Full wwPDB X-ray Structure Validation Report (i)

Jun 18, 2024 – 10:55 AM EDT

PDB ID	:	4JI5
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	:	3.85 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

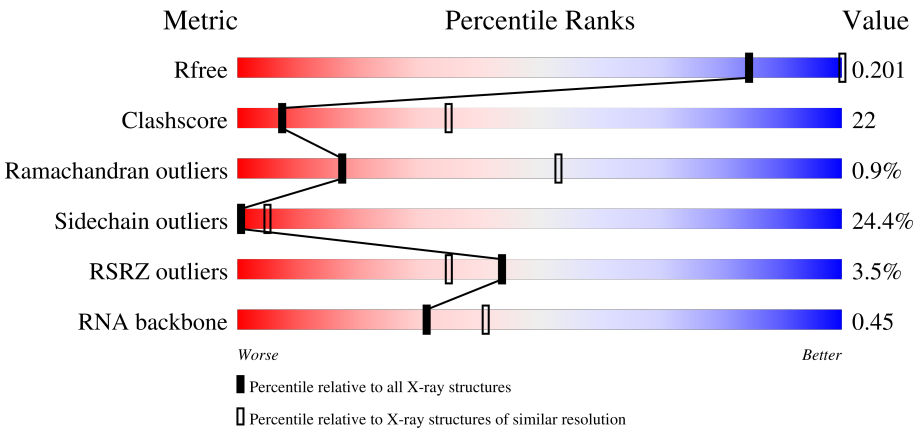
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.85 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1048 (4.10-3.62)
Clashscore	141614	1015 (4.08-3.64)
Ramachandran outliers	138981	1069 (4.10-3.62)
Sidechain outliers	138945	1062 (4.10-3.62)
RSRZ outliers	127900	1206 (4.12-3.60)
RNA backbone	3102	1039 (4.70-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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% 19% 39% 33% 9% •
2	B	256	% 42% 33% 14% • 9%
3	C	239	% 33% 40% 12% • 14%
4	D	209	9% 41% 44% 15%

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Mol	Chain	Length	Quality of chain
5	E	162	4% 36% 43% 12% • 7%
6	F	101	2% 38% 46% 17%
7	G	156	4% 53% 38% 9% •
8	H	138	41% 39% 20%
9	I	128	2% 40% 50% 9% ••
10	J	105	7% 30% 44% 16% • 7%
11	K	129	9% 47% 36% 7% 10%
12	L	135	7% 39% 42% 11% 8%
13	M	126	10% 39% 43% 11% • 6%
14	N	61	30% 44% 23% ••
15	O	89	34% 51% 13% •
16	P	88	9% 44% 43% 7% 6%
17	Q	105	5% 28% 48% 18% • 6%
18	R	88	3% 23% 41% 15% • 20%
19	S	93	4% 34% 34% 16% • 14%
20	T	106	% 39% 38% 16% • 7%
21	U	27	19% 59% 26% • 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
22	MG	A	1601	-	-	-	X
22	MG	A	1617	-	-	-	X
22	MG	A	1632	-	-	-	X
22	MG	A	1634	-	-	-	X
22	MG	A	1638	-	-	-	X
22	MG	A	1650	-	-	-	X
22	MG	A	1653	-	-	-	X
22	MG	A	1675	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	MG	A	1689	-	-	-	X
22	MG	A	1729	-	-	-	X
22	MG	A	1736	-	-	-	X
22	MG	A	1737	-	-	-	X
22	MG	A	1738	-	-	-	X
22	MG	A	1747	-	-	-	X
22	MG	A	1749	-	-	-	X
22	MG	A	1750	-	-	-	X
22	MG	A	1751	-	-	-	X
22	MG	A	1752	-	-	-	X
22	MG	A	1753	-	-	-	X
22	MG	A	1760	-	-	-	X
22	MG	A	1764	-	-	-	X
22	MG	E	201	-	-	-	X
22	MG	G	201	-	-	-	X

2 Entry composition (i)

There are 24 unique types of molecules in this entry. The entry contains 52228 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	1514	32687	14559	6046	10562	1520	0	6	0

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is a protein called RIBOSOMAL PROTEIN S2.

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

- Molecule 3 is a protein called RIBOSOMAL PROTEIN S3.

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

- Molecule 4 is a protein called RIBOSOMAL PROTEIN S4.

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

- Molecule 5 is a protein called RIBOSOMAL PROTEIN S5.

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

- Molecule 6 is a protein called RIBOSOMAL PROTEIN S6.

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

- Molecule 7 is a protein called RIBOSOMAL PROTEIN S7.

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

- Molecule 8 is a protein called RIBOSOMAL PROTEIN S8.

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

- Molecule 9 is a protein called RIBOSOMAL PROTEIN S9.

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

- Molecule 10 is a protein called RIBOSOMAL PROTEIN S10.

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

- Molecule 11 is a protein called RIBOSOMAL PROTEIN S11.

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

- Molecule 12 is a protein called RIBOSOMAL PROTEIN S12.

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

- Molecule 13 is a protein called RIBOSOMAL PROTEIN S13.

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

- Molecule 14 is a protein called RIBOSOMAL PROTEIN S14.

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

- Molecule 15 is a protein called RIBOSOMAL PROTEIN S15.

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

- Molecule 16 is a protein called RIBOSOMAL PROTEIN S16.

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

- Molecule 17 is a protein called RIBOSOMAL PROTEIN S17.

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

- Molecule 18 is a protein called RIBOSOMAL PROTEIN S18.

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

- Molecule 19 is a protein called RIBOSOMAL PROTEIN S19.

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

- Molecule 20 is a protein called RIBOSOMAL PROTEIN S20.

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

- Molecule 21 is a protein called RIBOSOMAL PROTEIN THX.

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
22	A	164	164	164	0	0
22	D	1	1	1	0	0
22	E	1	1	1	0	0
22	F	1	1	1	0	0
22	G	1	1	1	0	0
22	H	1	1	1	0	0
22	K	2	2	2	0	0
22	S	1	1	1	0	0

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

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

- Molecule 24 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
24	A	271	271	271	0	0

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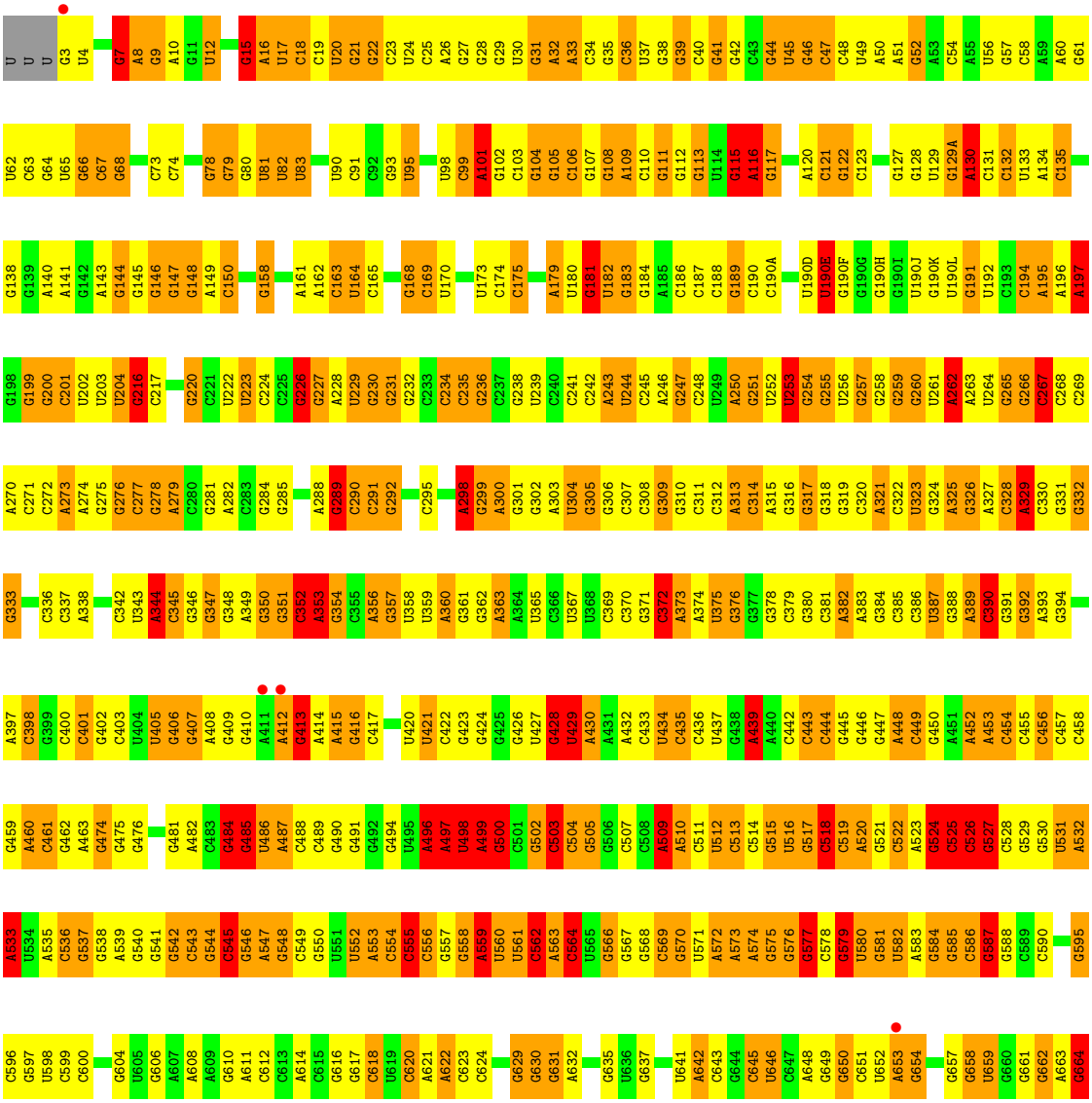
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	C	1	Total O 1 1	0	0
24	E	3	Total O 3 3	0	0
24	L	1	Total O 1 1	0	0
24	N	1	Total O 1 1	0	0
24	P	1	Total O 1 1	0	0
24	T	1	Total O 1 1	0	0

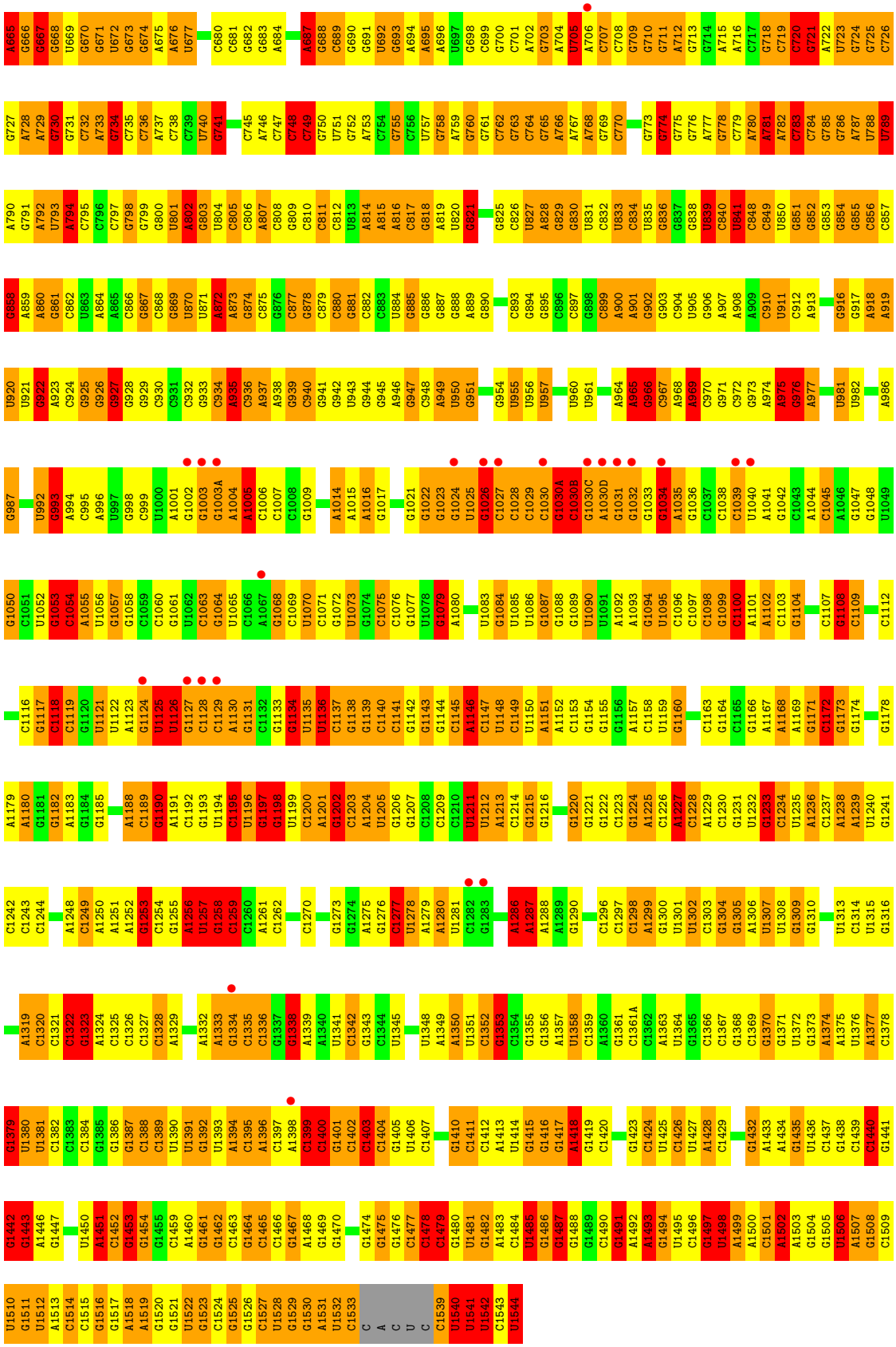
3 Residue-property plots (i)

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

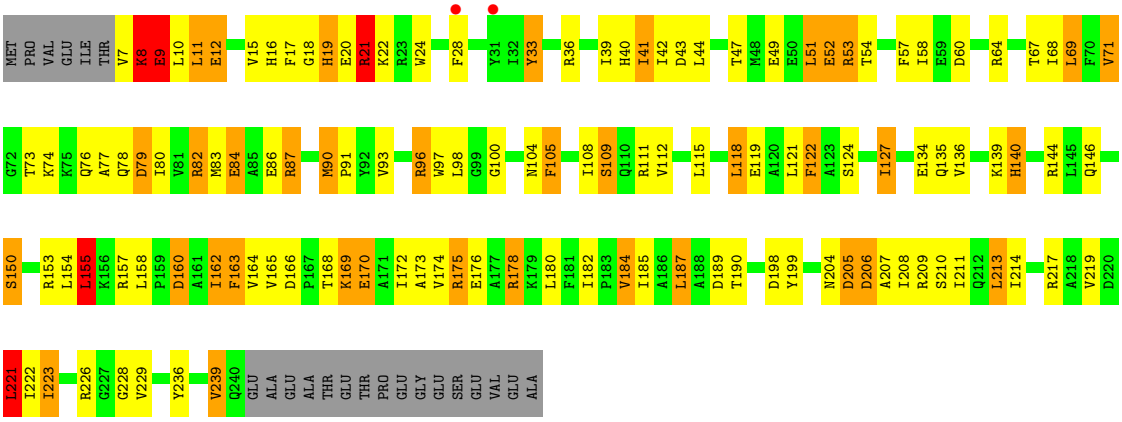
Chain A:





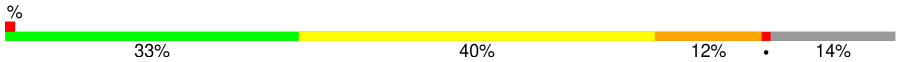
• Molecule 2: RIBOSOMAL PROTEIN S2

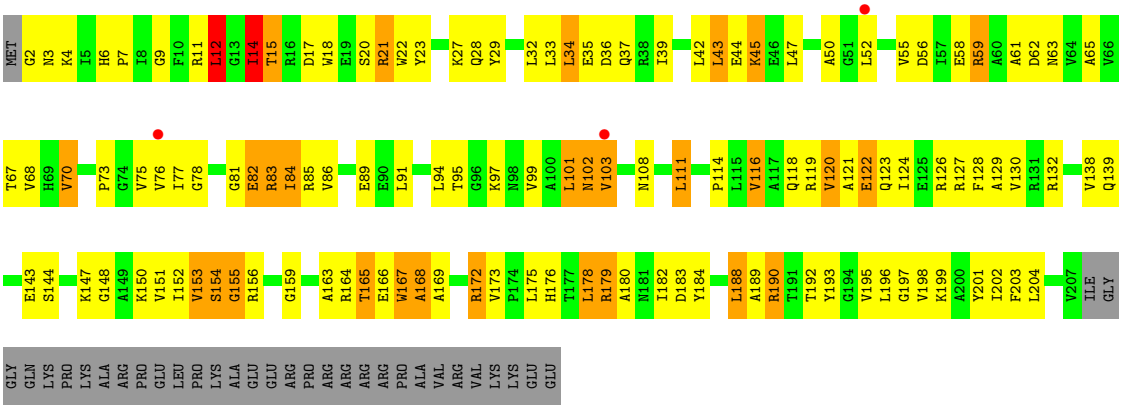
Chain B:



- Molecule 3: RIBOSOMAL PROTEIN S3

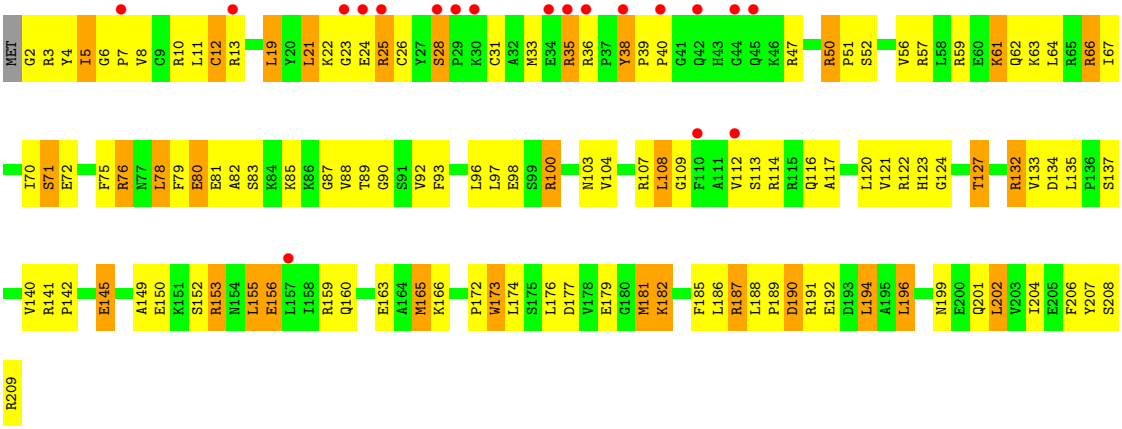
Chain C:





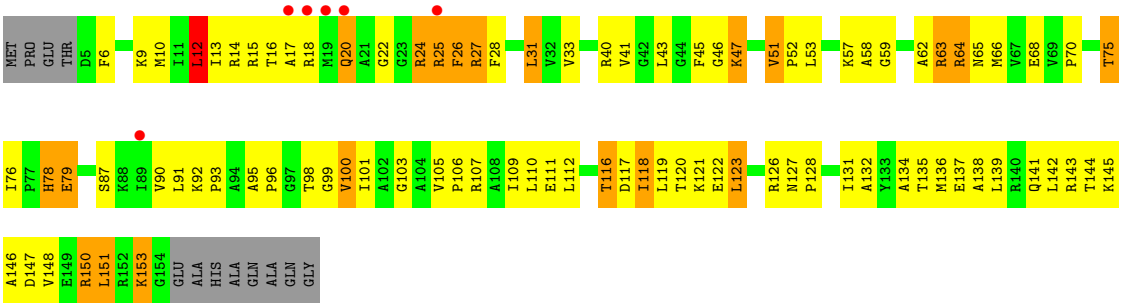
- Molecule 4: RIBOSOMAL PROTEIN S4

Chain D:



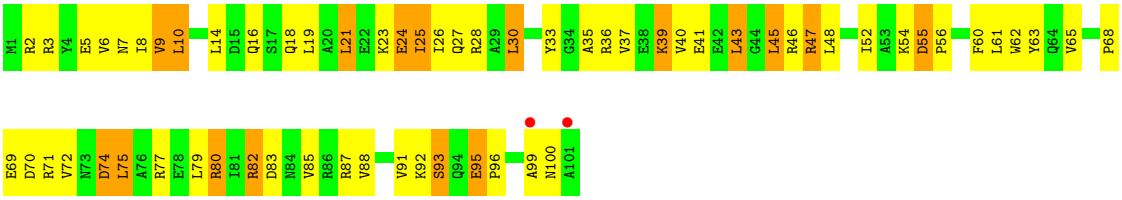
- Molecule 5: RIBOSOMAL PROTEIN S5

Chain E:



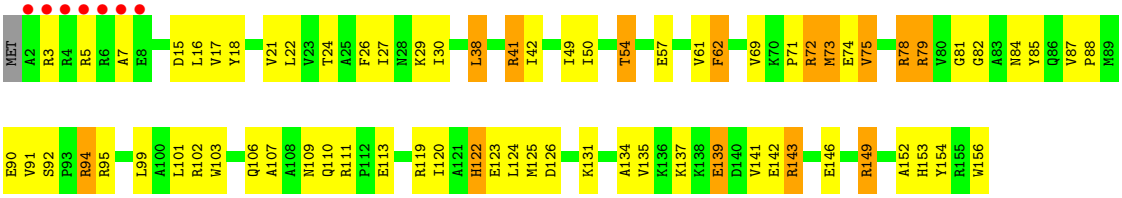
- Molecule 6: RIBOSOMAL PROTEIN S6

Chain F:



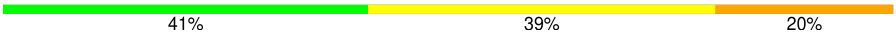
- Molecule 7: RIBOSOMAL PROTEIN S7

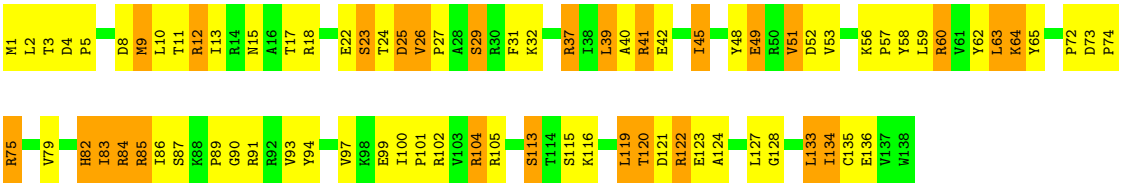
Chain G:



- Molecule 8: RIBOSOMAL PROTEIN S8

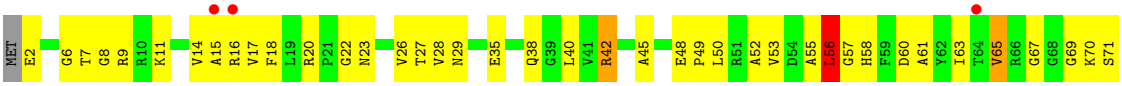
Chain H:





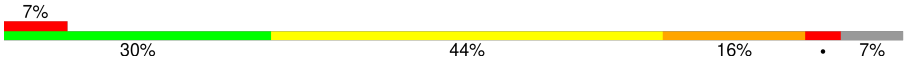
- Molecule 9: RIBOSOMAL PROTEIN S9

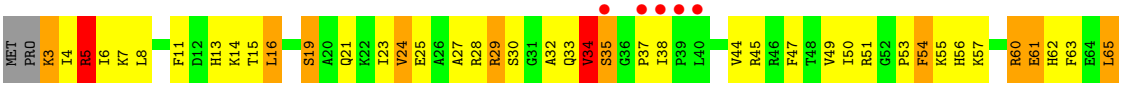
Chain I:

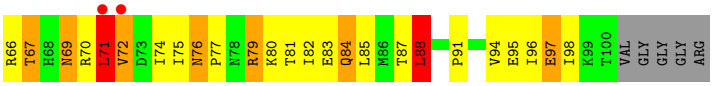


• Molecule 10: RIBOSOMAL PROTEIN S10

Chain J:

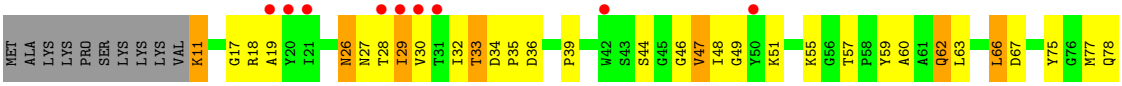


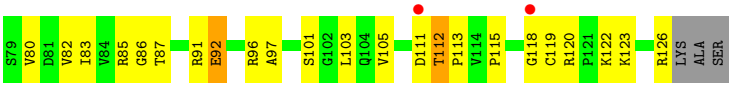




• Molecule 11: RIBOSOMAL PROTEIN S11

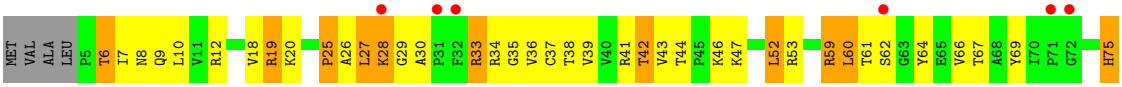
Chain K:

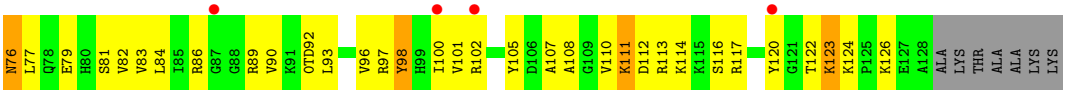




• Molecule 12: RIBOSOMAL PROTEIN S12

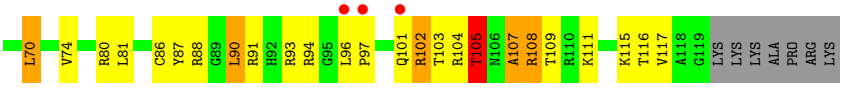
Chain L:





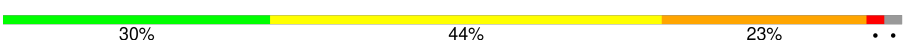
• Molecule 13: RIBOSOMAL PROTEIN S13

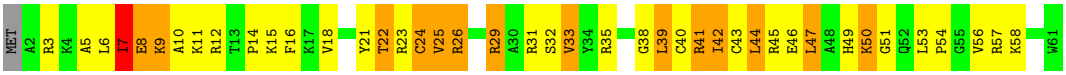
Chain M:



• Molecule 14: RIBOSOMAL PROTEIN S14

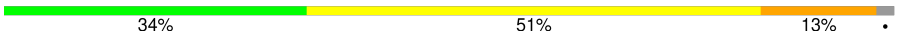
Chain N:

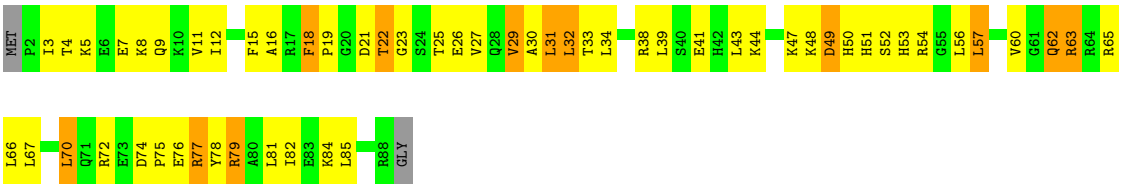




• Molecule 15: RIBOSOMAL PROTEIN S15

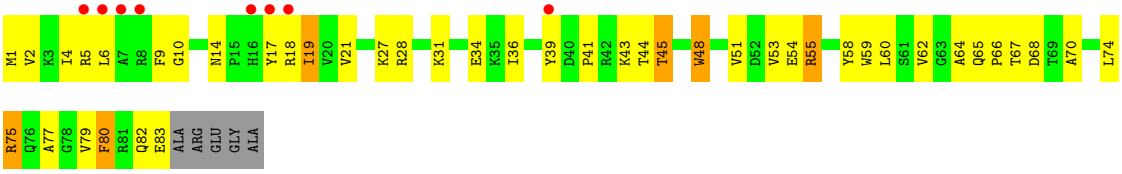
Chain O:





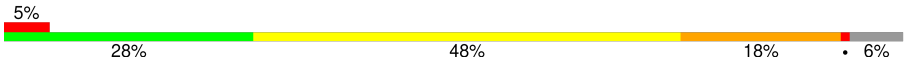
• Molecule 16: RIBOSOMAL PROTEIN S16

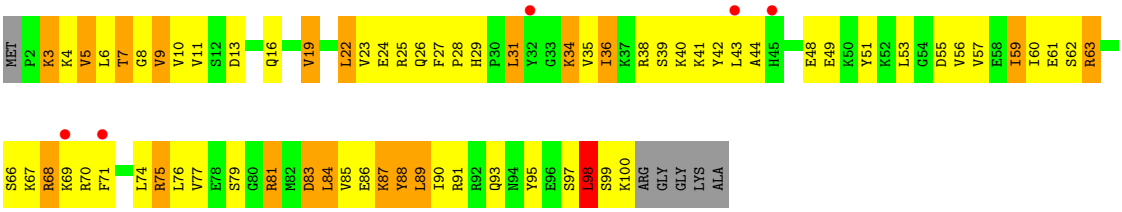
Chain P:



• Molecule 17: RIBOSOMAL PROTEIN S17

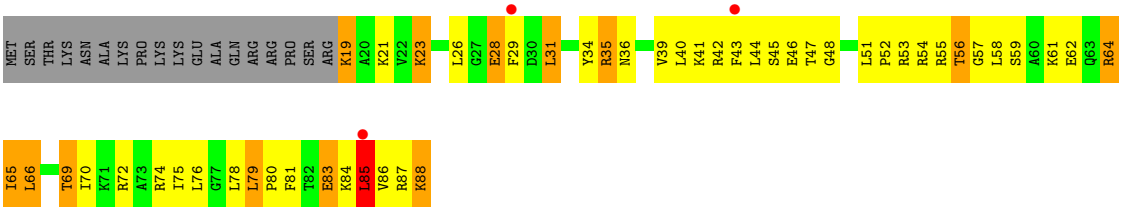
Chain Q:





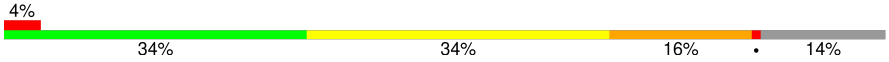
• Molecule 18: RIBOSOMAL PROTEIN S18

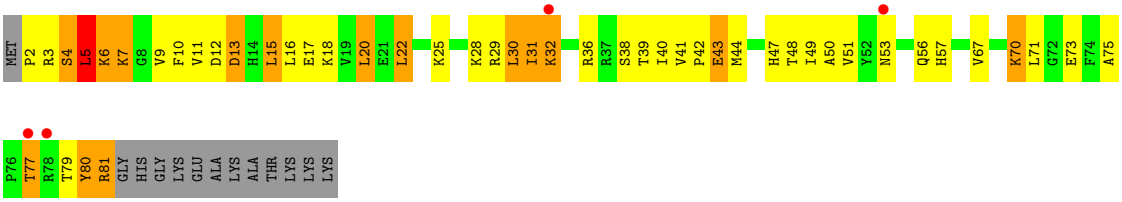
Chain R:



• Molecule 19: RIBOSOMAL PROTEIN S19

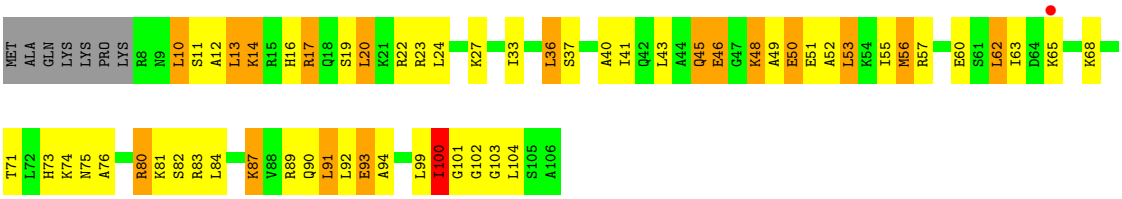
Chain S:





- 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	399.62Å 399.62Å 216.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.29 – 3.85 49.67 – 3.85	Depositor EDS
% Data completeness (in resolution range)	99.3 (47.29-3.85) 99.3 (49.67-3.85)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.47 (at 3.88Å)	Xtriage
Refinement program	PHENIX dev_1119	Depositor
R, R_{free}	0.153 , 0.202 0.154 , 0.201	Depositor DCC
R_{free} test set	8215 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	157.0	Xtriage
Anisotropy	0.232	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 166.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	52228	wwPDB-VP
Average B, all atoms (Å^2)	162.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.42% 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 (i)

5.1 Standard geometry (i)

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

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	1.18	129/36187 (0.4%)	2.02	1881/56471 (3.3%)
2	B	0.76	0/1935	1.00	6/2609 (0.2%)
3	C	0.79	0/1636	0.98	6/2205 (0.3%)
4	D	0.77	1/1733 (0.1%)	0.97	1/2318 (0.0%)
5	E	0.82	0/1162	1.05	4/1564 (0.3%)
6	F	0.83	0/856	1.02	3/1154 (0.3%)
7	G	0.73	0/1276	0.87	1/1709 (0.1%)
8	H	0.83	0/1136	0.98	0/1527
9	I	0.63	0/1029	0.88	1/1379 (0.1%)
10	J	0.77	0/805	1.03	4/1082 (0.4%)
11	K	0.71	0/879	0.91	0/1187
12	L	0.97	2/977 (0.2%)	1.15	2/1306 (0.2%)
13	M	0.59	0/947	0.84	0/1270
14	N	0.77	0/501	1.04	3/664 (0.5%)
15	O	0.69	0/740	0.94	0/987
16	P	0.74	0/716	0.92	0/963
17	Q	0.87	0/836	1.05	3/1117 (0.3%)
18	R	0.71	0/579	0.99	2/768 (0.3%)
19	S	0.60	0/661	1.01	4/890 (0.4%)
20	T	0.74	0/765	1.03	2/1007 (0.2%)
21	U	0.71	0/212	0.83	0/277
All	All	1.06	132/55568 (0.2%)	1.76	1923/82454 (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
8	H	0	1
9	I	0	2
10	J	0	2
13	M	0	3
14	N	0	1
16	P	0	1
20	T	0	3
All	All	0	18

All (132) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	672	U	C4-O4	8.76	1.30	1.23
1	A	563	A	N9-C4	-7.63	1.33	1.37
1	A	729	A	N3-C4	-7.49	1.30	1.34
1	A	1512	U	C4-O4	7.36	1.29	1.23
1	A	372	C	C2-O2	7.33	1.31	1.24
1	A	810	C	N3-C4	-7.31	1.28	1.33
1	A	1501	C	N1-C6	-6.93	1.32	1.37
1	A	1513	A	N9-C4	-6.92	1.33	1.37
1	A	802	A	N7-C5	-6.88	1.35	1.39
12	L	26	ALA	CA-CB	6.84	1.66	1.52
1	A	791	G	C6-O6	6.79	1.30	1.24
1	A	481	G	N7-C5	-6.78	1.35	1.39
1	A	922	G	C6-O6	6.78	1.30	1.24
1	A	792	A	N9-C4	-6.76	1.33	1.37
1	A	304	U	C4-O4	6.73	1.29	1.23
1	A	558	G	C6-O6	6.69	1.30	1.24
1	A	558	G	N3-C4	-6.62	1.30	1.35
1	A	642	A	N3-C4	-6.55	1.30	1.34
1	A	1392	G	C6-N1	-6.55	1.34	1.39
1	A	631	G	C6-N1	6.53	1.44	1.39
1	A	723	U	C2-N3	6.50	1.42	1.37
1	A	288	A	N9-C4	-6.49	1.33	1.37
1	A	523	A	N9-C4	-6.47	1.33	1.37
1	A	239	U	C4-O4	6.41	1.28	1.23
1	A	305	G	C6-O6	6.40	1.29	1.24
1	A	965	A	N9-C4	-6.40	1.34	1.37
1	A	790	A	N3-C4	-6.36	1.31	1.34
1	A	1335	C	N1-C2	6.35	1.46	1.40
1	A	1394	A	C6-N1	-6.33	1.31	1.35
1	A	1394	A	N3-C4	-6.32	1.31	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	715	A	N9-C4	-6.28	1.34	1.37
1	A	781	A	N9-C4	-6.27	1.34	1.37
1	A	484	G	C6-N1	-6.20	1.35	1.39
1	A	562	C	N1-C6	-6.19	1.33	1.37
1	A	509	A	N7-C5	-6.17	1.35	1.39
1	A	642	A	N9-C4	-6.16	1.34	1.37
1	A	1529	G	N7-C5	-6.15	1.35	1.39
1	A	32	A	N3-C4	-6.14	1.31	1.34
1	A	47	C	N3-C4	-6.08	1.29	1.33
1	A	439	A	N3-C4	-6.07	1.31	1.34
1	A	563	A	N3-C4	-6.05	1.31	1.34
1	A	238	G	N3-C4	-6.01	1.31	1.35
1	A	871	U	N1-C2	5.99	1.44	1.38
1	A	266	G	N9-C4	-5.99	1.33	1.38
1	A	550	G	C6-N1	-5.97	1.35	1.39
1	A	1230	C	C2-O2	5.97	1.29	1.24
1	A	26	A	N9-C4	-5.92	1.34	1.37
1	A	1005	A	N9-C4	5.91	1.41	1.37
1	A	1377	A	N9-C4	-5.86	1.34	1.37
1	A	309	G	C6-N1	5.86	1.43	1.39
1	A	50	A	N9-C4	-5.84	1.34	1.37
1	A	204	U	C2-N3	5.77	1.41	1.37
1	A	748	C	N1-C2	5.76	1.46	1.40
1	A	893	C	C2-O2	5.73	1.29	1.24
1	A	622	A	N9-C4	-5.73	1.34	1.37
1	A	1527	C	N3-C4	-5.73	1.29	1.33
1	A	1392	G	N1-C2	-5.72	1.33	1.37
1	A	262	A	N9-C4	-5.69	1.34	1.37
1	A	768	A	N9-C4	-5.68	1.34	1.37
12	L	98	TYR	CD2-CE2	5.68	1.47	1.39
1	A	267	C	N3-C4	-5.67	1.29	1.33
1	A	279	A	N9-C4	-5.65	1.34	1.37
1	A	382	A	C6-N1	-5.63	1.31	1.35
1	A	18	C	N1-C6	-5.63	1.33	1.37
1	A	250	A	C5-C4	5.62	1.42	1.38
1	A	859	A	N9-C4	-5.62	1.34	1.37
1	A	523	A	N3-C4	-5.60	1.31	1.34
1	A	108	G	N9-C4	-5.57	1.33	1.38
1	A	828	A	N9-C4	-5.55	1.34	1.37
1	A	878	G	C6-N1	-5.55	1.35	1.39
1	A	45	U	C4-O4	5.53	1.28	1.23
1	A	817	C	N1-C6	-5.53	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	728	A	N3-C4	-5.52	1.31	1.34
1	A	809	G	C5-C4	-5.52	1.34	1.38
1	A	357	G	C6-O6	5.52	1.29	1.24
1	A	32	A	C6-N1	-5.51	1.31	1.35
1	A	830	G	C6-O6	5.50	1.29	1.24
1	A	839	U	N1-C2	5.50	1.43	1.38
1	A	382	A	N3-C4	-5.49	1.31	1.34
1	A	108	G	N7-C5	-5.48	1.35	1.39
1	A	120	A	N7-C5	-5.47	1.35	1.39
1	A	505	G	C6-N1	-5.44	1.35	1.39
1	A	724	G	N7-C5	-5.44	1.35	1.39
1	A	969	A	N9-C4	-5.42	1.34	1.37
1	A	298	A	N3-C4	-5.41	1.31	1.34
1	A	553	A	N9-C4	-5.41	1.34	1.37
1	A	1531	A	N9-C8	5.40	1.42	1.37
4	D	173	TRP	CB-CG	-5.40	1.40	1.50
1	A	631	G	N1-C2	5.40	1.42	1.37
1	A	1124	G	C6-N1	5.40	1.43	1.39
1	A	1157	A	N9-C4	5.38	1.41	1.37
1	A	27	G	N7-C5	-5.38	1.36	1.39
1	A	1225	A	N3-C4	-5.37	1.31	1.34
1	A	375	U	C4-O4	5.36	1.27	1.23
1	A	703	G	C5-C6	5.36	1.47	1.42
1	A	919	A	C5-C4	-5.36	1.35	1.38
1	A	532	A	N3-C4	5.35	1.38	1.34
1	A	1493	A	N9-C4	5.33	1.41	1.37
1	A	964	A	N3-C4	-5.33	1.31	1.34
1	A	510	A	N3-C4	-5.31	1.31	1.34
1	A	47	C	N1-C6	-5.30	1.33	1.37
1	A	729	A	N7-C5	-5.30	1.36	1.39
1	A	1531	A	C5-C4	5.30	1.42	1.38
1	A	390	C	N1-C6	-5.29	1.33	1.37
1	A	9	G	N9-C8	-5.28	1.34	1.37
1	A	919	A	N7-C5	-5.25	1.36	1.39
1	A	122	G	C5-C4	-5.25	1.34	1.38
1	A	864	A	N3-C4	-5.23	1.31	1.34
1	A	325	A	N3-C4	-5.23	1.31	1.34
1	A	1530	G	C6-N1	5.23	1.43	1.39
1	A	1393	U	C4-O4	5.20	1.27	1.23
1	A	802	A	C5-C6	-5.20	1.36	1.41
1	A	67	C	N3-C4	-5.19	1.30	1.33
1	A	543	C	N1-C6	-5.19	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	704	A	N9-C4	-5.19	1.34	1.37
1	A	889	A	N3-C4	-5.18	1.31	1.34
1	A	1403	C	N1-C6	-5.18	1.34	1.37
1	A	1004	A	N9-C4	5.14	1.41	1.37
1	A	379	C	N1-C6	-5.14	1.34	1.37
1	A	357	G	C2-N3	-5.12	1.28	1.32
1	A	919	A	N9-C4	-5.09	1.34	1.37
1	A	791	G	N3-C4	-5.09	1.31	1.35
1	A	10	A	C6-N1	-5.09	1.31	1.35
1	A	728	A	C5-C6	-5.09	1.36	1.41
1	A	1506	U	N1-C2	5.08	1.43	1.38
1	A	1084	G	C6-O6	5.07	1.28	1.24
1	A	230	G	C6-O6	5.07	1.28	1.24
1	A	859	A	N3-C4	-5.06	1.31	1.34
1	A	964	A	N9-C4	-5.05	1.34	1.37
1	A	1084	G	C5-C6	5.05	1.47	1.42
1	A	66	G	N9-C4	-5.01	1.33	1.38
1	A	487	A	N9-C4	-5.00	1.34	1.37

