	MG	A	1855	1/1	0.87	0.87	128,128,128,128	0
22	MG	A	1799	1/1	0.87	0.26	84,84,84,84	0
22	MG	A	1754	1/1	0.88	0.10	156,156,156,156	0
22	MG	A	1772	1/1	0.88	1.46	120,120,120,120	0
22	MG	A	1755	1/1	0.88	0.38	122,122,122,122	0
22	MG	A	1701	1/1	0.88	0.32	138,138,138,138	0
22	MG	A	1661	1/1	0.88	0.45	87,87,87,87	0
22	MG	A	1874	1/1	0.88	0.20	431,431,431,431	0
22	MG	A	1718	1/1	0.88	0.16	92,92,92,92	0
22	MG	D	303	1/1	0.88	0.22	88,88,88,88	0
22	MG	D	304	1/1	0.88	0.56	110,110,110,110	0
22	MG	A	1806	1/1	0.88	0.29	414,414,414,414	0
22	MG	J	201	1/1	0.88	0.34	105,105,105,105	0
22	MG	A	1638	1/1	0.88	0.33	97,97,97,97	0
22	MG	A	1674	1/1	0.88	0.46	124,124,124,124	0
22	MG	A	1696	1/1	0.88	0.35	128,128,128,128	0
22	MG	C	302	1/1	0.89	0.12	129,129,129,129	0
22	MG	A	1852	1/1	0.89	0.50	108,108,108,108	0
22	MG	A	1778	1/1	0.89	0.15	157,157,157,157	0
22	MG	A	1619	1/1	0.89	0.63	106,106,106,106	0
22	MG	I	201	1/1	0.89	0.81	136,136,136,136	0
22	MG	A	1848	1/1	0.89	0.41	94,94,94,94	0
22	MG	A	1644	1/1	0.89	0.34	82,82,82,82	0
22	MG	A	1733	1/1	0.89	0.33	116,116,116,116	0
22	MG	A	1823	1/1	0.89	0.20	146,146,146,146	0
22	MG	A	1686	1/1	0.90	0.13	226,226,226,226	0
22	MG	A	1671	1/1	0.90	0.24	140,140,140,140	0
22	MG	A	1871	1/1	0.90	0.47	148,148,148,148	0
22	MG	A	1817	1/1	0.90	0.93	134,134,134,134	0
22	MG	A	1873	1/1	0.90	0.10	437,437,437,437	0
22	MG	A	1819	1/1	0.90	0.18	103,103,103,103	0
22	MG	A	1837	1/1	0.90	0.96	123,123,123,123	0
22	MG	A	1694	1/1	0.90	0.34	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	MG	A	1756	1/1	0.90	0.26	109,109,109,109	0
22	MG	A	1725	1/1	0.90	0.80	119,119,119,119	0
22	MG	A	1802	1/1	0.90	0.50	148,148,148,148	0
22	MG	A	1785	1/1	0.90	0.21	127,127,127,127	0
22	MG	A	1626	1/1	0.90	0.29	147,147,147,147	0
22	MG	A	1859	1/1	0.90	0.81	123,123,123,123	0
22	MG	A	1790	1/1	0.90	0.73	146,146,146,146	0
22	MG	A	1685	1/1	0.90	0.10	236,236,236,236	0
22	MG	A	1773	1/1	0.91	0.43	120,120,120,120	0
22	MG	A	1699	1/1	0.91	0.39	97,97,97,97	0
22	MG	B	302	1/1	0.91	0.15	111,111,111,111	0
22	MG	A	1673	1/1	0.91	0.10	120,120,120,120	0
22	MG	A	1800	1/1	0.91	0.09	132,132,132,132	0
22	MG	A	1789	1/1	0.91	0.11	96,96,96,96	0
22	MG	A	1863	1/1	0.91	0.31	101,101,101,101	0
22	MG	E	201	1/1	0.91	0.12	121,121,121,121	0
22	MG	A	1803	1/1	0.91	0.47	250,250,250,250	0
22	MG	A	1740	1/1	0.91	0.40	125,125,125,125	0