All (1923) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1528	U	O5'-P-OP2	-17.17	90.09	110.70
1	A	309	G	N1-C6-O6	16.92	130.05	119.90
1	A	922	G	N1-C6-O6	15.33	129.10	119.90
1	A	558	G	C5-C6-N1	-15.09	103.95	111.50
1	A	1335	C	N1-C2-O2	14.44	127.56	118.90
1	A	117	G	N1-C6-O6	14.31	128.49	119.90
1	A	791	G	C5-C6-N1	-13.57	104.72	111.50
1	A	325	A	N1-C6-N6	-13.50	110.50	118.60
1	A	922	G	C5-C6-N1	-13.29	104.86	111.50
1	A	970	C	N1-C2-O2	13.22	126.83	118.90
1	A	672	U	N3-C4-C5	-13.21	106.67	114.60
1	A	305	G	C5-C6-N1	-13.20	104.90	111.50
1	A	239	U	N3-C4-C5	-13.17	106.70	114.60
1	A	1512	U	N3-C4-C5	-13.00	106.80	114.60
1	A	1435	G	N1-C6-O6	12.82	127.59	119.90
1	A	541	G	N1-C6-O6	12.58	127.45	119.90
1	A	147	G	N1-C6-O6	12.50	127.40	119.90
1	A	1531	A	N7-C8-N9	12.41	120.01	113.80
1	A	58	C	C6-N1-C2	-12.22	115.41	120.30
1	A	1531	A	N1-C6-N6	12.19	125.91	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1531	A	C5-N7-C8	-12.04	97.88	103.90
1	A	304	U	N3-C4-C5	-11.95	107.43	114.60
1	A	730	G	C4-C5-N7	-11.91	106.04	110.80
1	A	518	C	N1-C2-O2	11.81	125.99	118.90
1	A	481	G	O5'-P-OP2	-11.75	95.13	105.70
1	A	871	U	N1-C2-O2	11.72	131.00	122.80
1	A	830	G	C5-C6-N1	-11.51	105.75	111.50
1	A	1064	G	C5-C6-O6	-11.50	121.70	128.60
1	A	1050	G	N1-C6-O6	11.43	126.76	119.90
1	A	1335	C	N3-C2-O2	-11.43	113.90	121.90
1	A	1530	G	N3-C4-C5	11.43	134.31	128.60
1	A	34	C	C6-N1-C2	11.40	124.86	120.30
1	A	309	G	C5-C6-O6	-11.38	121.78	128.60
1	A	1532	U	C5-C6-N1	11.23	128.32	122.70
1	A	285	G	C8-N9-C4	11.23	110.89	106.40
1	A	624	C	C6-N1-C2	11.23	124.79	120.30
1	A	27	G	N1-C6-O6	11.18	126.61	119.90
1	A	710	G	N1-C6-O6	11.13	126.58	119.90
1	A	1397	C	O5'-P-OP1	-11.08	95.73	105.70
1	A	1233	G	N1-C6-O6	11.06	126.53	119.90
1	A	254	G	O5'-P-OP1	-11.01	95.79	105.70
1	A	1124	G	C2-N3-C4	10.97	117.38	111.90
1	A	117	G	C6-C5-N7	-10.92	123.85	130.40
1	A	897	C	N3-C4-C5	10.91	126.27	121.90
1	A	769	G	O5'-P-OP2	-10.88	95.91	105.70
1	A	1514	C	C6-N1-C2	10.87	124.65	120.30
1	A	902	G	N1-C6-O6	10.78	126.36	119.90
1	A	718	G	C8-N9-C4	10.73	110.69	106.40
1	A	555	C	O5'-P-OP2	-10.66	96.11	105.70
1	A	1277	C	C6-N1-C2	-10.62	116.05	120.30
1	A	1125	U	N3-C2-O2	10.61	129.63	122.20
1	A	922	G	C4-C5-C6	10.61	125.17	118.80
1	A	1222	G	C5-C6-N1	-10.61	106.20	111.50
1	A	122	G	C8-N9-C4	10.58	110.63	106.40
1	A	54	C	C6-N1-C2	10.55	124.52	120.30
1	A	1064	G	N1-C6-O6	10.55	126.23	119.90
1	A	333	G	N1-C6-O6	10.50	126.20	119.90
1	A	1256	A	C8-N9-C4	10.43	109.97	105.80
1	A	1522	U	O5'-P-OP2	-10.40	96.34	105.70
1	A	893	C	N1-C2-N3	-10.37	111.94	119.20
1	A	357	G	C5-C6-N1	-10.32	106.34	111.50
1	A	710	G	C5-C6-N1	-10.31	106.35	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1227	A	N1-C6-N6	10.30	124.78	118.60
1	A	251	G	N1-C6-O6	10.17	126.00	119.90
1	A	314	C	C6-N1-C2	10.16	124.36	120.30
1	A	108	G	N1-C6-O6	10.15	125.99	119.90
1	A	975	A	C2-N3-C4	-10.11	105.54	110.60
1	A	300	A	N1-C6-N6	-10.11	112.54	118.60
1	A	522	C	C6-N1-C2	10.07	124.33	120.30
1	A	234	C	C6-N1-C2	10.06	124.32	120.30
1	A	1531	A	C4-C5-N7	10.04	115.72	110.70
1	A	204	U	C5-C6-N1	9.88	127.64	122.70
1	A	277	C	C6-N1-C2	9.84	124.24	120.30
1	A	325	A	N9-C4-C5	9.80	109.72	105.80
1	A	147	G	C5-C6-N1	-9.79	106.61	111.50
1	A	266	G	N3-C4-C5	9.78	133.49	128.60
1	A	724	G	N3-C4-C5	-9.77	123.72	128.60
1	A	1377	A	C2-N3-C4	-9.75	105.72	110.60
1	A	372	C	C6-N1-C2	9.72	124.19	120.30
1	A	372	C	N1-C2-N3	-9.72	112.39	119.20
1	A	814	A	C2-N3-C4	-9.72	105.74	110.60
1	A	830	G	N1-C6-O6	9.72	125.73	119.90
1	A	920	U	N3-C4-O4	-9.70	112.61	119.40
1	A	1233	G	C5-C6-N1	-9.66	106.67	111.50
1	A	922	G	N3-C2-N2	-9.66	113.14	119.90
1	A	309	G	C6-C5-N7	-9.64	124.61	130.40
1	A	332	G	N1-C6-O6	9.61	125.67	119.90
1	A	255	G	N1-C6-O6	9.61	125.66	119.90
1	A	1084	G	C4-C5-N7	-9.61	106.96	110.80
1	A	32	A	C6-N1-C2	-9.59	112.85	118.60
1	A	1531	A	C8-N9-C4	-9.51	101.99	105.80
1	A	557	G	N1-C6-O6	9.51	125.61	119.90
1	A	829	G	C8-N9-C4	9.50	110.20	106.40
1	A	855	G	C5-C6-N1	-9.50	106.75	111.50
1	A	27	G	C6-C5-N7	-9.49	124.71	130.40
1	A	113	G	N1-C6-O6	9.44	125.57	119.90
1	A	333	G	C5-C6-N1	-9.41	106.80	111.50
1	A	541	G	C5-C6-O6	-9.41	122.96	128.60
1	A	871	U	N3-C2-O2	-9.40	115.62	122.20
1	A	604	G	N1-C6-O6	9.39	125.53	119.90
1	A	325	A	C5-C6-N6	9.37	131.20	123.70
1	A	886	G	N1-C6-O6	9.36	125.52	119.90
1	A	298	A	C2-N3-C4	-9.34	105.93	110.60
1	A	855	G	C2-N3-C4	-9.29	107.25	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1054	C	N1-C2-O2	9.29	124.48	118.90
1	A	267	C	N3-C4-N4	-9.29	111.50	118.00
1	A	558	G	C5-C6-O6	9.26	134.16	128.60
1	A	518	C	N3-C2-O2	-9.23	115.44	121.90
1	A	635	G	N1-C6-O6	9.23	125.44	119.90
1	A	761	G	N1-C6-O6	9.23	125.44	119.90
1	A	562	C	N1-C2-O2	9.22	124.43	118.90
1	A	500	G	O5'-P-OP1	-9.21	97.41	105.70
1	A	893	C	N1-C2-O2	9.21	124.42	118.90
1	A	830	G	N3-C2-N2	-9.16	113.49	119.90
1	A	31	G	N3-C4-N9	9.15	131.49	126.00
1	A	313	A	N1-C6-N6	9.15	124.09	118.60
1	A	28	G	N1-C6-O6	9.14	125.39	119.90
1	A	398	C	C6-N1-C2	9.11	123.94	120.30
1	A	887	G	N1-C6-O6	9.11	125.36	119.90
1	A	610	G	C8-N9-C4	-9.09	102.76	106.40
1	A	1166	G	N3-C4-C5	-9.09	124.06	128.60
1	A	661	G	N1-C6-O6	9.08	125.35	119.90
1	A	810	C	N3-C4-N4	-9.08	111.65	118.00
1	A	1512	U	C5-C4-O4	9.07	131.34	125.90
1	A	27	G	O5'-P-OP1	-9.06	97.55	105.70
3	C	179	ARG	N-CA-C	-9.04	86.59	111.00
1	A	811	C	C5-C6-N1	-9.03	116.49	121.00
1	A	1426	C	C6-N1-C2	9.02	123.91	120.30
1	A	228	A	N1-C6-N6	-8.98	113.21	118.60
1	A	901	A	O5'-P-OP1	-8.98	97.62	105.70
1	A	1026	G	N7-C8-N9	8.98	117.59	113.10
1	A	1087	G	N1-C6-O6	8.98	125.29	119.90
1	A	381	C	C6-N1-C2	-8.98	116.71	120.30
1	A	1057	G	N3-C2-N2	-8.92	113.66	119.90
1	A	535	A	N1-C6-N6	-8.91	113.25	118.60
1	A	1070	U	O5'-P-OP2	-8.90	97.69	105.70
1	A	749	C	C6-N1-C2	-8.90	116.74	120.30
1	A	204	U	C2-N1-C1'	8.88	128.36	117.70
1	A	828	A	C8-N9-C4	8.88	109.35	105.80
1	A	1530	G	N3-C4-N9	-8.86	120.69	126.00
1	A	372	C	N3-C4-C5	8.83	125.43	121.90
1	A	19	C	O5'-P-OP2	-8.82	97.76	105.70
1	A	1004	A	O4'-C1'-N9	8.80	115.24	108.20
1	A	1277	C	C5-C6-N1	8.78	125.39	121.00
1	A	661	G	C5-C6-N1	-8.77	107.11	111.50
1	A	1479	C	C6-N1-C2	-8.76	116.80	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	113	G	C6-C5-N7	-8.76	125.14	130.40
1	A	400	C	C6-N1-C2	8.75	123.80	120.30
1	A	251	G	C5-C6-O6	-8.74	123.36	128.60
1	A	817	C	C2-N1-C1'	8.72	128.39	118.80
1	A	811	C	C6-N1-C2	8.72	123.79	120.30
1	A	544	G	C4-C5-N7	8.71	114.28	110.80
1	A	387	U	O5'-P-OP2	-8.71	97.86	105.70
1	A	590	C	C6-N1-C2	8.71	123.78	120.30
1	A	239	U	N3-C4-O4	8.70	125.49	119.40
1	A	664	G	C5-N7-C8	8.70	108.65	104.30
1	A	241	C	C6-N1-C2	8.70	123.78	120.30
1	A	265	G	N3-C4-N9	-8.70	120.78	126.00
1	A	557	G	C6-C5-N7	-8.70	125.18	130.40
1	A	1393	U	C4-C5-C6	8.69	124.92	119.70
1	A	1075	C	O5'-P-OP2	-8.69	97.88	105.70
1	A	1531	A	C6-C5-N7	-8.68	126.23	132.30
1	A	247	G	N1-C6-O6	8.66	125.10	119.90
1	A	484	G	N1-C2-N2	-8.65	108.41	116.20
1	A	113	G	N3-C4-N9	8.65	131.19	126.00
1	A	503	C	O5'-P-OP2	-8.65	97.92	105.70
1	A	1290	G	N1-C6-O6	8.63	125.08	119.90
1	A	31	G	C8-N9-C1'	-8.61	115.81	127.00
1	A	1516[A]	G	N3-C4-N9	-8.60	120.84	126.00
1	A	1516[B]	G	N3-C4-N9	-8.60	120.84	126.00
1	A	403	C	O5'-P-OP2	-8.60	97.96	105.70
1	A	927	G	O5'-P-OP1	-8.60	97.96	105.70
1	A	922	G	C6-C5-N7	-8.60	125.24	130.40
1	A	728	A	C8-N9-C4	-8.60	102.36	105.80
1	A	783	C	C6-N1-C2	8.59	123.73	120.30
1	A	731	G	C4-C5-N7	8.59	114.23	110.80
1	A	10	A	O5'-P-OP2	-8.58	97.98	105.70
1	A	113	G	C5-C6-O6	-8.57	123.45	128.60
1	A	1512	U	C6-N1-C2	-8.57	115.86	121.00
1	A	266	G	C5-N7-C8	-8.56	100.02	104.30
1	A	99	C	C6-N1-C2	-8.54	116.89	120.30
1	A	1256	A	N7-C8-N9	-8.52	109.54	113.80
1	A	1528	U	OP1-P-OP2	8.52	132.38	119.60
1	A	46	G	C8-N9-C4	-8.51	103.00	106.40
1	A	794	A	O5'-P-OP2	-8.51	98.04	105.70
1	A	108	G	C6-C5-N7	-8.49	125.30	130.40
1	A	1432	G	C8-N9-C4	-8.49	103.00	106.40
1	A	1026	G	C8-N9-C4	-8.48	103.01	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1432	G	C5-C6-N1	-8.45	107.27	111.50
1	A	1305	G	C8-N9-C4	-8.45	103.02	106.40
1	A	47	C	N3-C2-O2	-8.45	115.99	121.90
1	A	277	C	O5'-P-OP1	-8.44	98.10	105.70
1	A	664	G	C4-C5-N7	-8.44	107.43	110.80
1	A	121	C	C6-N1-C2	8.43	123.67	120.30
1	A	15	G	N1-C6-O6	8.42	124.95	119.90
1	A	284	G	N1-C6-O6	8.42	124.95	119.90
1	A	818	G	OP1-P-OP2	8.41	132.22	119.60
1	A	21	G	C6-C5-N7	-8.41	125.36	130.40
1	A	541	G	C6-C5-N7	-8.39	125.36	130.40
1	A	1087	G	C6-C5-N7	-8.38	125.37	130.40
1	A	372	C	N1-C2-O2	8.38	123.92	118.90
1	A	699	C	C6-N1-C2	8.37	123.65	120.30
1	A	729	A	OP1-P-O3'	8.37	123.62	105.20
1	A	500	G	N1-C6-O6	8.36	124.91	119.90
1	A	25	C	C6-N1-C2	8.34	123.64	120.30
1	A	485	G	C8-N9-C4	8.34	109.74	106.40
1	A	1205	U	N3-C4-C5	-8.33	109.60	114.60
1	A	526	C	O5'-P-OP1	8.32	120.69	110.70
1	A	122	G	N7-C8-N9	-8.30	108.95	113.10
1	A	987	G	N1-C6-O6	8.30	124.88	119.90
1	A	304	U	C4-C5-C6	8.29	124.67	119.70
1	A	774	G	C6-C5-N7	-8.28	125.43	130.40
1	A	1050	G	C5-C6-O6	-8.28	123.63	128.60
1	A	20	U	C5-C4-O4	-8.26	120.94	125.90
1	A	117	G	C5-C6-O6	-8.26	123.65	128.60
1	A	1211	U	C5-C6-N1	8.26	126.83	122.70
1	A	58	C	C5-C6-N1	8.24	125.12	121.00
1	A	724	G	C8-N9-C4	-8.24	103.11	106.40
1	A	45	U	N3-C4-C5	-8.23	109.66	114.60
1	A	122	G	N9-C4-C5	-8.22	102.11	105.40
1	A	113	G	C8-N9-C1'	-8.21	116.32	127.00
1	A	1393	U	N3-C4-C5	-8.21	109.67	114.60
1	A	408	A	C8-N9-C4	-8.20	102.52	105.80
1	A	906	G	N1-C6-O6	8.20	124.82	119.90
1	A	133	U	C5-C4-O4	8.19	130.81	125.90
1	A	239	U	C6-N1-C2	-8.19	116.09	121.00
1	A	766	A	O5'-P-OP2	-8.18	98.33	105.70
1	A	284	G	C2-N3-C4	-8.18	107.81	111.90
1	A	1230	C	C2-N3-C4	8.18	123.99	119.90
1	A	724	G	C6-C5-N7	-8.15	125.51	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	111	G	N3-C4-N9	-8.14	121.11	126.00
1	A	703	G	C8-N9-C1'	-8.14	116.41	127.00
1	A	730	G	C5-N7-C8	8.14	108.37	104.30
1	A	886	G	C2-N3-C4	-8.13	107.83	111.90
1	A	877	C	C6-N1-C2	-8.13	117.05	120.30
1	A	266	G	N3-C4-N9	-8.12	121.13	126.00
1	A	674	G	N1-C6-O6	8.12	124.77	119.90
1	A	819	A	N1-C6-N6	8.12	123.47	118.60
1	A	117	G	N9-C4-C5	-8.10	102.16	105.40
1	A	500	G	C8-N9-C4	8.09	109.64	106.40
1	A	7	G	C5-C6-O6	-8.09	123.75	128.60
1	A	306	G	N1-C6-O6	8.08	124.75	119.90
1	A	799	G	C6-C5-N7	-8.07	125.56	130.40
1	A	731	G	C5-N7-C8	-8.05	100.27	104.30
1	A	147	G	C6-C5-N7	-8.05	125.57	130.40
1	A	509	A	C8-N9-C4	-8.05	102.58	105.80
1	A	484	G	P-O3'-C3'	8.05	129.36	119.70
1	A	1435	G	C2-N3-C4	-8.05	107.88	111.90
1	A	1050	G	C6-C5-N7	-8.04	125.57	130.40
1	A	1064	G	C4-C5-N7	8.04	114.01	110.80
1	A	893	C	C2-N3-C4	8.03	123.92	119.90
1	A	1523	G	N1-C6-O6	8.03	124.72	119.90
1	A	1491	G	C8-N9-C4	-8.02	103.19	106.40
1	A	507	C	C6-N1-C2	8.02	123.51	120.30
1	A	785	G	N1-C6-O6	8.01	124.71	119.90
1	A	646	U	N3-C4-C5	-8.01	109.80	114.60
1	A	976	G	C5-C6-N1	-8.01	107.50	111.50
1	A	1173	G	C8-N9-C4	8.01	109.60	106.40
1	A	32	A	N1-C2-N3	8.00	133.30	129.30
1	A	1539	C	C6-N1-C2	-8.00	117.10	120.30
1	A	484	G	N1-C6-O6	-8.00	115.10	119.90
1	A	1202	G	N9-C4-C5	7.99	108.60	105.40
1	A	260	G	C8-N9-C4	-7.99	103.20	106.40
1	A	314	C	N3-C4-C5	7.99	125.09	121.90
1	A	906	G	C6-C5-N7	-7.99	125.61	130.40
1	A	133	U	N3-C2-O2	-7.98	116.61	122.20
1	A	791	G	C4-C5-C6	7.98	123.59	118.80
1	A	1131	G	N1-C6-O6	7.98	124.69	119.90
1	A	1202	G	N3-C4-N9	-7.97	121.22	126.00
1	A	27	G	C5-C6-O6	-7.97	123.82	128.60
1	A	333	G	N3-C2-N2	-7.95	114.33	119.90
17	Q	98	LEU	CA-CB-CG	7.95	133.59	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	190(H)	G	N1-C6-O6	7.95	124.67	119.90
1	A	290	C	O5'-P-OP2	-7.93	98.56	105.70
1	A	830	G	N3-C4-C5	7.93	132.57	128.60
1	A	104	G	C5-C6-N1	-7.93	107.53	111.50
1	A	1084	G	C5-C6-O6	7.93	133.36	128.60
1	A	799	G	N1-C6-O6	7.92	124.65	119.90
1	A	1304	G	C5-C6-N1	-7.92	107.54	111.50
1	A	1211	U	N1-C2-O2	7.92	128.34	122.80
1	A	257	G	N1-C6-O6	7.91	124.65	119.90
1	A	936	C	O5'-P-OP2	7.91	120.19	110.70
1	A	401	C	N3-C4-N4	7.91	123.53	118.00
1	A	1393	U	N3-C4-O4	7.89	124.93	119.40
1	A	102	G	C6-C5-N7	-7.89	125.66	130.40
1	A	1104	G	N1-C2-N3	7.89	128.63	123.90
1	A	1257	U	C2-N1-C1'	7.89	127.17	117.70
1	A	852	G	N1-C6-O6	7.89	124.63	119.90
1	A	481	G	C6-C5-N7	-7.89	125.67	130.40
1	A	1166	G	N3-C4-N9	7.89	130.73	126.00
1	A	276	G	N1-C2-N3	7.88	128.63	123.90
1	A	1189	C	C6-N1-C2	-7.88	117.15	120.30
1	A	288	A	C2-N3-C4	-7.88	106.66	110.60
1	A	1230	C	N1-C2-N3	-7.88	113.69	119.20
1	A	113	G	C4-N9-C1'	7.87	136.74	126.50
1	A	965	A	C8-N9-C4	7.87	108.95	105.80
1	A	204	U	C6-N1-C2	-7.86	116.28	121.00
1	A	579	G	N1-C6-O6	7.85	124.61	119.90
1	A	252	U	N1-C2-O2	-7.85	117.30	122.80
1	A	1079	G	N3-C4-C5	-7.84	124.68	128.60
1	A	674	G	C6-C5-N7	-7.83	125.70	130.40
1	A	329	A	O5'-P-OP1	-7.81	98.67	105.70
1	A	232	G	C6-C5-N7	-7.81	125.71	130.40
1	A	928	G	C5-C6-N1	-7.81	107.59	111.50
1	A	672	U	C4-C5-C6	7.80	124.38	119.70
1	A	49	U	N3-C2-O2	7.80	127.66	122.20
1	A	1532	U	C4-C5-C6	-7.80	115.02	119.70
1	A	254	G	OP2-P-O3'	7.79	122.35	105.20
1	A	558	G	N3-C4-N9	-7.79	121.33	126.00
1	A	562	C	C6-N1-C2	7.78	123.41	120.30
1	A	902	G	N9-C4-C5	-7.78	102.29	105.40
1	A	1516[A]	G	C2-N3-C4	-7.78	108.01	111.90
1	A	1516[B]	G	C2-N3-C4	-7.78	108.01	111.90
1	A	928	G	N1-C6-O6	7.77	124.56	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	401	C	N1-C2-O2	-7.77	114.24	118.90
1	A	830	G	N3-C4-N9	-7.77	121.34	126.00
1	A	646	U	C6-N1-C2	-7.77	116.34	121.00
1	A	1532	U	N3-C2-O2	7.77	127.64	122.20
1	A	1524	C	O5'-P-OP1	-7.76	98.72	105.70
1	A	761	G	C5-C6-N1	-7.75	107.62	111.50
1	A	789	U	N3-C4-C5	-7.75	109.95	114.60
1	A	902	G	C5-C6-O6	-7.75	123.95	128.60
1	A	976	G	N1-C6-O6	7.75	124.55	119.90
1	A	703	G	C5-C6-O6	7.74	133.25	128.60
1	A	1189	C	N3-C2-O2	-7.74	116.48	121.90
1	A	920	U	C5-C4-O4	7.73	130.54	125.90
1	A	864	A	N9-C4-C5	7.73	108.89	105.80
1	A	500	G	C5-C6-O6	-7.72	123.97	128.60
1	A	1502	A	C2-N3-C4	-7.71	106.74	110.60
1	A	761	G	C2-N3-C4	-7.71	108.05	111.90
1	A	746	A	C6-N1-C2	-7.71	113.97	118.60
1	A	1433	A	O5'-P-OP1	-7.71	98.76	105.70
1	A	372	C	C5-C4-N4	-7.70	114.81	120.20
1	A	1530	G	C4-N9-C1'	-7.70	116.49	126.50
1	A	830	G	C2-N3-C4	-7.70	108.05	111.90
1	A	659	U	N1-C2-N3	7.69	119.51	114.90
1	A	786	G	N1-C6-O6	7.68	124.51	119.90
1	A	251	G	C4-C5-N7	7.66	113.86	110.80
1	A	1124	G	N1-C2-N3	-7.66	119.31	123.90
1	A	239	U	C4-C5-C6	7.66	124.29	119.70
1	A	654	G	N3-C4-N9	-7.66	121.41	126.00
1	A	558	G	C4-C5-N7	-7.64	107.75	110.80
1	A	637	G	N1-C6-O6	7.64	124.48	119.90
1	A	120	A	C4-C5-C6	7.63	120.82	117.00
1	A	1100	C	C5-C6-N1	7.62	124.81	121.00
1	A	786	G	C5-C6-N1	-7.62	107.69	111.50
1	A	829	G	O5'-P-OP2	-7.60	98.86	105.70
1	A	1047	G	C5-C6-N1	-7.59	107.71	111.50
1	A	659	U	N3-C2-O2	-7.57	116.90	122.20
1	A	485	G	C5-C6-N1	-7.56	107.72	111.50
1	A	1182	G	N3-C4-C5	-7.55	124.82	128.60
1	A	392	G	C8-N9-C4	7.54	109.42	106.40
1	A	902	G	C6-C5-N7	-7.54	125.88	130.40
1	A	108	G	C2-N3-C4	-7.53	108.13	111.90
1	A	387	U	N3-C4-C5	-7.53	110.08	114.60
1	A	491	G	C5-C6-N1	-7.53	107.73	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1104	G	C2-N3-C4	-7.53	108.14	111.90
1	A	446	G	O5'-P-OP1	-7.53	98.93	105.70
1	A	1084	G	C5-N7-C8	7.53	108.06	104.30
1	A	117	G	C4-C5-N7	7.52	113.81	110.80
1	A	740	U	N1-C2-O2	-7.52	117.54	122.80
1	A	1129	C	C6-N1-C2	-7.52	117.29	120.30
1	A	1465	C	N1-C2-O2	7.51	123.41	118.90
1	A	1030(C)	G	C4-N9-C1'	7.51	136.26	126.50
2	B	71	VAL	CB-CA-C	-7.51	97.13	111.40
1	A	481	G	OP1-P-OP2	7.49	130.84	119.60
1	A	724	G	N3-C4-N9	7.49	130.50	126.00
1	A	1395	C	C6-N1-C2	7.49	123.30	120.30
1	A	1516[A]	G	N3-C4-C5	7.49	132.35	128.60
1	A	1516[B]	G	N3-C4-C5	7.49	132.35	128.60
1	A	494	G	C8-N9-C4	-7.49	103.40	106.40
1	A	120	A	N1-C2-N3	7.49	133.04	129.30
17	Q	84	LEU	CA-CB-CG	-7.49	98.08	115.30
1	A	833	U	N3-C4-C5	-7.48	110.11	114.60
1	A	1222	G	N1-C6-O6	7.48	124.39	119.90
1	A	494	G	O5'-P-OP1	-7.47	98.98	105.70
1	A	829	G	N7-C8-N9	-7.47	109.36	113.10
1	A	314	C	C2-N1-C1'	-7.47	110.59	118.80
1	A	774	G	N3-C4-N9	7.46	130.48	126.00
1	A	1539	C	C5-C6-N1	7.46	124.73	121.00
1	A	1075	C	C5-C6-N1	-7.45	117.27	121.00
1	A	1411	C	N1-C2-O2	7.45	123.37	118.90
1	A	309	G	N3-C2-N2	-7.44	114.69	119.90
1	A	689	C	N3-C2-O2	7.44	127.11	121.90
1	A	276	G	C2-N3-C4	-7.43	108.18	111.90
1	A	729	A	N9-C4-C5	7.43	108.77	105.80
1	A	26	A	C2-N3-C4	-7.43	106.89	110.60
1	A	535	A	N9-C4-C5	7.42	108.77	105.80
1	A	275	G	N1-C6-O6	7.42	124.35	119.90
1	A	746	A	N1-C2-N3	7.42	133.01	129.30
1	A	730	G	N9-C4-C5	7.42	108.37	105.40
1	A	1197	G	C4-N9-C1'	7.41	136.14	126.50
1	A	1420	C	C6-N1-C2	-7.41	117.34	120.30
1	A	244	U	N1-C2-N3	-7.41	110.45	114.90
1	A	108	G	C4-C5-N7	7.40	113.76	110.80
1	A	975	A	N7-C8-N9	7.40	117.50	113.80
2	B	11	LEU	CA-CB-CG	7.40	132.31	115.30
1	A	394	G	C5-C6-N1	-7.39	107.80	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	29	G	N1-C6-O6	7.39	124.34	119.90
1	A	715	A	C8-N9-C4	7.39	108.76	105.80
1	A	83	U	N1-C2-N3	-7.38	110.47	114.90
1	A	1121	U	C5-C6-N1	-7.38	119.01	122.70
1	A	1286	A	N1-C6-N6	7.38	123.03	118.60
1	A	1495	U	N3-C4-C5	-7.36	110.18	114.60
1	A	662	G	N9-C4-C5	-7.36	102.46	105.40
1	A	61	G	N1-C6-O6	7.36	124.31	119.90
1	A	499	A	N1-C6-N6	-7.36	114.19	118.60
1	A	549	C	C5-C6-N1	-7.36	117.32	121.00
1	A	1092	A	O5'-P-OP2	-7.35	99.09	105.70
1	A	1222	G	C2-N3-C4	-7.34	108.23	111.90
1	A	864	A	N1-C6-N6	-7.34	114.20	118.60
1	A	881	G	C8-N9-C4	7.34	109.33	106.40
1	A	672	U	C5-C4-O4	7.34	130.30	125.90
1	A	378	G	N1-C6-O6	7.33	124.30	119.90
1	A	66	G	N3-C4-C5	7.33	132.26	128.60
1	A	558	G	C6-N1-C2	7.32	129.49	125.10
1	A	1075	C	C4-C5-C6	7.32	121.06	117.40
1	A	197	A	N1-C6-N6	-7.30	114.22	118.60
1	A	730	G	C5-C6-O6	7.30	132.98	128.60
1	A	9	G	C8-N9-C4	7.30	109.32	106.40
1	A	1530	G	N1-C6-O6	7.30	124.28	119.90
1	A	818	G	C4-C5-N7	-7.29	107.88	110.80
1	A	741	G	C4-C5-N7	-7.29	107.89	110.80
1	A	446	G	C5-C6-O6	-7.28	124.23	128.60
1	A	122	G	N3-C4-N9	7.28	130.37	126.00
1	A	556	C	C5-C4-N4	-7.27	115.11	120.20
1	A	1183	A	N1-C6-N6	7.27	122.96	118.60
1	A	117	G	C5-C6-N1	-7.27	107.87	111.50
1	A	1125	U	C6-N1-C2	7.27	125.36	121.00
1	A	61	G	N3-C4-C5	7.26	132.23	128.60
1	A	27	G	C4-C5-N7	7.25	113.70	110.80
2	B	155	LEU	CA-CB-CG	7.25	131.97	115.30
1	A	300	A	N9-C4-C5	7.24	108.70	105.80
1	A	524	G	O5'-P-OP1	-7.24	99.18	105.70
1	A	1528	U	O5'-P-OP1	7.23	119.38	110.70
1	A	522	C	N3-C2-O2	7.23	126.96	121.90
1	A	902	G	C8-N9-C4	7.23	109.29	106.40
1	A	928	G	C2-N3-C4	-7.23	108.28	111.90
1	A	1212	U	O4'-C1'-N1	7.22	113.98	108.20
1	A	289	G	N1-C6-O6	7.22	124.23	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1490	C	C5-C6-N1	7.21	124.61	121.00
1	A	31	G	N9-C4-C5	-7.20	102.52	105.40
1	A	1328	C	C6-N1-C2	7.20	123.18	120.30
1	A	306	G	N3-C2-N2	-7.20	114.86	119.90
1	A	549	C	C6-N1-C2	7.20	123.18	120.30
1	A	885	G	C5-C6-N1	-7.20	107.90	111.50
1	A	47	C	C5-C6-N1	-7.19	117.40	121.00
1	A	894	G	C2-N3-C4	-7.19	108.30	111.90
1	A	181	G	C4-N9-C1'	7.18	135.83	126.50
1	A	66	G	N3-C4-N9	-7.17	121.70	126.00
1	A	611	A	N1-C6-N6	-7.17	114.30	118.60
1	A	889	A	N9-C4-C5	7.17	108.67	105.80
1	A	651	C	C6-N1-C2	7.17	123.17	120.30
1	A	235	C	C6-N1-C2	7.16	123.17	120.30
1	A	1258	G	C8-N9-C4	-7.16	103.54	106.40
1	A	674	G	C2-N3-C4	-7.16	108.32	111.90
1	A	833	U	C5-C4-O4	7.16	130.19	125.90
1	A	504	C	C6-N1-C2	-7.15	117.44	120.30
1	A	1435	G	C5-C6-O6	-7.14	124.32	128.60
1	A	1166	G	C4-N9-C1'	7.14	135.78	126.50
4	D	12	CYS	CA-CB-SG	7.14	126.85	114.00
1	A	584	G	N7-C8-N9	-7.14	109.53	113.10
1	A	729	A	C8-N9-C4	-7.14	102.94	105.80
1	A	1526	G	N3-C2-N2	-7.14	114.90	119.90
1	A	672	U	C2-N3-C4	7.13	131.28	127.00
1	A	522	C	C2-N1-C1'	-7.12	110.96	118.80
1	A	1513	A	C8-N9-C4	7.12	108.65	105.80
1	A	1432	G	N3-C4-N9	-7.11	121.73	126.00
1	A	299	G	C4-C5-C6	7.11	123.07	118.80
1	A	803	G	OP2-P-O3'	7.11	120.83	105.20
1	A	285	G	N9-C4-C5	-7.11	102.56	105.40
1	A	1104	G	N1-C2-N2	-7.11	109.81	116.20
1	A	735	C	C6-N1-C2	7.10	123.14	120.30
1	A	765	G	C8-N9-C4	7.10	109.24	106.40
1	A	20	U	C6-N1-C2	7.09	125.26	121.00
1	A	1392	G	N1-C6-O6	-7.09	115.64	119.90
1	A	789	U	N1-C2-N3	7.09	119.15	114.90
1	A	817	C	C6-N1-C1'	-7.08	112.30	120.80
1	A	230	G	C5-C6-N1	-7.08	107.96	111.50
1	A	630	G	C8-N9-C4	7.08	109.23	106.40
1	A	1155	G	C8-N9-C1'	-7.07	117.81	127.00
1	A	586	C	C5-C4-N4	-7.07	115.25	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	21	G	N3-C2-N2	7.07	124.85	119.90
1	A	1126	U	C5-C6-N1	7.07	126.23	122.70
1	A	1155	G	C5-C6-N1	-7.07	107.97	111.50
1	A	566	G	C8-N9-C4	7.07	109.23	106.40
1	A	494	G	O5'-P-OP2	7.06	119.17	110.70
1	A	497	A	N1-C6-N6	-7.06	114.37	118.60
1	A	748	C	C2-N1-C1'	7.05	126.56	118.80
1	A	1397	C	OP1-P-OP2	7.05	130.18	119.60
1	A	1155	G	C4-C5-C6	7.05	123.03	118.80
1	A	1257	U	C5-C6-N1	7.04	126.22	122.70
1	A	578	C	N3-C2-O2	-7.04	116.97	121.90
1	A	44	G	C6-C5-N7	-7.03	126.18	130.40
1	A	703	G	C4-N9-C1'	7.03	135.64	126.50
1	A	484	G	C5-C6-O6	7.03	132.82	128.60
1	A	299	G	C6-C5-N7	-7.03	126.18	130.40
1	A	22	G	N1-C6-O6	7.02	124.11	119.90
1	A	353	A	O5'-P-OP2	-7.01	99.39	105.70
1	A	1529	G	O5'-P-OP1	-7.01	99.39	105.70
1	A	674	G	N9-C4-C5	-7.01	102.60	105.40
1	A	1478	C	C5-C6-N1	7.00	124.50	121.00
1	A	95	U	N3-C4-C5	-7.00	110.40	114.60
1	A	734	G	C5-C6-O6	-7.00	124.40	128.60
1	A	746	A	N1-C6-N6	-7.00	114.40	118.60
1	A	232	G	N1-C6-O6	6.99	124.09	119.90
1	A	862	C	O5'-P-OP1	-6.99	99.41	105.70
1	A	949	A	N1-C6-N6	6.97	122.78	118.60
1	A	67	C	N3-C4-C5	6.97	124.69	121.90
1	A	523	A	C2-N3-C4	-6.96	107.12	110.60
1	A	854	G	C6-C5-N7	-6.96	126.22	130.40
1	A	308	C	N3-C4-N4	6.96	122.87	118.00
1	A	168	G	C5-C6-N1	-6.96	108.02	111.50
1	A	382	A	N1-C2-N3	6.96	132.78	129.30
1	A	940	C	C6-N1-C2	6.96	123.08	120.30
1	A	277	C	C2-N1-C1'	-6.95	111.15	118.80
1	A	784	C	O5'-P-OP2	-6.95	99.44	105.70
1	A	577	G	N3-C4-C5	6.95	132.07	128.60
1	A	859	A	C8-N9-C4	6.94	108.58	105.80
1	A	279	A	N7-C8-N9	6.94	117.27	113.80
1	A	1394	A	N1-C6-N6	-6.93	114.44	118.60
1	A	550	G	C2-N3-C4	-6.93	108.43	111.90
1	A	703	G	C4-C5-N7	-6.92	108.03	110.80
1	A	645	C	N3-C4-C5	6.92	124.67	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	955	U	N3-C4-C5	-6.92	110.45	114.60
1	A	587	G	C5-C6-N1	6.92	114.96	111.50
1	A	724	G	C4-C5-C6	6.91	122.94	118.80
1	A	880	C	C6-N1-C2	6.91	123.06	120.30
1	A	216	G	N3-C4-C5	6.90	132.05	128.60
1	A	667	G	N1-C6-O6	6.90	124.04	119.90
20	T	94	ALA	N-CA-C	-6.90	92.37	111.00
1	A	20	U	C5-C6-N1	-6.90	119.25	122.70
1	A	253	U	O5'-P-OP2	-6.89	99.50	105.70
1	A	584	G	C5-N7-C8	6.89	107.74	104.30
1	A	774	G	N9-C4-C5	-6.89	102.64	105.40
1	A	859	A	N1-C6-N6	6.89	122.73	118.60
1	A	734	G	C4-C5-N7	6.88	113.55	110.80
1	A	190(H)	G	C6-C5-N7	-6.88	126.27	130.40
1	A	1237	C	N3-C2-O2	-6.88	117.08	121.90
1	A	1373	G	N3-C4-C5	-6.88	125.16	128.60
1	A	817	C	C4-C5-C6	6.87	120.83	117.40
1	A	200	G	N1-C6-O6	6.86	124.02	119.90
1	A	873	A	O5'-P-OP2	-6.86	99.52	105.70
1	A	306	G	N3-C4-C5	6.86	132.03	128.60
9	I	56	LEU	CA-CB-CG	6.86	131.07	115.30
1	A	326	G	C5-C6-N1	-6.85	108.07	111.50
1	A	763	G	C5-C6-O6	-6.85	124.49	128.60
1	A	1432	G	N9-C4-C5	6.85	108.14	105.40
1	A	893	C	C4-C5-C6	-6.85	113.97	117.40
1	A	1094	G	N3-C4-C5	-6.85	125.18	128.60
1	A	555	C	O5'-P-OP1	6.85	118.92	110.70
1	A	1390	U	N3-C4-C5	-6.84	110.49	114.60
1	A	518	C	O5'-P-OP2	6.84	118.91	110.70
1	A	884	U	C4-C5-C6	6.84	123.80	119.70
1	A	1100	C	C2-N1-C1'	6.84	126.32	118.80
1	A	1197	G	O5'-P-OP2	6.83	118.90	110.70
1	A	481	G	C5-C6-O6	-6.83	124.50	128.60
1	A	799	G	C2-N3-C4	-6.83	108.48	111.90
1	A	1411	C	N3-C2-O2	-6.83	117.12	121.90
1	A	1155	G	C4-N9-C1'	6.83	135.38	126.50
1	A	1189	C	C2-N1-C1'	6.83	126.31	118.80
1	A	370	C	N1-C2-O2	6.83	123.00	118.90
1	A	429	U	O4'-C1'-N1	6.82	113.66	108.20
1	A	759	A	N1-C6-N6	-6.82	114.51	118.60
1	A	975	A	C5-C6-N1	-6.82	114.29	117.70
1	A	1435	G	C5-C6-N1	-6.82	108.09	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	544	G	C5-C6-O6	-6.82	124.51	128.60
1	A	1287	A	C8-N9-C4	-6.82	103.07	105.80
1	A	216	G	C4-N9-C1'	-6.81	117.65	126.50
1	A	230	G	C8-N9-C4	6.81	109.12	106.40
1	A	147	G	C4-C5-C6	6.81	122.89	118.80
1	A	758	G	N9-C4-C5	-6.80	102.68	105.40
1	A	548	G	N1-C6-O6	6.80	123.98	119.90
1	A	376	G	N7-C8-N9	-6.78	109.71	113.10
1	A	944	G	N3-C4-C5	-6.78	125.21	128.60
1	A	579	G	C6-C5-N7	-6.78	126.33	130.40
1	A	1088	G	C5-C6-O6	-6.78	124.53	128.60
1	A	688	G	C5-C6-N1	-6.77	108.11	111.50
1	A	308	C	C5-C4-N4	-6.77	115.46	120.20
1	A	190(L)	U	O5'-P-OP2	6.76	118.81	110.70
1	A	45	U	C4-C5-C6	6.76	123.75	119.70
1	A	579	G	C2-N3-C4	-6.76	108.52	111.90
1	A	1227	A	C6-C5-N7	-6.76	127.57	132.30
1	A	276	G	N1-C6-O6	6.75	123.95	119.90
1	A	357	G	C8-N9-C4	6.75	109.10	106.40
1	A	661	G	C2-N3-C4	-6.75	108.52	111.90
1	A	32	A	C5-C6-N1	6.75	121.08	117.70
1	A	174	C	OP2-P-O3'	6.75	120.05	105.20
1	A	729	A	C4-C5-C6	6.75	120.37	117.00
1	A	47	C	C2-N3-C4	-6.74	116.53	119.90
1	A	31	G	C4-N9-C1'	6.74	135.26	126.50
1	A	266	G	C4-C5-N7	6.74	113.50	110.80
1	A	289	G	C6-C5-N7	-6.74	126.36	130.40
1	A	783	C	N3-C2-O2	6.74	126.61	121.90
1	A	833	U	C4-C5-C6	6.74	123.74	119.70
1	A	899	C	C6-N1-C2	6.74	122.99	120.30
1	A	1435	G	C6-C5-N7	-6.73	126.36	130.40
1	A	1053	G	N3-C4-N9	-6.73	121.96	126.00
1	A	557	G	C4-C5-C6	6.72	122.83	118.80
1	A	718	G	N7-C8-N9	-6.72	109.74	113.10
1	A	1168	A	C2-N3-C4	6.72	113.96	110.60
1	A	1516[A]	G	N3-C2-N2	-6.72	115.19	119.90
1	A	1516[B]	G	N3-C2-N2	-6.72	115.19	119.90
1	A	1053	G	C4-N9-C1'	-6.72	117.77	126.50
1	A	260	G	N9-C4-C5	6.72	108.09	105.40
1	A	662	G	N1-C6-O6	6.71	123.93	119.90
19	S	81	ARG	NE-CZ-NH1	6.71	123.66	120.30
1	A	1527	C	C5-C6-N1	-6.71	117.64	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	46	G	C5-C6-N1	-6.71	108.14	111.50
1	A	791	G	C2-N3-C4	-6.71	108.55	111.90
1	A	789	U	C6-N1-C2	-6.71	116.98	121.00
1	A	144	G	N1-C6-O6	6.70	123.92	119.90
1	A	361	G	C8-N9-C4	6.70	109.08	106.40
1	A	631	G	N3-C4-C5	6.70	131.95	128.60
1	A	774	G	C4-C5-N7	6.70	113.48	110.80
1	A	1236	A	C8-N9-C4	6.70	108.48	105.80
1	A	906	G	C4-C5-N7	6.69	113.48	110.80
1	A	587	G	N1-C6-O6	-6.69	115.89	119.90
1	A	1498	UR3	P-O3'-C3'	6.69	127.73	119.70
1	A	50	A	C8-N9-C4	6.69	108.47	105.80
1	A	1286	A	C5-N7-C8	-6.68	100.56	103.90
1	A	922	G	C4-N9-C1'	6.67	135.18	126.50
1	A	1195	C	C6-N1-C2	-6.67	117.63	120.30
1	A	1370	G	C5-C6-N1	-6.67	108.16	111.50
1	A	169	C	C6-N1-C2	-6.67	117.63	120.30
1	A	304	U	N3-C4-O4	6.67	124.07	119.40
1	A	1442	G	C8-N9-C1'	-6.67	118.33	127.00
1	A	285	G	N3-C4-C5	6.67	131.93	128.60
1	A	736	C	N3-C2-O2	-6.66	117.24	121.90
1	A	309	G	C5-C6-N1	-6.66	108.17	111.50
1	A	257	G	C2-N3-C4	-6.65	108.57	111.90
1	A	1442	G	C4-N9-C1'	6.65	135.14	126.50
1	A	1487	G	N3-C4-N9	6.65	129.99	126.00
1	A	810	C	C5-C4-N4	6.64	124.85	120.20
1	A	317	G	C5-C6-O6	-6.64	124.62	128.60
1	A	376	G	C8-N9-C4	6.64	109.06	106.40
1	A	111	G	C5-C6-O6	6.64	132.58	128.60
1	A	407	G	O5'-P-OP1	-6.63	99.73	105.70
1	A	799	G	C4-C5-N7	6.63	113.45	110.80
1	A	1530	G	C8-N9-C1'	6.63	135.62	127.00
1	A	200	G	C2-N3-C4	-6.63	108.58	111.90
1	A	595	G	N3-C4-N9	6.63	129.98	126.00
1	A	731	G	N7-C8-N9	6.62	116.41	113.10
1	A	1394	A	N9-C4-C5	6.62	108.45	105.80
1	A	24	U	C5-C6-N1	-6.62	119.39	122.70
1	A	279	A	C5-N7-C8	-6.62	100.59	103.90
1	A	766	A	C5-N7-C8	-6.62	100.59	103.90
1	A	855	G	N1-C6-O6	6.62	123.87	119.90
1	A	120	A	C2-N3-C4	-6.61	107.29	110.60
1	A	721	G	C5-C6-N1	-6.61	108.19	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1228	C	N1-C2-O2	6.61	122.87	118.90
1	A	28	G	C6-C5-N7	-6.61	126.44	130.40
1	A	732	C	N3-C2-O2	-6.61	117.28	121.90
1	A	712	A	C6-N1-C2	-6.61	114.64	118.60
1	A	445	G	C8-N9-C4	-6.60	103.76	106.40
1	A	693	G	N3-C2-N2	-6.60	115.28	119.90
1	A	1512	U	N1-C2-N3	6.60	118.86	114.90
1	A	21	G	N9-C4-C5	-6.60	102.76	105.40
1	A	922	G	C8-N9-C1'	-6.60	118.42	127.00
1	A	1124	G	C5-C6-O6	-6.60	124.64	128.60
1	A	584	G	C8-N9-C4	6.59	109.04	106.40
1	A	570	G	C4-N9-C1'	6.59	135.07	126.50
1	A	1125	U	O5'-P-OP1	-6.59	99.77	105.70
1	A	1415	G	OP1-P-O3'	6.59	119.69	105.20
1	A	190(E)	U	N3-C2-O2	-6.59	117.59	122.20
1	A	288	A	N3-C4-C5	6.59	131.41	126.80
1	A	1527	C	O5'-P-OP2	-6.59	99.77	105.70
1	A	285	G	C2-N3-C4	-6.58	108.61	111.90
1	A	298	A	N1-C2-N3	6.58	132.59	129.30
1	A	428	G	P-O3'-C3'	6.58	127.59	119.70
1	A	1392	G	N1-C2-N2	-6.58	110.28	116.20
1	A	353	A	O5'-P-OP1	6.58	118.59	110.70
1	A	608	A	N1-C6-N6	-6.58	114.66	118.60
1	A	610	G	N7-C8-N9	6.57	116.38	113.10
1	A	616	G	C5-C6-N1	-6.57	108.22	111.50
1	A	1166	G	C6-C5-N7	-6.57	126.46	130.40
1	A	147	G	C2-N3-C4	-6.56	108.62	111.90
1	A	735	C	N3-C4-C5	6.56	124.53	121.90
1	A	761	G	C6-C5-N7	-6.56	126.46	130.40
1	A	46	G	O5'-P-OP1	-6.56	99.80	105.70
1	A	401	C	N3-C4-C5	-6.56	119.28	121.90
1	A	387	U	C5-C4-O4	6.56	129.83	125.90
1	A	757	U	C5-C4-O4	6.56	129.83	125.90
1	A	95	U	C5-C4-O4	6.55	129.83	125.90
1	A	200	G	C5-C6-N1	-6.55	108.22	111.50
1	A	955	U	C4-C5-C6	6.55	123.63	119.70
1	A	1452	C	C6-N1-C2	6.55	122.92	120.30
1	A	247	G	N3-C2-N2	-6.55	115.32	119.90
1	A	1092	A	C8-N9-C4	-6.55	103.18	105.80
1	A	158	G	C8-N9-C4	-6.55	103.78	106.40
1	A	403	C	C5-C6-N1	-6.55	117.73	121.00
1	A	618	C	C6-N1-C2	6.54	122.92	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	720	C	C5-C4-N4	-6.54	115.62	120.20
1	A	102	G	N1-C6-O6	6.53	123.82	119.90
1	A	741	G	C5-N7-C8	6.53	107.56	104.30
1	A	1075	C	C5-C4-N4	6.53	124.77	120.20
1	A	108	G	N3-C4-C5	6.52	131.86	128.60
1	A	26	A	N3-C4-C5	6.52	131.37	126.80
1	A	812	C	N1-C2-O2	6.52	122.81	118.90
1	A	1512	U	C4-C5-C6	6.52	123.61	119.70
1	A	849	C	C6-N1-C2	-6.52	117.69	120.30
1	A	631	G	C4-N9-C1'	-6.52	118.03	126.50
1	A	1231	G	N1-C6-O6	6.52	123.81	119.90
1	A	949	A	C4-C5-N7	6.51	113.96	110.70
1	A	1108	G	C5-C6-O6	6.51	132.51	128.60
3	C	14	ILE	CB-CA-C	-6.51	98.57	111.60
1	A	975	A	N1-C2-N3	6.51	132.56	129.30
1	A	529	G	O5'-P-OP2	-6.51	99.84	105.70
1	A	707	C	N1-C2-O2	6.51	122.81	118.90
1	A	1338	G	C4-N9-C1'	6.51	134.96	126.50
1	A	150	C	C6-N1-C2	6.51	122.90	120.30
1	A	248	C	C5-C6-N1	-6.51	117.75	121.00
1	A	1506	U	N1-C2-O2	6.51	127.36	122.80
1	A	1104	G	C6-C5-N7	-6.50	126.50	130.40
1	A	614	A	N1-C6-N6	6.50	122.50	118.60
1	A	413	G	O4'-C1'-N9	6.49	113.39	108.20
1	A	703	G	N3-C4-C5	-6.49	125.36	128.60
1	A	106	C	OP2-P-O3'	6.49	119.47	105.20
1	A	917	G	N1-C6-O6	-6.48	116.01	119.90
1	A	1531	A	C5-C6-N6	-6.48	118.52	123.70
1	A	724	G	C4-N9-C1'	6.48	134.93	126.50
1	A	677	U	O5'-P-OP2	-6.48	99.87	105.70
1	A	289	G	O5'-P-OP2	-6.47	99.87	105.70
1	A	579	G	N9-C4-C5	-6.47	102.81	105.40
1	A	577	G	C2-N3-C4	-6.47	108.67	111.90
1	A	1093	A	C5-C6-N1	6.47	120.94	117.70
1	A	21	G	N3-C4-N9	6.46	129.88	126.00
1	A	703	G	C5-N7-C8	6.46	107.53	104.30
1	A	710	G	C4-C5-C6	6.46	122.68	118.80
1	A	902	G	N1-C2-N3	6.46	127.78	123.90
1	A	1526	G	N1-C6-O6	6.46	123.78	119.90
1	A	809	G	C5-C6-N1	6.46	114.73	111.50
1	A	481	G	C4-C5-N7	6.45	113.38	110.80
1	A	975	A	C5-N7-C8	-6.45	100.67	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1166	G	C4-C5-C6	6.45	122.67	118.80
1	A	520	A	O5'-P-OP2	-6.45	99.89	105.70
1	A	535	A	O5'-P-OP2	-6.45	99.89	105.70
1	A	1432	G	O5'-P-OP2	-6.45	99.90	105.70
1	A	111	G	C5-C6-N1	-6.44	108.28	111.50
1	A	833	U	N1-C2-N3	6.44	118.77	114.90
1	A	893	C	C6-N1-C2	6.44	122.88	120.30
1	A	190(E)	U	O5'-P-OP2	-6.44	99.91	105.70
1	A	135	C	O5'-P-OP2	-6.43	99.91	105.70
1	A	314	C	N1-C2-O2	-6.43	115.04	118.90
1	A	517	G	C4-C5-N7	-6.43	108.23	110.80
1	A	723	U	N3-C4-C5	-6.43	110.74	114.60
1	A	726	C	O5'-P-OP1	-6.43	99.92	105.70
1	A	1050	G	C4-C5-N7	6.43	113.37	110.80
1	A	122	G	N3-C2-N2	6.42	124.40	119.90
1	A	484	G	N1-C2-N3	6.42	127.75	123.90
1	A	885	G	C4-C5-N7	-6.42	108.23	110.80
1	A	579	G	C8-N9-C4	6.42	108.97	106.40
1	A	1465	C	N3-C4-C5	6.41	124.46	121.90
1	A	1502	A	C5-N7-C8	-6.41	100.69	103.90
1	A	1525	G	C2-N3-C4	-6.41	108.69	111.90
1	A	631	G	N1-C2-N2	6.41	121.97	116.20
1	A	307	C	O5'-P-OP2	-6.41	99.93	105.70
1	A	1485	U	N1-C2-N3	6.41	118.74	114.90
1	A	449	C	N3-C4-C5	-6.40	119.34	121.90
1	A	617	G	N1-C2-N3	6.40	127.74	123.90
1	A	1512	U	C6-N1-C1'	6.40	130.15	121.20
1	A	255	G	C6-C5-N7	-6.39	126.56	130.40
1	A	981	U	N3-C4-O4	6.39	123.88	119.40
1	A	900	A	N1-C6-N6	6.39	122.44	118.60
1	A	857	C	N3-C2-O2	-6.39	117.43	121.90
1	A	285	G	N7-C8-N9	-6.39	109.91	113.10
1	A	871	U	C5-C6-N1	-6.39	119.51	122.70
1	A	910	C	N1-C2-O2	-6.39	115.07	118.90
1	A	313	A	N9-C4-C5	-6.39	103.25	105.80
1	A	1502	A	C4-C5-N7	6.38	113.89	110.70
1	A	232	G	C4-N9-C1'	6.38	134.79	126.50
1	A	265	G	N9-C4-C5	6.38	107.95	105.40
1	A	49	U	C6-N1-C2	6.38	124.83	121.00
19	S	81	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	A	535	A	C4-C5-N7	-6.37	107.52	110.70
1	A	657	G	N1-C6-O6	6.37	123.72	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1240	U	C5-C6-N1	-6.36	119.52	122.70
1	A	1341	U	C5-C4-O4	6.36	129.72	125.90
1	A	36	C	O5'-P-OP2	-6.36	99.98	105.70
1	A	1057	G	N1-C2-N2	6.36	121.92	116.20
1	A	1030(C)	G	C8-N9-C1'	-6.36	118.74	127.00
1	A	654	G	N3-C4-C5	6.35	131.78	128.60
1	A	190(L)	U	O5'-P-OP1	-6.35	99.98	105.70
1	A	779	C	C5-C6-N1	-6.35	117.83	121.00
1	A	927	G	N1-C6-O6	6.35	123.71	119.90
1	A	1087	G	C4-C5-C6	6.35	122.61	118.80
1	A	1442	G	N3-C4-N9	6.35	129.81	126.00
1	A	799	G	O5'-P-OP2	-6.34	99.99	105.70
1	A	700	G	C5-C6-N1	-6.34	108.33	111.50
1	A	965	A	N3-C4-C5	6.34	131.24	126.80
1	A	1058	G	C8-N9-C4	6.34	108.94	106.40
1	A	104	G	N1-C6-O6	6.34	123.70	119.90
1	A	1542	U	N1-C2-N3	-6.34	111.10	114.90
1	A	635	G	C6-C5-N7	-6.33	126.60	130.40
1	A	1197	G	C8-N9-C1'	-6.33	118.77	127.00
1	A	1374	A	N1-C2-N3	6.33	132.47	129.30
1	A	630	G	C6-C5-N7	6.33	134.20	130.40
1	A	725	G	C5-C6-O6	-6.33	124.80	128.60
1	A	1030(B)	C	C6-N1-C2	-6.33	117.77	120.30
1	A	507	C	N3-C4-C5	6.32	124.43	121.90
1	A	834	C	C6-N1-C2	6.32	122.83	120.30
1	A	1514	C	N3-C4-C5	6.32	124.43	121.90
1	A	1227	A	C5-N7-C8	-6.32	100.74	103.90
1	A	1506	U	O5'-P-OP2	-6.32	100.01	105.70
1	A	1512	U	C2-N3-C4	6.32	130.79	127.00
1	A	488	C	N3-C4-C5	6.31	124.43	121.90
1	A	517	G	C4-C5-C6	6.31	122.59	118.80
1	A	834	C	O5'-P-OP2	-6.31	100.02	105.70
1	A	950	U	C5-C4-O4	6.31	129.69	125.90
1	A	1197	G	O5'-P-OP1	-6.31	100.02	105.70
1	A	1338	G	N3-C4-C5	-6.31	125.44	128.60
1	A	1528	U	C6-N1-C2	6.31	124.79	121.00
1	A	703	G	N3-C4-N9	6.31	129.78	126.00
1	A	1390	U	C4-C5-C6	6.31	123.48	119.70
1	A	758	G	OP2-P-O3'	6.30	119.07	105.20
1	A	1544	U	C6-N1-C2	-6.30	117.22	121.00
1	A	816	A	N1-C6-N6	-6.30	114.82	118.60
1	A	309	G	C4-C5-C6	6.30	122.58	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1323	G	N1-C6-O6	6.30	123.68	119.90
1	A	654	G	C2-N3-C4	-6.29	108.75	111.90
1	A	1432	G	N3-C2-N2	-6.29	115.50	119.90
1	A	133	U	N1-C2-O2	6.29	127.20	122.80
1	A	314	C	C5-C6-N1	-6.29	117.86	121.00
1	A	314	C	N3-C4-N4	-6.29	113.60	118.00
1	A	266	G	C2-N3-C4	-6.29	108.76	111.90
1	A	1126	U	C6-N1-C2	-6.29	117.23	121.00
1	A	599	C	C6-N1-C2	6.28	122.81	120.30
1	A	535	A	C2-N3-C4	6.28	113.74	110.60
1	A	817	C	N3-C4-C5	-6.28	119.39	121.90
1	A	723	U	C6-N1-C2	-6.27	117.24	121.00
1	A	765	G	O5'-P-OP1	-6.27	100.06	105.70
1	A	835	U	N3-C2-O2	-6.27	117.81	122.20
1	A	890	G	C5-C6-O6	6.27	132.36	128.60
1	A	1397	C	N1-C2-O2	6.27	122.66	118.90
1	A	1525	G	N1-C2-N3	6.27	127.66	123.90
1	A	662	G	C8-N9-C1'	-6.26	118.86	127.00
1	A	1124	G	N1-C2-N2	6.26	121.84	116.20
1	A	710	G	C6-C5-N7	-6.25	126.65	130.40
1	A	916	G	N1-C6-O6	-6.25	116.15	119.90
1	A	1394	A	C5-C6-N6	6.24	128.69	123.70
1	A	113	G	N9-C4-C5	-6.24	102.90	105.40
1	A	818	G	O5'-P-OP1	-6.24	100.08	105.70
1	A	790	A	N1-C2-N3	6.24	132.42	129.30
3	C	155	GLY	N-CA-C	6.24	128.70	113.10
1	A	498	U	O5'-P-OP2	-6.24	100.09	105.70
1	A	889	A	N1-C6-N6	-6.24	114.86	118.60
1	A	401	C	N3-C2-O2	6.23	126.26	121.90
1	A	544	G	N9-C4-C5	-6.23	102.91	105.40
1	A	542	G	N3-C4-C5	-6.23	125.49	128.60
1	A	1334	G	C8-N9-C4	-6.22	103.91	106.40
1	A	117	G	C2-N3-C4	-6.22	108.79	111.90
1	A	192	U	N3-C2-O2	-6.22	117.84	122.20
1	A	975	A	C6-C5-N7	-6.22	127.94	132.30
1	A	504	C	C2-N1-C1'	6.22	125.64	118.80
1	A	815	A	OP1-P-OP2	-6.22	110.27	119.60
1	A	392	G	N7-C8-N9	-6.22	109.99	113.10
1	A	29	G	C5-C6-N1	-6.22	108.39	111.50
1	A	631	G	C8-N9-C1'	6.21	135.08	127.00
1	A	731	G	C8-N9-C4	-6.21	103.92	106.40
1	A	38	G	C5-C6-N1	-6.21	108.39	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1286	A	C4-C5-N7	6.21	113.81	110.70
1	A	497	A	C5-C6-N6	6.21	128.66	123.70
1	A	1401	G	C8-N9-C4	6.21	108.88	106.40
1	A	1513	A	N7-C8-N9	-6.21	110.70	113.80
1	A	641	U	C2-N1-C1'	6.20	125.14	117.70
1	A	1305	G	N7-C8-N9	6.20	116.20	113.10
1	A	385	C	O5'-P-OP1	-6.19	100.13	105.70
1	A	115	G	P-O3'-C3'	6.19	127.13	119.70
1	A	101	A	C2-N3-C4	-6.19	107.51	110.60
1	A	610	G	N9-C4-C5	6.19	107.88	105.40
1	A	832	C	OP2-P-O3'	6.19	118.81	105.20
1	A	1239	A	C8-N9-C4	6.18	108.27	105.80
1	A	148	G	N3-C4-N9	6.18	129.71	126.00
1	A	305	G	C4-C5-C6	6.18	122.51	118.80
1	A	733	A	N1-C2-N3	6.18	132.39	129.30
1	A	435	C	O5'-P-OP1	-6.18	100.14	105.70
1	A	836	G	N1-C6-O6	6.18	123.61	119.90
1	A	331	G	C6-C5-N7	-6.17	126.69	130.40
1	A	536	C	C6-N1-C2	-6.17	117.83	120.30
1	A	1094	G	N3-C4-N9	6.17	129.71	126.00
1	A	267	C	C5-C4-N4	6.17	124.52	120.20
1	A	652	U	N3-C4-C5	6.16	118.30	114.60
1	A	161	A	C5-C6-N6	6.16	128.63	123.70
1	A	104	G	C4-C5-C6	6.16	122.49	118.80
1	A	284	G	N3-C2-N2	-6.16	115.59	119.90
1	A	925	G	C2-N3-C4	-6.16	108.82	111.90
1	A	1079	G	N3-C4-N9	6.16	129.69	126.00
1	A	1341	U	N3-C4-O4	-6.16	115.09	119.40
1	A	232	G	C8-N9-C1'	-6.15	119.00	127.00
1	A	1259	C	N1-C2-O2	6.15	122.59	118.90
1	A	587	G	C2-N3-C4	6.15	114.97	111.90
1	A	774	G	C8-N9-C1'	-6.15	119.01	127.00
1	A	187	C	N3-C4-C5	-6.14	119.44	121.90
1	A	1206	G	C2-N3-C4	-6.14	108.83	111.90
1	A	1478	C	C6-N1-C2	-6.14	117.84	120.30
1	A	105	G	N1-C6-O6	6.14	123.59	119.90
1	A	255	G	C2-N3-C4	-6.14	108.83	111.90
1	A	1058	G	N1-C6-O6	6.14	123.59	119.90
1	A	1227	A	N9-C4-C5	-6.14	103.34	105.80
1	A	944	G	C4-N9-C1'	6.14	134.48	126.50
1	A	26	A	N3-C4-N9	-6.14	122.49	127.40
1	A	357	G	N1-C6-O6	6.14	123.58	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	406	G	C8-N9-C4	-6.14	103.94	106.40
1	A	564	C	C6-N1-C2	6.13	122.75	120.30
1	A	570	G	C8-N9-C4	-6.13	103.95	106.40
1	A	705	U	O5'-P-OP2	-6.13	100.18	105.70
1	A	375	U	N3-C4-C5	-6.13	110.92	114.60
1	A	352	C	N3-C4-C5	-6.12	119.45	121.90
1	A	1069	C	N3-C2-O2	6.12	126.19	121.90
1	A	1131	G	C5-C6-N1	-6.12	108.44	111.50
1	A	1125	U	N1-C2-N3	-6.12	111.23	114.90
1	A	61	G	O5'-P-OP1	-6.11	100.20	105.70
1	A	976	G	C8-N9-C4	6.11	108.84	106.40
1	A	631	G	N1-C2-N3	-6.11	120.23	123.90
1	A	776	G	OP1-P-O3'	6.10	118.63	105.20
1	A	1435	G	N3-C2-N2	-6.10	115.63	119.90
1	A	1490	C	C4-C5-C6	-6.10	114.35	117.40
1	A	562	C	C5-C6-N1	-6.10	117.95	121.00
1	A	1341	U	C5-C6-N1	-6.10	119.65	122.70
1	A	1530	G	O5'-P-OP2	-6.09	100.22	105.70
1	A	47	C	C4-C5-C6	6.09	120.44	117.40
1	A	773	G	N1-C2-N3	6.09	127.55	123.90
1	A	941	G	C8-N9-C4	6.08	108.83	106.40
1	A	1202	G	C8-N9-C4	-6.08	103.97	106.40
1	A	1342	C	N3-C4-C5	6.08	124.33	121.90
1	A	67	C	C2-N3-C4	-6.08	116.86	119.90
1	A	1528	U	OP1-P-O3'	6.08	118.57	105.20
1	A	517	G	N3-C4-C5	-6.08	125.56	128.60
1	A	819	A	N9-C4-C5	-6.07	103.37	105.80
1	A	1342	C	C6-N1-C2	6.07	122.73	120.30
1	A	1188	A	N1-C2-N3	6.07	132.34	129.30
1	A	945	G	C5-C6-N1	6.07	114.53	111.50
1	A	1454	G	C2-N3-C4	-6.07	108.87	111.90
1	A	778	G	C4-C5-C6	6.06	122.44	118.80
1	A	641	U	C6-N1-C1'	-6.06	112.72	121.20
1	A	707	C	N3-C2-O2	-6.06	117.66	121.90
1	A	774	G	C4-N9-C1'	6.05	134.37	126.50
1	A	652	U	C6-N1-C2	6.05	124.63	121.00
1	A	1054	C	C2-N1-C1'	6.05	125.45	118.80
1	A	710	G	C2-N3-C4	-6.05	108.88	111.90
1	A	513	C	C6-N1-C2	6.04	122.72	120.30
1	A	66	G	N3-C2-N2	-6.04	115.67	119.90
1	A	642	A	N1-C2-N3	6.04	132.32	129.30
1	A	105	G	C6-C5-N7	-6.04	126.78	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1227	A	O4'-C1'-N9	-6.04	103.37	108.20
1	A	10	A	C6-N1-C2	-6.03	114.98	118.60
1	A	698	G	N1-C6-O6	6.03	123.52	119.90
1	A	1491	G	N7-C8-N9	6.03	116.12	113.10
1	A	28	G	C4-C5-C6	6.03	122.42	118.80
1	A	325	A	C4-C5-N7	-6.03	107.69	110.70
1	A	1100	C	N1-C2-O2	6.03	122.52	118.90
1	A	1479	C	N3-C4-C5	-6.03	119.49	121.90
1	A	1530	G	N1-C2-N2	6.03	121.62	116.20
1	A	16	A	O5'-P-OP1	-6.02	100.28	105.70
1	A	1227	A	C5-C6-N6	-6.02	118.88	123.70
1	A	809	G	C2-N3-C4	6.02	114.91	111.90
1	A	234	C	C5-C6-N1	-6.02	117.99	121.00
1	A	584	G	C4-C5-N7	-6.02	108.39	110.80
1	A	811	C	C2-N3-C4	-6.02	116.89	119.90
1	A	1227	A	C4-C5-N7	6.02	113.71	110.70
1	A	1424	C	C6-N1-C2	6.02	122.71	120.30
1	A	1054	C	N3-C2-O2	-6.02	117.69	121.90