22	MG	A	1631	1/1	0.91	0.32	109,109,109,109	0
22	MG	A	1666	1/1	0.91	0.21	123,123,123,123	0
22	MG	A	1827	1/1	0.91	0.98	147,147,147,147	0
22	MG	A	1705	1/1	0.91	0.18	369,369,369,369	0
23	ZN	N	101	1/1	0.91	0.14	214,214,214,214	0
22	MG	A	1743	1/1	0.92	0.19	104,104,104,104	0
22	MG	A	1678	1/1	0.92	0.44	106,106,106,106	0
22	MG	A	1748	1/1	0.92	0.32	120,120,120,120	0
22	MG	A	1765	1/1	0.92	0.76	90,90,90,90	0
22	MG	A	1667	1/1	0.92	0.27	115,115,115,115	0
22	MG	A	1784	1/1	0.92	0.20	120,120,120,120	0
22	MG	A	1700	1/1	0.92	0.17	184,184,184,184	0
22	MG	A	1786	1/1	0.92	0.18	153,153,153,153	0
22	MG	D	302	1/1	0.92	0.19	103,103,103,103	0
22	MG	A	1768	1/1	0.92	0.13	147,147,147,147	0
22	MG	A	1814	1/1	0.92	0.56	131,131,131,131	0
22	MG	A	1752	1/1	0.92	0.50	89,89,89,89	0
22	MG	A	1689	1/1	0.92	0.76	170,170,170,170	0
22	MG	A	1738	1/1	0.92	0.54	100,100,100,100	0
22	MG	A	1739	1/1	0.92	0.49	74,74,74,74	0
22	MG	A	1864	1/1	0.92	0.43	122,122,122,122	0
22	MG	A	1774	1/1	0.92	0.51	112,112,112,112	0
22	MG	A	1639	1/1	0.92	0.31	216,216,216,216	0
22	MG	A	1758	1/1	0.92	0.28	109,109,109,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	MG	A	1664	1/1	0.93	0.44	101,101,101,101	0
22	MG	A	1653	1/1	0.93	0.17	113,113,113,113	0
22	MG	F	201	1/1	0.93	0.16	107,107,107,107	0
22	MG	A	1676	1/1	0.93	0.24	113,113,113,113	0
22	MG	A	1732	1/1	0.93	0.33	136,136,136,136	0
22	MG	A	1608	1/1	0.93	0.11	143,143,143,143	0
22	MG	A	1844	1/1	0.93	0.18	100,100,100,100	0
22	MG	A	1779	1/1	0.93	0.20	129,129,129,129	0
22	MG	A	1688	1/1	0.93	0.13	144,144,144,144	0
22	MG	A	1764	1/1	0.93	0.25	101,101,101,101	0
22	MG	A	1737	1/1	0.94	0.24	99,99,99,99	0
22	MG	A	1669	1/1	0.94	0.19	152,152,152,152	0
22	MG	A	1840	1/1	0.94	0.22	104,104,104,104	0
22	MG	A	1690	1/1	0.94	0.06	136,136,136,136	0
22	MG	A	1825	1/1	0.94	0.35	110,110,110,110	0
22	MG	A	1657	1/1	0.94	0.15	98,98,98,98	0
22	MG	A	1793	1/1	0.94	0.25	80,80,80,80	0
22	MG	A	1861	1/1	0.94	0.11	89,89,89,89	0
22	MG	A	1610	1/1	0.94	0.24	124,124,124,124	0
22	MG	A	1744	1/1	0.94	0.32	117,117,117,117	0
22	MG	A	1652	1/1	0.94	0.13	98,98,98,98	0
22	MG	A	1681	1/1	0.94	0.35	132,132,132,132	0
22	MG	A	1628	1/1	0.94	0.78	85,85,85,85	0
22	MG	A	1818	1/1	0.94	0.97	100,100,100,100	0
22	MG	A	1870	1/1	0.94	0.58	85,85,85,85	0
22	MG	A	1702	1/1	0.94	0.21	184,184,184,184	0
22	MG	A	1801	1/1	0.94	0.18	154,154,154,154	0