1	A	24	U	C2-N3-C4	-6.01	123.39	127.00
1	A	635	G	C5-C6-N1	-6.01	108.49	111.50
1	A	658	G	N1-C2-N3	6.01	127.50	123.90
1	A	1253	G	C8-N9-C4	-6.01	104.00	106.40
1	A	1437	C	C6-N1-C2	6.01	122.70	120.30
1	A	563	A	C2-N3-C4	-6.01	107.60	110.60
1	A	1053	G	C8-N9-C1'	6.00	134.81	127.00
1	A	1392	G	N3-C4-C5	-6.00	125.60	128.60
1	A	111	G	N9-C4-C5	6.00	107.80	105.40
1	A	234	C	N3-C4-C5	6.00	124.30	121.90
3	C	12	LEU	CA-CB-CG	-6.00	101.51	115.30
1	A	1453	G	N9-C4-C5	-6.00	103.00	105.40
1	A	1064	G	N9-C4-C5	-5.99	103.00	105.40
1	A	1167	A	C2-N3-C4	-5.99	107.61	110.60
1	A	22	G	C6-C5-N7	-5.99	126.81	130.40
1	A	864	A	C5-C6-N6	5.99	128.49	123.70
1	A	791	G	C8-N9-C1'	-5.99	119.22	127.00
1	A	1302	U	N3-C4-O4	-5.99	115.21	119.40
1	A	1054	C	O4'-C1'-N1	5.98	112.98	108.20
1	A	1522	U	O5'-P-OP1	5.98	117.88	110.70
1	A	549	C	C2-N3-C4	-5.98	116.91	119.90
1	A	557	G	C5-C6-N1	-5.98	108.51	111.50
1	A	228	A	C6-N1-C2	-5.97	115.02	118.60
1	A	553	A	C8-N9-C4	5.97	108.19	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1387	G	OP1-P-O3'	5.97	118.34	105.20
1	A	761	G	N1-C2-N3	5.97	127.48	123.90
1	A	385	C	O5'-P-OP2	5.97	117.86	110.70
1	A	970	C	C6-N1-C2	5.97	122.69	120.30
1	A	748	C	C6-N1-C2	-5.96	117.91	120.30
1	A	251	G	N9-C4-C5	-5.96	103.02	105.40
1	A	9	G	N7-C8-N9	-5.96	110.12	113.10
1	A	181	G	C8-N9-C1'	-5.96	119.25	127.00
1	A	724	G	N7-C8-N9	5.96	116.08	113.10
1	A	1149	C	N1-C2-O2	-5.96	115.33	118.90
1	A	474	G	N1-C6-O6	5.96	123.47	119.90
1	A	1211	U	C5-C4-O4	-5.96	122.33	125.90
1	A	1333	A	N1-C2-N3	5.95	132.28	129.30
1	A	1502	A	OP2-P-O3'	5.95	118.30	105.20
1	A	498	U	N1-C2-O2	-5.95	118.63	122.80
1	A	132	C	C5-C6-N1	-5.95	118.03	121.00
1	A	575	G	OP1-P-O3'	5.95	118.28	105.20
1	A	243	A	O5'-P-OP2	-5.95	100.35	105.70
1	A	481	G	N1-C6-O6	5.95	123.47	119.90
1	A	31	G	C6-C5-N7	-5.94	126.83	130.40
1	A	365	U	N3-C2-O2	-5.94	118.04	122.20
1	A	242	C	C5-C6-N1	-5.94	118.03	121.00
1	A	805	C	C5-C4-N4	-5.94	116.04	120.20
1	A	1396	A	OP1-P-OP2	5.94	128.51	119.60
12	L	27	LEU	CA-CB-CG	5.93	128.95	115.30
18	R	85	LEU	CA-CB-CG	5.93	128.94	115.30
1	A	1309	G	N1-C6-O6	-5.93	116.34	119.90
1	A	1061	G	N1-C6-O6	5.93	123.46	119.90
1	A	196	A	C4-C5-C6	-5.92	114.04	117.00
1	A	1026	G	C5-N7-C8	-5.92	101.34	104.30
1	A	168	G	N1-C6-O6	5.92	123.45	119.90
1	A	388	G	C8-N9-C4	5.92	108.77	106.40
1	A	957	U	N1-C2-N3	5.92	118.45	114.90
1	A	300	A	C5-C6-N6	5.92	128.43	123.70
1	A	1200	C	N1-C2-O2	-5.91	115.35	118.90
1	A	1516[A]	G	C8-N9-C1'	5.91	134.69	127.00
1	A	1516[B]	G	C8-N9-C1'	5.91	134.69	127.00
1	A	719	C	N3-C4-C5	-5.91	119.53	121.90
1	A	970	C	N3-C2-O2	-5.91	117.76	121.90
1	A	113	G	C4-C5-C6	5.91	122.35	118.80
1	A	381	C	C5-C6-N1	5.91	123.95	121.00
1	A	553	A	C2-N3-C4	-5.91	107.65	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	554	C	C4-C5-C6	5.91	120.35	117.40
1	A	174	C	C6-N1-C2	-5.90	117.94	120.30
1	A	886	G	C6-C5-N7	-5.90	126.86	130.40
1	A	1502	A	C6-C5-N7	-5.90	128.17	132.30
1	A	117	G	C4-C5-C6	5.90	122.34	118.80
1	A	641	U	N1-C2-O2	5.90	126.93	122.80
1	A	766	A	C4-C5-N7	5.90	113.65	110.70
1	A	650	G	C5-C6-O6	-5.89	125.06	128.60
1	A	133	U	N3-C4-C5	-5.89	111.06	114.60
1	A	357	G	N7-C8-N9	-5.89	110.15	113.10
1	A	791	G	C4-C5-N7	-5.89	108.44	110.80
1	A	858	G	N3-C4-N9	5.89	129.54	126.00
1	A	61	G	C5-N7-C8	-5.89	101.36	104.30
1	A	861	G	C4-C5-N7	5.89	113.16	110.80
1	A	313	A	C5-C6-N6	-5.89	118.99	123.70
1	A	712	A	N1-C2-N3	5.89	132.24	129.30
1	A	116	A	C2-N3-C4	-5.89	107.66	110.60
1	A	807	A	N1-C6-N6	5.89	122.13	118.60
1	A	216	G	N3-C4-N9	-5.88	122.47	126.00
1	A	630	G	N7-C8-N9	-5.88	110.16	113.10
1	A	1453	G	N3-C4-N9	5.88	129.53	126.00
1	A	485	G	O4'-C1'-N9	5.88	112.90	108.20
1	A	491	G	C4-C5-C6	5.87	122.32	118.80
1	A	993	G	C4-C5-N7	5.87	113.15	110.80
1	A	1054	C	C6-N1-C1'	-5.87	113.75	120.80
1	A	25	C	O5'-P-OP1	5.87	117.75	110.70
1	A	216	G	C8-N9-C4	5.87	108.75	106.40
1	A	1005	A	C4-C5-C6	5.87	119.94	117.00
1	A	45	U	N1-C2-N3	5.87	118.42	114.90
1	A	102	G	C5-C6-O6	-5.87	125.08	128.60
1	A	173	U	N3-C4-O4	-5.87	115.29	119.40
1	A	41	G	N1-C6-O6	5.87	123.42	119.90
1	A	400	C	N3-C2-O2	5.87	126.01	121.90
1	A	1287	A	N7-C8-N9	5.87	116.73	113.80
1	A	1463	C	C6-N1-C2	5.86	122.65	120.30
1	A	578	C	C2-N3-C4	-5.86	116.97	119.90
1	A	505	G	N1-C6-O6	-5.86	116.38	119.90
1	A	362	G	C5-C6-N1	-5.86	108.57	111.50
1	A	388	G	C5-C6-N1	-5.86	108.57	111.50
1	A	405	U	C5-C4-O4	5.86	129.41	125.90
1	A	657	G	N3-C2-N2	-5.86	115.80	119.90
1	A	778	G	C5-C6-N1	-5.86	108.57	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1524	C	N1-C2-O2	-5.86	115.39	118.90
1	A	887	G	N3-C2-N2	-5.85	115.80	119.90
1	A	1129	C	O4'-C1'-N1	5.85	112.88	108.20
1	A	15	G	C6-C5-N7	-5.85	126.89	130.40
1	A	251	G	C6-C5-N7	-5.85	126.89	130.40
1	A	1030(A)	G	C2-N3-C4	5.85	114.82	111.90
1	A	780	A	C5-C6-N1	5.84	120.62	117.70
1	A	317	G	N1-C6-O6	5.84	123.40	119.90
1	A	553	A	N1-C6-N6	5.84	122.10	118.60
1	A	1333	A	C6-N1-C2	-5.84	115.10	118.60
1	A	595	G	C8-N9-C1'	-5.83	119.42	127.00
1	A	719	C	N3-C4-N4	5.83	122.08	118.00
1	A	1198	G	C2-N3-C4	-5.83	108.98	111.90
1	A	188	C	N3-C4-C5	-5.83	119.57	121.90
1	A	284	G	N3-C4-C5	5.83	131.51	128.60
1	A	190(D)	U	C5-C6-N1	-5.83	119.79	122.70
1	A	1528	U	C5-C6-N1	-5.82	119.79	122.70
1	A	23	C	OP2-P-O3'	5.82	118.00	105.20
1	A	1205	U	N3-C4-O4	5.82	123.47	119.40
1	A	305	G	N1-C6-O6	5.82	123.39	119.90
6	F	21	LEU	CA-CB-CG	-5.82	101.92	115.30
1	A	572	A	N1-C6-N6	-5.81	115.11	118.60
1	A	1157	A	C8-N9-C4	-5.81	103.48	105.80
1	A	378	G	C5-C6-O6	-5.81	125.11	128.60
1	A	859	A	C5-C6-N1	-5.81	114.80	117.70
1	A	189	G	C8-N9-C4	5.80	108.72	106.40
1	A	810	C	N3-C2-O2	-5.80	117.84	121.90
1	A	260	G	C5-C6-N1	-5.80	108.60	111.50
1	A	1100	C	C5-C4-N4	-5.80	116.14	120.20
1	A	631	G	N3-C4-N9	-5.80	122.52	126.00
1	A	728	A	N7-C8-N9	5.80	116.70	113.80
1	A	877	C	N3-C4-N4	5.80	122.06	118.00
1	A	1205	U	C4-C5-C6	5.79	123.18	119.70
1	A	25	C	O5'-P-OP2	-5.79	100.49	105.70
1	A	1079	G	C8-N9-C4	-5.79	104.08	106.40
1	A	305	G	C2-N3-C4	-5.79	109.00	111.90
1	A	571	U	C6-N1-C2	-5.79	117.53	121.00
1	A	885	G	N3-C2-N2	-5.79	115.85	119.90
1	A	1220	G	N1-C6-O6	5.79	123.37	119.90
1	A	769	G	OP2-P-O3'	5.78	117.92	105.20
1	A	907	A	N1-C6-N6	-5.78	115.13	118.60
19	S	4	SER	N-CA-C	5.78	126.61	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	670	G	O5'-P-OP2	-5.78	100.50	105.70
1	A	720	C	N3-C4-C5	5.78	124.21	121.90
1	A	1470	G	C8-N9-C1'	-5.78	119.49	127.00
1	A	108	G	C5-C6-O6	-5.78	125.14	128.60
1	A	194	C	C6-N1-C2	5.78	122.61	120.30
1	A	548	G	C5-C6-O6	-5.78	125.14	128.60
1	A	562	C	C6-N1-C1'	-5.78	113.87	120.80
1	A	1182	G	N3-C4-N9	5.77	129.46	126.00
1	A	448	A	O5'-P-OP2	-5.77	100.51	105.70
1	A	703	G	N3-C2-N2	5.77	123.94	119.90
1	A	943	U	N3-C2-O2	5.77	126.24	122.20
1	A	1377	A	N1-C2-N3	5.77	132.18	129.30
1	A	79	G	C6-C5-N7	-5.76	126.94	130.40
1	A	485	G	N7-C8-N9	-5.76	110.22	113.10
1	A	1426	C	C5-C6-N1	-5.76	118.12	121.00
1	A	533	A	O5'-P-OP2	-5.76	100.52	105.70
1	A	122	G	O5'-P-OP1	-5.75	100.52	105.70
1	A	314	C	N3-C2-O2	5.75	125.93	121.90
1	A	1432	G	N7-C8-N9	5.75	115.98	113.10
1	A	821	G	C2-N3-C4	-5.75	109.03	111.90
1	A	1030(B)	C	C5-C6-N1	5.75	123.87	121.00
1	A	1053	G	C6-C5-N7	5.75	133.85	130.40
1	A	255	G	C5-C6-O6	-5.75	125.15	128.60
1	A	712	A	O5'-P-OP1	-5.74	100.53	105.70
1	A	637	G	C8-N9-C4	5.74	108.70	106.40
1	A	21	G	C4-C5-N7	5.74	113.10	110.80
1	A	1542	U	N1-C2-O2	5.74	126.82	122.80
1	A	664	G	N7-C8-N9	-5.74	110.23	113.10
1	A	562	C	N3-C2-O2	-5.74	117.89	121.90
1	A	61	G	C4-C5-N7	5.73	113.09	110.80
1	A	295	C	N3-C4-C5	5.73	124.19	121.90
1	A	1257	U	N1-C2-O2	5.73	126.81	122.80
1	A	104	G	C6-C5-N7	-5.72	126.97	130.40
1	A	566	G	N7-C8-N9	-5.72	110.24	113.10
1	A	817	C	N3-C2-O2	-5.72	117.89	121.90
1	A	31	G	N3-C2-N2	5.72	123.91	119.90
1	A	1487	G	N3-C4-C5	-5.72	125.74	128.60
1	A	791	G	N1-C6-O6	5.72	123.33	119.90
1	A	502	G	O5'-P-OP2	-5.72	100.55	105.70
1	A	164	U	O5'-P-OP1	-5.72	100.56	105.70
1	A	304	U	C6-N1-C2	-5.72	117.57	121.00
1	A	50	A	C2-N3-C4	-5.71	107.74	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	181	G	C6-C5-N7	-5.71	126.97	130.40
1	A	816	A	C4-C5-N7	-5.71	107.84	110.70
1	A	1100	C	C6-N1-C1'	-5.71	113.95	120.80
1	A	1230	C	C5-C6-N1	5.71	123.86	121.00
1	A	1083	U	C4-C5-C6	5.71	123.13	119.70
1	A	1193	G	C4-C5-C6	5.71	122.23	118.80
1	A	502	G	N3-C4-N9	-5.71	122.58	126.00
1	A	1514	C	C5-C6-N1	-5.71	118.15	121.00
1	A	381	C	N3-C4-C5	-5.70	119.62	121.90
1	A	541	G	N3-C2-N2	-5.70	115.91	119.90
1	A	1523	G	N3-C2-N2	-5.70	115.91	119.90
1	A	1125	U	N3-C4-O4	5.70	123.39	119.40
1	A	169	C	C5-C6-N1	5.70	123.85	121.00
1	A	1055	A	C4-C5-C6	5.70	119.85	117.00
1	A	1240	U	C2-N1-C1'	-5.70	110.87	117.70
1	A	381	C	C2-N1-C1'	5.69	125.06	118.80
1	A	146	G	O5'-P-OP1	-5.69	100.58	105.70
1	A	859	A	C2-N3-C4	-5.69	107.75	110.60
1	A	897	C	C2-N3-C4	-5.69	117.05	119.90
1	A	1470	G	C4-C5-C6	5.69	122.22	118.80
1	A	299	G	C8-N9-C1'	-5.69	119.60	127.00
1	A	729	A	N3-C4-C5	-5.69	122.82	126.80
1	A	558	G	N3-C4-C5	5.69	131.44	128.60
1	A	380	G	O5'-P-OP2	-5.69	100.58	105.70
1	A	555	C	N3-C4-C5	5.68	124.17	121.90
1	A	917	G	C8-N9-C4	-5.68	104.13	106.40
1	A	1139	G	N3-C4-C5	-5.68	125.76	128.60
1	A	229	U	C4-C5-C6	5.68	123.11	119.70
1	A	604	G	N3-C2-N2	-5.68	115.92	119.90
1	A	227	G	C6-C5-N7	-5.68	126.99	130.40
1	A	854	G	N1-C6-O6	5.68	123.31	119.90
1	A	1157	A	C2-N3-C4	5.68	113.44	110.60
1	A	1394	A	O5'-P-OP1	-5.67	100.59	105.70
1	A	1109	C	N3-C2-O2	-5.67	117.93	121.90
1	A	1232	U	N3-C4-O4	5.67	123.37	119.40
10	J	65	LEU	CA-CB-CG	5.67	128.34	115.30
1	A	7	G	N9-C4-C5	-5.67	103.13	105.40
1	A	830	G	N1-C2-N2	5.67	121.30	116.20
1	A	1432	G	C5-C6-O6	5.67	132.00	128.60
1	A	12	U	C2-N1-C1'	5.67	124.50	117.70
1	A	789	U	C5-C4-O4	5.67	129.30	125.90
1	A	1023	G	N9-C4-C5	-5.67	103.13	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	993	G	C6-C5-N7	-5.66	127.00	130.40
1	A	1286	A	N7-C8-N9	5.66	116.63	113.80
1	A	45	U	C5-C4-O4	5.66	129.30	125.90
1	A	485	G	OP2-P-O3'	5.66	117.65	105.20
1	A	1090	U	N3-C2-O2	-5.66	118.24	122.20
1	A	292	G	N1-C6-O6	5.66	123.30	119.90
1	A	289	G	C4-N9-C1'	5.66	133.85	126.50
1	A	902	G	C4-C5-N7	5.66	113.06	110.80
1	A	23	C	C2-N1-C1'	-5.66	112.58	118.80
1	A	242	C	C2-N3-C4	-5.66	117.07	119.90
1	A	709	G	N1-C6-O6	5.65	123.29	119.90
1	A	862	C	C6-N1-C2	5.65	122.56	120.30
1	A	790	A	C2-N3-C4	-5.65	107.78	110.60
1	A	499	A	OP1-P-O3'	5.65	117.63	105.20
1	A	566	G	C2-N3-C4	-5.65	109.08	111.90
1	A	635	G	C2-N3-C4	-5.65	109.08	111.90
1	A	752	G	C8-N9-C4	5.65	108.66	106.40
18	R	66	LEU	CA-CB-CG	-5.65	102.31	115.30
1	A	372	C	C6-N1-C1'	-5.65	114.03	120.80
1	A	1098	C	C6-N1-C2	5.64	122.56	120.30
1	A	265	G	C8-N9-C1'	5.64	134.33	127.00
1	A	394	G	N1-C6-O6	5.64	123.28	119.90
1	A	456	C	O5'-P-OP1	5.64	117.47	110.70
1	A	120	A	C8-N9-C4	-5.64	103.55	105.80
1	A	828	A	N9-C4-C5	-5.64	103.55	105.80
1	A	239	U	C2-N3-C4	5.63	130.38	127.00
1	A	911	U	C5-C4-O4	5.63	129.28	125.90
1	A	1204	A	N1-C6-N6	5.63	121.98	118.60
1	A	884	U	C5-C6-N1	-5.63	119.89	122.70
1	A	28	G	C5-C6-N1	-5.63	108.69	111.50
1	A	279	A	C8-N9-C4	-5.63	103.55	105.80
1	A	44	G	C4-C5-N7	5.63	113.05	110.80
1	A	1139	G	C4-C5-N7	-5.63	108.55	110.80
1	A	292	G	C4-C5-C6	5.62	122.17	118.80
1	A	484	G	N3-C2-N2	5.62	123.84	119.90
1	A	676	A	C8-N9-C4	5.62	108.05	105.80
1	A	1516[A]	G	C5-C6-N1	-5.62	108.69	111.50
1	A	1516[B]	G	C5-C6-N1	-5.62	108.69	111.50
1	A	1396	A	C2-N3-C4	-5.62	107.79	110.60
1	A	1462	G	N1-C6-O6	5.62	123.27	119.90
1	A	1461	G	N3-C4-C5	5.62	131.41	128.60
1	A	484	G	C4-N9-C1'	5.62	133.80	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1322	C	N3-C2-O2	5.62	125.83	121.90
14	N	39	LEU	CA-CB-CG	-5.62	102.38	115.30
1	A	34	C	N3-C2-O2	5.61	125.83	121.90
1	A	509	A	N7-C8-N9	5.61	116.61	113.80
1	A	662	G	C6-C5-N7	-5.61	127.03	130.40
1	A	752	G	N7-C8-N9	-5.61	110.29	113.10
1	A	774	G	N1-C6-O6	5.61	123.27	119.90
1	A	859	A	OP1-P-O3'	-5.61	92.85	105.20
1	A	347	G	N1-C6-O6	5.61	123.27	119.90
1	A	575	G	N1-C6-O6	-5.61	116.53	119.90
1	A	864	A	C8-N9-C4	-5.61	103.56	105.80
1	A	1451	A	N1-C6-N6	-5.61	115.23	118.60
1	A	22	G	OP2-P-O3'	5.61	117.53	105.20
1	A	672	U	C6-N1-C2	-5.61	117.64	121.00
1	A	945	G	O5'-P-OP2	-5.61	100.66	105.70
1	A	577	G	N3-C2-N2	-5.60	115.98	119.90
1	A	1530	G	C6-N1-C2	5.60	128.46	125.10
1	A	281	G	N1-C6-O6	5.60	123.26	119.90
1	A	361	G	N7-C8-N9	-5.60	110.30	113.10
1	A	579	G	C5-C6-N1	-5.60	108.70	111.50
1	A	815	A	C6-N1-C2	-5.60	115.24	118.60
1	A	888	G	C4-C5-N7	-5.60	108.56	110.80
1	A	1014	A	C2-N3-C4	5.60	113.40	110.60
1	A	1180	A	C8-N9-C4	-5.60	103.56	105.80
1	A	17	U	N3-C4-O4	5.60	123.32	119.40
1	A	574	A	C2-N3-C4	-5.60	107.80	110.60
1	A	802	A	N1-C6-N6	5.60	121.96	118.60
1	A	190(H)	G	C5-C6-O6	-5.60	125.24	128.60
1	A	1493	A	O4'-C1'-N9	5.60	112.68	108.20
1	A	552	U	C2-N3-C4	-5.59	123.64	127.00
1	A	901	A	C2-N3-C4	-5.59	107.80	110.60
1	A	928	G	N3-C2-N2	-5.59	115.98	119.90
1	A	949	A	C5-C6-N6	-5.59	119.23	123.70
1	A	1211	U	C2-N1-C1'	5.59	124.41	117.70
1	A	890	G	O4'-C1'-N9	5.59	112.67	108.20
1	A	266	G	N7-C8-N9	5.58	115.89	113.10
1	A	344	A	N7-C8-N9	5.58	116.59	113.80
1	A	791	G	C5-C6-O6	5.58	131.95	128.60
1	A	1485	U	C6-N1-C1'	5.58	129.02	121.20
1	A	488	C	C5-C4-N4	-5.58	116.29	120.20
1	A	550	G	C8-N9-C4	5.58	108.63	106.40
1	A	600	C	OP2-P-O3'	5.58	117.47	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	830	G	C6-N1-C2	5.58	128.44	125.10
1	A	360	A	C6-N1-C2	-5.57	115.26	118.60
1	A	1121	U	C2-N3-C4	-5.57	123.66	127.00
1	A	1373	G	C4-C5-C6	5.57	122.14	118.80
1	A	559	A	P-O3'-C3'	5.57	126.39	119.70
1	A	715	A	OP1-P-O3'	5.57	117.46	105.20
1	A	31	G	C8-N9-C4	5.57	108.63	106.40
1	A	362	G	C4-C5-N7	-5.57	108.57	110.80
1	A	805	C	C5-C6-N1	5.57	123.78	121.00
1	A	299	G	N1-C2-N2	-5.57	111.19	116.20
1	A	21	G	C4-N9-C1'	5.57	133.73	126.50
1	A	1117	G	N3-C4-N9	5.56	129.34	126.00
1	A	1166	G	C8-N9-C4	-5.56	104.17	106.40
1	A	575	G	C5-C6-N1	5.56	114.28	111.50
1	A	785	G	N9-C4-C5	-5.56	103.18	105.40
1	A	839	U	N1-C2-O2	5.56	126.69	122.80
1	A	872	A	N1-C2-N3	5.56	132.08	129.30
1	A	1134	G	C4-C5-N7	-5.56	108.58	110.80
1	A	27	G	C5-N7-C8	-5.56	101.52	104.30
1	A	279	A	O5'-P-OP2	-5.56	100.70	105.70
1	A	741	G	N3-C4-C5	-5.56	125.82	128.60
1	A	899	C	C2-N1-C1'	-5.56	112.69	118.80
1	A	733	A	C2-N3-C4	-5.56	107.82	110.60
1	A	604	G	C5-C6-N1	-5.55	108.72	111.50
1	A	761	G	N3-C2-N2	-5.55	116.01	119.90
1	A	783	C	N3-C4-C5	5.55	124.12	121.90
1	A	893	C	C5-C6-N1	5.55	123.78	121.00
1	A	1076	C	N3-C4-C5	5.55	124.12	121.90
17	Q	31	LEU	CA-CB-CG	-5.55	102.53	115.30
1	A	658	G	O5'-P-OP2	-5.55	100.70	105.70
1	A	1405	G	N1-C6-O6	5.55	123.23	119.90
1	A	299	G	C4-N9-C1'	5.55	133.71	126.50
1	A	1399	C	N3-C4-C5	-5.54	119.68	121.90
1	A	788	U	N3-C4-O4	5.54	123.28	119.40
1	A	1479	C	C5-C6-N1	5.54	123.77	121.00
19	S	5	LEU	N-CA-C	5.54	125.96	111.00
1	A	711	G	N1-C6-O6	5.54	123.22	119.90
1	A	332	G	N3-C2-N2	-5.53	116.03	119.90
1	A	1093	A	C6-N1-C2	-5.53	115.28	118.60
1	A	1124	G	C5-C6-N1	5.53	114.27	111.50
1	A	1147	C	C4-C5-C6	5.53	120.17	117.40
1	A	944	G	N3-C4-N9	5.53	129.32	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	66	G	O5'-P-OP1	-5.53	100.72	105.70
1	A	421	U	N1-C2-O2	5.53	126.67	122.80
1	A	905	U	C6-N1-C2	5.53	124.32	121.00
1	A	1380	U	P-O3'-C3'	5.53	126.33	119.70
1	A	1435	G	N3-C4-C5	5.53	131.36	128.60
1	A	1501	C	N3-C4-C5	5.53	124.11	121.90
7	G	120	ILE	CB-CA-C	-5.53	100.55	111.60
1	A	1323	G	C6-C5-N7	-5.52	127.09	130.40
1	A	121	C	O5'-P-OP2	-5.52	100.73	105.70
1	A	814	A	N1-C2-N3	5.52	132.06	129.30
1	A	1352	C	O5'-P-OP2	-5.52	100.73	105.70
1	A	21	G	C8-N9-C1'	-5.52	119.83	127.00
1	A	1188	A	C2-N3-C4	-5.52	107.84	110.60
1	A	1259	C	N3-C2-O2	-5.52	118.04	121.90
1	A	1053	G	N3-C4-C5	5.51	131.36	128.60
1	A	1529	G	C4-C5-C6	5.51	122.11	118.80
1	A	443	C	C6-N1-C2	5.51	122.50	120.30
1	A	23	C	N1-C2-O2	-5.51	115.59	118.90
1	A	1193	G	C4-N9-C1'	5.51	133.66	126.50
1	A	1160	G	N1-C6-O6	5.51	123.20	119.90
1	A	235	C	C5-C6-N1	-5.50	118.25	121.00
1	A	314	C	C2-N3-C4	-5.50	117.15	119.90
1	A	1197	G	C6-C5-N7	-5.50	127.10	130.40
1	A	1376	U	N3-C2-O2	-5.50	118.35	122.20
1	A	617	G	C2-N3-C4	-5.50	109.15	111.90
1	A	922	G	N1-C2-N3	5.50	127.20	123.90
1	A	829	G	OP1-P-OP2	5.50	127.84	119.60
1	A	1087	G	C4-N9-C1'	5.50	133.65	126.50
1	A	1121	U	C6-N1-C2	5.49	124.30	121.00
1	A	1139	G	C5-C6-O6	5.49	131.90	128.60
1	A	504	C	C5-C6-N1	5.49	123.75	121.00
1	A	445	G	C4-C5-N7	5.49	113.00	110.80
1	A	692	U	C6-N1-C2	5.49	124.30	121.00
1	A	902	G	C8-N9-C1'	-5.49	119.86	127.00
10	J	71	LEU	CA-CB-CG	-5.49	102.67	115.30
1	A	148	G	C6-C5-N7	-5.49	127.11	130.40
1	A	290	C	C5-C4-N4	-5.49	116.36	120.20
1	A	855	G	N1-C2-N3	5.49	127.19	123.90
1	A	1146	A	N1-C6-N6	5.49	121.89	118.60
1	A	1501	C	C6-N1-C1'	-5.49	114.21	120.80
1	A	780	A	C4-C5-C6	-5.49	114.26	117.00
1	A	928	G	N1-C2-N3	5.49	127.19	123.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1118	C	C6-N1-C2	-5.49	118.11	120.30
1	A	1388	C	N3-C4-C5	5.49	124.09	121.90
1	A	1485	U	C6-N1-C2	-5.49	117.71	121.00
1	A	732	C	C6-N1-C2	-5.48	118.11	120.30
1	A	284	G	C5-C6-N1	-5.48	108.76	111.50
1	A	323	U	O5'-P-OP2	-5.48	100.77	105.70
1	A	860	A	C8-N9-C4	5.48	107.99	105.80
1	A	748	C	P-O3'-C3'	5.47	126.27	119.70
1	A	975	A	C4-C5-C6	5.47	119.74	117.00
1	A	741	G	C8-N9-C1'	-5.47	119.89	127.00
1	A	325	A	N3-C4-N9	-5.47	123.03	127.40
1	A	1030(C)	G	N3-C4-C5	-5.47	125.86	128.60
1	A	1507	A	O5'-P-OP1	-5.47	100.78	105.70
5	E	12	LEU	CB-CG-CD1	-5.47	101.70	111.00
1	A	856	C	N1-C2-O2	-5.47	115.62	118.90
1	A	325	A	C6-C5-N7	5.47	136.13	132.30
1	A	975	A	C8-N9-C4	-5.47	103.61	105.80
1	A	33	A	O5'-P-OP2	-5.46	100.78	105.70
1	A	102	G	N3-C4-N9	5.46	129.28	126.00
1	A	1068	G	OP2-P-O3'	5.46	117.22	105.20
1	A	1256	A	C5-N7-C8	5.46	106.63	103.90
1	A	29	G	OP1-P-OP2	5.46	127.80	119.60
1	A	376	G	C5-N7-C8	5.46	107.03	104.30
1	A	668	G	C2-N3-C4	-5.46	109.17	111.90
1	A	251	G	C5-N7-C8	-5.46	101.57	104.30
1	A	434	U	C6-N1-C2	-5.46	117.72	121.00
1	A	538	G	N1-C6-O6	-5.46	116.62	119.90
1	A	1416	G	C8-N9-C4	-5.46	104.22	106.40
1	A	317	G	C4-C5-N7	5.46	112.98	110.80
1	A	542	G	N1-C6-O6	-5.46	116.62	119.90
1	A	814	A	OP1-P-O3'	5.46	117.21	105.20
1	A	728	A	C5-N7-C8	-5.46	101.17	103.90
1	A	867	G	O5'-P-OP2	-5.46	100.79	105.70
1	A	904	C	O5'-P-OP2	5.46	117.25	110.70
1	A	1193	G	N1-C2-N3	5.46	127.17	123.90
1	A	35	G	C8-N9-C4	5.45	108.58	106.40
1	A	1399	C	C4-C5-C6	5.45	120.13	117.40
1	A	957	U	C5-C4-O4	5.45	129.17	125.90
1	A	332	G	C5-C6-O6	-5.45	125.33	128.60
1	A	1131	G	C6-C5-N7	-5.45	127.13	130.40
1	A	1063	C	C4-C5-C6	5.45	120.12	117.40
1	A	570	G	N7-C8-N9	5.45	115.82	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	47	C	N1-C2-N3	5.45	123.01	119.20
1	A	108	G	C5-N7-C8	-5.45	101.58	104.30
1	A	199	G	C8-N9-C4	5.45	108.58	106.40
1	A	1350	A	O5'-P-OP2	-5.45	100.80	105.70
1	A	1511	G	C8-N9-C1'	-5.44	119.92	127.00
1	A	239	U	N1-C2-O2	-5.44	118.99	122.80
1	A	976	G	C2-N3-C4	-5.44	109.18	111.90
1	A	1230	C	N1-C2-O2	5.44	122.17	118.90
6	F	75	LEU	CA-CB-CG	5.44	127.81	115.30
1	A	871	U	C6-N1-C2	5.44	124.26	121.00
1	A	1467	G	C2-N3-C4	5.44	114.62	111.90
1	A	278	G	N3-C4-N9	-5.44	122.74	126.00
1	A	852	G	C2-N3-C4	-5.44	109.18	111.90
1	A	961	U	N3-C4-O4	5.44	123.20	119.40
1	A	935	A	OP1-P-OP2	5.43	127.75	119.60
1	A	234	C	C2-N1-C1'	-5.43	112.82	118.80
1	A	374	A	C8-N9-C4	5.43	107.97	105.80
1	A	976	G	O5'-P-OP1	-5.43	100.81	105.70
1	A	117	G	C8-N9-C1'	-5.43	119.94	127.00
1	A	1396	A	C8-N9-C4	5.43	107.97	105.80
1	A	564	C	C6-N1-C1'	-5.43	114.28	120.80
1	A	190(E)	U	N1-C2-O2	5.43	126.60	122.80
1	A	336	C	C6-N1-C2	5.43	122.47	120.30
1	A	224	C	N1-C2-O2	5.43	122.16	118.90
1	A	672	U	O4'-C1'-N1	5.43	112.54	108.20
1	A	839	U	N3-C2-O2	-5.43	118.40	122.20
1	A	1064	G	C6-C5-N7	-5.42	127.15	130.40
1	A	1249	C	C6-N1-C2	5.42	122.47	120.30
1	A	970	C	N1-C2-N3	-5.42	115.40	119.20
1	A	886	G	N3-C4-C5	5.42	131.31	128.60
1	A	947	G	N1-C6-O6	5.42	123.15	119.90
1	A	955	U	N1-C2-N3	5.42	118.15	114.90
14	N	7	ILE	CB-CA-C	5.42	122.44	111.60
1	A	877	C	C5-C6-N1	5.42	123.71	121.00
1	A	1377	A	N3-C4-C5	5.42	130.59	126.80
1	A	36	C	O5'-P-OP1	5.42	117.20	110.70
1	A	504	C	N3-C4-N4	5.42	121.79	118.00
1	A	820	U	C6-N1-C2	5.42	124.25	121.00
1	A	936	C	O5'-P-OP1	-5.42	100.82	105.70
1	A	170	U	N3-C4-O4	5.42	123.19	119.40
1	A	509	A	C4-C5-C6	5.42	119.71	117.00
1	A	785	G	C5-C6-O6	-5.42	125.35	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	902	G	C2-N3-C4	-5.41	109.19	111.90
1	A	41	G	C8-N9-C4	-5.41	104.23	106.40
1	A	1494	G	C4-N9-C1'	5.41	133.53	126.50
1	A	820	U	N3-C2-O2	5.41	125.98	122.20
1	A	113	G	N3-C4-C5	-5.40	125.90	128.60
1	A	316	G	C5-C6-O6	-5.40	125.36	128.60
1	A	1490	C	C2-N3-C4	5.40	122.60	119.90
1	A	161	A	N1-C6-N6	-5.40	115.36	118.60
1	A	661	G	N3-C2-N2	-5.40	116.12	119.90
1	A	819	A	C6-C5-N7	-5.40	128.52	132.30
1	A	1166	G	C8-N9-C1'	-5.40	119.98	127.00
1	A	590	C	C5-C6-N1	-5.40	118.30	121.00
1	A	234	C	N3-C4-N4	-5.40	114.22	118.00
1	A	102	G	C4-C5-C6	5.39	122.04	118.80
1	A	281	G	C6-C5-N7	-5.39	127.16	130.40
1	A	729	A	C6-N1-C2	-5.39	115.37	118.60
1	A	651	C	N3-C2-O2	5.39	125.67	121.90
1	A	817	C	O4'-C1'-N1	-5.39	103.89	108.20
1	A	890	G	OP2-P-O3'	5.39	117.05	105.20
1	A	54	C	OP1-P-O3'	5.38	117.05	105.20
1	A	792	A	C2-N3-C4	-5.38	107.91	110.60
1	A	1234	C	C6-N1-C2	5.38	122.45	120.30
1	A	276	G	C6-C5-N7	-5.38	127.17	130.40
1	A	445	G	C5-C6-O6	-5.38	125.37	128.60
1	A	1240	U	C5-C4-O4	5.38	129.13	125.90
1	A	444	C	N3-C2-O2	-5.38	118.13	121.90
1	A	934	C	C6-N1-C2	-5.38	118.15	120.30
1	A	525	C	C5-C6-N1	5.38	123.69	121.00
1	A	250	A	N1-C2-N3	5.37	131.99	129.30
1	A	659	U	C6-N1-C2	-5.37	117.78	121.00
1	A	1516[A]	G	C4-N9-C1'	-5.37	119.52	126.50
1	A	1516[B]	G	C4-N9-C1'	-5.37	119.52	126.50
1	A	175	C	O5'-P-OP1	5.37	117.14	110.70
1	A	1201	A	P-O3'-C3'	5.37	126.14	119.70
1	A	313	A	C6-C5-N7	-5.37	128.54	132.30
1	A	1239	A	N1-C6-N6	5.37	121.82	118.60
1	A	1304	G	C4-C5-C6	5.37	122.02	118.80
1	A	970	C	C6-N1-C1'	-5.37	114.36	120.80
1	A	1117	G	N3-C2-N2	5.37	123.66	119.90
20	T	13	LEU	CB-CG-CD1	5.37	120.12	111.00
1	A	161	A	N1-C2-N3	5.36	131.98	129.30
1	A	861	G	C5-N7-C8	-5.36	101.62	104.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	133	U	C4-C5-C6	5.36	122.92	119.70
1	A	517	G	C8-N9-C4	-5.36	104.25	106.40
1	A	496	A	O5'-P-OP2	5.36	117.13	110.70
1	A	1373	G	N3-C4-N9	5.36	129.22	126.00
1	A	769	G	O5'-P-OP1	5.36	117.13	110.70
1	A	1418	A	C8-N9-C4	-5.36	103.66	105.80
1	A	228	A	N9-C4-C5	5.36	107.94	105.80
1	A	284	G	OP2-P-O3'	5.36	116.98	105.20
1	A	446	G	N1-C6-O6	5.36	123.11	119.90
1	A	1118	C	C5-C6-N1	5.36	123.68	121.00
1	A	1440	C	N3-C4-N4	5.36	121.75	118.00
1	A	275	G	C6-C5-N7	-5.35	127.19	130.40
1	A	899	C	N3-C2-O2	5.35	125.65	121.90
1	A	216	G	N7-C8-N9	-5.35	110.42	113.10
1	A	497	A	N9-C4-C5	5.35	107.94	105.80
1	A	1139	G	C8-N9-C4	-5.35	104.26	106.40
1	A	1464	G	N1-C6-O6	5.35	123.11	119.90
1	A	148	G	C8-N9-C1'	-5.35	120.05	127.00
1	A	292	G	C5-C6-N1	-5.34	108.83	111.50
1	A	900	A	OP1-P-OP2	-5.34	111.58	119.60
1	A	446	G	N3-C2-N2	-5.34	116.16	119.90
1	A	818	G	C5-C6-O6	5.34	131.81	128.60
14	N	39	LEU	CB-CG-CD2	-5.34	101.92	111.00
1	A	238	G	O5'-P-OP2	-5.34	100.89	105.70
1	A	541	G	C4-C5-N7	5.34	112.94	110.80
1	A	886	G	C5-C6-N1	-5.34	108.83	111.50
2	B	122	PHE	N-CA-C	5.34	125.41	111.00
1	A	299	G	N1-C2-N3	5.34	127.10	123.90
1	A	1142	G	O5'-P-OP1	-5.34	100.90	105.70
1	A	1230	C	N3-C4-N4	5.34	121.74	118.00
1	A	853	G	C4-C5-C6	5.33	122.00	118.80
1	A	1233	G	C6-C5-N7	-5.33	127.20	130.40
1	A	265	G	C4-N9-C1'	-5.33	119.56	126.50
1	A	321	A	C8-N9-C4	5.33	107.93	105.80
1	A	1522	U	OP2-P-O3'	5.33	116.94	105.20
1	A	61	G	C2-N3-C4	-5.33	109.23	111.90
1	A	306	G	N1-C2-N2	5.33	121.00	116.20
1	A	363	A	C5-N7-C8	-5.33	101.23	103.90
1	A	148	G	C4-N9-C1'	5.33	133.43	126.50
1	A	573	A	OP2-P-O3'	5.33	116.92	105.20
1	A	893	C	C5-C4-N4	-5.33	116.47	120.20
1	A	197	A	C5-C6-N6	5.33	127.96	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	759	A	C2-N3-C4	5.33	113.26	110.60
1	A	1083	U	N3-C4-C5	-5.33	111.41	114.60
1	A	624	C	N1-C2-N3	-5.32	115.47	119.20
1	A	1353	G	C4-C5-N7	5.32	112.93	110.80
1	A	1507	A	OP1-P-O3'	5.32	116.91	105.20
10	J	54	PHE	N-CA-C	5.32	125.37	111.00
1	A	748	C	N3-C2-O2	-5.32	118.18	121.90
1	A	987	G	C5-C6-N1	-5.32	108.84	111.50
1	A	1478	C	C2-N3-C4	5.32	122.56	119.90
2	B	221	LEU	CA-CB-CG	5.32	127.54	115.30
1	A	436	C	O5'-P-OP1	-5.32	100.91	105.70
1	A	487	A	C2-N3-C4	-5.32	107.94	110.60
1	A	204	U	C2-N3-C4	5.32	130.19	127.00
1	A	265	G	N3-C4-C5	5.32	131.26	128.60
1	A	913	A	N1-C6-N6	-5.32	115.41	118.60
1	A	1440	C	C5-C4-N4	-5.32	116.48	120.20
1	A	52	G	N3-C4-N9	-5.31	122.81	126.00
1	A	120	A	N9-C4-C5	5.31	107.92	105.80
1	A	242	C	C6-N1-C2	5.31	122.42	120.30
1	A	299	G	C5-C6-N1	-5.31	108.85	111.50
1	A	583	A	C4-C5-C6	5.31	119.65	117.00
1	A	1005	A	C4-N9-C1'	5.31	135.85	126.30
1	A	1034	G	O4'-C1'-N9	5.31	112.44	108.20
1	A	1533	C	C5-C6-N1	5.31	123.65	121.00
1	A	313	A	O4'-C1'-N9	-5.31	103.95	108.20
1	A	1302	U	N3-C2-O2	-5.30	118.49	122.20
1	A	1369	C	N3-C4-C5	-5.30	119.78	121.90
1	A	66	G	N1-C2-N2	5.30	120.97	116.20
1	A	265	G	C4-C5-N7	-5.30	108.68	110.80
1	A	1077	G	N3-C4-C5	5.30	131.25	128.60
1	A	531	U	N3-C2-O2	-5.30	118.49	122.20
1	A	241	C	N3-C4-C5	5.30	124.02	121.90
1	A	515	G	C6-C5-N7	-5.30	127.22	130.40
1	A	1206	G	N1-C6-O6	5.30	123.08	119.90
1	A	1443	G	O4'-C1'-N9	-5.29	103.97	108.20
1	A	1497	G	N1-C2-N3	5.29	127.08	123.90
1	A	546	G	C8-N9-C4	-5.29	104.28	106.40
1	A	1393	U	O5'-P-OP1	5.29	117.05	110.70
1	A	243	A	O4'-C1'-N9	-5.29	103.97	108.20
1	A	676	A	N7-C8-N9	-5.29	111.16	113.80
6	F	9	VAL	CB-CA-C	-5.29	101.36	111.40
1	A	41	G	C5-C6-O6	-5.28	125.43	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	95	U	C4-C5-C6	5.28	122.87	119.70
1	A	1100	C	C4-C5-C6	-5.28	114.76	117.40
1	A	1215	G	N1-C6-O6	5.28	123.07	119.90
1	A	1530	G	C5-C6-N1	-5.28	108.86	111.50
1	A	190(A)	C	C5-C4-N4	-5.28	116.50	120.20
1	A	320	C	C6-N1-C2	5.28	122.41	120.30
1	A	1328	C	N3-C4-C5	5.28	124.01	121.90
1	A	763	G	C4-C5-N7	5.28	112.91	110.80
1	A	1125	U	N1-C2-O2	-5.28	119.11	122.80
1	A	1073	U	C6-N1-C2	-5.28	117.83	121.00
1	A	330	C	OP2-P-O3'	5.27	116.80	105.20
1	A	1099	G	N3-C4-N9	-5.27	122.84	126.00
1	A	1389	C	C6-N1-C2	-5.27	118.19	120.30
1	A	415	A	C8-N9-C4	-5.27	103.69	105.80
1	A	1084	G	C4-C5-C6	5.27	121.96	118.80
1	A	1172	C	C6-N1-C2	5.27	122.41	120.30
1	A	31	G	N3-C4-C5	-5.26	125.97	128.60
1	A	321	A	O5'-P-OP2	-5.26	100.96	105.70
1	A	687	A	OP1-P-O3'	5.26	116.78	105.20
1	A	36	C	C5-C6-N1	-5.26	118.37	121.00
1	A	282	A	C4-C5-N7	5.26	113.33	110.70
1	A	900	A	C5-C6-N6	-5.26	119.49	123.70
1	A	1508	G	N1-C2-N2	5.26	120.94	116.20
1	A	1396	A	C5-C6-N1	-5.26	115.07	117.70
1	A	200	G	C6-C5-N7	-5.26	127.25	130.40
1	A	1338	G	C4-C5-C6	5.26	121.95	118.80
1	A	108	G	C5-C6-N1	-5.25	108.87	111.50
1	A	344	A	C8-N9-C4	-5.25	103.70	105.80
1	A	348	G	C5-C6-O6	-5.25	125.45	128.60
1	A	387	U	C4-C5-C6	5.25	122.85	119.70
1	A	885	G	OP1-P-OP2	5.25	127.48	119.60
1	A	1358	U	C5-C6-N1	-5.25	120.07	122.70
1	A	127	G	N1-C6-O6	5.25	123.05	119.90
1	A	799	G	OP1-P-OP2	5.25	127.48	119.60
1	A	405	U	N3-C2-O2	-5.25	118.53	122.20
1	A	791	G	C4-N9-C1'	5.25	133.32	126.50
1	A	1304	G	N1-C6-O6	5.25	123.05	119.90
1	A	10	A	N1-C2-N3	5.25	131.92	129.30
1	A	587	G	C8-N9-C4	-5.25	104.30	106.40
1	A	1222	G	C4-C5-C6	5.24	121.95	118.80
1	A	689	C	N1-C2-O2	-5.24	115.76	118.90
1	A	993	G	C5-C6-O6	-5.24	125.46	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	908	A	N1-C6-N6	-5.24	115.46	118.60
1	A	977	A	C2-N3-C4	5.24	113.22	110.60
1	A	1391	U	C6-N1-C2	5.24	124.14	121.00
1	A	10	A	C5-C6-N1	5.24	120.32	117.70
1	A	348	G	N1-C6-O6	5.23	123.04	119.90
1	A	537	G	C8-N9-C4	5.23	108.49	106.40
1	A	1193	G	C5-C6-N1	-5.23	108.88	111.50
1	A	1261	A	N9-C4-C5	-5.23	103.71	105.80
2	B	41	ILE	CB-CA-C	-5.23	101.13	111.60
5	E	12	LEU	CA-CB-CG	5.23	127.33	115.30
1	A	254	G	C2-N3-C4	-5.23	109.28	111.90
1	A	853	G	C4-N9-C1'	5.23	133.30	126.50
1	A	1069	C	C5-C4-N4	-5.23	116.54	120.20
1	A	140	A	N1-C6-N6	5.23	121.74	118.60
1	A	1532	U	N1-C2-N3	-5.23	111.76	114.90
1	A	509	A	C6-C5-N7	-5.23	128.64	132.30
1	A	748	C	N1-C2-O2	5.23	122.04	118.90
1	A	1084	G	N3-C4-C5	-5.23	125.99	128.60
1	A	78	G	C5-C6-N1	-5.22	108.89	111.50
1	A	1359	C	N1-C2-O2	5.22	122.03	118.90
1	A	8	A	C2-N3-C4	-5.22	107.99	110.60
1	A	578	C	C5-C6-N1	-5.22	118.39	121.00
1	A	183	G	C6-C5-N7	-5.22	127.27	130.40
1	A	944	G	OP2-P-O3'	5.22	116.68	105.20
1	A	50	A	C5-C6-N6	5.22	127.88	123.70
1	A	597	G	C2-N3-C4	-5.22	109.29	111.90
1	A	712	A	N1-C6-N6	-5.22	115.47	118.60
1	A	673	G	C6-C5-N7	5.22	133.53	130.40
1	A	715	A	N7-C8-N9	-5.22	111.19	113.80
1	A	949	A	C6-C5-N7	-5.22	128.65	132.30
1	A	1124	G	O4'-C1'-N9	5.22	112.37	108.20
1	A	1125	U	OP2-P-O3'	5.22	116.68	105.20
1	A	1511	G	C8-N9-C4	5.22	108.49	106.40
1	A	61	G	C5-C6-O6	-5.21	125.47	128.60
1	A	267	C	N3-C4-C5	5.21	123.99	121.90
1	A	352	C	C2-N3-C4	5.21	122.51	119.90
1	A	284	G	N1-C2-N3	5.21	127.03	123.90
1	A	1195	C	N3-C4-C5	-5.21	119.81	121.90
1	A	1452	C	N1-C2-N3	-5.21	115.55	119.20
1	A	764	C	C2-N1-C1'	5.21	124.53	118.80
1	A	403	C	C4-C5-C6	5.21	120.00	117.40
1	A	1290	G	C6-C5-N7	-5.21	127.27	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	289	G	C8-N9-C1'	-5.21	120.23	127.00
1	A	852	G	C5-C6-N1	-5.21	108.90	111.50
1	A	791	G	N1-C2-N3	5.20	127.02	123.90
1	A	1055	A	C6-C5-N7	-5.20	128.66	132.30
1	A	1058	G	C2-N3-C4	-5.20	109.30	111.90
1	A	1079	G	C6-C5-N7	-5.20	127.28	130.40
1	A	1098	C	C5-C6-N1	-5.20	118.40	121.00
1	A	229	U	N3-C4-O4	5.20	123.04	119.40
1	A	144	G	C5-C6-N1	-5.20	108.90	111.50
1	A	255	G	N1-C2-N3	5.20	127.02	123.90
1	A	610	G	N3-C2-N2	-5.20	116.26	119.90
1	A	1087	G	N7-C8-N9	5.20	115.70	113.10
1	A	1119	C	N1-C2-O2	5.20	122.02	118.90
1	A	1143	G	C8-N9-C4	5.20	108.48	106.40
1	A	949	A	C5-N7-C8	-5.20	101.30	103.90
1	A	1129	C	C6-N1-C1'	5.20	127.04	120.80
1	A	1410	G	C8-N9-C4	5.20	108.48	106.40
1	A	513	C	N3-C4-C5	5.20	123.98	121.90
1	A	650	G	N1-C6-O6	5.20	123.02	119.90
1	A	1102	A	C8-N9-C4	-5.20	103.72	105.80
1	A	1190	G	C4-C5-N7	-5.20	108.72	110.80
1	A	1239	A	N9-C4-C5	-5.20	103.72	105.80
1	A	252	U	N3-C2-O2	5.19	125.84	122.20
1	A	1353	G	C6-C5-N7	-5.19	127.28	130.40
1	A	809	G	N1-C2-N3	-5.19	120.78	123.90
1	A	818	G	N9-C4-C5	5.19	107.48	105.40
1	A	1450	U	O5'-P-OP2	-5.19	101.03	105.70
1	A	439	A	N9-C4-C5	5.19	107.88	105.80
1	A	869	G	N1-C6-O6	-5.19	116.78	119.90
5	E	12	LEU	CB-CG-CD2	5.19	119.82	111.00
1	A	262	A	N3-C4-C5	5.19	130.43	126.80
1	A	556	C	N3-C4-N4	5.19	121.63	118.00
1	A	1229	A	C2-N3-C4	-5.19	108.01	110.60
1	A	1467	G	N3-C4-C5	-5.19	126.01	128.60
1	A	658	G	N1-C2-N2	-5.18	111.53	116.20
1	A	1087	G	C5-C6-N1	-5.18	108.91	111.50
1	A	305	G	C5-C6-O6	5.18	131.71	128.60
1	A	620	C	C6-N1-C2	5.18	122.37	120.30
1	A	672	U	N3-C4-O4	5.18	123.03	119.40
1	A	369	C	O5'-P-OP1	5.18	116.92	110.70
1	A	416	G	C8-N9-C4	-5.18	104.33	106.40
1	A	855	G	C4-C5-C6	5.18	121.91	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1158	C	N3-C2-O2	-5.18	118.28	121.90
1	A	1495	U	C6-N1-C2	-5.18	117.89	121.00
1	A	629	G	OP2-P-O3'	5.17	116.58	105.20
1	A	1128	C	N3-C4-C5	-5.17	119.83	121.90
1	A	247	G	C5-C6-O6	-5.17	125.50	128.60
1	A	20	U	C6-N1-C1'	-5.17	113.96	121.20
1	A	228	A	N1-C2-N3	5.17	131.89	129.30
1	A	244	U	N1-C2-O2	5.17	126.42	122.80
1	A	1261	A	C8-N9-C4	5.17	107.87	105.80
1	A	1155	G	N1-C2-N3	5.17	127.00	123.90
1	A	50	A	C5-C6-N1	-5.17	115.12	117.70
1	A	762	C	C2-N3-C4	-5.17	117.32	119.90
1	A	259	G	N1-C6-O6	5.17	123.00	119.90
1	A	668	G	N1-C6-O6	5.17	123.00	119.90
1	A	798	G	N1-C2-N3	-5.17	120.80	123.90
1	A	841	U	C5-C6-N1	5.16	125.28	122.70
1	A	910	C	N3-C2-O2	5.16	125.52	121.90
1	A	360	A	N1-C2-N3	5.16	131.88	129.30
1	A	444	C	N1-C2-O2	5.16	122.00	118.90
1	A	895	G	N1-C2-N3	5.16	127.00	123.90
1	A	147	G	N3-C2-N2	-5.16	116.29	119.90
1	A	254	G	C8-N9-C4	5.16	108.46	106.40
1	A	281	G	C2-N3-C4	-5.16	109.32	111.90
1	A	965	A	C4-C5-C6	-5.16	114.42	117.00
1	A	528	C	O5'-P-OP1	-5.16	101.06	105.70
1	A	818	G	C5-N7-C8	5.16	106.88	104.30
1	A	614	A	C4-C5-N7	5.15	113.28	110.70
1	A	226	G	N1-C6-O6	5.15	122.99	119.90
1	A	1099	G	C4-N9-C1'	-5.15	119.80	126.50
1	A	1522	U	C4-C5-C6	5.15	122.79	119.70
1	A	303	A	C8-N9-C4	-5.15	103.74	105.80
1	A	499	A	N9-C4-C5	5.14	107.86	105.80
1	A	553	A	OP2-P-O3'	5.14	116.52	105.20
1	A	590	C	N3-C4-C5	5.14	123.96	121.90
1	A	731	G	C5-C6-O6	-5.14	125.51	128.60
1	A	866	C	C5-C4-N4	5.14	123.80	120.20
1	A	1136	U	C5-C6-N1	5.14	125.27	122.70
1	A	257	G	C6-C5-N7	-5.14	127.31	130.40
1	A	1075	C	C2-N1-C1'	-5.14	113.14	118.80
1	A	1532	U	C2-N3-C4	5.14	130.09	127.00
1	A	273	A	C2-N3-C4	-5.14	108.03	110.60
1	A	570	G	C6-C5-N7	-5.14	127.32	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	502	G	C4-N9-C1'	-5.14	119.82	126.50
1	A	894	G	C5-C6-N1	-5.14	108.93	111.50
1	A	1084	G	C5-C6-N1	-5.14	108.93	111.50
1	A	382	A	N9-C4-C5	5.14	107.86	105.80
1	A	1510	U	O5'-P-OP1	-5.14	101.08	105.70
1	A	34	C	N1-C2-N3	-5.13	115.61	119.20
1	A	1394	A	C2-N3-C4	-5.13	108.03	110.60
1	A	577	G	N3-C4-N9	-5.13	122.92	126.00
1	A	799	G	C5-N7-C8	-5.13	101.73	104.30
1	A	612	C	C5-C4-N4	5.13	123.79	120.20
1	A	779	C	O5'-P-OP2	-5.13	101.08	105.70
1	A	908	A	N9-C4-C5	5.13	107.85	105.80
1	A	641	U	C5-C4-O4	-5.13	122.82	125.90
1	A	1278	U	O5'-P-OP2	-5.13	101.08	105.70
1	A	658	G	C6-N1-C2	-5.13	122.03	125.10
1	A	912	C	N1-C2-O2	-5.13	115.82	118.90
1	A	532	A	C8-N9-C4	5.12	107.85	105.80
1	A	734	G	C6-C5-N7	-5.12	127.33	130.40
1	A	821	G	N1-C2-N3	5.12	126.97	123.90
1	A	1453	G	C6-C5-N7	-5.12	127.33	130.40
1	A	792	A	C5-C6-N1	-5.12	115.14	117.70
1	A	1290	G	C5-C6-O6	-5.12	125.53	128.60
12	L	27	LEU	CB-CG-CD2	5.12	119.70	111.00
1	A	7	G	C8-N9-C4	5.12	108.45	106.40
1	A	740	U	C2-N1-C1'	-5.12	111.56	117.70
1	A	111	G	OP1-P-OP2	5.12	127.27	119.60
1	A	382	A	N1-C6-N6	-5.12	115.53	118.60
1	A	794	A	N1-C6-N6	-5.12	115.53	118.60
1	A	897	C	C6-N1-C2	5.12	122.35	120.30
1	A	453	A	C8-N9-C4	-5.11	103.75	105.80
1	A	851	G	N1-C6-O6	5.11	122.97	119.90
1	A	665	A	C2-N3-C4	5.11	113.16	110.60
1	A	1232	U	C2-N1-C1'	5.11	123.83	117.70
1	A	329	A	C5-C6-N6	5.11	127.79	123.70
1	A	1085	U	N1-C2-N3	-5.11	111.84	114.90
1	A	46	G	N9-C4-C5	5.11	107.44	105.40
1	A	631	G	C6-N1-C2	5.11	128.16	125.10
1	A	665	A	C5-C6-N1	5.11	120.25	117.70
1	A	512	U	C5-C4-O4	-5.10	122.84	125.90
1	A	130	A	N1-C6-N6	5.10	121.66	118.60
1	A	292	G	C6-C5-N7	-5.10	127.34	130.40
1	A	509	A	C2'-C3'-O3'	5.10	121.86	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	870	U	C5-C6-N1	-5.10	120.15	122.70
1	A	1257	U	C6-N1-C2	-5.10	117.94	121.00
1	A	68	G	N3-C4-N9	-5.10	122.94	126.00
1	A	674	G	C4-C5-N7	5.10	112.84	110.80
1	A	816	A	OP1-P-O3'	5.10	116.42	105.20
1	A	1128	C	C6-N1-C2	-5.10	118.26	120.30
1	A	1198	G	C5-C6-N1	-5.10	108.95	111.50
1	A	191	G	N3-C4-C5	-5.09	126.05	128.60
1	A	500	G	N9-C4-C5	-5.09	103.36	105.40
1	A	1399	C	N1-C2-N3	5.09	122.77	119.20
1	A	1525	G	N9-C1'-C2'	-5.09	106.40	112.00
1	A	1531	A	C2-N3-C4	-5.09	108.05	110.60
1	A	362	G	C5-N7-C8	5.09	106.85	104.30
1	A	585	G	N3-C4-C5	5.09	131.15	128.60
1	A	1299	A	N7-C8-N9	5.09	116.35	113.80
1	A	397	A	C8-N9-C4	-5.09	103.76	105.80
1	A	407	G	C2-N3-C4	-5.09	109.35	111.90
1	A	507	C	N3-C2-O2	5.09	125.46	121.90
1	A	1023	G	N3-C4-N9	5.09	129.06	126.00
1	A	148	G	N3-C4-C5	-5.09	126.06	128.60
1	A	184	G	C5-N7-C8	5.09	106.84	104.30
1	A	389	A	C8-N9-C4	-5.09	103.76	105.80
1	A	499	A	C5-C6-N6	5.09	127.77	123.70
1	A	900	A	C4-C5-N7	5.09	113.25	110.70
1	A	1529	G	C8-N9-C4	-5.09	104.36	106.40
1	A	872	A	C4-C5-C6	5.09	119.54	117.00
1	A	46	G	N7-C8-N9	5.09	115.64	113.10
1	A	889	A	C8-N9-C4	-5.09	103.77	105.80
1	A	331	G	N7-C8-N9	5.08	115.64	113.10
1	A	728	A	C6-C5-N7	-5.08	128.74	132.30
1	A	833	U	C6-N1-C1'	5.08	128.32	121.20
1	A	9	G	O5'-P-OP2	-5.08	101.12	105.70
1	A	747	C	C4-C5-C6	5.08	119.94	117.40
1	A	667	G	C5-C6-N1	-5.08	108.96	111.50
1	A	1379	G	C6-C5-N7	-5.08	127.35	130.40
1	A	502	G	N3-C4-C5	5.08	131.14	128.60
1	A	1079	G	C4-N9-C1'	5.08	133.10	126.50
1	A	1138	G	N3-C2-N2	-5.08	116.35	119.90
1	A	497	A	C4-C5-N7	-5.08	108.16	110.70
1	A	1416	G	N7-C8-N9	5.08	115.64	113.10
1	A	880	C	N1-C2-N3	-5.07	115.65	119.20
1	A	1322	C	OP1-P-OP2	-5.07	111.99	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	904	C	C6-N1-C2	5.07	122.33	120.30
1	A	223	U	C5-C6-N1	-5.07	120.17	122.70
1	A	917	G	C2-N3-C4	5.07	114.43	111.90
1	A	363	A	C5-C6-N6	-5.07	119.65	123.70
1	A	1502	A	N7-C8-N9	5.07	116.33	113.80
1	A	58	C	N3-C4-N4	5.07	121.55	118.00
1	A	60	A	C8-N9-C4	-5.07	103.77	105.80
1	A	435	C	O5'-P-OP2	5.07	116.78	110.70
1	A	887	G	C5-C6-N1	-5.07	108.97	111.50
3	C	14	ILE	CG1-CB-CG2	5.07	122.54	111.40
3	C	21	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	A	116	A	OP1-P-OP2	5.06	127.20	119.60
1	A	857	C	OP2-P-O3'	5.06	116.34	105.20
1	A	881	G	N9-C4-C5	-5.06	103.37	105.40
1	A	612	C	N3-C4-N4	-5.06	114.46	118.00
1	A	820	U	C5-C6-N1	-5.06	120.17	122.70
1	A	148	G	C4-C5-C6	5.06	121.84	118.80
1	A	231	G	O5'-P-OP2	5.06	116.77	110.70
1	A	1240	U	N3-C4-O4	-5.06	115.86	119.40
1	A	248	C	C2-N3-C4	-5.06	117.37	119.90
1	A	504	C	N3-C4-C5	-5.06	119.88	121.90
1	A	934	C	O5'-P-OP2	-5.06	101.15	105.70
1	A	277	C	N3-C4-C5	5.06	123.92	121.90
1	A	406	G	N7-C8-N9	5.06	115.63	113.10
1	A	599	C	N3-C2-O2	5.06	125.44	121.90
1	A	300	A	C4-C5-N7	-5.06	108.17	110.70
1	A	595	G	N3-C2-N2	5.05	123.44	119.90
10	J	5	ARG	CG-CD-NE	5.05	122.41	111.80
1	A	564	C	N1-C2-O2	5.05	121.93	118.90
1	A	788	U	N3-C4-C5	-5.05	111.57	114.60
1	A	1193	G	OP1-P-OP2	5.05	127.18	119.60
1	A	1373	G	C4-N9-C1'	5.05	133.06	126.50
1	A	688	G	N1-C6-O6	5.05	122.93	119.90
1	A	993	G	N3-C4-N9	5.05	129.03	126.00
1	A	382	A	C5-C6-N6	5.05	127.74	123.70
1	A	500	G	C2-N3-C4	-5.05	109.38	111.90
1	A	546	G	N7-C8-N9	5.05	115.62	113.10
1	A	1125	U	C2-N1-C1'	-5.05	111.64	117.70
1	A	1494	G	C8-N9-C1'	-5.04	120.44	127.00
1	A	316	G	N3-C4-N9	5.04	129.03	126.00
1	A	224	C	N3-C2-O2	-5.04	118.37	121.90
1	A	535	A	C5-N7-C8	5.04	106.42	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1166	G	N7-C8-N9	5.04	115.62	113.10
1	A	1338	G	C8-N9-C1'	-5.04	120.45	127.00
1	A	1397	C	N3-C4-C5	5.04	123.92	121.90
1	A	1304	G	C4-N9-C1'	5.04	133.05	126.50
1	A	1391	U	C2-N1-C1'	-5.04	111.65	117.70
1	A	585	G	N3-C4-N9	-5.04	122.98	126.00
1	A	879	C	C2-N1-C1'	-5.04	113.26	118.80
1	A	918	A	C5-C6-N6	-5.04	119.67	123.70
1	A	232	G	N3-C4-N9	5.04	129.02	126.00
1	A	787	A	C6-N1-C2	-5.04	115.58	118.60
1	A	1370	G	C2-N3-C4	-5.04	109.38	111.90
1	A	1524	C	OP2-P-O3'	5.04	116.28	105.20
1	A	517	G	C5-C6-N1	-5.03	108.98	111.50
1	A	580	U	N3-C4-C5	-5.03	111.58	114.60
1	A	834	C	N3-C4-C5	5.03	123.91	121.90
1	A	1227	A	O5'-P-OP1	-5.03	101.17	105.70
1	A	375	U	N3-C4-O4	5.03	122.92	119.40
1	A	918	A	C5-C6-N1	5.03	120.22	117.70
1	A	79	G	N1-C6-O6	5.03	122.92	119.90
1	A	545	C	OP1-P-OP2	5.03	127.14	119.60
5	E	123	LEU	CB-CG-CD2	-5.03	102.45	111.00
1	A	951	G	N1-C6-O6	5.03	122.92	119.90
1	A	1386	G	O5'-P-OP2	-5.03	101.18	105.70
1	A	575	G	N3-C2-N2	5.02	123.42	119.90
1	A	542	G	C5-C6-N1	5.02	114.01	111.50
1	A	28	G	O5'-P-OP1	-5.02	101.18	105.70
1	A	42	G	N3-C2-N2	-5.02	116.39	119.90
1	A	1397	C	N3-C2-O2	-5.02	118.39	121.90
1	A	1526	G	C2-N3-C4	-5.02	109.39	111.90
1	A	352	C	C5-C6-N1	5.02	123.51	121.00
1	A	1148	U	N3-C2-O2	-5.02	118.69	122.20
1	A	1395	C	N3-C2-O2	5.02	125.41	121.90
1	A	582	U	C4-C5-C6	5.02	122.71	119.70
1	A	406	G	C6-C5-N7	-5.01	127.39	130.40
1	A	517	G	N9-C4-C5	5.01	107.41	105.40
1	A	786	G	C4-C5-C6	5.01	121.81	118.80
1	A	1202	G	C8-N9-C1'	5.01	133.52	127.00
1	A	886	G	C4-C5-N7	5.01	112.80	110.80
1	A	906	G	C5-C6-O6	-5.01	125.59	128.60
1	A	646	U	C2-N3-C4	5.01	130.00	127.00
1	A	1417	G	O4'-C1'-N9	5.01	112.21	108.20
1	A	1435	G	C4-C5-N7	5.01	112.80	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	710	G	N3-C2-N2	-5.01	116.39	119.90
1	A	1494	G	N3-C4-N9	5.01	129.00	126.00
1	A	1495	U	C2-N3-C4	5.01	130.00	127.00
1	A	357	G	C6-N1-C2	5.00	128.10	125.10
1	A	654	G	OP2-P-O3'	5.00	116.21	105.20
1	A	190(H)	G	C8-N9-C1'	-5.00	120.49	127.00
1	A	869	G	N3-C4-N9	5.00	129.00	126.00
1	A	332	G	C5-C6-N1	-5.00	109.00	111.50
1	A	518	C	C2-N1-C1'	5.00	124.30	118.80
1	A	662	G	C5-C6-N1	-5.00	109.00	111.50
1	A	770	C	N1-C2-O2	5.00	121.90	118.90
1	A	786	G	C8-N9-C1'	-5.00	120.50	127.00
1	A	1079	G	C6-N1-C2	-5.00	122.10	125.10

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	8	LYS	Peptide
2	B	9	GLU	Peptide
3	C	154	SER	Peptide
3	C	166	GLU	Peptide
3	C	168	ALA	Peptide
8	H	90	GLY	Peptide
9	I	56	LEU	Peptide
9	I	57	GLY	Peptide
10	J	34	VAL	Peptide
10	J	88	LEU	Peptide
13	M	105	THR	Peptide
13	M	107	ALA	Peptide
13	M	62	ASN	Peptide
14	N	7	ILE	Peptide
16	P	19	ILE	Peptide
20	T	12	ALA	Peptide
20	T	92	LEU	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	32687	0	16528	920	0
2	B	1900	0	1951	96	0
3	C	1612	0	1677	97	0
4	D	1703	0	1763	104	0
5	E	1146	0	1207	78	0
6	F	843	0	857	62	0
7	G	1257	0	1296	69	0
8	H	1116	0	1177	74	0
9	I	1010	0	1037	65	0
10	J	792	0	835	73	0
11	K	864	0	881	44	0
12	L	972	0	1058	59	0
13	M	937	0	995	59	0
14	N	492	0	529	47	0
15	O	729	0	768	49	0
16	P	700	0	720	34	0
17	Q	823	0	891	55	0
18	R	574	0	644	49	0
19	S	647	0	673	48	0
20	T	763	0	861	51	0
21	U	208	0	221	9	0
22	A	164	0	0	0	0
22	D	1	0	0	0	0
22	E	1	0	0	0	0
22	F	1	0	0	0	0
22	G	1	0	0	0	0
22	H	1	0	0	0	0
22	K	2	0	0	0	0
22	S	1	0	0	0	0
23	D	1	0	0	0	0
23	N	1	0	0	0	0
24	A	271	0	0	14	0
24	C	1	0	0	0	0
24	E	3	0	0	0	0
24	L	1	0	0	0	0
24	N	1	0	0	0	0
24	P	1	0	0	0	0
24	T	1	0	0	0	0
All	All	52228	0	36569	1946	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 22.