22	MG	B	301	1/1	0.95	0.20	99,99,99,99	0
22	MG	A	1816	1/1	0.95	0.41	105,105,105,105	0
22	MG	A	1831	1/1	0.95	0.33	52,52,52,52	0
22	MG	A	1714	1/1	0.95	0.21	219,219,219,219	0
22	MG	A	1862	1/1	0.95	0.32	127,127,127,127	0
22	MG	A	1649	1/1	0.95	0.48	116,116,116,116	0
22	MG	A	1650	1/1	0.95	0.24	90,90,90,90	0
22	MG	A	1635	1/1	0.95	0.12	99,99,99,99	0
22	MG	A	1710	1/1	0.95	0.41	114,114,114,114	0
22	MG	A	1722	1/1	0.95	0.24	155,155,155,155	0
22	MG	A	1723	1/1	0.95	0.16	102,102,102,102	0
22	MG	A	1692	1/1	0.95	0.27	150,150,150,150	0
22	MG	A	1727	1/1	0.95	0.74	140,140,140,140	0
22	MG	A	1728	1/1	0.95	0.05	214,214,214,214	0
22	MG	A	1828	1/1	0.95	0.28	447,447,447,447	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	MG	A	1646	1/1	0.95	0.40	91,91,91,91	0
22	MG	A	1795	1/1	0.96	0.52	117,117,117,117	0
22	MG	A	1645	1/1	0.96	0.06	91,91,91,91	0
22	MG	A	1624	1/1	0.96	0.25	117,117,117,117	0
22	MG	A	1875	1/1	0.96	0.07	228,228,228,228	0
22	MG	A	1659	1/1	0.96	0.12	121,121,121,121	0
22	MG	A	1647	1/1	0.96	0.44	182,182,182,182	0
22	MG	A	1648	1/1	0.96	0.14	164,164,164,164	0
22	MG	A	1603	1/1	0.96	0.23	84,84,84,84	0
22	MG	A	1726	1/1	0.96	0.41	134,134,134,134	0
22	MG	A	1643	1/1	0.96	0.15	90,90,90,90	0
22	MG	A	1805	1/1	0.96	0.12	203,203,203,203	0
22	MG	A	1741	1/1	0.96	0.17	76,76,76,76	0
22	MG	A	1807	1/1	0.96	0.12	278,278,278,278	0
22	MG	A	1742	1/1	0.96	0.31	116,116,116,116	0
22	MG	A	1697	1/1	0.96	0.33	127,127,127,127	0
22	MG	A	1792	1/1	0.96	0.13	97,97,97,97	0
22	MG	A	1675	1/1	0.96	0.21	116,116,116,116	0
22	MG	A	1869	1/1	0.96	0.19	106,106,106,106	0
22	MG	A	1813	1/1	0.96	0.19	122,122,122,122	0
22	MG	A	1612	1/1	0.96	0.12	164,164,164,164	0
22	MG	A	1615	1/1	0.97	0.12	99,99,99,99	0
22	MG	A	1730	1/1	0.97	0.26	110,110,110,110	0
22	MG	A	1707	1/1	0.97	0.07	167,167,167,167	0
22	MG	A	1804	1/1	0.97	0.11	194,194,194,194	0
22	MG	A	1621	1/1	0.97	0.31	123,123,123,123	0
22	MG	A	1771	1/1	0.97	0.67	83,83,83,83	0
22	MG	A	1654	1/1	0.97	0.10	49,49,49,49	0
22	MG	A	1747	1/1	0.97	0.07	105,105,105,105	0
22	MG	A	1734	1/1	0.97	0.26	129,129,129,129	0
22	MG	A	1820	1/1	0.97	0.06	91,91,91,91	0
22	MG	A	1658	1/1	0.98	0.18	130,130,130,130	0
22	MG	A	1602	1/1	0.98	0.21	130,130,130,130	0
22	MG	A	1706	1/1	0.98	0.36	97,97,97,97	0
22	MG	A	1604	1/1	0.98	0.12	100,100,100,100	0
22	MG	A	1613	1/1	0.98	0.21	121,121,121,121	0