All (1946) 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)
9:I:8:GLY:HA2	9:I:79:LEU:HD13	1.48	0.95
8:H:10:LEU:HD22	8:H:83:ILE:HD11	1.49	0.94
1:A:664:G:H22	1:A:741:G:H1	1.17	0.92
1:A:1002:G:N1	1:A:1003(A):G:O6	2.04	0.91
4:D:187:ARG:HH22	4:D:188:LEU:HD12	1.36	0.91
1:A:1026:G:H8	1:A:1027:C:H5"	1.34	0.90
1:A:1003:G:O2'	1:A:1003(A):G:N7	2.04	0.90
1:A:1366:C:O2'	10:J:60:ARG:NH2	2.05	0.89
15:O:5:LYS:H	15:O:5:LYS:HZ3	1.18	0.88
13:M:48:LEU:HD12	13:M:53:VAL:HG22	1.55	0.88
19:S:18:LYS:HG2	19:S:31:ILE:HD11	1.55	0.87
7:G:85:TYR:HD1	7:G:154:TYR:HE1	1.23	0.87
8:H:113:SER:HB3	8:H:134:ILE:HD11	1.56	0.87
11:K:57:THR:HG22	11:K:59:TYR:H	1.40	0.85
2:B:17:PHE:HD1	2:B:18:GLY:H	1.22	0.85
1:A:1443:G:H4'	1:A:1446:A:H5'	1.59	0.85
1:A:677:U:H3	1:A:713:G:H22	1.23	0.85
7:G:122:HIS:HA	7:G:125:MET:HB2	1.57	0.84
1:A:1028:C:H6	1:A:1033:G:H22	1.25	0.84
10:J:55:LYS:HG2	10:J:56:HIS:H	1.44	0.83
1:A:598:U:H4'	8:H:94:TYR:CD1	2.13	0.82
8:H:9:MET:HG3	8:H:26:VAL:HG21	1.60	0.82
4:D:187:ARG:CZ	4:D:188:LEU:H	1.93	0.82
1:A:1026:G:C8	1:A:1027:C:H5"	2.15	0.81
15:O:70:LEU:HD11	15:O:77:ARG:HB2	1.61	0.81
15:O:32:LEU:HD12	15:O:63:ARG:HB3	1.63	0.81
1:A:1543:C:H2'	1:A:1544:U:H5"	1.63	0.80
19:S:39:THR:HG22	19:S:70:LYS:HD2	1.61	0.80
1:A:1238:A:H5'	1:A:1336:C:H41	1.47	0.79
1:A:1425:U:H3	1:A:1475:G:H1	1.26	0.79
6:F:2:ARG:HH11	6:F:69:GLU:HG2	1.47	0.79
1:A:1527:C:H2'	1:A:1528:U:C6	2.17	0.79
1:A:103:C:OP1	20:T:17:ARG:NH1	2.15	0.79
12:L:27:LEU:O	12:L:29:GLY:N	2.16	0.79
1:A:1178:G:OP1	9:I:93:ARG:NH1	2.16	0.78
4:D:98:GLU:OE1	4:D:103:ASN:ND2	2.16	0.78
3:C:155:GLY:HA3	3:C:163:ALA:HB1	1.65	0.78
2:B:16:HIS:HB3	2:B:210:SER:HB2	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:123:GLN:HB2	3:C:128:PHE:HD1	1.47	0.78
11:K:85:ARG:HD3	11:K:113:PRO:HD3	1.65	0.78
1:A:298:A:N6	24:A:1868:HOH:O	2.18	0.77
1:A:254:G:H2'	1:A:255:G:H8	1.48	0.77
1:A:758:G:N7	24:A:2070:HOH:O	2.17	0.77
3:C:95:THR:HB	3:C:97:LYS:HG2	1.67	0.77
4:D:153:ARG:HD3	4:D:181:MET:HG3	1.67	0.76
1:A:677:U:O4	1:A:713:G:N1	2.15	0.76
19:S:80:TYR:CE1	19:S:81:ARG:HD3	2.20	0.76
1:A:1262:C:H42	1:A:1273:G:H1	1.31	0.76
2:B:91:PRO:HG3	2:B:155:LEU:HB3	1.67	0.76
18:R:79:LEU:HD23	18:R:80:PRO:HD2	1.66	0.76
1:A:1001:A:H61	1:A:1039:C:H42	1.34	0.76
3:C:35:GLU:OE1	3:C:59:ARG:NH1	2.18	0.76
7:G:27:ILE:HA	7:G:30:ILE:HD12	1.66	0.76
1:A:1073:U:OP2	5:E:57:LYS:NZ	2.18	0.75
1:A:1249:C:O2'	9:I:73:GLN:NE2	2.20	0.75
15:O:62:GLN:HG2	15:O:65:ARG:HH21	1.52	0.75
1:A:673:G:H2'	1:A:674:G:C8	2.21	0.75
1:A:902:G:H2'	1:A:903:G:H8	1.50	0.75
5:E:64:ARG:HE	5:E:65:ASN:HB2	1.51	0.75
20:T:40:ALA:HB2	20:T:55:ILE:HG22	1.68	0.75
18:R:34:TYR:HB3	18:R:69:THR:HG22	1.69	0.75
1:A:695:A:H2'	1:A:696:A:C8	2.21	0.74
4:D:57:ARG:HG3	4:D:202:LEU:HD12	1.68	0.74
8:H:40:ALA:HB2	8:H:45:ILE:HD13	1.68	0.74
1:A:967:5MC:O2'	9:I:128:ARG:NH1	2.20	0.74
16:P:9:PHE:CD1	16:P:18:ARG:HD2	2.23	0.74
7:G:85:TYR:HD1	7:G:154:TYR:CE1	2.05	0.74
1:A:299:G:N1	24:A:1868:HOH:O	2.19	0.74
4:D:149:ALA:HB3	4:D:152:SER:HB3	1.69	0.74
11:K:92:GLU:HB3	11:K:96:ARG:HH21	1.52	0.74
1:A:1236:A:H4'	1:A:1304:G:H4'	1.70	0.73
1:A:669:U:H2'	1:A:670:G:C8	2.24	0.73
1:A:1367:C:H5'	10:J:60:ARG:HH21	1.53	0.73
1:A:1423:G:N2	1:A:1477:C:O2	2.19	0.73
1:A:562:C:H4'	1:A:563:A:H5"	1.71	0.73
1:A:1026:G:OP1	1:A:1030(D):A:O2'	2.07	0.73
1:A:1316:G:H4'	14:N:18:VAL:HG11	1.71	0.73
9:I:29:ASN:HD21	9:I:65:VAL:HB	1.52	0.73
1:A:925:G:O2'	1:A:927:G:OP1	2.07	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:5:GLU:HB3	6:F:62:TRP:HE1	1.53	0.73
12:L:25:PRO:C	12:L:27:LEU:H	1.91	0.73
1:A:920:U:H2'	1:A:921:U:C6	2.23	0.72
6:F:14:LEU:HD13	6:F:19:LEU:HA	1.71	0.72
8:H:11:THR:O	8:H:15:ASN:ND2	2.21	0.72
20:T:53:LEU:HD13	20:T:103:GLY:H	1.55	0.72
1:A:1033:G:H3'	1:A:1034:G:H5'	1.70	0.72
3:C:50:ALA:HB2	3:C:75:VAL:HB	1.71	0.72
1:A:669:U:OP1	15:O:48:LYS:NZ	2.15	0.72
2:B:15:VAL:HG13	2:B:209:ARG:HG3	1.72	0.72
1:A:62:U:H2'	1:A:63:C:H6	1.55	0.72
1:A:413:G:H8	1:A:428:G:H21	1.35	0.72
2:B:178:ARG:HB2	2:B:178:ARG:HH11	1.55	0.71
5:E:79:GLU:HG3	8:H:105:ARG:HG2	1.72	0.71
15:O:56:LEU:O	15:O:60:VAL:HG23	1.90	0.71
1:A:1258:G:H2'	1:A:1259:C:H5'	1.72	0.71
1:A:1316:G:N1	1:A:1319:A:OP2	2.22	0.71
20:T:50:GLU:HB2	20:T:99:LEU:HD23	1.70	0.71
1:A:45:U:H2'	1:A:46:G:C8	2.25	0.71
1:A:108:G:H5'	1:A:109:A:H5'	1.72	0.71
1:A:1348:U:H4'	9:I:120:ARG:HG3	1.71	0.71
20:T:57:ARG:HH22	20:T:100:ILE:HD12	1.55	0.71
1:A:1288:A:N3	1:A:1352:C:O2'	2.24	0.71
7:G:113:GLU:HG2	7:G:119:ARG:HG2	1.73	0.71
7:G:111:ARG:HH21	7:G:123:GLU:HA	1.56	0.70
3:C:77:ILE:HG22	3:C:81:GLY:HA2	1.73	0.70
4:D:155:LEU:HD23	4:D:156:GLU:H	1.56	0.70
11:K:85:ARG:HE	11:K:111:ASP:HB3	1.55	0.70
1:A:390:C:H2'	1:A:391:G:C8	2.26	0.70
1:A:975:A:H4'	1:A:976:G:H5"	1.71	0.70
8:H:41:ARG:HH12	8:H:42:GLU:HG2	1.56	0.70
4:D:186:LEU:HD23	4:D:186:LEU:H	1.56	0.70
6:F:77:ARG:HA	6:F:80:ARG:HG2	1.74	0.70
1:A:337:C:H2'	1:A:338:A:H8	1.57	0.70
1:A:981:U:H5'	14:N:21:TYR:CE1	2.27	0.70
8:H:124:ALA:O	8:H:128:GLY:N	2.25	0.70
10:J:57:LYS:HG3	10:J:60:ARG:HH12	1.57	0.69
1:A:1005:A:N7	1:A:1025:U:H1'	2.07	0.69
17:Q:3:LYS:NZ	17:Q:61:GLU:O	2.24	0.69
1:A:337:C:H2'	1:A:338:A:C8	2.27	0.69
4:D:23:GLY:HA3	4:D:112:VAL:HG12	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:44:SER:H	11:K:47:VAL:HB	1.55	0.69
1:A:343:U:O2'	1:A:346:G:O6	2.09	0.69
1:A:878:G:H5'	8:H:89:PRO:HG2	1.74	0.69
14:N:32:SER:O	14:N:40:CYS:HA	1.91	0.69
1:A:1320:C:O2	19:S:36:ARG:NH1	2.26	0.69
11:K:86:GLY:N	11:K:112:THR:OG1	2.20	0.69
16:P:60:LEU:HD23	16:P:64:ALA:HB3	1.75	0.69
1:A:948:C:H42	1:A:1233:G:H1	1.41	0.69
6:F:33:TYR:HB2	6:F:75:LEU:HD23	1.75	0.69
1:A:253:U:H2'	1:A:254:G:H8	1.59	0.68
1:A:1391:U:H2'	1:A:1392:G:C8	2.28	0.68
2:B:136:VAL:HA	2:B:139:LYS:HZ2	1.58	0.68
10:J:34:VAL:HG13	10:J:74:ILE:HA	1.75	0.68
13:M:12:ASN:H	13:M:45:VAL:CG1	2.05	0.68
15:O:16:ALA:HB1	15:O:21:ASP:HB3	1.73	0.68
17:Q:9:VAL:HG23	17:Q:56:VAL:HG22	1.74	0.68
9:I:50:LEU:HA	9:I:53:VAL:HG22	1.75	0.68
1:A:1128:C:O2'	1:A:1130:A:OP1	2.09	0.68
1:A:1147:C:O2	9:I:16:ARG:NH1	2.26	0.68
2:B:79:ASP:HA	2:B:82:ARG:HG2	1.75	0.68
1:A:259:G:H1	1:A:267:C:H42	1.42	0.68
17:Q:61:GLU:HA	17:Q:71:PHE:CE2	2.29	0.68
1:A:770:C:H1'	1:A:899:C:H42	1.57	0.68
1:A:1366:C:H2'	1:A:1367:C:C6	2.28	0.68
19:S:49:ILE:HG21	19:S:71:LEU:HD11	1.74	0.68
2:B:77:ALA:HB2	2:B:211:ILE:HD13	1.74	0.68
4:D:76:ARG:HB2	4:D:207:TYR:HE2	1.59	0.68
6:F:14:LEU:HD22	6:F:18:GLN:HB3	1.76	0.67
1:A:1030(D):A:H5"	1:A:1031:G:H5"	1.77	0.67
2:B:90:MET:N	2:B:90:MET:SD	2.67	0.67
1:A:310:G:H2'	1:A:311:C:H6	1.59	0.67
2:B:96:ARG:HG3	2:B:97:TRP:N	2.09	0.67
1:A:17:U:H2'	1:A:18:C:C6	2.30	0.67
1:A:527:7MG:H5"	1:A:527:7MG:H81	1.76	0.67
1:A:669:U:H2'	1:A:670:G:H8	1.56	0.67
2:B:76:GLN:HE22	2:B:206:ASP:HB3	1.58	0.67
1:A:664:G:N2	1:A:741:G:H1	1.92	0.67
11:K:80:VAL:HG13	11:K:103:LEU:HD21	1.76	0.67
1:A:967:5MC:H4'	9:I:128:ARG:HG3	1.76	0.66
1:A:1367:C:H5'	10:J:60:ARG:NH2	2.10	0.66
3:C:14:ILE:HB	3:C:15:THR:HG23	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1427:U:H2'	1:A:1428:A:C8	2.29	0.66
15:O:29:VAL:HG11	15:O:81:LEU:HD11	1.77	0.66
1:A:1343:G:H4'	9:I:122:ALA:HB3	1.75	0.66
2:B:119:GLU:OE2	2:B:153:ARG:NH2	2.29	0.66
1:A:720:C:H5"	1:A:721:G:H5"	1.77	0.66
1:A:1326:C:H5"	21:U:12:LYS:HE3	1.78	0.66
8:H:29:SER:HG	8:H:32:LYS:H	1.43	0.66
5:E:31:LEU:HG	5:E:45:PHE:HD1	1.61	0.66
13:M:4:ILE:HD12	13:M:22:ILE:HD11	1.78	0.66
20:T:53:LEU:HD22	20:T:56:MET:HG2	1.77	0.66
1:A:1127:G:H1	1:A:1145:C:H42	1.40	0.66
6:F:30:LEU:HA	6:F:75:LEU:HD21	1.77	0.66
1:A:514:C:H2'	1:A:515:G:H8	1.60	0.66
8:H:11:THR:HG23	8:H:15:ASN:HD21	1.60	0.66
13:M:96:LEU:HB3	13:M:97:PRO:HD2	1.78	0.66
17:Q:6:LEU:H	17:Q:59:ILE:HG22	1.59	0.66
1:A:1035:A:H2'	1:A:1036:G:H8	1.59	0.66
13:M:8:GLU:N	13:M:8:GLU:OE2	2.29	0.66
6:F:91:VAL:HG13	18:R:72:ARG:HH22	1.61	0.65
6:F:8:ILE:HD11	6:F:79:LEU:HD13	1.78	0.65
8:H:4:ASP:OD2	8:H:85:ARG:NH1	2.29	0.65
6:F:91:VAL:HG12	6:F:92:LYS:O	1.95	0.65
7:G:95:ARG:HG3	7:G:99:LEU:HD12	1.77	0.65
16:P:74:LEU:HD22	16:P:79:VAL:HG21	1.79	0.65
1:A:1527:C:H2'	1:A:1528:U:H6	1.58	0.65
4:D:206:PHE:HD2	4:D:207:TYR:CE1	2.15	0.65
3:C:164:ARG:HG2	3:C:165:THR:H	1.61	0.65
5:E:99:GLY:N	5:E:117:ASP:OD1	2.29	0.65
1:A:259:G:OP2	20:T:83:ARG:NH1	2.29	0.65
1:A:1332:A:H2'	1:A:1333:A:H8	1.61	0.65
1:A:1226:C:OP2	13:M:91:ARG:NH2	2.30	0.65
9:I:118:LYS:O	9:I:120:ARG:N	2.30	0.65
8:H:25:ASP:OD1	8:H:25:ASP:N	2.30	0.64
10:J:29:ARG:NH2	10:J:84:GLN:OE1	2.30	0.64
1:A:1130:A:OP1	1:A:1130:A:H8	1.79	0.64
11:K:17:GLY:HA2	11:K:35:PRO:HD3	1.80	0.64
15:O:26:GLU:O	15:O:29:VAL:HG12	1.97	0.64
1:A:1320:C:H4'	19:S:73:GLU:HG3	1.80	0.64
1:A:1541:PSU:H5'	1:A:1542:U:OP1	1.97	0.64
9:I:6:GLY:HA3	9:I:83:ARG:HG3	1.79	0.64
10:J:4:ILE:HB	10:J:74:ILE:CG1	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:7:THR:O	17:Q:23:VAL:HG13	1.97	0.64
17:Q:88:TYR:HA	17:Q:91:ARG:HD3	1.79	0.64
1:A:312:C:H2'	1:A:313:A:C8	2.32	0.64
1:A:537:G:OP1	12:L:113:ARG:NH2	2.30	0.64
13:M:22:ILE:HG21	13:M:66:LEU:HD13	1.79	0.64
14:N:25:VAL:HG12	14:N:38:GLY:O	1.97	0.64
1:A:579:G:H4'	15:O:54:ARG:HH21	1.63	0.64
5:E:116:THR:OG1	5:E:117:ASP:OD2	2.16	0.64
6:F:45:LEU:O	6:F:46:ARG:NH1	2.31	0.64
14:N:47:LEU:O	14:N:50:LYS:N	2.31	0.64
1:A:793:U:O2	1:A:1516[A]:G:H4'	1.96	0.64
4:D:199:ASN:HB3	4:D:202:LEU:HD23	1.78	0.64
12:L:27:LEU:HG	12:L:28:LYS:H	1.62	0.64
1:A:352:C:H5'	24:A:2004:HOH:O	1.97	0.64
1:A:62:U:H2'	1:A:63:C:C6	2.33	0.64
1:A:426:G:OP1	4:D:36:ARG:NH1	2.31	0.64
1:A:1125:U:O2'	1:A:1126:U:OP2	2.12	0.64
1:A:1258:G:OP2	1:A:1258:G:H8	1.80	0.64
2:B:68:ILE:H	2:B:90:MET:HG3	1.63	0.64
7:G:78:ARG:HH12	7:G:156:TRP:HB2	1.63	0.64
15:O:15:PHE:CE2	15:O:84:LYS:HG2	2.33	0.64
1:A:937:A:H5"	1:A:938:A:OP2	1.98	0.63
1:A:1121:U:H2'	1:A:1122:U:C6	2.33	0.63
3:C:76:VAL:O	3:C:83:ARG:HG2	1.98	0.63
7:G:15:ASP:OD2	7:G:18:TYR:N	2.29	0.63
9:I:77:ILE:O	9:I:81:ILE:HG12	1.98	0.63
1:A:1146:A:H2'	1:A:1147:C:O4'	1.98	0.63
1:A:1418:A:H2'	1:A:1419:G:O4'	1.99	0.63
14:N:42:ILE:O	14:N:46:GLU:HG3	1.99	0.63
15:O:18:PHE:CE2	15:O:21:ASP:HB2	2.32	0.63
18:R:26:LEU:HD11	18:R:42:ARG:HD3	1.81	0.63
18:R:56:THR:OG1	18:R:57:GLY:N	2.28	0.63
1:A:1171:G:O2'	1:A:1172:C:H5'	1.98	0.63
1:A:1366:C:H2'	1:A:1367:C:H6	1.62	0.63
1:A:1510:U:H2'	1:A:1511:G:C8	2.32	0.63
4:D:31:CYS:C	4:D:33:MET:H	2.02	0.63
12:L:66:VAL:HG21	12:L:98:TYR:CE1	2.33	0.63
19:S:13:ASP:OD2	19:S:13:ASP:N	2.28	0.63
1:A:444:C:O2	1:A:490:G:N2	2.27	0.63
1:A:940:C:OP1	7:G:29:LYS:NZ	2.31	0.63
1:A:115:G:O2'	1:A:116:A:OP2	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1342:C:H2'	1:A:1343:G:C8	2.33	0.63
10:J:88:LEU:HD22	10:J:88:LEU:N	2.12	0.63
1:A:711:G:H2'	1:A:712:A:H8	1.64	0.63
4:D:71:SER:OG	4:D:72:GLU:N	2.32	0.63
5:E:151:LEU:HD11	8:H:79:VAL:HA	1.80	0.63
10:J:4:ILE:HG13	10:J:77:PRO:HG2	1.81	0.63
20:T:49:ALA:O	20:T:53:LEU:HB2	1.99	0.63
1:A:782:A:OP1	1:A:1521:G:N2	2.31	0.63
7:G:72:ARG:NE	7:G:142:GLU:OE1	2.20	0.63
20:T:63:ILE:HD13	20:T:80:ARG:HB3	1.81	0.63
1:A:664:G:OP1	18:R:64:ARG:HD2	1.99	0.63
10:J:53:PRO:HA	14:N:41:ARG:HH21	1.64	0.63
1:A:1057:G:H4'	3:C:197:GLY:H	1.64	0.62
2:B:16:HIS:CB	2:B:210:SER:HB2	2.28	0.62
7:G:85:TYR:CD1	7:G:154:TYR:HE1	2.10	0.62
1:A:881:G:OP2	12:L:12:ARG:NH2	2.30	0.62
1:A:1523:G:OP1	11:K:123:LYS:NZ	2.18	0.62
6:F:9:VAL:HG22	6:F:60:PHE:CD2	2.34	0.62
13:M:5:ALA:HA	13:M:61:GLU:HG3	1.80	0.62
3:C:91:LEU:HB3	3:C:99:VAL:HG21	1.81	0.62
7:G:41:ARG:NH1	7:G:41:ARG:HB2	2.15	0.62
2:B:236:TYR:O	2:B:239:VAL:HG23	2.00	0.62
1:A:750:G:H1'	15:O:23:GLY:H	1.65	0.62
1:A:1388:C:H2'	1:A:1389:C:H6	1.64	0.62
1:A:1481:U:H2'	1:A:1482:G:C8	2.35	0.62
4:D:36:ARG:HD2	4:D:38:TYR:CE2	2.33	0.62
1:A:489:C:H2'	1:A:490:G:H8	1.63	0.62
1:A:880:C:OP1	12:L:8:ASN:ND2	2.33	0.62
21:U:10:ARG:HA	21:U:13:ILE:HB	1.82	0.62
3:C:153:VAL:HG23	3:C:198:VAL:HG22	1.81	0.62
5:E:33:VAL:HG11	5:E:109:ILE:HA	1.81	0.62
10:J:88:LEU:HD22	10:J:88:LEU:H	1.65	0.62
11:K:26:ASN:O	11:K:26:ASN:ND2	2.30	0.62
1:A:390:C:O3'	16:P:28:ARG:NH2	2.32	0.62
2:B:19:HIS:CE1	2:B:206:ASP:HB2	2.35	0.62
2:B:80:ILE:HG21	2:B:211:ILE:HG22	1.80	0.62
3:C:121:ALA:HA	3:C:124:ILE:HD12	1.81	0.62
5:E:18:ARG:HG2	5:E:25:ARG:O	1.99	0.61
10:J:8:LEU:HD22	10:J:96:ILE:HG22	1.81	0.61
1:A:1196:U:H3'	24:A:1871:HOH:O	1.99	0.61
2:B:9:GLU:OE2	2:B:12:GLU:N	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:116:LYS:HG3	8:H:127:LEU:HD11	1.82	0.61
1:A:861:G:HO2'	1:A:874:G:HO2'	1.47	0.61
4:D:21:LEU:HD12	4:D:22:LYS:H	1.65	0.61
9:I:50:LEU:HD11	9:I:81:ILE:HG21	1.81	0.61
1:A:1228:C:OP1	13:M:108:ARG:NH2	2.33	0.61
1:A:1258:G:C2'	1:A:1259:C:H5'	2.30	0.61
1:A:1060:C:C5	3:C:2:GLY:HA2	2.35	0.61
1:A:1368:G:OP2	9:I:112:LYS:NZ	2.27	0.61
1:A:1504:G:OP1	1:A:1507:A:H4'	2.00	0.61
7:G:146:GLU:HA	7:G:149:ARG:HB2	1.80	0.61
13:M:4:ILE:HD11	13:M:10:PRO:HG3	1.81	0.61
15:O:5:LYS:H	15:O:5:LYS:NZ	1.97	0.61
15:O:18:PHE:CD2	15:O:21:ASP:HB2	2.35	0.61
18:R:87:ARG:O	18:R:88:LYS:HB2	2.00	0.61
1:A:322:C:H4'	20:T:23:ARG:HD2	1.82	0.61
1:A:955:U:H1'	1:A:1227:A:H61	1.66	0.61
1:A:1060:C:OP1	14:N:45:ARG:NH2	2.33	0.61
13:M:5:ALA:N	13:M:8:GLU:OE1	2.34	0.61
1:A:643:C:H5'	8:H:31:PHE:CD1	2.36	0.61
8:H:85:ARG:NE	8:H:87:SER:O	2.34	0.61
14:N:29:ARG:HH22	14:N:41:ARG:HH12	1.49	0.61
1:A:264:U:H2'	1:A:265:G:O4'	2.00	0.61
1:A:737:A:H2'	1:A:738:C:C6	2.36	0.61
1:A:1127:G:O6	1:A:1144:G:N1	2.30	0.61
1:A:1505:G:H4'	1:A:1506:U:H5"	1.82	0.61
1:A:1511:G:H2'	1:A:1512:U:O4'	2.01	0.61
3:C:6:HIS:CD2	3:C:9:GLY:H	2.19	0.61
19:S:47:HIS:HB3	19:S:49:ILE:HD11	1.82	0.61
1:A:1243:C:H2'	1:A:1244:C:C6	2.36	0.61
1:A:1321:C:H5"	1:A:1322:C:H5"	1.82	0.61
12:L:83:VAL:HG21	12:L:100:ILE:HD13	1.83	0.61
15:O:22:THR:O	15:O:27:VAL:HG11	2.00	0.61
1:A:1491:G:C6	1:A:1493:A:H2	2.19	0.60
3:C:150:LYS:HB3	3:C:201:TYR:HB2	1.82	0.60
6:F:91:VAL:HG13	18:R:72:ARG:NH2	2.17	0.60
12:L:77:LEU:HD21	12:L:107:ALA:HA	1.82	0.60
1:A:1425:U:H2'	1:A:1426:C:C6	2.36	0.60
8:H:23:SER:HB2	8:H:62:TYR:HA	1.82	0.60
1:A:310:G:OP2	16:P:27:LYS:NZ	2.35	0.60
1:A:1103:C:H5"	2:B:98:LEU:HD22	1.84	0.60
1:A:1435:G:H2'	1:A:1436:U:C6	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:155:LEU:HD23	4:D:156:GLU:N	2.16	0.60
3:C:18:TRP:CD1	14:N:54:PRO:HA	2.36	0.60
18:R:39:VAL:HG13	18:R:40:LEU:HD23	1.84	0.60
1:A:253:U:H2'	1:A:254:G:C8	2.35	0.60
1:A:976:G:H5'	1:A:1358:U:O2'	2.02	0.60
1:A:1307:U:H2'	1:A:1308:U:C6	2.37	0.60
11:K:48:ILE:HG22	11:K:49:GLY:H	1.66	0.60
1:A:1124:G:H5'	10:J:35:SER:HB2	1.83	0.60
2:B:178:ARG:HD3	8:H:72:PRO:HA	1.82	0.60
3:C:188:LEU:HD11	3:C:195:VAL:HG13	1.84	0.60
1:A:448:A:OP2	1:A:485:G:N2	2.31	0.60
1:A:499:A:H4'	1:A:500:G:OP1	2.01	0.60
1:A:1134:G:H2'	1:A:1135:U:O4'	2.01	0.60
5:E:64:ARG:NE	5:E:65:ASN:HB2	2.16	0.60
6:F:2:ARG:HD2	6:F:69:GLU:HG2	1.83	0.60
1:A:197:A:H5"	24:A:1993:HOH:O	2.01	0.60
1:A:1255:G:H2'	1:A:1258:G:H21	1.67	0.60
2:B:213:LEU:HD23	2:B:214:ILE:HD13	1.84	0.60
7:G:38:LEU:O	7:G:42:ILE:HG13	2.02	0.60
10:J:61:GLU:OE2	14:N:49:HIS:NE2	2.34	0.60
20:T:87:LYS:O	20:T:91:LEU:HB2	2.02	0.60
1:A:1144:G:H2'	1:A:1145:C:C5	2.36	0.60
10:J:24:VAL:HG21	10:J:37:PRO:HG3	1.84	0.60
11:K:92:GLU:HB3	11:K:96:ARG:NH2	2.16	0.60
17:Q:87:LYS:HE3	17:Q:88:TYR:N	2.16	0.60
1:A:434:U:H2'	1:A:435:C:H6	1.66	0.59
1:A:1518[B]:MA6:H8	1:A:1518[B]:MA6:O5'	2.01	0.59
2:B:9:GLU:HG2	2:B:10:LEU:N	2.16	0.59
7:G:102:ARG:O	7:G:106:GLN:HG3	2.01	0.59
1:A:447:G:H2'	1:A:485:G:N2	2.17	0.59
20:T:10:LEU:HD22	20:T:11:SER:N	2.16	0.59
20:T:33:ILE:HG13	20:T:62:LEU:HD13	1.83	0.59
3:C:12:LEU:HD21	14:N:51:GLY:HA2	1.83	0.59
1:A:1096:C:H2'	1:A:1097:C:H6	1.66	0.59
10:J:50:ILE:HD12	10:J:50:ILE:N	2.17	0.59
4:D:104:VAL:HG21	4:D:140:VAL:HG21	1.85	0.59
1:A:447:G:H1	1:A:485:G:HO2'	1.50	0.59
1:A:1338:G:H2'	1:A:1339:A:C8	2.38	0.59
3:C:6:HIS:CD2	14:N:49:HIS:HB3	2.38	0.59
4:D:187:ARG:NH2	4:D:188:LEU:HB2	2.16	0.59
13:M:50:GLU:HA	13:M:53:VAL:HB	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:A:N7	4:D:208:SER:OG	2.36	0.59
4:D:206:PHE:HD2	4:D:207:TYR:CD1	2.20	0.59
1:A:514:C:O2'	1:A:515:G:H5'	2.03	0.59
2:B:180:LEU:HB2	2:B:182:ILE:HG13	1.84	0.59
9:I:26:VAL:HG13	9:I:61:ALA:HB3	1.83	0.59
9:I:65:VAL:HG11	9:I:73:GLN:OE1	2.03	0.59
1:A:948:C:H5'	1:A:1306:A:O2'	2.02	0.59
1:A:1399:C:H4'	1:A:1400:5MC:H5"	1.84	0.59
2:B:189:ASP:OD1	2:B:190:THR:N	2.30	0.59
4:D:196:LEU:HD23	4:D:196:LEU:H	1.67	0.59
16:P:19:ILE:HG22	16:P:36:ILE:HG13	1.85	0.59
1:A:579:G:H5'	1:A:728:A:H1'	1.84	0.58
1:A:1190:G:H5'	3:C:176:HIS:CE1	2.38	0.58
6:F:5:GLU:HB3	6:F:62:TRP:NE1	2.18	0.58
8:H:64:LYS:HG2	8:H:79:VAL:HG21	1.84	0.58
1:A:1099:G:H2'	1:A:1100:C:C6	2.38	0.58
8:H:51:VAL:HG12	8:H:58:TYR:O	2.03	0.58
2:B:74:LYS:NZ	2:B:74:LYS:HB3	2.18	0.58
6:F:39:LYS:HD3	6:F:40:VAL:N	2.18	0.58
6:F:41:GLU:OE1	18:R:35:ARG:NH2	2.36	0.58
6:F:77:ARG:O	6:F:77:ARG:HG2	2.04	0.58
1:A:234:C:H2'	1:A:235:C:C6	2.39	0.58
1:A:243:A:C2	1:A:246:A:C8	2.91	0.58
1:A:457:C:H2'	1:A:458:C:H6	1.68	0.58
1:A:1027:C:O2	1:A:1028:C:N4	2.36	0.58
1:A:1332:A:H2'	1:A:1333:A:C8	2.38	0.58
18:R:87:ARG:HG2	18:R:88:LYS:H	1.67	0.58
1:A:437:U:HO2'	4:D:123:HIS:HD1	1.50	0.58
2:B:121:LEU:O	2:B:124:SER:OG	2.21	0.58
2:B:170:GLU:O	2:B:173:ALA:N	2.37	0.58
6:F:33:TYR:HD2	6:F:71:ARG:HD2	1.68	0.58
17:Q:22:LEU:HD11	17:Q:39:SER:HB2	1.85	0.58
20:T:14:LYS:HA	20:T:17:ARG:HG3	1.86	0.58
1:A:1003(A):G:N2	1:A:1038:C:O2	2.36	0.58
1:A:1234:C:H1'	1:A:1364:U:O2	2.03	0.58
21:U:5:ASP:O	21:U:11:GLY:HA3	2.02	0.58
2:B:158:LEU:H	2:B:158:LEU:HD12	1.69	0.58
3:C:21:ARG:HH11	3:C:21:ARG:HG3	1.69	0.58
4:D:21:LEU:O	4:D:113:SER:HB2	2.04	0.58
1:A:426:G:OP1	4:D:38:TYR:OH	2.14	0.58
3:C:28:GLN:HB3	3:C:32:LEU:HD13	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:35:GLU:HA	9:I:38:GLN:HB2	1.85	0.58
10:J:53:PRO:HA	14:N:41:ARG:NH2	2.18	0.58
18:R:51:LEU:HD13	18:R:55:ARG:HE	1.69	0.58
1:A:132:C:O3'	20:T:74:LYS:NZ	2.37	0.58
1:A:190(J):U:H2'	1:A:190(K):G:C8	2.39	0.58
3:C:9:GLY:HA2	3:C:12:LEU:HD13	1.84	0.58
13:M:23:TYR:HB3	13:M:67:GLU:HA	1.85	0.58
13:M:40:ASN:HB3	13:M:43:THR:HG23	1.86	0.58
1:A:390:C:H2'	1:A:391:G:H8	1.65	0.57
1:A:811:C:H4'	1:A:900:A:N6	2.19	0.57
1:A:1005:A:H3'	1:A:1006:C:C6	2.39	0.57
6:F:100:ASN:ND2	18:R:23:LYS:O	2.36	0.57
8:H:65:TYR:HA	8:H:79:VAL:HG23	1.86	0.57
2:B:122:PHE:CD2	2:B:127:ILE:HG21	2.38	0.57
11:K:62:GLN:HG2	11:K:63:LEU:HD23	1.86	0.57
12:L:19:ARG:H	12:L:19:ARG:CZ	2.16	0.57
15:O:25:THR:HG21	15:O:70:LEU:HD23	1.87	0.57
19:S:12:ASP:O	19:S:15:LEU:HD23	2.04	0.57
1:A:353:A:H5'	1:A:353:A:H8	1.70	0.57
1:A:1310:G:OP2	13:M:88:ARG:NH2	2.24	0.57
1:A:1531:A:O5'	1:A:1531:A:H8	1.87	0.57
4:D:78:LEU:HD21	4:D:96:LEU:HB3	1.86	0.57
9:I:102:LEU:H	9:I:102:LEU:HD12	1.69	0.57
12:L:66:VAL:HG22	12:L:67:THR:N	2.20	0.57
1:A:606:G:H1'	1:A:632:A:H61	1.69	0.57
1:A:665:A:H3'	1:A:725:G:N2	2.18	0.57
1:A:1412:C:H2'	1:A:1413:A:C8	2.40	0.57
5:E:107:ARG:HG3	5:E:111:GLU:HG3	1.85	0.57
15:O:18:PHE:HB2	15:O:19:PRO:HD2	1.87	0.57
17:Q:83:ASP:OD2	17:Q:83:ASP:N	2.36	0.57
1:A:509:A:C8	1:A:509:A:H3'	2.40	0.57
1:A:1392:G:H21	1:A:1502:A:H8	1.50	0.57
8:H:82:HIS:NE2	8:H:84:ARG:HD2	2.19	0.57
9:I:106:ALA:O	9:I:108:VAL:HG22	2.04	0.57
12:L:7:ILE:O	12:L:10:LEU:N	2.37	0.57
17:Q:74:LEU:HG	17:Q:75:ARG:HG2	1.85	0.57
1:A:1314:C:H5	19:S:6:LYS:HZ2	1.52	0.57
2:B:33:TYR:CD2	2:B:43:ASP:HA	2.40	0.57
2:B:97:TRP:HH2	2:B:176:GLU:CD	2.07	0.57
3:C:17:ASP:OD1	3:C:18:TRP:N	2.37	0.57
6:F:46:ARG:HB2	6:F:60:PHE:CE1	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:922:G:H4'	5:E:20:GLN:HA	1.87	0.57
2:B:7:VAL:N	2:B:8:LYS:HD2	2.19	0.57
18:R:45:SER:OG	18:R:46:GLU:N	2.38	0.57
16:P:34:GLU:OE1	16:P:55:ARG:NH1	2.38	0.57
17:Q:10:VAL:HG23	17:Q:55:ASP:O	2.05	0.57
1:A:517:G:N2	1:A:533:A:OP2	2.33	0.57
1:A:807:A:H2'	1:A:808:C:C6	2.39	0.57
1:A:1118:C:H1'	1:A:1179:A:C4	2.40	0.57
1:A:1226:C:H4'	1:A:1227:A:OP1	2.05	0.57
1:A:201:C:H42	1:A:216:G:H1	1.53	0.56
1:A:527:7MG:H5"	1:A:527:7MG:C8	2.40	0.56
16:P:10:GLY:HA3	16:P:14:ASN:O	2.05	0.56
1:A:1032:G:H2'	1:A:1033:G:H5'	1.86	0.56
1:A:1280:A:O2'	1:A:1281:U:H5'	2.05	0.56
4:D:52:SER:O	4:D:56:VAL:HG23	2.04	0.56
10:J:5:ARG:O	10:J:98:ILE:HA	2.04	0.56
18:R:29:PHE:HZ	18:R:43:PHE:HE1	1.52	0.56
1:A:922:G:H2'	1:A:923:A:C8	2.39	0.56
1:A:1033:G:H2'	1:A:1033:G:N3	2.20	0.56
1:A:1041:A:H2'	1:A:1042:G:O4'	2.05	0.56
2:B:21:ARG:HA	2:B:39:ILE:HA	1.86	0.56
2:B:80:ILE:O	2:B:84:GLU:HB2	2.06	0.56
4:D:8:VAL:HG12	4:D:21:LEU:HD22	1.87	0.56
6:F:41:GLU:HB3	6:F:43:LEU:HD11	1.87	0.56
20:T:37:SER:HB3	20:T:84:LEU:HD13	1.87	0.56
2:B:84:GLU:OE1	2:B:87:ARG:NH2	2.37	0.56
4:D:176:LEU:HD12	4:D:177:ASP:N	2.20	0.56
6:F:47:ARG:NH1	6:F:48:LEU:O	2.37	0.56
7:G:73:MET:HG3	7:G:90:GLU:HA	1.86	0.56
1:A:269:C:H2'	1:A:270:A:C8	2.40	0.56
1:A:485:G:O2'	1:A:486:U:P	2.63	0.56
1:A:693:G:H2'	1:A:694:A:C8	2.41	0.56
1:A:838:G:H1	1:A:848:C:H42	1.54	0.56
9:I:50:LEU:HD23	9:I:55:ALA:HB3	1.87	0.56
9:I:79:LEU:O	9:I:83:ARG:HG2	2.06	0.56
6:F:80:ARG:NE	6:F:88:VAL:HB	2.20	0.56
1:A:129:U:O3'	1:A:129(A):G:H3'	2.05	0.56
1:A:676:A:H1'	11:K:115:PRO:HB3	1.88	0.56
2:B:208:ILE:H	2:B:208:ILE:HD12	1.71	0.56
1:A:277:C:H5'	17:Q:68:ARG:NH1	2.21	0.56
5:E:138:ALA:O	5:E:141:GLN:HB2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:75:LEU:HD13	6:F:79:LEU:HD11	1.86	0.56
15:O:33:THR:OG1	15:O:63:ARG:NH1	2.39	0.56
16:P:74:LEU:O	16:P:77:ALA:HB3	2.06	0.56
17:Q:19:VAL:HG22	17:Q:44:ALA:HB3	1.85	0.56
1:A:40:C:H2'	1:A:41:G:O4'	2.06	0.56
1:A:254:G:H2'	1:A:255:G:C8	2.36	0.56
1:A:691:G:H2'	1:A:692:U:H6	1.71	0.56
1:A:841:U:C6	1:A:848:C:H5'	2.41	0.56
12:L:27:LEU:C	12:L:29:GLY:H	2.04	0.56
2:B:118:LEU:O	2:B:121:LEU:HB3	2.06	0.56
16:P:58:TYR:O	16:P:62:VAL:HG13	2.06	0.56
20:T:74:LYS:HB2	20:T:76:ALA:H	1.69	0.56
1:A:496:A:H4'	1:A:497:A:H5'	1.87	0.55
1:A:680:C:H42	1:A:710:G:H1	1.55	0.55
2:B:22:LYS:HE2	2:B:40:HIS:HE1	1.71	0.55
4:D:82:ALA:HB1	4:D:92:VAL:HG13	1.87	0.55
15:O:50:HIS:O	15:O:53:HIS:HB3	2.06	0.55
1:A:141:A:H1'	1:A:182:U:O2	2.06	0.55
1:A:975:A:H5'	1:A:975:A:H8	1.71	0.55
1:A:1030(A):G:H2'	1:A:1030(B):C:H5"	1.89	0.55
1:A:1414:U:H2'	1:A:1415:G:C8	2.41	0.55
1:A:1501:C:N4	1:A:1504:G:C2	2.73	0.55
2:B:9:GLU:HG2	2:B:10:LEU:H	1.70	0.55
2:B:82:ARG:NH2	2:B:86:GLU:OE2	2.39	0.55
4:D:159:ARG:O	4:D:163:GLU:HB2	2.06	0.55
18:R:36:ASN:OD1	18:R:39:VAL:HG12	2.06	0.55
18:R:52:PRO:HG3	18:R:54:ARG:NH2	2.20	0.55
1:A:553:A:O2'	12:L:29:GLY:O	2.23	0.55
1:A:1060:C:H5"	10:J:51:ARG:HG2	1.88	0.55
7:G:79:ARG:HA	7:G:84:ASN:HB3	1.88	0.55
1:A:922:G:H1	1:A:1395:C:H42	1.53	0.55
3:C:77:ILE:HD11	3:C:103:VAL:HG21	1.88	0.55
10:J:49:VAL:HG13	14:N:41:ARG:HG3	1.88	0.55
16:P:59:TRP:HB3	16:P:64:ALA:HB2	1.89	0.55
1:A:1211:U:O2'	1:A:1213:A:N3	2.34	0.55
3:C:36:ASP:HA	3:C:39:ILE:HD12	1.88	0.55
9:I:79:LEU:HD22	9:I:83:ARG:NE	2.22	0.55
1:A:1118:C:OP1	9:I:9:ARG:HD2	2.06	0.55
12:L:75:HIS:HA	12:L:102:ARG:HH22	1.72	0.55
18:R:51:LEU:HD22	18:R:52:PRO:HD2	1.88	0.55
18:R:85:LEU:HD11	18:R:88:LYS:HG2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:7:LYS:HE2	19:S:7:LYS:O	2.06	0.55
19:S:31:ILE:HA	19:S:32:LYS:HZ3	1.70	0.55
1:A:1040:U:O4	1:A:1041:A:N6	2.40	0.55
1:A:1194:U:H4'	5:E:22:GLY:HA2	1.89	0.55
6:F:75:LEU:O	6:F:79:LEU:HG	2.06	0.55
1:A:106:C:O2'	1:A:107:G:H5'	2.07	0.55
1:A:1275:A:H2'	1:A:1276:G:O4'	2.07	0.55
1:A:1287:A:H2'	1:A:1288:A:C8	2.42	0.55
4:D:12:CYS:HA	4:D:19:LEU:HG	1.89	0.55
4:D:174:LEU:HD23	4:D:185:PHE:HA	1.89	0.55
5:E:20:GLN:OE1	5:E:25:ARG:NH2	2.28	0.55
5:E:27:ARG:NH1	5:E:27:ARG:HB2	2.22	0.55
1:A:20:U:H1'	1:A:916:G:N2	2.22	0.55
1:A:706:A:H1'	11:K:29:ILE:HD11	1.89	0.55
1:A:1089:G:C5	1:A:1090:U:C5	2.95	0.55
1:A:1322:C:H4'	1:A:1323:G:OP1	2.06	0.55
3:C:95:THR:C	3:C:97:LYS:H	2.10	0.55
4:D:4:TYR:OH	4:D:7:PRO:O	2.21	0.55
7:G:26:PHE:HA	7:G:101:LEU:HD23	1.89	0.55
9:I:28:VAL:HG12	9:I:29:ASN:HD22	1.72	0.55
1:A:881:G:P	12:L:12:ARG:HH22	2.30	0.54
1:A:976:G:OP2	1:A:1358:U:O2'	2.24	0.54
15:O:15:PHE:HE2	15:O:84:LYS:HG2	1.72	0.54
15:O:15:PHE:HD1	15:O:30:ALA:HB2	1.72	0.54
1:A:325:A:H2'	1:A:326:G:O4'	2.07	0.54
1:A:563:A:H2'	1:A:567:G:C8	2.42	0.54
4:D:70:ILE:HG22	4:D:71:SER:N	2.21	0.54
12:L:28:LYS:HD2	12:L:33:ARG:CZ	2.37	0.54
12:L:93:LEU:HB3	12:L:96:VAL:HG21	1.88	0.54
21:U:5:ASP:HB3	21:U:8:THR:HG23	1.90	0.54
1:A:1443:G:C4'	1:A:1446:A:H5'	2.34	0.54
4:D:100:ARG:HD2	4:D:137:SER:HA	1.90	0.54
1:A:299:G:C6	1:A:300:A:C6	2.96	0.54
4:D:70:ILE:HG22	4:D:71:SER:H	1.72	0.54
2:B:79:ASP:OD2	2:B:79:ASP:N	2.31	0.54
4:D:187:ARG:NH2	4:D:188:LEU:HD12	2.15	0.54
4:D:196:LEU:HD23	4:D:196:LEU:N	2.22	0.54
7:G:139:GLU:HG3	7:G:143:ARG:HH22	1.71	0.54
9:I:96:LEU:HG	9:I:101:PHE:HD1	1.72	0.54
19:S:40:ILE:HB	19:S:67:VAL:O	2.08	0.54
1:A:375:U:C2	1:A:376:G:C8	2.96	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:668:G:O4'	15:O:49:ASP:HB2	2.08	0.54
1:A:1499:A:H1'	1:A:1520[B]:G:OP1	2.07	0.54
2:B:71:VAL:O	2:B:164:VAL:HA	2.06	0.54
5:E:93:PRO:HG2	8:H:105:ARG:NH1	2.22	0.54
10:J:4:ILE:HB	10:J:74:ILE:HD11	1.90	0.54
1:A:560:U:H4'	1:A:561:U:H5"	1.88	0.54
1:A:1286:A:H2'	1:A:1287:A:H4'	1.88	0.54
12:L:76:ASN:OD1	12:L:108:ALA:N	2.38	0.54
13:M:11:ARG:HA	13:M:45:VAL:HG11	1.90	0.54
1:A:216:G:O2'	1:A:217:C:O5'	2.26	0.54
1:A:292:G:N2	1:A:309:G:C4	2.76	0.54
1:A:620:C:H2'	1:A:621:A:O4'	2.08	0.54
1:A:986:A:C2	1:A:1220:G:C2	2.96	0.54
2:B:19:HIS:NE2	2:B:206:ASP:HB2	2.22	0.54
16:P:6:LEU:HD23	16:P:17:TYR:CG	2.42	0.54
1:A:81:U:H2'	1:A:82:U:H5"	1.89	0.54
1:A:691:G:O2'	1:A:797:C:H4'	2.08	0.54
1:A:1016:A:H2'	1:A:1017:G:O4'	2.07	0.54
1:A:1496:C:O2	1:A:1517[A]:G:N2	2.41	0.54
3:C:156:ARG:H	3:C:163:ALA:HA	1.73	0.54
7:G:109:ASN:OD1	7:G:119:ARG:NH2	2.40	0.54
13:M:91:ARG:NH2	13:M:103:THR:HG21	2.23	0.54
21:U:6:ARG:HG2	21:U:15:ARG:HH21	1.73	0.54
1:A:182:U:H6	1:A:182:U:H5'	1.72	0.53
1:A:950:U:H2'	1:A:951:G:C8	2.43	0.53
7:G:50:ILE:HD11	7:G:124:LEU:HD11	1.89	0.53
10:J:84:GLN:HA	10:J:84:GLN:HE21	1.73	0.53
1:A:356:A:H2'	1:A:357:G:O4'	2.09	0.53
3:C:73:PRO:O	3:C:77:ILE:HG12	2.08	0.53
5:E:137:GLU:O	5:E:141:GLN:HG2	2.08	0.53
1:A:1465:C:H2'	1:A:1466:C:O4'	2.08	0.53
3:C:68:VAL:HG12	3:C:70:VAL:HG22	1.91	0.53
5:E:15:ARG:HH11	5:E:15:ARG:HG3	1.72	0.53
10:J:76:ASN:N	10:J:77:PRO:HD3	2.22	0.53
11:K:85:ARG:NE	11:K:111:ASP:HB3	2.21	0.53
12:L:90:VAL:HG23	12:L:93:LEU:HB2	1.90	0.53
13:M:2:ALA:O	13:M:10:PRO:HD2	2.09	0.53
13:M:2:ALA:N	13:M:9:ILE:HG23	2.23	0.53
1:A:1095:U:N3	1:A:1096:C:C4	2.77	0.53
1:A:1361:G:H2'	1:A:1361(A):C:C6	2.43	0.53
12:L:28:LYS:HB2	12:L:33:ARG:HE	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:547:A:OP2	4:D:2:GLY:N	2.42	0.53
1:A:1190:G:H5'	3:C:176:HIS:NE2	2.24	0.53
1:A:1202:G:N2	14:N:43:CYS:SG	2.81	0.53
1:A:1425:U:H2'	1:A:1426:C:H6	1.74	0.53
4:D:36:ARG:HD2	4:D:38:TYR:HE2	1.71	0.53
4:D:152:SER:O	4:D:152:SER:OG	2.25	0.53
7:G:113:GLU:CG	7:G:119:ARG:HG2	2.38	0.53
12:L:84:LEU:HD23	12:L:101:VAL:HG21	1.90	0.53
1:A:44:G:H5"	1:A:44:G:H8	1.73	0.53
1:A:147:G:C2	1:A:148:G:C8	2.96	0.53
1:A:1502:A:H2	1:A:1505:G:H1	1.57	0.53
8:H:23:SER:HA	8:H:63:LEU:HD13	1.89	0.53
9:I:71:SER:O	9:I:74:ILE:HB	2.08	0.53
10:J:79:ARG:O	10:J:82:ILE:N	2.42	0.53
18:R:51:LEU:HD11	18:R:55:ARG:HH21	1.74	0.53
20:T:33:ILE:HD11	20:T:63:ILE:HA	1.91	0.53
1:A:258:G:H2'	1:A:259:G:H8	1.73	0.53
1:A:514:C:H2'	1:A:515:G:C8	2.42	0.53
1:A:1119:C:H42	1:A:1154:G:H1	1.55	0.53
1:A:1163:C:H2'	1:A:1164:G:O4'	2.09	0.53
4:D:127:THR:HG21	4:D:150:GLU:OE1	2.08	0.53
5:E:27:ARG:HB2	5:E:27:ARG:HH11	1.74	0.53
5:E:43:LEU:HB2	5:E:136:MET:HG3	1.91	0.53
16:P:6:LEU:HB3	16:P:17:TYR:CD2	2.44	0.53
1:A:658:G:H2'	1:A:659:U:O4'	2.08	0.53
1:A:734:G:N2	18:R:75:ILE:HD11	2.23	0.53
1:A:770:C:O2'	1:A:899:C:N3	2.39	0.53
1:A:965:A:C2	1:A:969:A:C2	2.96	0.53
2:B:84:GLU:O	2:B:219:VAL:HG21	2.09	0.53
13:M:62:ASN:OD1	13:M:62:ASN:N	2.41	0.53
1:A:130:A:H1'	1:A:263:A:O2'	2.09	0.53
1:A:375:U:H2'	1:A:376:G:H8	1.74	0.53
1:A:671:G:C2	1:A:672:U:H1'	2.44	0.53
1:A:778:G:H8	1:A:778:G:O5'	1.91	0.53
5:E:40:ARG:HH21	5:E:66:MET:HG3	1.73	0.53
5:E:144:THR:HB	5:E:147:ASP:H	1.74	0.53
9:I:17:VAL:HG21	9:I:80:GLY:HA3	1.91	0.53
12:L:25:PRO:C	12:L:27:LEU:N	2.61	0.53
20:T:20:LEU:HD22	20:T:20:LEU:H	1.73	0.53
1:A:276:G:O2'	17:Q:68:ARG:NH1	2.42	0.53
1:A:1241:G:H2'	1:A:1242:C:H6	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:103:GLY:O	5:E:106:PRO:HD2	2.09	0.53
1:A:123:C:OP1	1:A:311:C:O2'	2.25	0.52
1:A:569:C:H42	1:A:881:G:H1	1.55	0.52
4:D:187:ARG:HH22	4:D:188:LEU:CD1	2.17	0.52
5:E:150:ARG:NH1	5:E:150:ARG:HB2	2.25	0.52
6:F:30:LEU:HD23	6:F:35:ALA:HB3	1.90	0.52
12:L:84:LEU:HB3	12:L:101:VAL:CG2	2.39	0.52
13:M:108:ARG:O	13:M:111:LYS:N	2.42	0.52
1:A:414:A:H3'	24:A:1969:HOH:O	2.10	0.52
1:A:881:G:H2'	1:A:882:C:O4'	2.09	0.52
1:A:975:A:H5'	1:A:975:A:C8	2.43	0.52
1:A:1144:G:H2'	1:A:1145:C:C6	2.44	0.52
5:E:144:THR:HG22	5:E:146:ALA:H	1.74	0.52
9:I:48:GLU:N	9:I:49:PRO:HD2	2.24	0.52
10:J:34:VAL:HG13	10:J:74:ILE:HG22	1.90	0.52
20:T:53:LEU:HD12	20:T:101:GLY:H	1.74	0.52
1:A:1491:G:C6	1:A:1493:A:C2	2.98	0.52
7:G:99:LEU:O	7:G:103:TRP:HB2	2.10	0.52
10:J:65:LEU:HD12	14:N:56:VAL:HG22	1.91	0.52
17:Q:97:SER:O	17:Q:98:LEU:HD12	2.09	0.52
1:A:254:G:OP1	17:Q:67:LYS:O	2.27	0.52
2:B:60:ASP:O	2:B:64:ARG:HG3	2.10	0.52
21:U:10:ARG:HA	21:U:13:ILE:HD12	1.92	0.52
1:A:279:A:OP2	17:Q:95:TYR:OH	2.17	0.52
1:A:946:A:H2'	1:A:947:G:C8	2.45	0.52
1:A:1031:G:O2'	1:A:1032:G:N2	2.43	0.52
1:A:1476:G:C2'	1:A:1477:C:H5'	2.39	0.52
2:B:93:VAL:HG21	2:B:97:TRP:CD1	2.44	0.52
4:D:142:PRO:HA	4:D:185:PHE:HD2	1.74	0.52
9:I:18:PHE:HB3	9:I:20:ARG:HH12	1.74	0.52
1:A:926:G:C6	1:A:1505:G:C6	2.97	0.52
1:A:1148:U:H2'	1:A:1149:C:O4'	2.10	0.52
1:A:1313:U:H5	19:S:4:SER:HB2	1.74	0.52
2:B:47:THR:O	2:B:51:LEU:HB2	2.10	0.52
6:F:47:ARG:CZ	6:F:47:ARG:HB2	2.33	0.52
16:P:58:TYR:CZ	16:P:62:VAL:HG11	2.45	0.52
1:A:78:G:C2	1:A:79:G:C8	2.97	0.52
1:A:474:G:O2'	1:A:475:G:H5'	2.09	0.52
1:A:562:C:H4'	1:A:563:A:C5'	2.40	0.52
1:A:877:C:O2	8:H:3:THR:HG21	2.09	0.52
17:Q:34:LYS:HG2	17:Q:35:VAL:H	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:58:LEU:HB3	18:R:62:GLU:HB3	1.91	0.52
1:A:164:U:H2'	1:A:165:C:C6	2.44	0.52
1:A:563:A:H5'	1:A:564:C:OP1	2.09	0.52
1:A:1313:U:OP2	19:S:6:LYS:HA	2.09	0.52
1:A:1451:A:H5"	1:A:1452:C:C5	2.45	0.52
1:A:1483:A:H2'	1:A:1483:A:N3	2.23	0.52
1:A:1518[B]:MA6:O2'	1:A:1519[B]:MA6:OP1	2.27	0.52
5:E:40:ARG:HE	5:E:66:MET:HE2	1.75	0.52
7:G:41:ARG:HB2	7:G:41:ARG:HH11	1.74	0.52
12:L:6:THR:HG23	12:L:9:GLN:OE1	2.09	0.52
15:O:72:ARG:NH1	15:O:72:ARG:HB3	2.25	0.52
1:A:143:A:O3'	1:A:144:G:H8	1.93	0.52
1:A:924:C:O2'	1:A:1502:A:N6	2.43	0.52
1:A:1124:G:OP1	10:J:33:GLN:NE2	2.43	0.52
1:A:1192:C:OP2	3:C:4:LYS:NZ	2.42	0.52
1:A:1234:C:H2'	1:A:1235:U:H6	1.74	0.52
1:A:1324:A:H2'	1:A:1325:C:O4'	2.09	0.52
2:B:189:ASP:HB2	2:B:205:ASP:H	1.75	0.52
14:N:33:VAL:HA	14:N:39:LEU:O	2.10	0.52
1:A:474:G:OP2	16:P:75:ARG:HD2	2.10	0.52
1:A:1277:C:H3'	1:A:1277:C:C6	2.44	0.52
1:A:1342:C:H2'	1:A:1343:G:H8	1.75	0.52
5:E:43:LEU:O	5:E:62:ALA:HA	2.10	0.52
7:G:99:LEU:HD22	7:G:103:TRP:CH2	2.45	0.52
14:N:26:ARG:HH22	14:N:47:LEU:HD13	1.74	0.52
18:R:36:ASN:O	18:R:40:LEU:HG	2.10	0.52
19:S:18:LYS:O	19:S:22:LEU:HG	2.10	0.52
1:A:17:U:H2'	1:A:18:C:H6	1.73	0.51
1:A:924:C:O2'	1:A:925:G:H5'	2.09	0.51
5:E:78:HIS:HB2	8:H:104:ARG:HG2	1.91	0.51
6:F:69:GLU:O	6:F:72:VAL:HG23	2.10	0.51
12:L:25:PRO:HB2	12:L:64:TYR:CE2	2.45	0.51
1:A:279:A:C6	17:Q:98:LEU:HD13	2.45	0.51
1:A:671:G:N2	1:A:672:U:H1'	2.25	0.51
1:A:814:A:N7	1:A:816:A:C4	2.79	0.51
1:A:830:G:C6	1:A:831:U:C4	2.98	0.51
1:A:1023:G:H3'	1:A:1024:G:H5"	1.91	0.51
1:A:1134:G:H1	1:A:1140:C:H42	1.57	0.51
1:A:1321:C:C5'	1:A:1322:C:H5"	2.39	0.51
2:B:97:TRP:CH2	2:B:173:ALA:HA	2.46	0.51
10:J:85:LEU:HA	10:J:88:LEU:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:57:THR:HB	11:K:60:ALA:H	1.76	0.51
14:N:14:PRO:O	14:N:15:LYS:HB3	2.09	0.51
19:S:31:ILE:HG22	19:S:49:ILE:HA	1.92	0.51
1:A:39:G:O2'	1:A:40:C:H5'	2.10	0.51
1:A:168:G:C2	1:A:169:C:C5	2.98	0.51
1:A:547:A:H4'	1:A:548:G:O5'	2.09	0.51
1:A:667:G:C2	1:A:740:U:O2	2.63	0.51
1:A:839:U:O2	1:A:839:U:H3'	2.11	0.51
1:A:1005:A:H1'	1:A:1026:G:H1	1.75	0.51
2:B:105:PHE:CE1	2:B:109:SER:HB3	2.45	0.51
1:A:181:G:H4'	1:A:182:U:C5'	2.41	0.51
1:A:1323:G:H2'	1:A:1324:A:C8	2.45	0.51
1:A:1366:C:O3'	10:J:60:ARG:NH2	2.42	0.51
1:A:1403:C:C2	1:A:1404:5MC:HM52	2.45	0.51
12:L:110:VAL:O	12:L:122:THR:HG21	2.11	0.51
19:S:11:VAL:HG12	19:S:15:LEU:HD21	1.92	0.51
20:T:43:LEU:HA	20:T:46:GLU:HB2	1.93	0.51
1:A:734:G:H21	18:R:75:ILE:HD11	1.76	0.51
1:A:951:G:OP2	13:M:102:ARG:NH2	2.44	0.51
1:A:956:U:H2'	1:A:957:U:O4'	2.11	0.51
1:A:1169:A:C5	1:A:1171:G:H1'	2.45	0.51
1:A:1216:G:H5"	14:N:5:ALA:CB	2.40	0.51
1:A:1493:A:HO2'	1:A:1494:G:H8	1.58	0.51
8:H:86:ILE:HG22	8:H:93:VAL:HG21	1.92	0.51
13:M:10:PRO:O	13:M:45:VAL:HG21	2.11	0.51
18:R:47:THR:HB	18:R:83:GLU:O	2.10	0.51
1:A:708:C:H2'	1:A:709:G:H8	1.76	0.51
1:A:781:A:H2'	1:A:782:A:H5'	1.92	0.51
10:J:50:ILE:HD12	10:J:50:ILE:H	1.76	0.51
10:J:55:LYS:HG2	10:J:56:HIS:N	2.22	0.51
18:R:61:LYS:O	18:R:65:ILE:HG12	2.09	0.51
19:S:50:ALA:HB1	19:S:57:HIS:HB3	1.92	0.51
20:T:43:LEU:HB2	20:T:52:ALA:HB2	1.93	0.51
1:A:8:A:N6	4:D:209:ARG:HB2	2.26	0.51
1:A:143:A:H2	1:A:220:G:H22	1.58	0.51
1:A:825:G:H21	8:H:11:THR:HG21	1.76	0.51
2:B:22:LYS:HE2	2:B:40:HIS:CE1	2.46	0.51
2:B:160:ASP:OD2	2:B:160:ASP:N	2.37	0.51
4:D:145:GLU:OE2	4:D:182:LYS:NZ	2.43	0.51
1:A:546:G:P	4:D:72:GLU:HB3	2.51	0.51
1:A:710:G:H2'	1:A:711:G:H8	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:860:A:H2'	1:A:861:G:O4'	2.10	0.51
1:A:1057:G:H5"	3:C:154:SER:HB2	1.93	0.51
1:A:1403:C:O2	1:A:1403:C:H2'	2.11	0.51
2:B:53:ARG:HG3	2:B:54:THR:N	2.25	0.51
4:D:57:ARG:HB3	4:D:206:PHE:HB2	1.91	0.51
5:E:131:ILE:O	5:E:134:ALA:HB3	2.11	0.51
8:H:73:ASP:OD2	8:H:75:ARG:HG3	2.11	0.51
1:A:439:A:C4	1:A:497:A:C2	2.99	0.51
2:B:17:PHE:CD1	2:B:18:GLY:N	2.77	0.51
3:C:159:GLY:HA2	3:C:193:TYR:CD1	2.46	0.51
17:Q:89:LEU:O	17:Q:93:GLN:HG3	2.11	0.51
1:A:748:C:H6	1:A:748:C:O5'	1.93	0.51
1:A:858:G:O6	1:A:869:G:H3'	2.10	0.51
1:A:1064:G:H1'	1:A:1190:G:N2	2.25	0.51
1:A:1070:U:H2'	1:A:1071:C:C6	2.46	0.51
1:A:1313:U:C5	19:S:4:SER:HB2	2.46	0.51
4:D:156:GLU:O	4:D:160:GLN:HG3	2.10	0.51
5:E:101:ILE:O	5:E:120:THR:HB	2.11	0.51
10:J:19:SER:HB2	10:J:91:PRO:HG2	1.93	0.51
16:P:48:TRP:N	16:P:48:TRP:CD1	2.79	0.51
20:T:93:GLU:N	20:T:93:GLU:OE2	2.44	0.51
1:A:1238:A:OP2	1:A:1335:C:O2	2.29	0.50
1:A:1299:A:C8	1:A:1301:U:H1'	2.46	0.50
1:A:1372:U:OP2	9:I:11:LYS:NZ	2.35	0.50
2:B:105:PHE:O	2:B:108:ILE:N	2.44	0.50
8:H:27:PRO:HG3	8:H:58:TYR:CE2	2.46	0.50
1:A:1133:G:H1	1:A:1141:C:H42	1.59	0.50
1:A:1189:C:H5'	14:N:58:LYS:HZ1	1.77	0.50
3:C:130:VAL:HG11	3:C:153:VAL:HG11	1.93	0.50
12:L:113:ARG:HH11	12:L:116:SER:H	1.58	0.50
19:S:41:VAL:HG23	19:S:43:GLU:HG2	1.92	0.50
1:A:116:A:O5'	1:A:116:A:H8	1.94	0.50
1:A:235:C:O2'	1:A:236:G:H5'	2.11	0.50
1:A:1029:C:N3	1:A:1030:C:N4	2.55	0.50
1:A:1122:U:O2'	1:A:1123:A:H5'	2.11	0.50
1:A:1223:C:H3'	1:A:1224:G:H5"	1.92	0.50
3:C:150:LYS:HA	3:C:169:ALA:HA	1.94	0.50
10:J:16:LEU:HD22	10:J:94:VAL:HG23	1.93	0.50
13:M:14:ARG:HB2	13:M:17:VAL:HG22	1.92	0.50
1:A:836:G:C6	1:A:851:G:C6	3.00	0.50
1:A:1001:A:H61	1:A:1039:C:N4	2.06	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1238:A:N7	1:A:1303:C:H1'	2.26	0.50
1:A:1426:C:H2'	1:A:1427:U:C6	2.46	0.50
4:D:12:CYS:SG	4:D:21:LEU:HD11	2.51	0.50
8:H:51:VAL:HG22	8:H:52:ASP:H	1.76	0.50
19:S:31:ILE:HG21	19:S:49:ILE:HD12	1.93	0.50
1:A:512:U:H2'	1:A:513:C:H6	1.76	0.50
1:A:665:A:H1'	1:A:733:A:O4'	2.12	0.50
1:A:811:C:H4'	1:A:900:A:H61	1.76	0.50
1:A:1194:U:H2'	1:A:1195:C:C6	2.46	0.50
1:A:1504:G:H4'	1:A:1505:G:O5'	2.11	0.50
3:C:7:PRO:O	3:C:11:ARG:HD2	2.11	0.50
3:C:85:ARG:HH11	3:C:86:VAL:HG23	1.77	0.50
3:C:139:GLN:HG3	3:C:143:GLU:OE1	2.10	0.50
11:K:11:LYS:HB2	11:K:11:LYS:NZ	2.27	0.50
16:P:9:PHE:HD1	16:P:18:ARG:HD2	1.72	0.50
18:R:19:LYS:O	18:R:21:LYS:NZ	2.45	0.50
1:A:774:G:C4	1:A:775:G:C8	2.99	0.50
1:A:804:U:H5"	1:A:805:C:OP2	2.11	0.50
1:A:1221:G:H4'	19:S:77:THR:HG21	1.93	0.50
3:C:184:TYR:OH	3:C:199:LYS:HD3	2.11	0.50
16:P:51:VAL:HG11	16:P:77:ALA:HB1	1.93	0.50
1:A:134:A:H2'	1:A:135:C:O4'	2.12	0.50
1:A:227:G:O2'	24:A:1959:HOH:O	2.20	0.50
1:A:310:G:H2'	1:A:311:C:C6	2.43	0.50
1:A:1073:U:P	5:E:57:LYS:HZ1	2.34	0.50
1:A:1451:A:H5"	1:A:1452:C:H5	1.77	0.50
4:D:163:GLU:OE1	4:D:166:LYS:HE2	2.11	0.50
6:F:33:TYR:CD2	6:F:71:ARG:HD2	2.46	0.50
9:I:22:GLY:HA3	9:I:60:ASP:N	2.26	0.50
9:I:79:LEU:HD22	9:I:83:ARG:HE	1.77	0.50
12:L:6:THR:O	12:L:9:GLN:HB2	2.12	0.50
12:L:19:ARG:H	12:L:19:ARG:NE	2.09	0.50
16:P:58:TYR:CE2	16:P:62:VAL:HG11	2.46	0.50
17:Q:83:ASP:OD2	17:Q:84:LEU:HG	2.12	0.50
1:A:179:A:H2'	1:A:180:U:C6	2.47	0.50
1:A:350:G:H5"	1:A:350:G:H8	1.77	0.50
1:A:410:G:C2	1:A:429:U:C2	3.00	0.50
1:A:681:C:N4	1:A:682:G:O6	2.45	0.50
2:B:204:ASN:HB3	2:B:206:ASP:O	2.12	0.50
4:D:172:PRO:HD2	4:D:173:TRP:CE3	2.47	0.50
6:F:39:LYS:HD3	6:F:40:VAL:H	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:G:C2	1:A:226:G:N3	2.80	0.50
1:A:736:C:H2'	1:A:737:A:C8	2.46	0.50
1:A:1349:A:H1'	1:A:1374:A:N6	2.27	0.50
1:A:1410:G:H2'	1:A:1411:C:C6	2.46	0.50
5:E:99:GLY:O	5:E:101:ILE:HG13	2.11	0.50
9:I:50:LEU:HD12	9:I:50:LEU:H	1.77	0.50
9:I:124:GLN:HG3	9:I:125:TYR:N	2.26	0.50
18:R:74:ARG:HB3	18:R:81:PHE:CE2	2.46	0.50
1:A:259:G:H2'	1:A:260:G:O4'	2.12	0.49
1:A:1502:A:H2	1:A:1505:G:H22	1.54	0.49
6:F:82:ARG:HB2	6:F:85:VAL:HG23	1.93	0.49
9:I:81:ILE:HG22	9:I:85:LEU:HD22	1.94	0.49
1:A:763:G:H2'	1:A:764:C:H6	1.77	0.49
1:A:966:M2G:HM22	1:A:967:5MC:O2	2.12	0.49
1:A:975:A:N6	1:A:1366:C:O2'	2.41	0.49
1:A:1133:G:H1	1:A:1141:C:N4	2.10	0.49
1:A:1352:C:H2'	1:A:1353:G:C8	2.47	0.49
12:L:35:GLY:HA3	12:L:59:ARG:O	2.12	0.49
17:Q:26:GLN:HA	17:Q:36:ILE:O	2.13	0.49
1:A:278:G:C6	17:Q:95:TYR:CD2	3.00	0.49
1:A:346:G:H2'	1:A:347:G:O4'	2.13	0.49
1:A:727:G:N2	1:A:730:G:OP2	2.45	0.49
2:B:146:GLN:O	2:B:150:SER:HB2	2.11	0.49
13:M:11:ARG:HD2	13:M:45:VAL:HG11	1.94	0.49
1:A:260:G:H2'	1:A:261:U:C6	2.47	0.49
1:A:1095:U:C4	1:A:1096:C:N4	2.80	0.49
1:A:1400:5MC:H3'	1:A:1401:G:H5'	1.93	0.49
12:L:66:VAL:HG21	12:L:98:TYR:HE1	1.75	0.49
13:M:34:LEU:HD13	13:M:41:PRO:HA	1.94	0.49
15:O:18:PHE:CD2	15:O:18:PHE:N	2.80	0.49
20:T:57:ARG:HH22	20:T:100:ILE:CD1	2.25	0.49
1:A:191:G:O2'	20:T:101:GLY:O	2.30	0.49
1:A:270:A:H2'	1:A:271:C:O4'	2.13	0.49
1:A:767:A:H2'	1:A:768:A:O4'	2.13	0.49
1:A:1112:C:O2	3:C:179:ARG:HB2	2.13	0.49
1:A:1112:C:N3	3:C:178:LEU:HD12	2.27	0.49
3:C:116:VAL:HG21	3:C:202:ILE:HD11	1.94	0.49
4:D:31:CYS:O	4:D:31:CYS:SG	2.71	0.49
5:E:15:ARG:HG3	5:E:15:ARG:NH1	2.27	0.49
10:J:3:LYS:NZ	10:J:3:LYS:HB3	2.27	0.49
15:O:18:PHE:N	15:O:18:PHE:HD2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:U:C2	1:A:63:C:C5	3.01	0.49
1:A:460:A:O2'	1:A:461:C:H5'	2.13	0.49
1:A:522:C:OP2	12:L:69:TYR:OH	2.24	0.49
1:A:927:G:O2'	1:A:1503:A:N7	2.44	0.49
3:C:150:LYS:HG3	3:C:169:ALA:HB2	1.93	0.49
4:D:173:TRP:O	4:D:186:LEU:HD23	2.13	0.49
5:E:76:ILE:HD13	5:E:76:ILE:N	2.27	0.49
3:C:67:THR:HA	3:C:102:ASN:OD1	2.13	0.49
5:E:14:ARG:O	5:E:28:PHE:HD2	1.95	0.49
9:I:118:LYS:C	9:I:120:ARG:H	2.16	0.49
10:J:15:THR:O	10:J:19:SER:HB3	2.13	0.49
10:J:61:GLU:OE1	14:N:58:LYS:HD2	2.13	0.49
11:K:48:ILE:HD13	11:K:63:LEU:HB2	1.93	0.49
13:M:10:PRO:HB2	13:M:18:ALA:HB1	1.95	0.49
13:M:50:GLU:HG3	13:M:53:VAL:HB	1.93	0.49
19:S:11:VAL:HG13	19:S:38:SER:HB3	1.95	0.49
1:A:680:C:N3	1:A:710:G:N2	2.46	0.49
1:A:718:G:O6	18:R:74:ARG:NH1	2.46	0.49
1:A:770:C:N4	24:A:1934:HOH:O	2.18	0.49
1:A:933:G:N2	1:A:1384:C:O2	2.40	0.49
1:A:1442:G:N1	1:A:1446:A:N6	2.60	0.49
11:K:80:VAL:HG22	11:K:103:LEU:HD22	1.93	0.49
20:T:16:HIS:O	20:T:20:LEU:HD22	2.13	0.49
1:A:106:C:C2'	1:A:107:G:H5'	2.43	0.49
1:A:116:A:H61	1:A:313:A:H1'	1.77	0.49
1:A:432:A:H2'	1:A:433:C:O4'	2.13	0.49
1:A:1505:G:H5'	24:A:1809:HOH:O	2.12	0.49
13:M:19:LEU:HD11	13:M:56:LEU:HD11	1.94	0.49
1:A:642:A:H2'	1:A:643:C:C6	2.48	0.49
1:A:725:G:C5	1:A:726:C:C5	3.01	0.49
1:A:939:G:C6	1:A:940:C:N4	2.81	0.49
1:A:1345:U:C4	1:A:1377:A:C2	3.01	0.49
5:E:92:LYS:HB3	5:E:119:LEU:HB2	1.94	0.49
8:H:116:LYS:CG	8:H:127:LEU:HD11	2.43	0.49
14:N:35:ARG:HG2	14:N:35:ARG:HH11	1.77	0.49
16:P:53:VAL:HG23	16:P:54:GLU:H	1.77	0.49
17:Q:5:VAL:HB	17:Q:60:ILE:CD1	2.43	0.49
18:R:29:PHE:HZ	18:R:43:PHE:CE1	2.30	0.49
18:R:46:GLU:N	18:R:46:GLU:OE2	2.37	0.49
1:A:350:G:O2'	1:A:351:G:H5'	2.13	0.48
1:A:358:U:H2'	1:A:359:U:H6	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:642:A:N7	8:H:115:SER:HA	2.28	0.48
3:C:164:ARG:HG2	3:C:165:THR:N	2.27	0.48
13:M:91:ARG:HH21	13:M:103:THR:HG21	1.77	0.48
1:A:7:G:C5	1:A:298:A:C2	3.01	0.48
3:C:121:ALA:O	3:C:124:ILE:HB	2.13	0.48
6:F:30:LEU:HD21	6:F:65:VAL:HG11	1.95	0.48
7:G:69:VAL:HG11	7:G:134:ALA:HB1	1.95	0.48
7:G:78:ARG:NH1	7:G:154:TYR:O	2.46	0.48
10:J:13:HIS:CD2	10:J:14:LYS:N	2.80	0.48
17:Q:40:LYS:HD3	17:Q:42:TYR:CZ	2.48	0.48
1:A:291:C:O2	1:A:291:C:H2'	2.12	0.48
1:A:730:G:N2	1:A:765:G:H5"	2.27	0.48
1:A:826:C:H2'	1:A:827:U:H6	1.78	0.48
1:A:1461:G:H2'	1:A:1462:G:H8	1.77	0.48
2:B:76:GLN:NE2	2:B:206:ASP:HB3	2.27	0.48
5:E:51:VAL:N	5:E:52:PRO:HD2	2.28	0.48
6:F:99:ALA:HB2	18:R:31:LEU:HG	1.94	0.48
13:M:87:TYR:HA	13:M:90:LEU:HD22	1.95	0.48
1:A:1118:C:OP1	9:I:104:ARG:NE	2.45	0.48
1:A:1378:C:N4	1:A:1379:G:N3	2.62	0.48
1:A:1378:C:C5	1:A:1379:G:C8	3.02	0.48
1:A:1481:U:H2'	1:A:1482:G:H8	1.76	0.48
2:B:69:LEU:HB3	2:B:162:ILE:HD11	1.95	0.48
2:B:178:ARG:CD	8:H:72:PRO:HA	2.44	0.48
3:C:147:LYS:NZ	3:C:172:ARG:HE	2.10	0.48
5:E:121:LYS:HG3	5:E:122:GLU:O	2.13	0.48
6:F:25:ILE:HA	6:F:28:ARG:HG2	1.94	0.48
7:G:88:PRO:HG2	7:G:152:ALA:HA	1.95	0.48
13:M:12:ASN:H	13:M:45:VAL:HG12	1.76	0.48
15:O:3:ILE:HA	15:O:7:GLU:OE1	2.13	0.48
16:P:19:ILE:HD11	16:P:39:TYR:HB2	1.95	0.48
1:A:15:G:H5'	1:A:1396:A:O2'	2.14	0.48
1:A:44:G:H2'	1:A:45:U:O4'	2.13	0.48
1:A:414:A:H2'	1:A:415:A:C8	2.48	0.48
1:A:1025:U:H5	1:A:1034:G:H1	1.62	0.48
1:A:1168:A:H2'	1:A:1169:A:C8	2.48	0.48
1:A:1371:G:O3'	9:I:69:GLY:HA3	2.13	0.48
2:B:28:PHE:CE2	2:B:190:THR:HG22	2.49	0.48
1:A:389:A:C6	1:A:390:C:H1'	2.49	0.48
1:A:648:A:H2'	1:A:649:G:O4'	2.14	0.48
1:A:1026:G:C8	1:A:1026:G:H3'	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1508:G:C5	1:A:1509:C:C5	3.02	0.48
5:E:78:HIS:CE1	5:E:143:ARG:H	2.31	0.48
20:T:55:ILE:HA	20:T:55:ILE:HD13	1.72	0.48
1:A:323:U:H2'	1:A:324:G:O4'	2.12	0.48
1:A:539:A:H2'	1:A:540:G:C8	2.49	0.48
1:A:745:C:H5"	1:A:851:G:O2'	2.13	0.48
1:A:806:C:O2'	1:A:807:A:H5'	2.13	0.48
1:A:1029:C:OP1	1:A:1033:G:N2	2.47	0.48
1:A:1138:G:H3'	1:A:1138:G:N3	2.29	0.48
2:B:93:VAL:HG21	2:B:97:TRP:HD1	1.79	0.48
3:C:108:ASN:ND2	3:C:111:LEU:HD22	2.29	0.48
1:A:109:A:C6	1:A:326:G:C6	3.02	0.48
1:A:463:A:O2'	16:P:82:GLN:HG2	2.14	0.48
1:A:780:A:OP2	11:K:122:LYS:HE3	2.13	0.48
1:A:1096:C:H2'	1:A:1097:C:C6	2.48	0.48
1:A:1152:A:H5"	10:J:13:HIS:HB2	1.94	0.48
1:A:1374:A:C4	1:A:1375:A:C8	3.01	0.48
2:B:10:LEU:O	2:B:12:GLU:N	2.47	0.48
4:D:72:GLU:O	4:D:75:PHE:N	2.47	0.48
12:L:113:ARG:NH1	12:L:116:SER:H	2.11	0.48
13:M:101:GLN:OE1	13:M:101:GLN:N	2.46	0.48
1:A:485:G:O2'	1:A:486:U:OP2	2.29	0.48
1:A:586:C:C2'	1:A:587:G:H5'	2.44	0.48
1:A:662:G:H2'	1:A:663:A:C8	2.49	0.48
1:A:683:G:H3'	1:A:684:A:H8	1.78	0.48
1:A:691:G:H2'	1:A:692:U:C6	2.48	0.48
1:A:1070:U:H2'	1:A:1071:C:H6	1.77	0.48
1:A:1150:U:C2'	1:A:1151:A:H5'	2.43	0.48
1:A:1195:C:O3'	1:A:1196:U:H4'	2.14	0.48
1:A:1224:G:O2'	1:A:1322:C:OP1	2.20	0.48
1:A:1238:A:H5'	1:A:1336:C:N4	2.23	0.48
4:D:201:GLN:HG2	4:D:204:ILE:HD12	1.96	0.48
5:E:9:LYS:HG2	5:E:112:LEU:HD11	1.95	0.48
7:G:17:VAL:HG12	7:G:18:TYR:CD1	2.49	0.48
9:I:90:PRO:O	9:I:93:ARG:HG3	2.14	0.48
16:P:6:LEU:HD23	16:P:17:TYR:CD2	2.49	0.48
17:Q:75:ARG:NH1	17:Q:75:ARG:HB2	2.29	0.48
19:S:11:VAL:HG12	19:S:12:ASP:H	1.79	0.48
20:T:57:ARG:NH1	20:T:100:ILE:HG21	2.29	0.48
1:A:558:G:H3'	1:A:559:A:H3'	1.96	0.48
1:A:682:G:C2	1:A:683:G:C8	3.02	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:716:A:N3	11:K:118:GLY:HA2	2.29	0.48
1:A:949:A:C2	1:A:1233:G:N3	2.82	0.48
1:A:1044:A:C6	1:A:1045:C:H1'	2.49	0.48
3:C:20:SER:HB3	3:C:22:TRP:HE1	1.79	0.48
3:C:120:VAL:HG12	3:C:198:VAL:HG11	1.95	0.48
7:G:50:ILE:O	7:G:54:THR:OG1	2.23	0.48
16:P:44:THR:OG1	16:P:45:THR:HG22	2.13	0.48
18:R:45:SER:HB2	18:R:51:LEU:HD21	1.96	0.48
1:A:98:U:O2'	1:A:99:C:H5'	2.14	0.47
1:A:429:U:H1'	1:A:430:A:H5"	1.96	0.47
1:A:512:U:H2'	1:A:513:C:C6	2.49	0.47
1:A:622:A:C8	1:A:623:C:C5	3.02	0.47
1:A:910:C:C4	1:A:911:U:C5	3.03	0.47
1:A:918:A:H2'	1:A:919:A:C8	2.48	0.47
1:A:1137:C:O2	1:A:1138:G:N1	2.45	0.47
3:C:43:LEU:HD13	3:C:47:LEU:HD22	1.95	0.47
4:D:38:TYR:H	4:D:38:TYR:HD2	1.62	0.47
17:Q:66:SER:OG	17:Q:69:LYS:HB2	2.14	0.47
19:S:5:LEU:HD22	19:S:6:LYS:NZ	2.29	0.47
1:A:416:G:C6	1:A:417:C:N3	2.82	0.47
1:A:705:U:H5"	1:A:706:A:OP2	2.14	0.47
1:A:1086:U:O5'	1:A:1086:U:H6	1.96	0.47
1:A:1381:U:O2'	1:A:1382:C:H5'	2.14	0.47
2:B:178:ARG:HH21	8:H:74:PRO:HG3	1.78	0.47
5:E:40:ARG:HB3	5:E:66:MET:CE	2.43	0.47
7:G:16:LEU:HD22	9:I:42:ARG:HA	1.96	0.47
11:K:126:ARG:HH11	11:K:126:ARG:HG3	1.79	0.47
18:R:46:GLU:OE2	18:R:55:ARG:NH2	2.47	0.47
1:A:149:A:H2'	1:A:150:C:C6	2.49	0.47
1:A:344:A:C5'	1:A:345:C:H5	2.28	0.47
1:A:454:C:H5"	1:A:455:C:C5	2.49	0.47
1:A:709:G:H2'	1:A:710:G:H8	1.79	0.47
1:A:725:G:H2'	1:A:726:C:H6	1.79	0.47
1:A:1075:C:O3'	2:B:175:ARG:NH2	2.47	0.47
1:A:1304:G:C6	1:A:1305:G:N1	2.82	0.47
3:C:34:LEU:HD23	14:N:25:VAL:HG21	1.96	0.47
10:J:6:ILE:HB	10:J:72:VAL:CG2	2.44	0.47
13:M:48:LEU:H	13:M:48:LEU:HG	1.42	0.47
15:O:11:VAL:HG21	15:O:34:LEU:HD22	1.95	0.47
19:S:39:THR:HA	19:S:70:LYS:HA	1.95	0.47
1:A:434:U:H2'	1:A:435:C:C6	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:737:A:H2'	1:A:738:C:H6	1.79	0.47
1:A:1233:G:N2	1:A:1234:C:N3	2.62	0.47
1:A:1519[B]:MA6:C5	1:A:1520[B]:G:H1'	2.44	0.47
2:B:54:THR:OG1	2:B:199:TYR:HB3	2.13	0.47
14:N:9:LYS:HD3	14:N:10:ALA:N	2.29	0.47
18:R:69:THR:O	18:R:72:ARG:HB2	2.14	0.47
1:A:107:G:C2	1:A:108:G:H1'	2.50	0.47
1:A:109:A:C4	1:A:327:A:C2	3.02	0.47
1:A:448:A:C4	1:A:487:A:C2	3.03	0.47
1:A:452:A:C2	1:A:453:A:C4	3.03	0.47
1:A:1191:A:H2'	1:A:1192:C:C6	2.49	0.47
2:B:109:SER:O	2:B:112:VAL:HB	2.14	0.47
3:C:148:GLY:HA3	3:C:172:ARG:O	2.14	0.47
4:D:190:ASP:OD2	4:D:192:GLU:N	2.39	0.47
9:I:52:ALA:O	9:I:95:LYS:HD3	2.15	0.47
10:J:6:ILE:HB	10:J:72:VAL:HG23	1.96	0.47
11:K:62:GLN:O	11:K:66:LEU:HB2	2.14	0.47
13:M:49:THR:OG1	13:M:52:GLU:HG3	2.14	0.47
1:A:37:U:O2'	1:A:500:G:H4'	2.14	0.47
1:A:1309:G:C6	1:A:1329:A:C2	3.02	0.47
2:B:112:VAL:O	2:B:115:LEU:HB3	2.15	0.47
3:C:151:VAL:O	3:C:152:ILE:HD13	2.14	0.47
12:L:117:ARG:NH2	12:L:124:LYS:HB2	2.29	0.47
13:M:23:TYR:CE2	13:M:70:LEU:HD13	2.50	0.47
13:M:108:ARG:NH2	13:M:111:LYS:HG2	2.30	0.47
21:U:8:THR:HG1	21:U:11:GLY:H	1.61	0.47
1:A:375:U:H2'	1:A:376:G:C8	2.50	0.47
1:A:729:A:C2'	1:A:730:G:H5'	2.44	0.47
1:A:975:A:H4'	1:A:976:G:C5'	2.40	0.47
1:A:1057:G:O6	1:A:1203:C:N4	2.44	0.47
1:A:1127:G:N2	1:A:1145:C:N3	2.62	0.47
1:A:1315:U:H2'	1:A:1316:G:O4'	2.15	0.47
1:A:1327:C:H2'	1:A:1328:C:C6	2.50	0.47
3:C:20:SER:O	14:N:54:PRO:HB3	2.15	0.47
3:C:126:ARG:O	3:C:127:ARG:HG2	2.15	0.47
3:C:182:ILE:HD12	3:C:203:PHE:HB2	1.96	0.47
8:H:10:LEU:O	8:H:13:ILE:HB	2.15	0.47
8:H:39:LEU:HA	8:H:39:LEU:HD22	1.54	0.47
10:J:87:THR:C	10:J:88:LEU:HD13	2.34	0.47
11:K:120:ARG:HH22	11:K:126:ARG:HH12	1.62	0.47
15:O:15:PHE:HD1	15:O:30:ALA:CB	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:G:C2	1:A:309:G:C2	3.03	0.47
1:A:376:G:H5"	16:P:5:ARG:HD2	1.96	0.47
1:A:564:C:C5	17:Q:31:LEU:HD21	2.50	0.47
1:A:710:G:H5"	6:F:54:LYS:HE3	1.97	0.47
1:A:1508:G:H2'	1:A:1509:C:O4'	2.15	0.47
2:B:18:GLY:H	2:B:41:ILE:HG23	1.80	0.47
3:C:167:TRP:HE3	3:C:168:ALA:H	1.59	0.47
12:L:36:VAL:HG12	12:L:37:CYS:O	2.15	0.47
1:A:475:G:H2'	1:A:476:G:H8	1.80	0.47
1:A:674:G:H2'	1:A:675:A:C8	2.49	0.47
1:A:902:G:O2'	1:A:903:G:H5'	2.15	0.47
3:C:23:TYR:HD1	10:J:11:PHE:CE2	2.33	0.47
5:E:59:GLY:C	5:E:63:ARG:HH21	2.18	0.47
6:F:14:LEU:HA	6:F:18:GLN:OE1	2.14	0.47
8:H:51:VAL:HG11	8:H:60:ARG:NH1	2.30	0.47
11:K:27:ASN:OD1	11:K:28:THR:N	2.47	0.47
13:M:53:VAL:O	13:M:57:ARG:HB2	2.14	0.47
14:N:6:LEU:HD13	14:N:23:ARG:HH22	1.80	0.47
1:A:263:A:O2'	1:A:264:U:H5'	2.15	0.47
1:A:500:G:C5	1:A:546:G:N2	2.83	0.47
4:D:206:PHE:CD2	4:D:207:TYR:CE1	2.99	0.47
5:E:100:VAL:HA	5:E:118:ILE:HG22	1.97	0.47
5:E:106:PRO:O	5:E:110:LEU:HG	2.14	0.47
7:G:62:PHE:HD1	7:G:124:LEU:HD22	1.80	0.47
11:K:19:ALA:HB2	11:K:32:ILE:HG23	1.96	0.47
13:M:4:ILE:CD1	13:M:22:ILE:HD11	2.44	0.47
16:P:67:THR:O	16:P:70:ALA:HB3	2.15	0.47
1:A:405:U:C2	1:A:498:U:C5	3.03	0.46
1:A:530:G:H2'	1:A:530:G:N3	2.30	0.46
1:A:1377:A:N6	7:G:5:ARG:HH22	2.14	0.46
2:B:163:PHE:CE2	2:B:185:ILE:HG22	2.50	0.46
6:F:52:ILE:O	6:F:55:ASP:HB2	2.15	0.46
11:K:17:GLY:O	11:K:80:VAL:HA	2.15	0.46
19:S:51:VAL:O	19:S:57:HIS:HA	2.16	0.46
1:A:595:G:H1'	1:A:596:C:H5	1.80	0.46
1:A:750:G:N3	15:O:23:GLY:HA3	2.30	0.46
1:A:1057:G:N2	1:A:1204:A:H1'	2.30	0.46
1:A:1172:C:H2'	1:A:1173:G:H8	1.80	0.46
1:A:1226:C:C5	13:M:104:ARG:HA	2.50	0.46
3:C:18:TRP:O	3:C:21:ARG:NH1	2.49	0.46
3:C:102:ASN:OD1	3:C:102:ASN:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:26:ILE:O	6:F:30:LEU:HB2	2.15	0.46
8:H:49:GLU:HB2	8:H:62:TYR:CE2	2.50	0.46
12:L:123:LYS:H	12:L:123:LYS:HG2	1.27	0.46
19:S:53:ASN:O	19:S:77:THR:HG22	2.15	0.46
20:T:50:GLU:CB	20:T:99:LEU:HD23	2.42	0.46
1:A:3:G:H1	4:D:87:GLY:H	1.64	0.46
1:A:17:U:C2	1:A:18:C:C5	3.04	0.46
1:A:66:G:N3	1:A:66:G:H2'	2.29	0.46
1:A:128:G:H4'	17:Q:3:LYS:HG2	1.97	0.46
1:A:710:G:C2	1:A:711:G:C5	3.03	0.46
1:A:949:A:H1'	1:A:1364:U:N3	2.30	0.46
1:A:1310:G:C2	1:A:1328:C:N3	2.84	0.46
1:A:1310:G:N7	19:S:2:PRO:HD3	2.30	0.46
1:A:1487:G:C5	1:A:1488:G:C8	3.03	0.46
1:A:1539:C:H5"	7:G:82:GLY:CA	2.46	0.46
2:B:223:ILE:CD1	2:B:228:GLY:HA3	2.45	0.46
5:E:33:VAL:HG22	5:E:43:LEU:HD13	1.98	0.46
8:H:1:MET:HG2	8:H:2:LEU:H	1.79	0.46
9:I:63:ILE:HG21	9:I:77:ILE:HD11	1.96	0.46
16:P:21:VAL:HG21	16:P:59:TRP:CD1	2.50	0.46
1:A:138:G:C2	1:A:226:G:C2	3.03	0.46
1:A:442:C:H2'	1:A:443:C:C6	2.50	0.46
1:A:452:A:O2'	1:A:453:A:H8	1.97	0.46
1:A:948:C:OP2	13:M:108:ARG:HB2	2.16	0.46
2:B:223:ILE:HD12	2:B:228:GLY:HA3	1.97	0.46
3:C:11:ARG:HH12	3:C:180:ALA:HB3	1.81	0.46
6:F:43:LEU:HD22	6:F:43:LEU:H	1.80	0.46
8:H:87:SER:HB2	8:H:93:VAL:HG22	1.95	0.46
11:K:66:LEU:HD23	11:K:97:ALA:HB1	1.97	0.46
20:T:43:LEU:HD13	20:T:51:GLU:HB3	1.97	0.46
1:A:448:A:P	1:A:485:G:H22	2.38	0.46
1:A:1048:G:H1	1:A:1209:C:H42	1.63	0.46
1:A:1248:A:O2'	9:I:70:LYS:NZ	2.28	0.46
1:A:1438:G:H2'	1:A:1439:C:H6	1.80	0.46
1:A:1491:G:C2'	1:A:1492:A:H5'	2.45	0.46
2:B:69:LEU:HD23	2:B:91:PRO:O	2.15	0.46
7:G:95:ARG:CZ	7:G:99:LEU:HD11	2.46	0.46
13:M:90:LEU:HA	13:M:93:ARG:HB3	1.98	0.46
1:A:463:A:H2'	1:A:474:G:O4'	2.15	0.46
1:A:500:G:C6	1:A:546:G:C2	3.04	0.46
1:A:502:G:OP1	12:L:117:ARG:N	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544:G:OP1	4:D:59:ARG:NH2	2.33	0.46
1:A:833:U:H2'	1:A:834:C:C6	2.50	0.46
1:A:935:A:N6	7:G:3:ARG:HG3	2.31	0.46
1:A:992:U:H3	1:A:1044:A:H62	1.63	0.46
1:A:1499:A:H1'	1:A:1520[A]:G:H5'	1.98	0.46
2:B:36:ARG:HB3	2:B:41:ILE:HD11	1.96	0.46
3:C:129:ALA:HB3	3:C:132:ARG:HD2	1.97	0.46
3:C:195:VAL:C	3:C:196:LEU:HD12	2.35	0.46
10:J:4:ILE:HB	10:J:74:ILE:CD1	2.46	0.46
14:N:23:ARG:HD3	14:N:29:ARG:O	2.16	0.46
14:N:41:ARG:HG2	14:N:42:ILE:HG23	1.97	0.46
15:O:50:HIS:O	15:O:53:HIS:N	2.48	0.46
20:T:53:LEU:CD2	20:T:56:MET:HG2	2.46	0.46
21:U:6:ARG:HG2	21:U:15:ARG:NH2	2.31	0.46
1:A:229:U:H2'	1:A:230:G:H8	1.81	0.46
1:A:542:G:H2'	1:A:543:C:H6	1.80	0.46
1:A:693:G:O2'	7:G:81:GLY:O	2.25	0.46
1:A:867:G:O2'	1:A:868:C:H5'	2.15	0.46
1:A:869:G:C8	24:A:2036:HOH:O	2.68	0.46
1:A:1079:G:C6	1:A:1080:A:N6	2.84	0.46
1:A:1333:A:H2'	1:A:1334:G:O4'	2.15	0.46
3:C:81:GLY:O	3:C:84:ILE:HG22	2.16	0.46
4:D:202:LEU:HD13	4:D:202:LEU:HA	1.80	0.46
7:G:101:LEU:N	7:G:101:LEU:HD12	2.31	0.46
10:J:32:ALA:HB3	10:J:75:ILE:HB	1.97	0.46
13:M:12:ASN:H	13:M:45:VAL:HG11	1.79	0.46
15:O:85:LEU:HD23	15:O:85:LEU:HA	1.54	0.46
1:A:310:G:C5	1:A:311:C:C5	3.04	0.46
1:A:448:A:C2	1:A:449:C:C2	3.03	0.46
1:A:872:A:C5	1:A:874:G:C8	3.04	0.46
1:A:1443:G:H5"	1:A:1443:G:H8	1.81	0.46
1:A:1502:A:H5"	1:A:1504:G:N7	2.31	0.46
4:D:19:LEU:HB2	4:D:21:LEU:HD23	1.98	0.46
7:G:50:ILE:HD13	7:G:61:VAL:HG11	1.98	0.46
7:G:87:VAL:HA	7:G:88:PRO:HD2	1.75	0.46
9:I:86:VAL:HA	9:I:89:ASN:O	2.16	0.46
18:R:66:LEU:O	18:R:70:ILE:HG13	2.15	0.46
19:S:53:ASN:HB2	19:S:56:GLN:O	2.15	0.46
1:A:93:G:H2'	1:A:95:U:O4'	2.16	0.46
1:A:690:G:N7	11:K:55:LYS:NZ	2.63	0.46
1:A:839:U:H5"	1:A:840:C:OP2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:920:U:O4'	1:A:1080:A:C2	2.68	0.46
1:A:1035:A:C4	1:A:1036:G:N7	2.84	0.46
1:A:1367:C:N3	1:A:1368:G:C8	2.84	0.46
1:A:1486:G:H2'	1:A:1487:G:O4'	2.16	0.46
3:C:150:LYS:HD2	3:C:173:VAL:HG21	1.98	0.46
5:E:12:LEU:HD23	5:E:13:ILE:CA	2.46	0.46
5:E:135:THR:O	5:E:138:ALA:HB3	2.16	0.46
7:G:75:VAL:HA	7:G:87:VAL:O	2.16	0.46
12:L:10:LEU:HD23	12:L:10:LEU:HA	1.57	0.46
12:L:117:ARG:HB3	12:L:122:THR:OG1	2.16	0.46
17:Q:31:LEU:HD12	17:Q:31:LEU:HA	1.65	0.46
18:R:53:ARG:HA	18:R:56:THR:HG23	1.98	0.46
20:T:89:ARG:HH21	20:T:104:LEU:HD22	1.81	0.46
1:A:401:C:H2'	1:A:402:G:H8	1.81	0.46
1:A:499:A:N6	1:A:547:A:C8	2.84	0.46
1:A:520:A:OP1	12:L:52:LEU:HD12	2.16	0.46
1:A:800:G:O2'	1:A:801:U:H5'	2.16	0.46
1:A:1151:A:H1'	1:A:1152:A:C8	2.51	0.46
1:A:1487:G:H2'	1:A:1488:G:H5'	1.97	0.46
17:Q:8:GLY:HA3	17:Q:22:LEU:O	2.16	0.46
17:Q:60:ILE:HA	17:Q:60:ILE:HD12	1.68	0.46
1:A:7:G:H5'	1:A:298:A:O4'	2.16	0.45
1:A:56:U:O2'	1:A:57:G:H5'	2.16	0.45
1:A:130:A:H4'	1:A:190(F):G:C2	2.51	0.45
1:A:515:G:H2'	1:A:516:PSU:O4'	2.16	0.45
1:A:645:C:H2'	1:A:646:U:O4'	2.15	0.45
1:A:1491:G:N1	1:A:1493:A:H2	2.14	0.45
5:E:12:LEU:HD21	5:E:14:ARG:HB3	1.98	0.45
8:H:120:THR:HG23	8:H:123:GLU:HG3	1.99	0.45
10:J:3:LYS:N	10:J:74:ILE:O	2.50	0.45
19:S:25:LYS:HE3	19:S:25:LYS:HB3	1.75	0.45
1:A:352:C:H6	1:A:352:C:H5"	1.81	0.45
1:A:401:C:H2'	1:A:402:G:C8	2.51	0.45
1:A:452:A:HO2'	1:A:453:A:H8	1.64	0.45
1:A:689:C:P	11:K:46:GLY:HA3	2.56	0.45
1:A:728:A:H2'	1:A:729:A:O4'	2.16	0.45
1:A:938:A:C6	1:A:939:G:C5	3.04	0.45
1:A:942:G:C2	1:A:1342:C:C2	3.05	0.45
1:A:1171:G:H2'	1:A:1172:C:C6	2.51	0.45
1:A:1309:G:N2	1:A:1329:A:H1'	2.31	0.45
1:A:1378:C:N4	1:A:1379:G:C4	2.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:80:ARG:HB3	13:M:80:ARG:CZ	2.45	0.45
17:Q:70:ARG:O	17:Q:71:PHE:HD2	1.99	0.45
1:A:496:A:C2	1:A:497:A:C5	3.04	0.45
1:A:581:G:C2	1:A:582:U:C5	3.04	0.45
1:A:581:G:N2	1:A:760:G:N7	2.63	0.45
1:A:665:A:C5	1:A:733:A:C5	3.04	0.45
1:A:682:G:H1	1:A:708:C:H42	1.65	0.45
1:A:993:G:H2'	1:A:995:C:H41	1.81	0.45
1:A:1126:U:C4	1:A:1127:G:C2	3.04	0.45
1:A:1402:4OC:O2	1:A:1500:A:N1	2.49	0.45
3:C:122:GLU:OE1	3:C:126:ARG:HD2	2.16	0.45
6:F:23:LYS:O	6:F:26:ILE:HB	2.17	0.45
17:Q:81:ARG:HE	17:Q:81:ARG:HB3	1.45	0.45
17:Q:85:VAL:O	17:Q:89:LEU:HB2	2.17	0.45
18:R:83:GLU:OE1	18:R:84:LYS:HG3	2.16	0.45
1:A:665:A:H3'	1:A:725:G:H21	1.82	0.45
1:A:1234:C:H2'	1:A:1235:U:C6	2.49	0.45
1:A:1461:G:H2'	1:A:1462:G:C8	2.51	0.45
7:G:5:ARG:HE	7:G:7:ALA:HA	1.81	0.45
8:H:9:MET:O	8:H:13:ILE:HD12	2.17	0.45
8:H:29:SER:OG	8:H:32:LYS:N	2.31	0.45
8:H:100:ILE:HA	8:H:101:PRO:HD2	1.77	0.45
10:J:8:LEU:CD2	10:J:96:ILE:HG22	2.44	0.45
17:Q:4:LYS:HE2	17:Q:6:LEU:HD21	1.98	0.45
1:A:222:U:H2'	1:A:223:U:C6	2.51	0.45
1:A:342:C:H42	1:A:347:G:H1	1.62	0.45
1:A:561:U:HO2'	1:A:562:C:P	2.40	0.45
1:A:584:G:H2'	1:A:585:G:C8	2.51	0.45
1:A:709:G:H2'	1:A:710:G:C8	2.52	0.45
1:A:1119:C:N4	1:A:1154:G:H1	2.13	0.45
1:A:1256:A:H4'	1:A:1257:U:O5'	2.16	0.45
6:F:40:VAL:HG22	6:F:63:TYR:HD2	1.80	0.45
8:H:121:ASP:OD2	8:H:122:ARG:N	2.49	0.45
10:J:6:ILE:HA	10:J:97:GLU:O	2.17	0.45
11:K:18:ARG:HG3	11:K:33:THR:HG23	1.99	0.45
15:O:70:LEU:HD22	15:O:70:LEU:HA	1.68	0.45
17:Q:95:TYR:O	17:Q:98:LEU:HD12	2.17	0.45
20:T:53:LEU:HD23	20:T:53:LEU:HA	1.82	0.45
20:T:100:ILE:HG22	20:T:102:GLY:H	1.81	0.45
21:U:6:ARG:H	21:U:6:ARG:HG3	1.57	0.45
1:A:629:G:H2'	1:A:630:G:O4'	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:710:G:H2'	1:A:711:G:C8	2.50	0.45
1:A:899:C:H2'	1:A:900:A:O4'	2.16	0.45
1:A:1510:U:H2'	1:A:1511:G:N7	2.32	0.45
1:A:1518[B]:MA6:HO2'	1:A:1519[B]:MA6:P	2.40	0.45
2:B:184:VAL:O	2:B:198:ASP:HB2	2.16	0.45
7:G:71:PRO:HG3	7:G:103:TRP:HZ3	1.81	0.45
7:G:107:ALA:HA	7:G:110:GLN:HG2	1.99	0.45
7:G:139:GLU:CG	7:G:143:ARG:HH22	2.28	0.45
8:H:86:ILE:HG21	8:H:133:LEU:HD13	1.99	0.45
9:I:111:ARG:O	9:I:111:ARG:HG3	2.16	0.45
16:P:41:PRO:O	16:P:43:LYS:HD2	2.17	0.45
19:S:16:LEU:HD11	19:S:20:LEU:HD23	1.98	0.45
1:A:509:A:C8	1:A:509:A:C3'	3.00	0.45
1:A:542:G:O2'	1:A:543:C:H5'	2.16	0.45
1:A:725:G:C4	1:A:726:C:C5	3.05	0.45
1:A:782:A:H2'	1:A:783:C:O4'	2.17	0.45
1:A:1403:C:N4	1:A:1544:U:OP1	2.50	0.45
1:A:1414:U:H2'	1:A:1415:G:H8	1.82	0.45
1:A:1503:A:N6	1:A:1532:U:O2'	2.49	0.45
3:C:182:ILE:HG22	3:C:183:ASP:O	2.16	0.45
4:D:35:ARG:O	4:D:36:ARG:HG2	2.15	0.45
4:D:63:LYS:O	4:D:67:ILE:HG13	2.17	0.45
5:E:17:ALA:HB2	5:E:26:PHE:CD2	2.52	0.45
5:E:79:GLU:HG3	8:H:105:ARG:CG	2.45	0.45
10:J:6:ILE:O	10:J:72:VAL:HG23	2.17	0.45
15:O:41:GLU:OE2	15:O:44:LYS:HD3	2.16	0.45
1:A:112:G:H21	1:A:354:G:C4'	2.30	0.45
1:A:502:G:H2'	1:A:503:C:O4'	2.16	0.45
1:A:933:G:N1	1:A:935:A:H1'	2.32	0.45
1:A:966:M2G:C8	1:A:967:5MC:HM52	2.52	0.45
1:A:1233:G:C2	1:A:1234:C:C4	3.05	0.45
1:A:1514:C:H2'	1:A:1515[A]:C:O4'	2.16	0.45
4:D:10:ARG:HG3	4:D:40:PRO:HG3	1.98	0.45
8:H:51:VAL:HG11	8:H:60:ARG:HH12	1.82	0.45
1:A:950:U:H2'	1:A:951:G:H8	1.82	0.45
1:A:1015:A:H2'	1:A:1016:A:C8	2.52	0.45
1:A:1349:A:OP1	9:I:120:ARG:HB2	2.16	0.45
1:A:1518[A]:MA6:N6	1:A:1519[A]:MA6:H103	2.32	0.45
1:A:1539:C:H5"	7:G:82:GLY:HA2	1.99	0.45
3:C:150:LYS:CG	3:C:169:ALA:HB2	2.46	0.45
5:E:75:THR:C	5:E:76:ILE:HD13	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:7:ASN:HD22	6:F:7:ASN:N	2.14	0.45
20:T:10:LEU:HD22	20:T:11:SER:H	1.82	0.45
1:A:499:A:C6	1:A:547:A:C8	3.05	0.45
1:A:711:G:N3	1:A:712:A:C8	2.85	0.45
1:A:1377:A:OP2	7:G:94:ARG:NE	2.50	0.45
7:G:99:LEU:HD22	7:G:103:TRP:CZ3	2.52	0.45
14:N:6:LEU:HA	14:N:6:LEU:HD23	1.63	0.45
14:N:31:ARG:O	14:N:33:VAL:HG22	2.17	0.45
1:A:73:C:O2'	1:A:74:C:H5'	2.17	0.44
1:A:874:G:C6	1:A:875:C:C4	3.04	0.44
1:A:936:C:H2'	1:A:937:A:O4'	2.17	0.44
1:A:1392:G:H8	1:A:1392:G:O5'	2.01	0.44
1:A:1481:U:O2'	1:A:1482:G:H5'	2.17	0.44
4:D:107:ARG:NH1	4:D:114:ARG:HH22	2.15	0.44
5:E:46:GLY:N	5:E:58:ALA:HB2	2.31	0.44
11:K:33:THR:OG1	11:K:34:ASP:N	2.49	0.44
12:L:38:THR:HB	12:L:39:VAL:H	1.66	0.44
12:L:111:LYS:O	12:L:112:ASP:HB2	2.17	0.44
14:N:32:SER:HB2	14:N:41:ARG:HB3	1.98	0.44
15:O:49:ASP:OD1	15:O:52:SER:OG	2.22	0.44
17:Q:29:HIS:HB2	17:Q:36:ILE:HD12	2.00	0.44
19:S:5:LEU:C	19:S:6:LYS:HZ3	2.20	0.44
1:A:226:G:C2	1:A:227:G:C8	3.05	0.44
1:A:489:C:H2'	1:A:490:G:C8	2.48	0.44
1:A:711:G:H2'	1:A:712:A:C8	2.49	0.44
1:A:792:A:H4'	1:A:793:U:H5"	1.99	0.44
1:A:1250:A:H4'	9:I:67:GLY:HA2	2.00	0.44
1:A:1307:U:H2'	1:A:1308:U:H6	1.82	0.44
1:A:1416:G:H2'	1:A:1417:G:H5'	1.99	0.44
1:A:1506:U:N3	1:A:1522:U:OP1	2.29	0.44
2:B:221:LEU:HD13	2:B:222:ILE:N	2.32	0.44
5:E:28:PHE:O	5:E:47:LYS:HA	2.16	0.44
5:E:91:LEU:HA	5:E:91:LEU:HD23	1.59	0.44
5:E:127:ASN:HA	5:E:128:PRO:HD2	1.81	0.44
6:F:3:ARG:HG2	6:F:93:SER:HB2	1.99	0.44
8:H:119:LEU:N	8:H:119:LEU:HD12	2.33	0.44
9:I:48:GLU:HB3	9:I:101:PHE:CZ	2.52	0.44
12:L:28:LYS:HD2	12:L:33:ARG:NE	2.32	0.44
15:O:51:HIS:O	15:O:54:ARG:HB3	2.18	0.44
15:O:74:ASP:HA	15:O:75:PRO:HD2	1.85	0.44
17:Q:27:PHE:HA	17:Q:28:PRO:HD3	1.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:7:LYS:H	19:S:7:LYS:HZ3	1.65	0.44
20:T:36:LEU:HD22	20:T:36:LEU:HA	1.83	0.44
20:T:65:LYS:O	20:T:68:LYS:HB2	2.18	0.44
1:A:106:C:H2'	1:A:107:G:H8	1.81	0.44
1:A:414:A:OP2	1:A:428:G:N2	2.43	0.44
1:A:785:G:C2	1:A:786:G:C8	3.06	0.44
1:A:929:G:C5	1:A:930:C:C5	3.05	0.44
1:A:1086:U:O2'	1:A:1087:G:H5'	2.18	0.44
1:A:1143:G:H2'	1:A:1144:G:C8	2.53	0.44
1:A:1254:C:O4'	1:A:1356:G:H5"	2.17	0.44
1:A:1356:G:H2'	1:A:1357:A:C8	2.52	0.44
1:A:1539:C:H2'	1:A:1540:PSU:H5"	1.98	0.44
3:C:123:GLN:HB2	3:C:128:PHE:CD1	2.37	0.44
4:D:61:LYS:HG3	4:D:62:GLN:N	2.27	0.44
4:D:177:ASP:OD2	4:D:179:GLU:HG2	2.17	0.44
9:I:28:VAL:HG22	9:I:63:ILE:HB	1.98	0.44
10:J:38:ILE:HG13	10:J:71:LEU:HB2	1.99	0.44
17:Q:57:VAL:HG12	17:Q:76:LEU:HA	1.98	0.44
1:A:147:G:H1	1:A:175:C:H42	1.65	0.44
1:A:412:A:N6	4:D:35:ARG:HB3	2.33	0.44
1:A:484:G:H5'	1:A:486:U:O4'	2.17	0.44
1:A:486:U:H2'	1:A:487:A:H8	1.82	0.44
1:A:762:C:H2'	1:A:763:G:H8	1.83	0.44
1:A:1053:G:C3'	1:A:1054:C:H5'	2.47	0.44
1:A:1438:G:H2'	1:A:1439:C:C6	2.52	0.44
1:A:1476:G:O2'	1:A:1477:C:H5'	2.17	0.44
1:A:1496:C:H2'	1:A:1497:G:O4'	2.18	0.44
2:B:71:VAL:HG13	2:B:93:VAL:HB	2.00	0.44
4:D:172:PRO:HD2	4:D:173:TRP:CZ3	2.53	0.44
6:F:40:VAL:HG22	6:F:63:TYR:CD2	2.52	0.44
6:F:68:PRO:HG2	6:F:71:ARG:NH2	2.33	0.44
14:N:23:ARG:HA	14:N:29:ARG:O	2.16	0.44
1:A:138:G:N2	1:A:226:G:N3	2.66	0.44
1:A:255:G:C2	1:A:256:U:C4	3.05	0.44
1:A:372:C:H4'	1:A:373:A:OP1	2.17	0.44
1:A:1387:G:C6	1:A:1388:C:N4	2.85	0.44
2:B:136:VAL:O	2:B:140:HIS:HB2	2.17	0.44
4:D:190:ASP:OD2	4:D:190:ASP:C	2.56	0.44
6:F:10:LEU:H	6:F:10:LEU:HD12	1.82	0.44
7:G:74:GLU:HG2	7:G:91:VAL:HG11	2.00	0.44
8:H:52:ASP:OD1	8:H:56:LYS:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:7:LYS:O	10:J:8:LEU:HD23	2.18	0.44
13:M:91:ARG:HA	13:M:91:ARG:HD2	1.81	0.44
1:A:79:G:C2	1:A:80:G:C8	3.06	0.44
1:A:194:C:H2'	1:A:195:A:H5"	1.99	0.44
1:A:386:C:H2'	1:A:387:U:H5'	1.99	0.44
1:A:693:G:H2'	1:A:694:A:H8	1.82	0.44
1:A:764:C:H5"	1:A:765:G:OP2	2.18	0.44
1:A:1072:G:C5	1:A:1073:U:C4	3.06	0.44
1:A:1241:G:H2'	1:A:1242:C:C6	2.52	0.44
1:A:1484:C:H2'	1:A:1485:U:O4'	2.17	0.44
2:B:166:ASP:HB3	2:B:169:LYS:HB3	2.00	0.44
9:I:7:THR:HG22	9:I:8:GLY:N	2.32	0.44
10:J:25:GLU:HA	10:J:28:ARG:HB2	2.00	0.44
17:Q:59:ILE:HD13	17:Q:59:ILE:HA	1.77	0.44
1:A:622:A:C8	1:A:623:C:C6	3.05	0.44
1:A:826:C:H5'	8:H:12:ARG:CZ	2.47	0.44
1:A:1221:G:H4'	19:S:77:THR:CG2	2.48	0.44
1:A:1417:G:H2'	1:A:1482:G:N2	2.33	0.44
1:A:1484:C:C4	1:A:1485:U:O2	2.71	0.44
3:C:11:ARG:O	3:C:14:ILE:O	2.34	0.44
5:E:116:THR:OG1	5:E:117:ASP:N	2.51	0.44
8:H:86:ILE:HG21	8:H:133:LEU:HD22	1.99	0.44
9:I:48:GLU:HB3	9:I:101:PHE:HZ	1.83	0.44
17:Q:29:HIS:HB2	17:Q:36:ILE:CD1	2.48	0.44
1:A:544:G:P	4:D:59:ARG:HH22	2.39	0.44
1:A:932:C:H2'	1:A:933:G:C8	2.52	0.44
3:C:35:GLU:HG3	3:C:95:THR:HG21	1.99	0.44
7:G:17:VAL:HG12	7:G:18:TYR:HD1	1.83	0.44
8:H:56:LYS:HA	8:H:57:PRO:HD3	1.80	0.44
13:M:14:ARG:HB3	13:M:41:PRO:O	2.17	0.44
13:M:86:CYS:O	13:M:90:LEU:HD22	2.18	0.44
15:O:57:LEU:HA	15:O:57:LEU:HD13	1.45	0.44
1:A:254:G:N3	1:A:255:G:C8	2.86	0.44
1:A:427:U:C4	1:A:428:G:C6	3.06	0.44
1:A:803:G:H2'	1:A:804:U:O4'	2.18	0.44
1:A:1459:C:H2'	1:A:1460:A:O4'	2.18	0.44
1:A:1478:C:H2'	1:A:1479:C:O4'	2.18	0.44
4:D:104:VAL:O	4:D:108:LEU:HB2	2.18	0.44
8:H:13:ILE:O	8:H:17:THR:HG23	2.18	0.44
8:H:40:ALA:O	8:H:42:GLU:N	2.51	0.44
11:K:59:TYR:CE2	11:K:63:LEU:HD11	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:15:LYS:HB3	14:N:15:LYS:HE2	1.74	0.44
17:Q:26:GLN:O	17:Q:27:PHE:HB3	2.18	0.44
20:T:87:LYS:HE2	20:T:87:LYS:HB2	1.91	0.44
1:A:67:C:H2'	1:A:68:G:C8	2.53	0.43
1:A:113:G:H1	1:A:314:C:H42	1.66	0.43
1:A:670:G:H1	1:A:736:C:H42	1.66	0.43
1:A:967:5MC:H2'	1:A:968:A:C8	2.53	0.43
4:D:194:LEU:HB3	4:D:196:LEU:CD2	2.48	0.43
8:H:86:ILE:HG21	8:H:133:LEU:HB3	1.99	0.43
10:J:57:LYS:HG3	10:J:57:LYS:O	2.18	0.43
13:M:29:ARG:HB3	13:M:64:TRP:CZ3	2.53	0.43
19:S:39:THR:HG22	19:S:70:LYS:CD	2.42	0.43
1:A:235:C:N4	24:A:1842:HOH:O	2.51	0.43
1:A:518:C:H2'	1:A:530:G:C8	2.53	0.43
1:A:707:C:OP1	11:K:85:ARG:NH1	2.51	0.43
1:A:954:G:H2'	1:A:955:U:C6	2.54	0.43
1:A:1104:G:H5"	1:A:1104:G:H8	1.82	0.43
1:A:1399:C:O2	1:A:1401:G:C5	2.71	0.43
2:B:57:PHE:CG	2:B:199:TYR:CE1	3.06	0.43
8:H:63:LEU:HD13	8:H:63:LEU:H	1.83	0.43
10:J:57:LYS:HG3	10:J:60:ARG:NH1	2.29	0.43
12:L:33:ARG:HG2	12:L:62:SER:HB3	2.00	0.43
13:M:94:ARG:HB3	13:M:96:LEU:HD12	2.00	0.43
14:N:11:LYS:HE2	14:N:11:LYS:HB3	1.78	0.43
17:Q:43:LEU:HD23	17:Q:68:ARG:NH2	2.32	0.43
1:A:64:G:H4'	1:A:65:U:H3'	2.00	0.43
1:A:104:G:C2	1:A:105:G:C8	3.06	0.43
1:A:277:C:OP2	17:Q:41:LYS:HE3	2.19	0.43
1:A:382:A:C2	1:A:383:A:C4	3.06	0.43
1:A:673:G:H5"	6:F:87:ARG:NH1	2.33	0.43
1:A:841:U:H6	1:A:848:C:H5'	1.82	0.43
1:A:1297:C:H4'	1:A:1298:C:H5'	2.00	0.43
4:D:117:ALA:O	4:D:121:VAL:HG23	2.18	0.43
5:E:142:LEU:O	5:E:143:ARG:HD3	2.17	0.43
9:I:65:VAL:HG11	9:I:73:GLN:CD	2.38	0.43
9:I:117:HIS:HB2	9:I:121:ARG:HG2	2.00	0.43
12:L:33:ARG:HB3	12:L:60:LEU:CD1	2.49	0.43
1:A:186:C:O3'	20:T:82:SER:HB2	2.19	0.43
1:A:392:G:H2'	1:A:393:A:C8	2.54	0.43
1:A:949:A:N1	1:A:1233:G:N3	2.67	0.43
1:A:1005:A:C2	1:A:1006:C:C2	3.07	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1022:G:H2'	1:A:1023:G:O4'	2.17	0.43
1:A:1052:U:O4	1:A:1200:C:C2	2.71	0.43
1:A:1198:G:C6	1:A:1199:U:C4	3.07	0.43
1:A:1468:A:O5'	1:A:1468:A:H8	2.02	0.43
1:A:1519[B]:MA6:N7	1:A:1520[B]:G:H1'	2.33	0.43
4:D:5:ILE:O	4:D:5:ILE:HG12	2.19	0.43
8:H:23:SER:HA	8:H:63:LEU:CD1	2.48	0.43
13:M:87:TYR:HA	13:M:90:LEU:CD2	2.48	0.43
15:O:79:ARG:HE	15:O:79:ARG:HB2	1.56	0.43
16:P:34:GLU:OE2	16:P:55:ARG:HD2	2.18	0.43
17:Q:24:GLU:HA	17:Q:38:ARG:O	2.18	0.43
17:Q:68:ARG:N	17:Q:70:ARG:HH12	2.16	0.43
18:R:23:LYS:HE3	18:R:57:GLY:O	2.17	0.43
1:A:261:U:O2	1:A:263:A:C8	2.71	0.43
1:A:358:U:H2'	1:A:359:U:C6	2.53	0.43
1:A:778:G:H1	1:A:804:U:H3	1.67	0.43
1:A:947:G:H1	1:A:1234:C:H42	1.65	0.43
1:A:1124:G:H22	1:A:1280:A:N6	2.17	0.43
3:C:114:PRO:O	3:C:118:GLN:HG3	2.19	0.43
4:D:31:CYS:C	4:D:33:MET:N	2.71	0.43
4:D:79:PHE:HA	4:D:93:PHE:CE2	2.53	0.43
9:I:49:PRO:HG2	9:I:50:LEU:HD12	1.99	0.43
11:K:77:MET:O	11:K:78:GLN:NE2	2.43	0.43
1:A:200:G:H2'	1:A:201:C:O4'	2.19	0.43
1:A:352:C:O2'	1:A:354:G:OP1	2.33	0.43
1:A:585:G:O5'	1:A:585:G:H8	2.00	0.43
1:A:674:G:H2'	1:A:675:A:H8	1.83	0.43
1:A:1213:A:C4	1:A:1215:G:C8	3.07	0.43
1:A:1256:A:N3	1:A:1256:A:O4'	2.51	0.43
3:C:101:LEU:HD23	3:C:101:LEU:HA	1.77	0.43
6:F:99:ALA:O	18:R:28:GLU:HG3	2.19	0.43
7:G:111:ARG:HB3	7:G:113:GLU:OE2	2.19	0.43
10:J:50:ILE:H	10:J:50:ILE:CD1	2.31	0.43
20:T:48:LYS:H	20:T:48:LYS:HG2	1.39	0.43
1:A:110:C:H2'	1:A:111:G:O4'	2.19	0.43
1:A:229:U:H2'	1:A:230:G:C8	2.54	0.43
1:A:332:G:H2'	1:A:333:G:H8	1.83	0.43
1:A:429:U:O3'	4:D:22:LYS:HE3	2.18	0.43
1:A:443:C:H2'	1:A:444:C:H6	1.82	0.43
1:A:925:G:O2'	1:A:926:G:H5"	2.18	0.43
1:A:1172:C:H2'	1:A:1173:G:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1192:C:P	3:C:4:LYS:HZ1	2.41	0.43
1:A:1220:G:H2'	1:A:1221:G:H8	1.84	0.43
1:A:1427:U:H2'	1:A:1428:A:H8	1.80	0.43
3:C:188:LEU:CD1	3:C:195:VAL:HG13	2.49	0.43
4:D:25:ARG:HA	4:D:28:SER:HB3	2.00	0.43
11:K:91:ARG:HB3	11:K:92:GLU:OE1	2.19	0.43
12:L:28:LYS:HB3	12:L:30:ALA:CB	2.49	0.43
15:O:32:LEU:HD22	15:O:32:LEU:HA	1.64	0.43
20:T:10:LEU:HD13	20:T:13:LEU:H	1.84	0.43
1:A:162:A:C5	1:A:163:C:H1'	2.54	0.43
1:A:1095:U:C4	1:A:1096:C:C4	3.06	0.43
1:A:1179:A:O3'	9:I:103:THR:HG23	2.19	0.43
1:A:1196:U:O2'	1:A:1197:G:OP1	2.33	0.43
1:A:1233:G:N2	1:A:1234:C:C2	2.87	0.43
1:A:1480:G:C6	1:A:1481:U:C4	3.06	0.43
1:A:1485:U:C6	1:A:1486:G:N7	2.87	0.43
3:C:23:TYR:CD1	10:J:11:PHE:CE2	3.07	0.43
4:D:90:GLY:N	4:D:204:ILE:HD11	2.34	0.43
5:E:79:GLU:HG3	5:E:79:GLU:H	1.48	0.43
6:F:21:LEU:HD12	6:F:21:LEU:HA	1.78	0.43
10:J:69:ASN:O	10:J:70:ARG:HG3	2.18	0.43
17:Q:29:HIS:O	17:Q:31:LEU:N	2.51	0.43
1:A:262:A:C6	1:A:263:A:C6	3.06	0.43
1:A:349:A:H2'	1:A:350:G:H5"	2.00	0.43
1:A:429:U:H4'	1:A:430:A:O5'	2.18	0.43
1:A:869:G:N7	24:A:2036:HOH:O	2.36	0.43
1:A:1525:G:C8	1:A:1525:G:H3'	2.54	0.43
3:C:91:LEU:HD23	3:C:99:VAL:HG21	2.00	0.43
10:J:50:ILE:N	10:J:50:ILE:CD1	2.81	0.43
12:L:84:LEU:HD13	12:L:105:TYR:HE1	1.84	0.43
16:P:80:PHE:N	16:P:80:PHE:CD1	2.87	0.43
1:A:449:C:C5	1:A:450:G:C5	3.06	0.43
1:A:695:A:H2'	1:A:696:A:H8	1.78	0.43
1:A:780:A:P	11:K:122:LYS:HG3	2.58	0.43
1:A:947:G:H2'	1:A:948:C:O4'	2.19	0.43
1:A:973:G:OP1	10:J:57:LYS:HD3	2.19	0.43
1:A:1124:G:H4'	1:A:1125:U:OP1	2.19	0.43
1:A:1152:A:H2'	1:A:1153:C:C6	2.54	0.43
1:A:1233:G:OP2	9:I:124:GLN:HB3	2.18	0.43
3:C:33:LEU:HD21	14:N:53:LEU:HD22	1.99	0.43
3:C:78:GLY:HA3	3:C:83:ARG:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:80:GLU:O	4:D:83:SER:N	2.50	0.43
6:F:8:ILE:HG21	6:F:26:ILE:HD11	2.01	0.43
12:L:28:LYS:HB3	12:L:30:ALA:H	1.84	0.43
14:N:26:ARG:HH12	14:N:47:LEU:HD22	1.82	0.43
15:O:8:LYS:O	15:O:12:ILE:HG13	2.19	0.43
18:R:64:ARG:HE	18:R:64:ARG:HB2	1.50	0.43
1:A:554:C:C2'	1:A:555:C:H5'	2.49	0.42
1:A:788:U:H2'	1:A:789:U:C6	2.54	0.42
1:A:1023:G:H2'	1:A:1023:G:N3	2.33	0.42
1:A:1361:G:H2'	1:A:1361(A):C:H6	1.84	0.42
2:B:49:GLU:O	2:B:52:GLU:HB3	2.19	0.42
4:D:67:ILE:O	4:D:114:ARG:HD2	2.18	0.42
10:J:47:PHE:HB2	10:J:63:PHE:HB2	2.01	0.42
13:M:22:ILE:HB	13:M:25:ILE:HB	2.01	0.42
14:N:22:THR:OG1	14:N:33:VAL:HG21	2.19	0.42
14:N:24:CYS:HB3	14:N:29:ARG:HB2	2.01	0.42
18:R:58:LEU:HD22	18:R:62:GLU:HB3	2.00	0.42
19:S:41:VAL:HB	19:S:42:PRO:HD2	2.01	0.42
1:A:267:C:H2'	1:A:268:C:H6	1.85	0.42
1:A:576:G:H3'	1:A:577:G:H5"	2.01	0.42
1:A:1029:C:H1'	1:A:1033:G:H1'	2.01	0.42
1:A:1039:C:H2'	1:A:1040:U:C6	2.54	0.42
1:A:1063:C:N4	1:A:1064:G:C2	2.87	0.42
1:A:1188:A:N7	1:A:1189:C:C5	2.87	0.42
3:C:152:ILE:HB	3:C:199:LYS:HB2	2.01	0.42
4:D:13:ARG:NH1	4:D:38:TYR:O	2.52	0.42
8:H:119:LEU:HD12	8:H:119:LEU:H	1.83	0.42
9:I:17:VAL:HG22	9:I:63:ILE:HD12	2.01	0.42
11:K:29:ILE:HD12	11:K:30:VAL:N	2.34	0.42
12:L:102:ARG:HE	12:L:102:ARG:HB3	1.52	0.42
17:Q:89:LEU:HA	17:Q:89:LEU:HD22	1.78	0.42
18:R:44:LEU:HD12	18:R:48:GLY:O	2.18	0.42
18:R:53:ARG:NH1	18:R:59:SER:HA	2.33	0.42
19:S:30:LEU:O	19:S:31:ILE:HB	2.18	0.42
1:A:148:G:H2'	1:A:149:A:H8	1.85	0.42
1:A:304:U:O2'	1:A:305:G:H5'	2.18	0.42
1:A:575:G:O2'	1:A:821:G:OP2	2.24	0.42
1:A:1178:G:N2	1:A:1180:A:H3'	2.34	0.42
6:F:95:GLU:HA	6:F:96:PRO:HD3	1.79	0.42
7:G:57:GLU:O	7:G:61:VAL:HG23	2.19	0.42
7:G:95:ARG:HG3	7:G:99:LEU:CD1	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:28:LYS:HB3	12:L:30:ALA:HB2	2.01	0.42
19:S:10:PHE:O	19:S:39:THR:HG23	2.18	0.42
20:T:20:LEU:HD13	20:T:20:LEU:N	2.34	0.42
20:T:60:GLU:HG3	20:T:81:LYS:HD2	2.01	0.42
1:A:52:G:C5	1:A:360:A:C2	3.07	0.42
1:A:134:A:C6	1:A:135:C:C2	3.08	0.42
1:A:328:C:H4'	1:A:329:A:H5'	2.00	0.42
1:A:526:C:H3'	1:A:527:7MG:O4'	2.19	0.42
1:A:561:U:O2'	1:A:562:C:P	2.78	0.42
1:A:1502:A:C2	1:A:1504:G:C2	3.07	0.42
2:B:17:PHE:HA	2:B:44:LEU:HD21	2.01	0.42
4:D:187:ARG:HD2	4:D:187:ARG:HA	1.35	0.42
5:E:63:ARG:HE	5:E:63:ARG:HB2	1.53	0.42
8:H:83:ILE:HA	8:H:136:GLU:O	2.18	0.42
9:I:40:LEU:CD1	9:I:70:LYS:HD2	2.50	0.42
12:L:66:VAL:HG22	12:L:67:THR:H	1.82	0.42
14:N:40:CYS:O	14:N:44:LEU:HB3	2.20	0.42
1:A:122:G:O2'	1:A:123:C:H5'	2.19	0.42
2:B:21:ARG:H	2:B:21:ARG:HG2	1.51	0.42
3:C:61:ALA:O	3:C:63:ASN:N	2.53	0.42
4:D:24:GLU:O	4:D:25:ARG:HB3	2.19	0.42
4:D:109:GLY:HA3	4:D:165:MET:SD	2.59	0.42
5:E:24:ARG:O	5:E:25:ARG:HG2	2.20	0.42
5:E:139:LEU:HA	5:E:142:LEU:HG	2.02	0.42
6:F:9:VAL:HG22	6:F:60:PHE:CE2	2.55	0.42
8:H:120:THR:OG1	8:H:122:ARG:HG3	2.20	0.42
9:I:124:GLN:HE21	9:I:124:GLN:HB2	1.57	0.42
20:T:13:LEU:HD12	20:T:14:LYS:N	2.34	0.42
1:A:115:G:H1'	1:A:116:A:N7	2.34	0.42
1:A:719:C:C5	1:A:720:C:C4	3.07	0.42
1:A:749:C:O2'	1:A:750:G:H5'	2.20	0.42
1:A:986:A:H2'	1:A:987:G:O4'	2.19	0.42
1:A:1130:A:OP1	1:A:1130:A:C8	2.67	0.42
1:A:1532:U:H3'	1:A:1532:U:H6	1.83	0.42
5:E:78:HIS:NE2	5:E:142:LEU:HA	2.35	0.42
6:F:16:GLN:OE1	6:F:16:GLN:HA	2.18	0.42
14:N:57:ARG:HG2	14:N:58:LYS:N	2.34	0.42
15:O:70:LEU:HD12	15:O:78:TYR:N	2.34	0.42
17:Q:87:LYS:O	17:Q:90:ILE:N	2.52	0.42
20:T:100:ILE:HG22	20:T:102:GLY:N	2.34	0.42
1:A:99:C:H2'	1:A:101:A:C8	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:G:P	24:A:1801:HOH:O	2.77	0.42
1:A:437:U:H5"	4:D:155:LEU:HD11	2.01	0.42
1:A:620:C:C2	4:D:135:LEU:HD22	2.54	0.42
1:A:687:A:H2'	1:A:701:C:H41	1.84	0.42
4:D:186:LEU:HD23	4:D:186:LEU:N	2.30	0.42
5:E:43:LEU:HD21	5:E:132:ALA:HB1	2.01	0.42
5:E:153:LYS:O	5:E:153:LYS:HG2	2.20	0.42
7:G:38:LEU:O	7:G:41:ARG:HB3	2.18	0.42
8:H:40:ALA:HB2	8:H:45:ILE:CD1	2.44	0.42
11:K:126:ARG:HG3	11:K:126:ARG:NH1	2.35	0.42
13:M:3:ARG:O	13:M:57:ARG:NE	2.50	0.42
14:N:43:CYS:O	14:N:46:GLU:N	2.53	0.42
16:P:36:ILE:HD13	16:P:36:ILE:HG21	1.76	0.42
20:T:74:LYS:HE2	20:T:74:LYS:HA	2.02	0.42
1:A:642:A:H2'	1:A:643:C:H6	1.84	0.42
1:A:653:A:O4'	8:H:56:LYS:HD3	2.19	0.42
1:A:807:A:C6	1:A:808:C:N4	2.87	0.42
1:A:1239:A:C4	1:A:1298:C:N4	2.88	0.42
1:A:1251:A:H2'	1:A:1252:A:C8	2.55	0.42
4:D:89:THR:O	4:D:92:VAL:HG12	2.20	0.42
4:D:108:LEU:HD23	4:D:108:LEU:HA	1.89	0.42
5:E:64:ARG:O	5:E:65:ASN:HB3	2.19	0.42
6:F:47:ARG:HH22	6:F:56:PRO:HB3	1.85	0.42
7:G:5:ARG:HH21	7:G:7:ALA:HA	1.84	0.42
9:I:69:GLY:O	9:I:73:GLN:HG3	2.19	0.42
10:J:23:ILE:HD12	10:J:72:VAL:HG21	2.01	0.42
10:J:88:LEU:N	10:J:88:LEU:CD2	2.80	0.42
19:S:70:LYS:HE3	19:S:70:LYS:HB3	1.76	0.42
1:A:363:A:OP2	12:L:34:ARG:NH1	2.52	0.42
1:A:390:C:H4'	16:P:28:ARG:HH21	1.85	0.42
1:A:514:C:C2'	1:A:515:G:H5'	2.49	0.42
1:A:849:C:H2'	1:A:850:U:H6	1.84	0.42
1:A:1309:G:N1	1:A:1329:A:C4	2.88	0.42
1:A:1518[A]:MA6:C6	1:A:1519[A]:MA6:H103	2.50	0.42
5:E:15:ARG:HA	5:E:28:PHE:CE2	2.55	0.42
5:E:26:PHE:CD1	5:E:26:PHE:N	2.88	0.42
7:G:38:LEU:HD23	7:G:38:LEU:HA	1.85	0.42
14:N:14:PRO:C	14:N:16:PHE:H	2.23	0.42
1:A:36:C:O2'	12:L:117:ARG:NH2	2.53	0.42
1:A:519:C:H2'	1:A:520:A:C8	2.55	0.42
1:A:1097:C:H2'	1:A:1098:C:C6	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1127:G:H8	1:A:1127:G:H3'	1.83	0.42
1:A:1316:G:O6	19:S:5:LEU:HD21	2.20	0.42
2:B:69:LEU:HB3	2:B:162:ILE:CD1	2.50	0.42
5:E:98:THR:N	5:E:117:ASP:OD1	2.53	0.42
6:F:37:VAL:HG12	6:F:39:LYS:O	2.20	0.42
15:O:4:THR:OG1	15:O:7:GLU:HG3	2.20	0.42
18:R:78:LEU:H	18:R:78:LEU:HG	1.60	0.42
1:A:579:G:H2'	1:A:580:U:C6	2.55	0.41
1:A:1108:G:H2'	1:A:1109:C:H5'	2.02	0.41
1:A:1112:C:C4	3:C:178:LEU:HD12	2.55	0.41
1:A:1226:C:H5"	19:S:80:TYR:CE2	2.54	0.41
1:A:1326:C:H2'	1:A:1327:C:C6	2.55	0.41
1:A:1350:A:H2'	1:A:1351:U:C6	2.55	0.41
2:B:209:ARG:HD3	2:B:239:VAL:HG11	2.02	0.41
5:E:95:ALA:HB1	5:E:96:PRO:HD2	2.01	0.41
9:I:7:THR:O	9:I:15:ALA:O	2.38	0.41
20:T:89:ARG:HG2	20:T:90:GLN:N	2.35	0.41
1:A:257:G:C2	1:A:270:A:C2	3.08	0.41
1:A:373:A:C2	1:A:482:A:C6	3.08	0.41
1:A:671:G:N3	1:A:671:G:H2'	2.34	0.41
1:A:801:U:H2'	1:A:802:A:C8	2.55	0.41
1:A:829:G:N2	1:A:830:G:H1'	2.35	0.41
1:A:1107:C:OP1	3:C:172:ARG:HB2	2.20	0.41
1:A:1136:U:H6	1:A:1136:U:H2'	1.61	0.41
1:A:1453:G:H2'	1:A:1454:G:O4'	2.20	0.41
1:A:1497:G:C2'	1:A:1498:UR3:H5'	2.50	0.41
2:B:74:LYS:NZ	2:B:76:GLN:HG3	2.35	0.41
2:B:100:GLY:O	2:B:104:ASN:N	2.50	0.41
2:B:213:LEU:O	2:B:217:ARG:HG2	2.20	0.41
5:E:90:VAL:O	5:E:120:THR:HA	2.20	0.41
8:H:5:PRO:O	8:H:8:ASP:HB3	2.19	0.41
15:O:29:VAL:HG21	15:O:67:LEU:HG	2.03	0.41
1:A:33:A:O2'	1:A:363:A:H1'	2.20	0.41
1:A:146:G:C2	1:A:147:G:C8	3.09	0.41
1:A:273:A:N6	1:A:274:A:C6	2.89	0.41
1:A:289:G:N2	1:A:290:C:C2	2.88	0.41
1:A:552:U:O2'	12:L:86:ARG:O	2.34	0.41
1:A:672:U:H2'	1:A:673:G:H8	1.86	0.41
1:A:1026:G:C8	1:A:1026:G:C3'	3.02	0.41
6:F:74:ASP:HA	6:F:77:ARG:HH11	1.85	0.41
8:H:99:GLU:O	8:H:101:PRO:HD3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:80:LYS:HG2	10:J:83:GLU:OE2	2.21	0.41
13:M:37:THR:HG21	13:M:56:LEU:HA	2.01	0.41
13:M:90:LEU:O	13:M:93:ARG:HB3	2.21	0.41
1:A:563:A:N7	1:A:567:G:H1'	2.36	0.41
1:A:670:G:C4	1:A:671:G:C8	3.08	0.41
1:A:688:G:H5'	11:K:46:GLY:O	2.19	0.41
1:A:1071:C:H2'	1:A:1072:G:C8	2.55	0.41
1:A:1516[A]:G:H2'	1:A:1518[A]:MA6:OP2	2.20	0.41
3:C:75:VAL:O	3:C:83:ARG:HD3	2.21	0.41
4:D:13:ARG:HD2	4:D:36:ARG:O	2.21	0.41
4:D:124:GLY:HA3	4:D:132:ARG:NH1	2.35	0.41
5:E:43:LEU:HD12	5:E:43:LEU:HA	1.72	0.41
5:E:110:LEU:HD13	5:E:118:ILE:HD13	2.01	0.41
7:G:101:LEU:HD12	7:G:101:LEU:H	1.84	0.41
8:H:101:PRO:HG3	8:H:133:LEU:HD11	2.00	0.41
12:L:98:TYR:CD1	12:L:98:TYR:N	2.89	0.41
1:A:486:U:C2	1:A:487:A:C8	3.08	0.41
1:A:524:G:C6	1:A:525:C:N4	2.89	0.41
1:A:667:G:H4'	15:O:51:HIS:CE1	2.55	0.41
1:A:996:A:N1	1:A:1045:C:O2'	2.47	0.41
1:A:1104:G:H4'	2:B:111:ARG:HD3	2.03	0.41
2:B:187:LEU:HA	2:B:187:LEU:HD23	1.81	0.41
3:C:77:ILE:CG2	3:C:81:GLY:HA2	2.47	0.41
3:C:95:THR:O	3:C:97:LYS:N	2.53	0.41
4:D:4:TYR:CE2	4:D:11:LEU:HD11	2.54	0.41
6:F:24:GLU:O	6:F:27:GLN:N	2.53	0.41
10:J:34:VAL:CG1	10:J:74:ILE:HG22	2.49	0.41
10:J:75:ILE:HG22	10:J:76:ASN:OD1	2.21	0.41
13:M:105:THR:O	13:M:107:ALA:N	2.53	0.41
19:S:36:ARG:HG2	19:S:51:VAL:HG12	2.02	0.41
1:A:103:C:P	20:T:17:ARG:HH12	2.41	0.41
1:A:179:A:H2'	1:A:180:U:H6	1.86	0.41
1:A:1417:G:N2	1:A:1484:C:N4	2.69	0.41
4:D:6:GLY:O	4:D:8:VAL:HG23	2.20	0.41
7:G:26:PHE:CA	7:G:101:LEU:HD23	2.50	0.41
1:A:21:G:H2'	1:A:22:G:C8	2.55	0.41
1:A:344:A:H5'	1:A:345:C:H5	1.85	0.41
1:A:666:G:C2	1:A:741:G:C4	3.08	0.41
1:A:682:G:N1	1:A:709:G:C6	2.89	0.41
1:A:833:U:O2	1:A:854:G:C2	2.73	0.41
1:A:1220:G:H2'	1:A:1221:G:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1367:C:C2	1:A:1368:G:C8	3.08	0.41
1:A:1469:G:H8	1:A:1469:G:O5'	2.03	0.41
2:B:52:GLU:HG3	2:B:53:ARG:N	2.35	0.41
3:C:45:LYS:NZ	3:C:45:LYS:HA	2.36	0.41
4:D:206:PHE:CD2	4:D:207:TYR:CD1	3.07	0.41
7:G:18:TYR:N	7:G:18:TYR:CD1	2.88	0.41
12:L:42:THR:HA	12:L:53:ARG:O	2.21	0.41
18:R:87:ARG:CG	18:R:88:LYS:H	2.30	0.41
19:S:18:LYS:HE3	19:S:31:ILE:HG12	2.01	0.41
1:A:254:G:C4	1:A:255:G:C8	3.09	0.41
1:A:264:U:O2'	17:Q:63:ARG:HG2	2.20	0.41
1:A:353:A:H5'	1:A:353:A:C8	2.52	0.41
1:A:682:G:N3	1:A:683:G:C8	2.88	0.41
1:A:806:C:H2'	1:A:807:A:C8	2.56	0.41
1:A:1023:G:H3'	1:A:1024:G:C5'	2.49	0.41
1:A:1134:G:N2	1:A:1140:C:N3	2.54	0.41
1:A:1189:C:H5'	14:N:58:LYS:NZ	2.35	0.41
1:A:1277:C:H3'	1:A:1277:C:H6	1.84	0.41
1:A:1403:C:H3'	1:A:1404:5MC:HM51	2.02	0.41
1:A:1464:G:O2'	1:A:1465:C:H5'	2.21	0.41
10:J:23:ILE:HD13	10:J:23:ILE:HG21	1.86	0.41
10:J:55:LYS:CG	10:J:56:HIS:H	2.19	0.41
18:R:36:ASN:CG	18:R:39:VAL:HG12	2.41	0.41
20:T:45:GLN:HB2	20:T:91:LEU:HG	2.01	0.41
1:A:190(J):U:H2'	1:A:190(K):G:H8	1.84	0.41
1:A:199:G:O2'	1:A:200:G:H5'	2.21	0.41
1:A:420:U:O2'	1:A:423:G:O6	2.30	0.41
1:A:475:G:H2'	1:A:476:G:C8	2.56	0.41
1:A:519:C:H41	1:A:533:A:N6	2.18	0.41
1:A:587:G:O2'	1:A:588:G:OP2	2.32	0.41
1:A:665:A:C2	1:A:732:C:C2	3.09	0.41
1:A:794:A:H2'	1:A:795:C:C6	2.55	0.41
1:A:875:C:H1'	8:H:15:ASN:OD1	2.21	0.41
1:A:939:G:H5'	7:G:102:ARG:NH1	2.36	0.41
1:A:1068:G:N3	1:A:1191:A:C2	2.89	0.41
1:A:1326:C:H2'	1:A:1327:C:H6	1.86	0.41
1:A:1428:A:H2'	1:A:1429:C:C6	2.55	0.41
1:A:1442:G:N1	1:A:1446:A:C6	2.89	0.41
2:B:74:LYS:HB3	2:B:74:LYS:HZ2	1.84	0.41
2:B:76:GLN:OE1	2:B:207:ALA:N	2.54	0.41
3:C:85:ARG:NH1	3:C:86:VAL:HG23	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:68:GLU:OE1	5:E:68:GLU:N	2.54	0.41
5:E:123:LEU:HA	5:E:123:LEU:HD23	1.73	0.41
7:G:15:ASP:HB3	7:G:24:THR:HG23	2.02	0.41
7:G:22:LEU:HD23	7:G:62:PHE:HE2	1.85	0.41
7:G:149:ARG:HD2	11:K:59:TYR:CD1	2.55	0.41
8:H:4:ASP:HA	8:H:5:PRO:HD2	1.91	0.41
8:H:24:THR:O	8:H:24:THR:HG23	2.21	0.41
10:J:8:LEU:O	10:J:69:ASN:HA	2.20	0.41
10:J:57:LYS:O	10:J:60:ARG:NH1	2.53	0.41
13:M:15:VAL:CG1	13:M:34:LEU:HD21	2.51	0.41
13:M:59:TYR:O	13:M:60:VAL:C	2.59	0.41
13:M:64:TRP:CD1	13:M:64:TRP:N	2.84	0.41
17:Q:51:TYR:CD1	17:Q:51:TYR:N	2.89	0.41
1:A:189:G:H2'	1:A:190:C:O4'	2.21	0.41
1:A:696:A:H8	1:A:696:A:O5'	2.04	0.41
1:A:1039:C:O2'	1:A:1040:U:O4'	2.36	0.41
1:A:1350:A:OP2	9:I:118:LYS:NZ	2.35	0.41
1:A:1406:U:H4'	1:A:1518[B]:MA6:H1'	2.03	0.41
1:A:1415:G:O6	1:A:1485:U:C4	2.74	0.41
1:A:1424:C:C4	1:A:1425:U:C5	3.08	0.41
2:B:60:ASP:OD2	2:B:64:ARG:HD2	2.21	0.41
3:C:190:ARG:H	3:C:190:ARG:HG2	1.65	0.41
4:D:11:LEU:HD13	4:D:66:ARG:HG2	2.03	0.41
6:F:6:VAL:HB	6:F:63:TYR:HB2	2.03	0.41
10:J:11:PHE:HE2	10:J:67:THR:HG23	1.86	0.41
10:J:27:ALA:O	10:J:30:SER:N	2.54	0.41
12:L:111:LYS:HE2	12:L:111:LYS:HB2	1.83	0.41
19:S:36:ARG:NH2	19:S:75:ALA:O	2.54	0.41
20:T:52:ALA:O	20:T:56:MET:HB3	2.20	0.41
1:A:90:U:H2'	1:A:91:C:C6	2.56	0.40
1:A:459:G:H8	1:A:459:G:O5'	2.04	0.40
1:A:569:C:H1'	1:A:574:A:C4	2.56	0.40
1:A:755:G:OP2	15:O:65:ARG:HD2	2.21	0.40
1:A:855:G:C6	1:A:856:C:C4	3.09	0.40
1:A:901:A:C5	1:A:902:G:H1'	2.57	0.40
1:A:939:G:OP1	7:G:102:ARG:NH1	2.50	0.40
1:A:1014:A:H2'	1:A:1015:A:C8	2.56	0.40
1:A:1084:G:H5'	1:A:1102:A:OP2	2.22	0.40
1:A:1116:C:C2'	1:A:1117:G:H5'	2.51	0.40
3:C:121:ALA:HB1	3:C:189:ALA:HB2	2.02	0.40
5:E:12:LEU:HD23	5:E:13:ILE:C	2.41	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:70:LEU:O	13:M:74:VAL:HG23	2.21	0.40
17:Q:56:VAL:O	17:Q:77:VAL:HB	2.21	0.40
1:A:544:G:C6	1:A:545:C:C4	3.09	0.40
1:A:993:G:H4'	1:A:994:A:OP2	2.20	0.40
1:A:1096:C:C2	1:A:1097:C:C5	3.10	0.40
1:A:1116:C:C2	1:A:1185:G:C2	3.09	0.40
1:A:1253:G:H1'	1:A:1355:G:O2'	2.21	0.40
1:A:1434:A:H61	1:A:1467:G:H1'	1.86	0.40
2:B:41:ILE:HG22	2:B:42:ILE:N	2.36	0.40
3:C:58:GLU:HB2	3:C:65:ALA:HB2	2.03	0.40
4:D:189:PRO:HB2	4:D:194:LEU:HD22	2.03	0.40
6:F:77:ARG:O	6:F:80:ARG:HB2	2.21	0.40
7:G:26:PHE:CD2	7:G:62:PHE:HE1	2.39	0.40
11:K:33:THR:HB	11:K:39:PRO:HA	2.03	0.40
12:L:120:TYR:O	12:L:122:THR:HG23	2.22	0.40
20:T:73:HIS:HB3	20:T:74:LYS:H	1.66	0.40
1:A:725:G:O2'	1:A:726:C:H5'	2.20	0.40
1:A:763:G:H2'	1:A:764:C:C6	2.57	0.40
1:A:1375:A:H4'	7:G:29:LYS:HE2	2.02	0.40
1:A:1416:G:N2	1:A:1485:U:O2'	2.55	0.40
1:A:1440:C:H5"	1:A:1441:G:OP2	2.21	0.40
1:A:1515[B]:C:N4	1:A:1520[B]:G:O6	2.51	0.40
2:B:54:THR:O	2:B:58:ILE:HG13	2.21	0.40
3:C:152:ILE:HD13	3:C:152:ILE:HA	1.70	0.40
4:D:50:ARG:HA	4:D:51:PRO:HD3	1.59	0.40
6:F:62:TRP:HB2	18:R:35:ARG:NH1	2.36	0.40
7:G:16:LEU:HD23	9:I:45:ALA:HB2	2.02	0.40
9:I:8:GLY:N	9:I:83:ARG:HD2	2.36	0.40
15:O:43:LEU:HA	15:O:43:LEU:HD23	1.83	0.40
1:A:190(E):U:C2	17:Q:63:ARG:NH1	2.89	0.40
1:A:317:G:C2'	1:A:318:G:H5'	2.51	0.40
1:A:407:G:H4'	4:D:116:GLN:HA	2.04	0.40
1:A:721:G:H8	1:A:721:G:O5'	2.04	0.40
1:A:1133:G:H2'	1:A:1134:G:O4'	2.21	0.40
3:C:44:GLU:HA	3:C:52:LEU:HD21	2.03	0.40
3:C:82:GLU:OE2	3:C:83:ARG:N	2.54	0.40
5:E:53:LEU:HA	5:E:53:LEU:HD13	1.63	0.40
5:E:118:ILE:O	5:E:119:LEU:HD23	2.21	0.40
7:G:74:GLU:OE2	7:G:95:ARG:NH2	2.49	0.40
8:H:37:ARG:HH11	8:H:37:ARG:HB3	1.86	0.40
8:H:41:ARG:NH1	8:H:42:GLU:HG2	2.27	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:54:PHE:O	10:J:55:LYS:HB3	2.21	0.40
14:N:8:GLU:O	14:N:11:LYS:HB3	2.21	0.40
15:O:5:LYS:O	15:O:9:GLN:HB2	2.22	0.40
15:O:27:VAL:HG12	15:O:31:LEU:HD22	2.04	0.40
17:Q:66:SER:O	17:Q:70:ARG:NH1	2.54	0.40
19:S:31:ILE:HA	19:S:32:LYS:NZ	2.36	0.40
19:S:40:ILE:HG23	19:S:44:MET:SD	2.62	0.40
1:A:134:A:C6	1:A:135:C:N3	2.89	0.40
1:A:148:G:C2	1:A:149:A:C5	3.10	0.40
1:A:302:G:N3	1:A:556:C:H4'	2.37	0.40
1:A:392:G:H2'	1:A:393:A:H8	1.85	0.40
1:A:463:A:OP2	16:P:75:ARG:NH1	2.54	0.40
1:A:673:G:H5"	6:F:87:ARG:CZ	2.51	0.40
1:A:745:C:O5'	1:A:745:C:H6	2.04	0.40
1:A:965:A:OP1	1:A:1198:G:H5"	2.21	0.40
1:A:1072:G:C6	1:A:1073:U:N3	2.89	0.40
1:A:1127:G:H3'	1:A:1127:G:C8	2.57	0.40
10:J:91:PRO:O	10:J:94:VAL:HG12	2.21	0.40
11:K:120:ARG:HH22	11:K:126:ARG:NH1	2.19	0.40
14:N:12:ARG:NH1	14:N:21:TYR:O	2.55	0.40
16:P:4:ILE:H	16:P:66:PRO:HA	1.86	0.40
18:R:46:GLU:CD	18:R:55:ARG:HH22	2.24	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%)	198 (85%)	29 (12%)	5 (2%)	6 37
3	C	204/239 (85%)	175 (86%)	27 (13%)	2 (1%)	15 51
4	D	206/209 (99%)	190 (92%)	16 (8%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	148/162 (91%)	139 (94%)	6 (4%)	3 (2%)	7	39
6	F	99/101 (98%)	97 (98%)	2 (2%)	0	100	100
7	G	153/156 (98%)	137 (90%)	16 (10%)	0	100	100
8	H	136/138 (99%)	127 (93%)	9 (7%)	0	100	100
9	I	125/128 (98%)	111 (89%)	12 (10%)	2 (2%)	9	43
10	J	96/105 (91%)	81 (84%)	13 (14%)	2 (2%)	7	38
11	K	114/129 (88%)	99 (87%)	15 (13%)	0	100	100
12	L	121/135 (90%)	106 (88%)	12 (10%)	3 (2%)	5	35
13	M	116/126 (92%)	94 (81%)	21 (18%)	1 (1%)	17	53
14	N	58/61 (95%)	48 (83%)	10 (17%)	0	100	100
15	O	85/89 (96%)	78 (92%)	7 (8%)	0	100	100
16	P	81/88 (92%)	70 (86%)	11 (14%)	0	100	100
17	Q	97/105 (92%)	89 (92%)	8 (8%)	0	100	100
18	R	68/88 (77%)	59 (87%)	9 (13%)	0	100	100
19	S	78/93 (84%)	67 (86%)	9 (12%)	2 (3%)	5	35
20	T	97/106 (92%)	79 (81%)	16 (16%)	2 (2%)	7	38
21	U	22/27 (82%)	21 (96%)	1 (4%)	0	100	100
All	All	2336/2541 (92%)	2065 (88%)	249 (11%)	22 (1%)	17	53