22	MG	A	1614	1/1	0.98	0.18	135,135,135,135	0
22	MG	A	1691	1/1	0.98	0.38	155,155,155,155	0
22	MG	A	1713	1/1	0.98	0.32	431,431,431,431	0
22	MG	A	1876	1/1	0.98	0.24	399,399,399,399	0
22	MG	A	1609	1/1	0.98	0.18	94,94,94,94	0
22	MG	A	1760	1/1	0.98	0.20	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	MG	A	1616	1/1	0.98	0.18	66,66,66,66	0
22	MG	A	1762	1/1	0.98	0.30	83,83,83,83	0
22	MG	A	1695	1/1	0.98	0.11	81,81,81,81	0
22	MG	A	1717	1/1	0.98	0.24	94,94,94,94	0
22	MG	A	1788	1/1	0.98	0.51	77,77,77,77	0
22	MG	A	1627	1/1	0.98	0.83	79,79,79,79	0
22	MG	A	1860	1/1	0.98	0.56	123,123,123,123	0
22	MG	A	1680	1/1	0.98	0.29	136,136,136,136	0
22	MG	A	1617	1/1	0.98	0.29	56,56,56,56	0
22	MG	A	1668	1/1	0.98	0.12	136,136,136,136	0
22	MG	N	102	1/1	0.98	0.30	225,225,225,225	0
22	MG	A	1724	1/1	0.98	0.37	92,92,92,92	0
22	MG	A	1656	1/1	0.98	0.14	178,178,178,178	0
22	MG	A	1670	1/1	0.98	0.10	140,140,140,140	0
23	ZN	D	301	1/1	0.98	0.28	122,122,122,122	0
22	MG	A	1618	1/1	0.98	0.35	94,94,94,94	0
22	MG	A	1623	1/1	0.99	0.14	135,135,135,135	0
22	MG	A	1651	1/1	0.99	0.15	61,61,61,61	0
22	MG	A	1606	1/1	0.99	0.11	96,96,96,96	0
22	MG	A	1640	1/1	0.99	0.16	72,72,72,72	0
22	MG	A	1757	1/1	0.99	0.09	80,80,80,80	0
22	MG	A	1698	1/1	0.99	0.36	182,182,182,182	0
22	MG	A	1641	1/1	0.99	0.12	99,99,99,99	0
22	MG	A	1655	1/1	0.99	0.14	131,131,131,131	0
22	MG	B	303	1/1	0.99	0.18	184,184,184,184	0
22	MG	A	1719	1/1	0.99	0.19	139,139,139,139	0
22	MG	A	1630	1/1	0.99	0.24	83,83,83,83	0
22	MG	A	1620	1/1	0.99	0.10	83,83,83,83	0
22	MG	A	1632	1/1	0.99	0.14	128,128,128,128	0
22	MG	A	1611	1/1	0.99	0.12	92,92,92,92	0
22	MG	A	1812	1/1	0.99	0.16	99,99,99,99	0
22	MG	A	1634	1/1	0.99	0.20	235,235,235,235	0
22	MG	A	1607	1/1	0.99	0.20	91,91,91,91	0
22	MG	A	1746	1/1	0.99	0.17	101,101,101,101	0
22	MG	A	1636	1/1	0.99	0.12	69,69,69,69	0
22	MG	A	1708	1/1	0.99	0.18	120,120,120,120	0
22	MG	A	1709	1/1	0.99	0.11	140,140,140,140	0
22	MG	A	1750	1/1	0.99	0.23	123,123,123,123	0
22	MG	A	1637	1/1	0.99	0.37	85,85,85,85	0
22	MG	A	1693	1/1	0.99	0.15	133,133,133,133	0
22	MG	A	1775	1/1	0.99	0.12	121,121,121,121	0
22	MG	A	1663	1/1	1.00	0.09	127,127,127,127	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	MG	A	1721	1/1	1.00	0.20	46,46,46,46	0

6.5 Other polymers (i)

There are no such residues in this entry.