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	21	ARG
12	L	28	LYS
19	S	31	ILE
2	B	9	GLU
3	C	62	ASP
9	I	58	HIS
2	B	11	LEU
5	E	16	THR
9	I	119	ALA
12	L	25	PRO
2	B	78	GLN
3	C	27	LYS
5	E	118	ILE
10	J	35	SER

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Mol	Chain	Res	Type
20	T	71	THR
12	L	79	GLU
19	S	30	LEU
10	J	34	VAL
13	M	7	VAL
5	E	70	PRO
2	B	229	VAL
20	T	100	ILE

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%)	150 (74%)	52 (26%)	0 4
3	C	160/188 (85%)	121 (76%)	39 (24%)	0 5
4	D	180/181 (99%)	135 (75%)	45 (25%)	0 5
5	E	115/123 (94%)	88 (76%)	27 (24%)	1 5
6	F	90/90 (100%)	72 (80%)	18 (20%)	1 9
7	G	126/127 (99%)	103 (82%)	23 (18%)	1 11
8	H	119/119 (100%)	83 (70%)	36 (30%)	0 2
9	I	98/99 (99%)	77 (79%)	21 (21%)	1 7
10	J	87/92 (95%)	63 (72%)	24 (28%)	0 3
11	K	88/99 (89%)	69 (78%)	19 (22%)	1 7
12	L	103/110 (94%)	78 (76%)	25 (24%)	0 5
13	M	94/101 (93%)	71 (76%)	23 (24%)	0 5
14	N	49/50 (98%)	34 (69%)	15 (31%)	0 2
15	O	79/80 (99%)	61 (77%)	18 (23%)	1 6
16	P	72/74 (97%)	61 (85%)	11 (15%)	2 17
17	Q	94/97 (97%)	64 (68%)	30 (32%)	0 2
18	R	61/77 (79%)	45 (74%)	16 (26%)	0 4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
19	S	71/80 (89%)	52 (73%)	19 (27%)	0 4
20	T	76/82 (93%)	54 (71%)	22 (29%)	0 2
21	U	19/22 (86%)	18 (95%)	1 (5%)	22 52
All	All	1983/2111 (94%)	1499 (76%)	484 (24%)	0 5

All (484) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	8	LYS
2	B	12	GLU
2	B	19	HIS
2	B	20	GLU
2	B	21	ARG
2	B	24	TRP
2	B	33	TYR
2	B	51	LEU
2	B	52	GLU
2	B	53	ARG
2	B	67	THR
2	B	69	LEU
2	B	73	THR
2	B	79	ASP
2	B	82	ARG
2	B	83	MET
2	B	84	GLU
2	B	87	ARG
2	B	90	MET
2	B	96	ARG
2	B	105	PHE
2	B	109	SER
2	B	118	LEU
2	B	127	ILE
2	B	134	GLU
2	B	135	GLN
2	B	140	HIS
2	B	144	ARG
2	B	150	SER
2	B	154	LEU
2	B	155	LEU
2	B	157	ARG
2	B	160	ASP

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Mol	Chain	Res	Type
2	B	162	ILE
2	B	163	PHE
2	B	165	VAL
2	B	168	THR
2	B	169	LYS
2	B	170	GLU
2	B	172	ILE
2	B	174	VAL
2	B	175	ARG
2	B	178	ARG
2	B	184	VAL
2	B	187	LEU
2	B	205	ASP
2	B	206	ASP
2	B	213	LEU
2	B	221	LEU
2	B	223	ILE
2	B	226	ARG
2	B	239	VAL
3	C	3	ASN
3	C	12	LEU
3	C	14	ILE
3	C	15	THR
3	C	29	TYR
3	C	34	LEU
3	C	37	GLN
3	C	42	LEU
3	C	43	LEU
3	C	45	LYS
3	C	55	VAL
3	C	56	ASP
3	C	59	ARG
3	C	70	VAL
3	C	82	GLU
3	C	83	ARG
3	C	84	ILE
3	C	89	GLU
3	C	94	LEU
3	C	101	LEU
3	C	102	ASN
3	C	103	VAL
3	C	111	LEU

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Mol	Chain	Res	Type
3	C	116	VAL
3	C	119	ARG
3	C	120	VAL
3	C	122	GLU
3	C	138	VAL
3	C	144	SER
3	C	153	VAL
3	C	165	THR
3	C	167	TRP
3	C	172	ARG
3	C	175	LEU
3	C	178	LEU
3	C	188	LEU
3	C	190	ARG
3	C	192	THR
3	C	204	LEU
4	D	3	ARG
4	D	5	ILE
4	D	19	LEU
4	D	21	LEU
4	D	25	ARG
4	D	26	CYS
4	D	28	SER
4	D	35	ARG
4	D	38	TYR
4	D	39	PRO
4	D	47	ARG
4	D	50	ARG
4	D	61	LYS
4	D	64	LEU
4	D	66	ARG
4	D	71	SER
4	D	76	ARG
4	D	78	LEU
4	D	80	GLU
4	D	81	GLU
4	D	85	LYS
4	D	88	VAL
4	D	97	LEU
4	D	100	ARG
4	D	108	LEU
4	D	120	LEU

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Mol	Chain	Res	Type
4	D	122	ARG
4	D	127	THR
4	D	132	ARG
4	D	133	VAL
4	D	134	ASP
4	D	141	ARG
4	D	145	GLU
4	D	153	ARG
4	D	155	LEU
4	D	156	GLU
4	D	165	MET
4	D	181	MET
4	D	182	LYS
4	D	187	ARG
4	D	190	ASP
4	D	191	ARG
4	D	194	LEU
4	D	196	LEU
4	D	202	LEU
5	E	6	PHE
5	E	10	MET
5	E	12	LEU
5	E	20	GLN
5	E	24	ARG
5	E	25	ARG
5	E	26	PHE
5	E	27	ARG
5	E	31	LEU
5	E	41	VAL
5	E	47	LYS
5	E	51	VAL
5	E	63	ARG
5	E	64	ARG
5	E	75	THR
5	E	78	HIS
5	E	79	GLU
5	E	87	SER
5	E	100	VAL
5	E	105	VAL
5	E	116	THR
5	E	126	ARG
5	E	145	LYS

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Mol	Chain	Res	Type
5	E	148	VAL
5	E	150	ARG
5	E	151	LEU
5	E	153	LYS
6	F	10	LEU
6	F	24	GLU
6	F	25	ILE
6	F	30	LEU
6	F	36	ARG
6	F	39	LYS
6	F	43	LEU
6	F	45	LEU
6	F	47	ARG
6	F	55	ASP
6	F	61	LEU
6	F	70	ASP
6	F	74	ASP
6	F	80	ARG
6	F	82	ARG
6	F	83	ASP
6	F	93	SER
6	F	95	GLU
7	G	21	VAL
7	G	38	LEU
7	G	41	ARG
7	G	49	ILE
7	G	54	THR
7	G	62	PHE
7	G	72	ARG
7	G	73	MET
7	G	75	VAL
7	G	78	ARG
7	G	79	ARG
7	G	92	SER
7	G	94	ARG
7	G	122	HIS
7	G	126	ASP
7	G	131	LYS
7	G	135	VAL
7	G	137	LYS
7	G	139	GLU
7	G	141	VAL

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Mol	Chain	Res	Type
7	G	143	ARG
7	G	149	ARG
7	G	153	HIS
8	H	9	MET
8	H	12	ARG
8	H	18	ARG
8	H	22	GLU
8	H	23	SER
8	H	25	ASP
8	H	26	VAL
8	H	29	SER
8	H	37	ARG
8	H	39	LEU
8	H	41	ARG
8	H	45	ILE
8	H	48	TYR
8	H	49	GLU
8	H	51	VAL
8	H	53	VAL
8	H	59	LEU
8	H	60	ARG
8	H	63	LEU
8	H	64	LYS
8	H	75	ARG
8	H	82	HIS
8	H	83	ILE
8	H	84	ARG
8	H	85	ARG
8	H	91	ARG
8	H	97	VAL
8	H	102	ARG
8	H	104	ARG
8	H	113	SER
8	H	119	LEU
8	H	120	THR
8	H	122	ARG
8	H	133	LEU
8	H	134	ILE
8	H	135	CYS
9	I	2	GLU
9	I	14	VAL
9	I	23	ASN

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Mol	Chain	Res	Type
9	I	27	THR
9	I	42	ARG
9	I	56	LEU
9	I	65	VAL
9	I	79	LEU
9	I	85	LEU
9	I	91	ASP
9	I	96	LEU
9	I	102	LEU
9	I	108	VAL
9	I	111	ARG
9	I	113	LYS
9	I	116	LYS
9	I	118	LYS
9	I	121	ARG
9	I	124	GLN
9	I	126	SER
9	I	127	LYS
10	J	3	LYS
10	J	5	ARG
10	J	16	LEU
10	J	19	SER
10	J	21	GLN
10	J	24	VAL
10	J	29	ARG
10	J	44	VAL
10	J	45	ARG
10	J	60	ARG
10	J	61	GLU
10	J	62	HIS
10	J	66	ARG
10	J	67	THR
10	J	69	ASN
10	J	71	LEU
10	J	72	VAL
10	J	76	ASN
10	J	79	ARG
10	J	81	THR
10	J	84	GLN
10	J	88	LEU
10	J	95	GLU
10	J	97	GLU

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Mol	Chain	Res	Type
11	K	11	LYS
11	K	26	ASN
11	K	29	ILE
11	K	33	THR
11	K	36	ASP
11	K	47	VAL
11	K	51	LYS
11	K	62	GLN
11	K	66	LEU
11	K	67	ASP
11	K	75	TYR
11	K	82	VAL
11	K	83	ILE
11	K	87	THR
11	K	92	GLU
11	K	101	SER
11	K	105	VAL
11	K	112	THR
11	K	119	CYS
12	L	6	THR
12	L	18	VAL
12	L	19	ARG
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	46	LYS
12	L	47	LYS
12	L	52	LEU
12	L	59	ARG
12	L	60	LEU
12	L	61	THR
12	L	75	HIS
12	L	76	ASN
12	L	81	SER
12	L	82	VAL
12	L	89	ARG
12	L	97	ARG
12	L	111	LYS
12	L	114	LYS

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Mol	Chain	Res	Type
12	L	123	LYS
12	L	126	LYS
13	M	3	ARG
13	M	4	ILE
13	M	29	ARG
13	M	35	GLU
13	M	45	VAL
13	M	46	LYS
13	M	48	LEU
13	M	50	GLU
13	M	54	VAL
13	M	63	THR
13	M	64	TRP
13	M	65	LYS
13	M	66	LEU
13	M	70	LEU
13	M	81	LEU
13	M	90	LEU
13	M	102	ARG
13	M	105	THR
13	M	108	ARG
13	M	109	THR
13	M	115	LYS
13	M	116	THR
13	M	117	VAL
14	N	3	ARG
14	N	7	ILE
14	N	8	GLU
14	N	9	LYS
14	N	22	THR
14	N	24	CYS
14	N	25	VAL
14	N	26	ARG
14	N	29	ARG
14	N	33	VAL
14	N	41	ARG
14	N	42	ILE
14	N	44	LEU
14	N	47	LEU
14	N	50	LYS
15	O	18	PHE
15	O	22	THR

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Mol	Chain	Res	Type
15	O	29	VAL
15	O	31	LEU
15	O	32	LEU
15	O	38	ARG
15	O	39	LEU
15	O	47	LYS
15	O	49	ASP
15	O	57	LEU
15	O	62	GLN
15	O	63	ARG
15	O	66	LEU
15	O	70	LEU
15	O	76	GLU
15	O	77	ARG
15	O	79	ARG
15	O	82	ILE
16	P	1	MET
16	P	2	VAL
16	P	31	LYS
16	P	45	THR
16	P	48	TRP
16	P	55	ARG
16	P	65	GLN
16	P	68	ASP
16	P	75	ARG
16	P	80	PHE
16	P	83	GLU
17	Q	3	LYS
17	Q	5	VAL
17	Q	7	THR
17	Q	9	VAL
17	Q	11	VAL
17	Q	13	ASP
17	Q	16	GLN
17	Q	19	VAL
17	Q	22	LEU
17	Q	25	ARG
17	Q	34	LYS
17	Q	36	ILE
17	Q	48	GLU
17	Q	49	GLU
17	Q	53	LEU

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Mol	Chain	Res	Type
17	Q	59	ILE
17	Q	62	SER
17	Q	63	ARG
17	Q	68	ARG
17	Q	75	ARG
17	Q	79	SER
17	Q	81	ARG
17	Q	83	ASP
17	Q	86	GLU
17	Q	87	LYS
17	Q	88	TYR
17	Q	89	LEU
17	Q	98	LEU
17	Q	99	SER
17	Q	100	LYS
18	R	19	LYS
18	R	23	LYS
18	R	28	GLU
18	R	31	LEU
18	R	35	ARG
18	R	41	LYS
18	R	56	THR
18	R	64	ARG
18	R	65	ILE
18	R	69	THR
18	R	76	LEU
18	R	79	LEU
18	R	83	GLU
18	R	85	LEU
18	R	86	VAL
18	R	88	LYS
19	S	3	ARG
19	S	5	LEU
19	S	6	LYS
19	S	7	LYS
19	S	9	VAL
19	S	13	ASP
19	S	15	LEU
19	S	17	GLU
19	S	20	LEU
19	S	22	LEU
19	S	28	LYS

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Mol	Chain	Res	Type
19	S	29	ARG
19	S	32	LYS
19	S	43	GLU
19	S	48	THR
19	S	70	LYS
19	S	77	THR
19	S	79	THR
19	S	80	TYR
20	T	10	LEU
20	T	14	LYS
20	T	17	ARG
20	T	19	SER
20	T	20	LEU
20	T	22	ARG
20	T	24	LEU
20	T	27	LYS
20	T	36	LEU
20	T	41	ILE
20	T	45	GLN
20	T	46	GLU
20	T	48	LYS
20	T	50	GLU
20	T	53	LEU
20	T	56	MET
20	T	62	LEU
20	T	75	ASN
20	T	80	ARG
20	T	87	LYS
20	T	91	LEU
20	T	100	ILE
21	U	10	ARG

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

Mol	Chain	Res	Type
2	B	19	HIS
2	B	40	HIS
3	C	6	HIS
7	G	110	GLN
9	I	29	ASN
9	I	73	GLN
9	I	124	GLN

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Mol	Chain	Res	Type
10	J	13	HIS
10	J	33	GLN
15	O	62	GLN
20	T	16	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1505/1522 (98%)	357 (23%)	27 (1%)

All (357) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	4	U
1	A	7	G
1	A	9	G
1	A	12	U
1	A	15	G
1	A	16	A
1	A	30	U
1	A	31	G
1	A	32	A
1	A	39	G
1	A	47	C
1	A	48	C
1	A	51	A
1	A	81	U
1	A	82	U
1	A	83	U
1	A	101	A
1	A	109	A
1	A	115	G
1	A	116	A
1	A	117	G
1	A	121	C
1	A	129(A)	G
1	A	130	A
1	A	131	C
1	A	145	G
1	A	158	G
1	A	163	C

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Mol	Chain	Res	Type
1	A	179	A
1	A	182	U
1	A	183	G
1	A	190(E)	U
1	A	195	A
1	A	197	A
1	A	201	C
1	A	202	U
1	A	203	U
1	A	204	U
1	A	216	G
1	A	220	G
1	A	226	G
1	A	231	G
1	A	236	G
1	A	244	U
1	A	245	C
1	A	247	G
1	A	251	G
1	A	253	U
1	A	262	A
1	A	266	G
1	A	267	C
1	A	272	C
1	A	289	G
1	A	291	C
1	A	298	A
1	A	301	G
1	A	315	A
1	A	319	G
1	A	321	A
1	A	328	C
1	A	329	A
1	A	344	A
1	A	345	C
1	A	350	G
1	A	351	G
1	A	352	C
1	A	353	A
1	A	354	G
1	A	356	A
1	A	367	U

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Mol	Chain	Res	Type
1	A	371	G
1	A	372	C
1	A	373	A
1	A	384	G
1	A	390	C
1	A	398	C
1	A	406	G
1	A	409	G
1	A	412	A
1	A	413	G
1	A	421	U
1	A	422	C
1	A	424	G
1	A	429	U
1	A	430	A
1	A	439	A
1	A	452	A
1	A	454	C
1	A	456	C
1	A	460	A
1	A	461	C
1	A	462	G
1	A	484	G
1	A	485	G
1	A	486	U
1	A	496	A
1	A	497	A
1	A	498	U
1	A	500	G
1	A	503	C
1	A	504	C
1	A	505	G
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	524	G
1	A	526	C
1	A	527	7MG
1	A	531	U

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Mol	Chain	Res	Type
1	A	532	A
1	A	533	A
1	A	536	C
1	A	545	C
1	A	547	A
1	A	555	C
1	A	559	A
1	A	560	U
1	A	561	U
1	A	562	C
1	A	564	C
1	A	566	G
1	A	568	G
1	A	569	C
1	A	570	G
1	A	572	A
1	A	573	A
1	A	576	G
1	A	577	G
1	A	579	G
1	A	581	G
1	A	587	G
1	A	618	C
1	A	631	G
1	A	650	G
1	A	653	A
1	A	654	G
1	A	664	G
1	A	665	A
1	A	666	G
1	A	667	G
1	A	671	G
1	A	687	A
1	A	695	A
1	A	702	A
1	A	703	G
1	A	705	U
1	A	720	C
1	A	721	G
1	A	722	A
1	A	723	U
1	A	724	G

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Mol	Chain	Res	Type
1	A	730	G
1	A	734	G
1	A	741	G
1	A	749	C
1	A	751	U
1	A	753	A
1	A	755	G
1	A	760	G
1	A	766	A
1	A	774	G
1	A	777	A
1	A	781	A
1	A	782	A
1	A	783	C
1	A	784	C
1	A	787	A
1	A	789	U
1	A	793	U
1	A	794	A
1	A	798	G
1	A	801	U
1	A	802	A
1	A	815	A
1	A	817	C
1	A	818	G
1	A	821	G
1	A	827	U
1	A	828	A
1	A	839	U
1	A	840	C
1	A	841	U
1	A	848	C
1	A	852	G
1	A	858	G
1	A	870	U
1	A	872	A
1	A	873	A
1	A	874	G
1	A	885	G
1	A	922	G
1	A	926	G
1	A	927	G

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Mol	Chain	Res	Type
1	A	934	C
1	A	935	A
1	A	937	A
1	A	939	G
1	A	960	U
1	A	965	A
1	A	966	M2G
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	982	U
1	A	993	G
1	A	998	G
1	A	999	C
1	A	1003	G
1	A	1003(A)	G
1	A	1004	A
1	A	1005	A
1	A	1007	C
1	A	1009	G
1	A	1016	A
1	A	1021	G
1	A	1022	G
1	A	1024	G
1	A	1025	U
1	A	1026	G
1	A	1027	C
1	A	1028	C
1	A	1029	C
1	A	1030	C
1	A	1030(A)	G
1	A	1030(B)	C
1	A	1030(C)	G
1	A	1030(D)	A
1	A	1031	G
1	A	1032	G
1	A	1034	G
1	A	1035	A

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Mol	Chain	Res	Type
1	A	1039	C
1	A	1045	C
1	A	1050	G
1	A	1053	G
1	A	1054	C
1	A	1055	A
1	A	1056	U
1	A	1065	U
1	A	1079	G
1	A	1094	G
1	A	1095	U
1	A	1100	C
1	A	1101	A
1	A	1108	G
1	A	1118	C
1	A	1125	U
1	A	1126	U
1	A	1127	G
1	A	1129	C
1	A	1130	A
1	A	1131	G
1	A	1134	G
1	A	1135	U
1	A	1136	U
1	A	1137	C
1	A	1139	G
1	A	1140	C
1	A	1141	C
1	A	1145	C
1	A	1146	A
1	A	1151	A
1	A	1159	U
1	A	1160	G
1	A	1171	G
1	A	1172	C
1	A	1174	G
1	A	1182	G
1	A	1190	G
1	A	1196	U
1	A	1197	G
1	A	1198	G
1	A	1201	A

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Mol	Chain	Res	Type
1	A	1202	G
1	A	1203	C
1	A	1205	U
1	A	1211	U
1	A	1212	U
1	A	1213	A
1	A	1214	C
1	A	1224	G
1	A	1225	A
1	A	1227	A
1	A	1233	G
1	A	1238	A
1	A	1253	G
1	A	1256	A
1	A	1257	U
1	A	1258	G
1	A	1259	C
1	A	1270	C
1	A	1277	C
1	A	1278	U
1	A	1279	A
1	A	1280	A
1	A	1286	A
1	A	1287	A
1	A	1296	C
1	A	1298	C
1	A	1300	G
1	A	1302	U
1	A	1307	U
1	A	1320	C
1	A	1322	C
1	A	1323	G
1	A	1336	C
1	A	1338	G
1	A	1353	G
1	A	1363	A
1	A	1370	G
1	A	1379	G
1	A	1381	U
1	A	1394	A
1	A	1398	A
1	A	1399	C

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Mol	Chain	Res	Type
1	A	1400	5MC
1	A	1403	C
1	A	1418	A
1	A	1428	A
1	A	1432	G
1	A	1440	C
1	A	1442	G
1	A	1443	G
1	A	1447	G
1	A	1451	A
1	A	1453	G
1	A	1474	G
1	A	1475	G
1	A	1477	C
1	A	1478	C
1	A	1479	C
1	A	1481	U
1	A	1482	G
1	A	1485	U
1	A	1486	G
1	A	1487	G
1	A	1491	G
1	A	1493	A
1	A	1497	G
1	A	1498	UR3
1	A	1499	A
1	A	1502	A
1	A	1506	U
1	A	1529	G
1	A	1530	G
1	A	1533	C
1	A	1540	PSU
1	A	1541	PSU
1	A	1542	U
1	A	1544	U

All (27) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	115	G
1	A	129(A)	G
1	A	181	G

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Mol	Chain	Res	Type
1	A	204	U
1	A	250	A
1	A	350	G
1	A	428	G
1	A	429	U
1	A	484	G
1	A	485	G
1	A	499	A
1	A	509	A
1	A	518	C
1	A	525	C
1	A	559	A
1	A	748	C
1	A	793	U
1	A	992	U
1	A	1125	U
1	A	1126	U
1	A	1195	C
1	A	1201	A
1	A	1256	A
1	A	1277	C
1	A	1319	A
1	A	1380	U
1	A	1529	G

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	5MC	A	967	1	19,22,23	1.14	2 (10%)	26,32,35	1.15	3 (11%)
1	5MC	A	1404	1	19,22,23	1.40	3 (15%)	26,32,35	1.15	3 (11%)
1	MA6	A	1519[A]	1	19,26,27	1.23	3 (15%)	18,38,41	0.89	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	5MC	A	1407	1	19,22,23	1.08	2 (10%)	26,32,35	1.29	2 (7%)
12	0TD	L	92	12	8,9,10	1.58	1 (12%)	6,11,13	2.34	2 (33%)
1	M2G	A	966	1	20,27,28	1.57	2 (10%)	19,40,43	1.51	2 (10%)
1	PSU	A	516	22,1	18,21,22	1.28	3 (16%)	21,30,33	1.14	3 (14%)
1	5MC	A	1400	1	19,22,23	1.56	5 (26%)	26,32,35	1.15	4 (15%)
1	7MG	A	527	1	23,26,27	3.88	6 (26%)	27,39,42	2.37	8 (29%)
1	UR3	A	1498	1	19,22,23	1.33	3 (15%)	26,32,35	1.42	4 (15%)
1	MA6	A	1518[A]	1	19,26,27	1.24	1 (5%)	18,38,41	0.83	1 (5%)
1	MA6	A	1519[B]	1	19,26,27	1.86	5 (26%)	18,38,41	0.76	0
1	2MG	A	1207	22,1	18,26,27	1.39	2 (11%)	16,38,41	1.23	2 (12%)
1	PSU	A	1540	1	18,21,22	1.01	1 (5%)	21,30,33	1.64	3 (14%)
1	PSU	A	1541	1	18,21,22	1.08	3 (16%)	21,30,33	1.94	6 (28%)
1	4OC	A	1402	1	20,23,24	1.14	2 (10%)	25,32,35	0.98	2 (8%)
1	MA6	A	1518[B]	1	19,26,27	1.43	4 (21%)	18,38,41	0.82	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	A	967	1	-	0/7/25/26	0/2/2/2
1	5MC	A	1404	1	-	0/7/25/26	0/2/2/2
1	MA6	A	1519[A]	1	-	4/7/29/30	0/3/3/3
1	5MC	A	1407	1	-	0/7/25/26	0/2/2/2
12	0TD	L	92	12	-	3/7/12/14	-
1	M2G	A	966	1	-	2/7/29/30	0/3/3/3
1	PSU	A	516	22,1	-	0/7/25/26	0/2/2/2
1	5MC	A	1400	1	-	2/7/25/26	0/2/2/2
1	7MG	A	527	1	-	1/7/37/38	0/3/3/3
1	UR3	A	1498	1	-	0/7/25/26	0/2/2/2
1	MA6	A	1518[A]	1	-	3/7/29/30	0/3/3/3
1	MA6	A	1519[B]	1	-	4/7/29/30	0/3/3/3
1	2MG	A	1207	22,1	-	0/5/27/28	0/3/3/3
1	PSU	A	1540	1	-	0/7/25/26	0/2/2/2
1	PSU	A	1541	1	-	3/7/25/26	0/2/2/2
1	4OC	A	1402	1	-	2/9/29/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MA6	A	1518[B]	1	-	6/7/29/30	0/3/3/3

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	527	7MG	C8-N9	-16.46	1.35	1.45
1	A	1519[B]	MA6	C6-N1	5.09	1.39	1.32
1	A	527	7MG	C5-N7	4.67	1.41	1.35
1	A	1518[A]	MA6	C6-C5	-4.57	1.37	1.44
1	A	1207	2MG	C5-C6	-4.27	1.39	1.47
1	A	966	M2G	C2-N2	4.23	1.42	1.35
1	A	1518[B]	MA6	C6-N1	4.01	1.38	1.32
1	A	527	7MG	C6-N1	-3.83	1.31	1.38
1	A	1400	5MC	C2-N1	3.81	1.48	1.40
1	A	966	M2G	C2-N3	3.74	1.35	1.30
1	A	527	7MG	C2-N1	-3.49	1.29	1.37
12	L	92	0TD	CB-CA	-3.44	1.53	1.54
1	A	516	PSU	C6-C5	3.40	1.39	1.35
1	A	1540	PSU	C6-C5	3.26	1.38	1.35
1	A	1519[B]	MA6	C2-N1	3.26	1.39	1.33
1	A	1400	5MC	C2-N3	3.21	1.42	1.36
1	A	1402	4OC	O2-C2	-3.10	1.17	1.23
1	A	1519[B]	MA6	C6-N6	3.10	1.44	1.37
1	A	527	7MG	C2-N2	3.00	1.41	1.34
1	A	967	5MC	C5-C4	-2.98	1.41	1.44
1	A	1498	UR3	C3U-N3	-2.97	1.41	1.47
1	A	1519[B]	MA6	C2-N3	2.94	1.36	1.32
1	A	1404	5MC	O2-C2	-2.90	1.18	1.23
1	A	1404	5MC	C2-N3	2.82	1.41	1.36
1	A	1519[A]	MA6	C6-N1	2.74	1.36	1.32
1	A	1541	PSU	C6-C5	2.74	1.38	1.35
1	A	1400	5MC	C6-N1	-2.73	1.33	1.38
1	A	1402	4OC	C6-N1	-2.71	1.31	1.38
1	A	1519[A]	MA6	C2-N1	2.64	1.38	1.33
1	A	1519[B]	MA6	C4-N3	2.57	1.39	1.35
1	A	1400	5MC	C5-C4	-2.47	1.42	1.44
1	A	967	5MC	C2-N1	2.43	1.45	1.40
1	A	1518[B]	MA6	C6-N6	2.40	1.43	1.37
1	A	1498	UR3	O4-C4	2.39	1.28	1.23
1	A	1404	5MC	C5-C4	-2.36	1.42	1.44
1	A	516	PSU	O4'-C1'	-2.35	1.40	1.43
1	A	1519[A]	MA6	C6-C5	-2.28	1.41	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1407	5MC	C5-C4	-2.27	1.42	1.44
1	A	516	PSU	C4-C5	-2.27	1.38	1.44
1	A	1541	PSU	O4'-C1'	-2.24	1.40	1.43
1	A	1518[B]	MA6	C2-N1	2.23	1.37	1.33
1	A	1518[B]	MA6	C2-N3	2.22	1.35	1.32
1	A	1207	2MG	C2-N2	2.20	1.38	1.33
1	A	1407	5MC	C2-N3	2.20	1.40	1.36
1	A	1498	UR3	C4-N3	-2.19	1.36	1.40
1	A	1400	5MC	O2-C2	2.10	1.27	1.23
1	A	1541	PSU	C4-C5	-2.04	1.38	1.44
1	A	527	7MG	C8-N7	-2.01	1.32	1.42

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	527	7MG	C5-C6-N1	5.06	119.84	110.94
12	L	92	0TD	CSB-SB-CB	-4.67	93.96	102.36
1	A	527	7MG	N9-C8-N7	4.66	109.97	103.37
1	A	527	7MG	C2-N3-C4	4.54	120.12	112.30
1	A	527	7MG	C5-C4-N3	-4.43	119.81	128.13
1	A	1540	PSU	C4-N3-C2	-4.42	120.28	126.37
1	A	527	7MG	N9-C4-N3	4.37	131.87	125.46
1	A	1541	PSU	C4-N3-C2	-4.15	120.65	126.37
1	A	966	M2G	O6-C6-N1	-3.96	115.92	120.62
1	A	1541	PSU	N1-C2-N3	3.96	119.34	115.17
1	A	1541	PSU	O2-C2-N1	-3.88	118.78	122.79
1	A	966	M2G	O6-C6-C5	3.82	131.90	124.32
1	A	1540	PSU	N1-C2-N3	3.79	119.16	115.17
1	A	527	7MG	C6-C5-C4	-3.38	116.45	122.40
1	A	1541	PSU	C6-C5-C4	3.33	120.42	118.17
1	A	1407	5MC	C1'-N1-C6	-3.32	115.68	121.15
1	A	1207	2MG	O6-C6-N1	-3.18	116.85	120.62
1	A	527	7MG	C6-C5-N7	3.09	136.72	131.93
1	A	1498	UR3	O3'-C3'-C2'	3.08	121.69	111.82
1	A	527	7MG	C2-N1-C6	-2.89	119.86	125.11
1	A	516	PSU	C4-N3-C2	-2.89	122.38	126.37
1	A	1207	2MG	O6-C6-C5	2.81	129.90	124.32
1	A	1498	UR3	C6-N1-C2	-2.67	119.62	121.80
1	A	967	5MC	C5-C4-N3	2.59	124.41	121.75
1	A	1400	5MC	C1'-N1-C6	-2.57	116.92	121.15
1	A	1407	5MC	C5-C4-N3	2.49	124.31	121.75
1	A	1400	5MC	O2-C2-N1	2.44	123.67	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1404	5MC	C1'-N1-C2	2.42	123.78	118.44
1	A	1541	PSU	O4'-C1'-C2'	2.36	108.42	105.15
1	A	1541	PSU	C6-N1-C2	-2.34	120.52	122.69
1	A	1402	4OC	C2'-C1'-N1	-2.34	109.80	114.24
1	A	1540	PSU	C6-N1-C2	-2.23	120.62	122.69
1	A	1498	UR3	C4-N3-C2	2.22	126.36	124.58
1	A	967	5MC	C4-N3-C2	-2.19	117.77	120.81
1	A	1404	5MC	C4-N3-C2	-2.18	117.78	120.81
1	A	1404	5MC	C1'-N1-C6	-2.18	117.56	121.15
1	A	516	PSU	O4'-C1'-C2'	2.17	108.16	105.15
1	A	1402	4OC	C5-C4-N4	-2.16	117.65	122.40
1	A	967	5MC	N4-C4-N3	-2.13	114.65	118.51
1	A	1400	5MC	C1'-N1-C2	2.08	123.04	118.44
1	A	1518[A]	MA6	N1-C6-N6	-2.06	114.45	116.83
1	A	1400	5MC	N4-C4-N3	-2.06	114.77	118.51
1	A	1498	UR3	C5-C4-N3	-2.03	112.36	115.04
1	A	516	PSU	O4-C4-C5	-2.03	118.96	124.01
12	L	92	0TD	CB-CA-N	-2.03	104.98	109.10

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	966	M2G	O4'-C4'-C5'-O5'
1	A	1402	4OC	O4'-C4'-C5'-O5'
1	A	1402	4OC	C3'-C4'-C5'-O5'
1	A	1518[A]	MA6	O4'-C4'-C5'-O5'
1	A	1518[A]	MA6	C3'-C4'-C5'-O5'
1	A	1518[B]	MA6	O4'-C4'-C5'-O5'
1	A	1518[B]	MA6	C3'-C4'-C5'-O5'
1	A	1518[B]	MA6	C5-C6-N6-C9
1	A	1518[B]	MA6	C5-C6-N6-C10
1	A	1518[B]	MA6	N1-C6-N6-C9
1	A	1518[B]	MA6	N1-C6-N6-C10
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-C10
12	L	92	0TD	O-C-CA-CB
1	A	1400	5MC	O4'-C4'-C5'-O5'
1	A	1519[B]	MA6	C3'-C4'-C5'-O5'
1	A	1541	PSU	O4'-C4'-C5'-O5'
1	A	527	7MG	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
1	A	1519[A]	MA6	C4'-C5'-O5'-P
1	A	966	M2G	C3'-C4'-C5'-O5'
1	A	1519[B]	MA6	N1-C6-N6-C9
1	A	1519[B]	MA6	O4'-C4'-C5'-O5'
1	A	1400	5MC	C3'-C4'-C5'-O5'
1	A	1541	PSU	C3'-C4'-C5'-O5'
12	L	92	0TD	CG-CB-SB-CSB
1	A	1518[A]	MA6	C5-C6-N6-C10
1	A	1519[B]	MA6	C5-C6-N6-C9
12	L	92	0TD	SB-CB-CG-OD1
1	A	1541	PSU	O4'-C1'-C5-C4

There are no ring outliers.

14 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	967	5MC	5	0
1	A	1404	5MC	2	0
1	A	1519[A]	MA6	2	0
1	A	966	M2G	2	0
1	A	516	PSU	1	0
1	A	1400	5MC	2	0
1	A	527	7MG	3	0
1	A	1498	UR3	1	0
1	A	1518[A]	MA6	3	0
1	A	1519[B]	MA6	4	0
1	A	1540	PSU	1	0
1	A	1541	PSU	1	0
1	A	1402	4OC	1	0
1	A	1518[B]	MA6	4	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 174 ligands modelled in this entry, 174 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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	1500/1522 (98%)	0.01	28 (1%)	66	58	107, 152, 229, 333	0
2	B	234/256 (91%)	-0.15	2 (0%)	84	78	122, 170, 240, 274	0
3	C	206/239 (86%)	-0.05	3 (1%)	73	65	121, 156, 199, 229	0
4	D	208/209 (99%)	0.13	19 (9%)	9	7	104, 151, 206, 237	0
5	E	150/162 (92%)	-0.01	6 (4%)	38	31	93, 132, 172, 216	0
6	F	101/101 (100%)	-0.43	2 (1%)	65	56	135, 171, 201, 254	0
7	G	155/156 (99%)	-0.37	7 (4%)	33	27	145, 183, 228, 254	0
8	H	138/138 (100%)	-0.25	0	100	100	114, 143, 181, 226	0
9	I	127/128 (99%)	-0.35	3 (2%)	59	49	149, 182, 222, 246	0
10	J	98/105 (93%)	0.10	7 (7%)	16	12	136, 186, 225, 252	0
11	K	116/129 (89%)	0.35	11 (9%)	8	7	134, 168, 207, 226	0
12	L	123/135 (91%)	0.38	10 (8%)	12	9	106, 137, 168, 224	0
13	M	118/126 (93%)	0.48	12 (10%)	6	6	149, 192, 225, 299	0
14	N	60/61 (98%)	-0.41	0	100	100	133, 161, 214, 240	0
15	O	87/89 (97%)	-0.16	0	100	100	128, 160, 194, 201	0
16	P	83/88 (94%)	0.61	8 (9%)	8	6	126, 148, 181, 205	0
17	Q	99/105 (94%)	0.07	5 (5%)	28	24	120, 144, 178, 199	0
18	R	70/88 (79%)	0.20	3 (4%)	35	29	131, 165, 237, 266	0
19	S	80/93 (86%)	0.39	4 (5%)	28	24	157, 197, 240, 268	0
20	T	99/106 (93%)	-0.32	1 (1%)	82	75	123, 154, 196, 214	0
21	U	24/27 (88%)	1.28	5 (20%)	1	1	172, 194, 241, 254	0
All	All	3876/4063 (95%)	0.01	136 (3%)	44	35	93, 159, 221, 333	0

All (136) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1129	C	5.9
4	D	35	ARG	5.7
1	A	1030(D)	A	5.5
1	A	1003	G	5.3
6	F	101	ALA	4.7
13	M	2	ALA	4.6
11	K	31	THR	4.5
21	U	18	TYR	4.2
1	A	412	A	4.2
7	G	2	ALA	4.1
5	E	19	MET	4.1
7	G	3	ARG	4.1
4	D	45	GLN	4.1
1	A	1283	G	4.0
1	A	1003(A)	G	3.9
5	E	20	GLN	3.9
11	K	19	ALA	3.8
1	A	1031	G	3.7
16	P	39	TYR	3.6
10	J	71	LEU	3.6
12	L	72	GLY	3.5
13	M	3	ARG	3.5
11	K	21	ILE	3.5
13	M	4	ILE	3.4
4	D	42	GLN	3.4
4	D	25	ARG	3.4
4	D	24	GLU	3.3
1	A	1024	G	3.3
4	D	40	PRO	3.3
11	K	118	GLY	3.3
4	D	29	PRO	3.2
21	U	17	THR	3.2
13	M	10	PRO	3.2
10	J	39	PRO	3.2
16	P	17	TYR	3.1
10	J	72	VAL	3.1
5	E	18	ARG	3.0
1	A	1002	G	3.0
5	E	25	ARG	3.0
10	J	38	ILE	3.0
16	P	16	HIS	3.0
19	S	53	ASN	3.0
11	K	42	TRP	2.9

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Mol	Chain	Res	Type	RSRZ
7	G	7	ALA	2.8
4	D	30	LYS	2.8
1	A	1027	C	2.8
12	L	62	SER	2.8
4	D	13	ARG	2.8
19	S	77	THR	2.8
16	P	6	LEU	2.8
21	U	24	ARG	2.8
4	D	38	TYR	2.7
6	F	99	ALA	2.7
7	G	6	ARG	2.7
12	L	71	PRO	2.7
1	A	1282	C	2.7
1	A	1030(C)	G	2.6
16	P	7	ALA	2.6
1	A	1128	C	2.6
1	A	653	A	2.6
12	L	28	LYS	2.6
4	D	36	ARG	2.6
1	A	1334	G	2.5
16	P	18	ARG	2.5
1	A	1040	U	2.5
1	A	1030	C	2.5
1	A	706	A	2.5
19	S	78	ARG	2.5
17	Q	45	HIS	2.5
1	A	1032	G	2.5
18	R	29	PHE	2.5
5	E	89	ILE	2.5
11	K	30	VAL	2.5
17	Q	43	LEU	2.4
9	I	16	ARG	2.4
3	C	76	VAL	2.4
12	L	31	PRO	2.4
4	D	28	SER	2.4
7	G	4	ARG	2.4
13	M	96	LEU	2.4
4	D	110	PHE	2.4
1	A	1398	A	2.4
4	D	44	GLY	2.4
13	M	9	ILE	2.4
1	A	1026	G	2.4

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Mol	Chain	Res	Type	RSRZ
4	D	23	GLY	2.4
7	G	8	GLU	2.3
10	J	37	PRO	2.3
12	L	102	ARG	2.3
10	J	35	SER	2.3
19	S	32	LYS	2.3
21	U	25	LYS	2.3
1	A	1124	G	2.3
1	A	1039	C	2.3
13	M	97	PRO	2.3
4	D	34	GLU	2.3
1	A	1127	G	2.3
11	K	111	ASP	2.3
1	A	1034	G	2.3
2	B	28	PHE	2.3
1	A	411	A	2.3
11	K	29	ILE	2.3
13	M	19	LEU	2.3
12	L	120	TYR	2.2
5	E	17	ALA	2.2
11	K	28	THR	2.2
4	D	112	VAL	2.2
3	C	52	LEU	2.2
11	K	20	TYR	2.2
1	A	3	G	2.2
1	A	1067	A	2.2
10	J	40	LEU	2.2
13	M	15	VAL	2.2
21	U	21	TYR	2.1
12	L	87	GLY	2.1
13	M	45	VAL	2.1
12	L	32	PHE	2.1
4	D	157	LEU	2.1
13	M	11	ARG	2.1
17	Q	32	TYR	2.1
7	G	5	ARG	2.1
9	I	15	ALA	2.1
20	T	65	LYS	2.1
13	M	101	GLN	2.1
17	Q	69	LYS	2.1
16	P	5	ARG	2.0
18	R	85	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
17	Q	71	PHE	2.0
2	B	31	TYR	2.0
9	I	64	THR	2.0
12	L	100	ILE	2.0
4	D	7	PRO	2.0
16	P	8	ARG	2.0
3	C	103	VAL	2.0
11	K	50	TYR	2.0
18	R	43	PHE	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, 95th 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	0.87	0.34	234,259,275,280	0
1	7MG	A	527	24/25	0.88	0.25	127,137,152,160	0
1	5MC	A	1404	21/22	0.89	0.36	132,137,141,146	0
1	PSU	A	1541	20/21	0.89	0.21	232,243,250,252	0
1	MA6	A	1518[A]	24/25	0.90	0.28	109,121,135,142	24
1	MA6	A	1518[B]	24/25	0.90	0.28	126,134,140,141	24
1	4OC	A	1402	22/23	0.91	0.26	117,134,153,154	0
1	PSU	A	516	20/21	0.91	0.15	143,152,163,165	0
1	MA6	A	1519[B]	24/25	0.94	0.38	105,117,131,134	24
1	5MC	A	1400	21/22	0.94	0.16	106,127,151,157	0
1	MA6	A	1519[A]	24/25	0.94	0.38	104,118,124,129	24
1	M2G	A	966	25/26	0.95	0.21	120,145,181,186	0
1	5MC	A	1407	21/22	0.95	0.19	140,145,154,161	0
1	UR3	A	1498	21/22	0.95	0.32	115,130,138,144	0
1	2MG	A	1207	24/25	0.97	0.10	148,156,161,163	0
1	5MC	A	967	21/22	0.97	0.15	134,149,157,162	0
12	0TD	L	92	10/11	0.98	0.39	130,141,148,274	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, 95th 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	G	201	1/1	0.09	1.05	157,157,157,157	0
22	MG	A	1732	1/1	0.11	0.14	161,161,161,161	0
22	MG	A	1675	1/1	0.24	1.45	95,95,95,95	0
22	MG	A	1632	1/1	0.33	0.58	161,161,161,161	0
22	MG	A	1728	1/1	0.41	0.15	120,120,120,120	0
22	MG	A	1756	1/1	0.45	0.17	132,132,132,132	0
22	MG	A	1754	1/1	0.47	0.35	121,121,121,121	0
22	MG	A	1736	1/1	0.52	0.53	112,112,112,112	0
22	MG	A	1750	1/1	0.53	1.45	137,137,137,137	0
22	MG	A	1751	1/1	0.56	1.18	170,170,170,170	0
22	MG	A	1747	1/1	0.56	0.83	102,102,102,102	0
22	MG	A	1752	1/1	0.58	0.61	156,156,156,156	0
22	MG	A	1722	1/1	0.59	0.34	73,73,73,73	0
22	MG	A	1653	1/1	0.60	1.57	100,100,100,100	0
22	MG	A	1601	1/1	0.61	0.64	96,96,96,96	0
22	MG	A	1737	1/1	0.62	0.60	143,143,143,143	0
22	MG	A	1634	1/1	0.63	0.56	113,113,113,113	0
22	MG	S	101	1/1	0.63	0.24	137,137,137,137	0
22	MG	A	1628	1/1	0.65	0.28	127,127,127,127	0
22	MG	A	1729	1/1	0.68	0.78	94,94,94,94	0
22	MG	A	1760	1/1	0.68	0.47	121,121,121,121	0
22	MG	A	1741	1/1	0.71	0.29	111,111,111,111	0
22	MG	A	1738	1/1	0.71	0.73	126,126,126,126	0
22	MG	E	201	1/1	0.74	0.42	95,95,95,95	0
22	MG	A	1650	1/1	0.74	0.43	120,120,120,120	0
22	MG	A	1762	1/1	0.74	0.27	136,136,136,136	0
22	MG	A	1742	1/1	0.75	0.32	97,97,97,97	0
22	MG	A	1689	1/1	0.75	1.29	107,107,107,107	0
22	MG	A	1755	1/1	0.75	0.21	148,148,148,148	0
22	MG	A	1734	1/1	0.77	0.19	136,136,136,136	0
22	MG	A	1605	1/1	0.77	0.24	293,293,293,293	0
22	MG	A	1674	1/1	0.77	0.31	114,114,114,114	0
22	MG	A	1749	1/1	0.78	1.28	134,134,134,134	0
22	MG	A	1735	1/1	0.78	0.32	143,143,143,143	0
22	MG	A	1619	1/1	0.79	0.16	132,132,132,132	0
22	MG	A	1753	1/1	0.79	0.71	118,118,118,118	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	MG	A	1617	1/1	0.79	0.53	109,109,109,109	0
22	MG	A	1638	1/1	0.79	0.55	95,95,95,95	0
22	MG	A	1646	1/1	0.79	0.20	153,153,153,153	0
22	MG	A	1706	1/1	0.80	0.16	400,400,400,400	0
22	MG	A	1764	1/1	0.80	0.51	132,132,132,132	0
22	MG	A	1744	1/1	0.80	0.15	115,115,115,115	0
22	MG	A	1707	1/1	0.80	0.11	411,411,411,411	0
22	MG	A	1698	1/1	0.80	0.12	424,424,424,424	0
22	MG	A	1630	1/1	0.81	1.23	127,127,127,127	0
22	MG	A	1614	1/1	0.81	0.87	113,113,113,113	0
22	MG	A	1622	1/1	0.82	0.53	88,88,88,88	0
22	MG	A	1715	1/1	0.83	0.09	167,167,167,167	0
22	MG	A	1701	1/1	0.83	0.24	383,383,383,383	0
22	MG	A	1613	1/1	0.83	0.80	88,88,88,88	0
22	MG	A	1673	1/1	0.83	0.32	121,121,121,121	0
22	MG	A	1672	1/1	0.84	0.43	129,129,129,129	0
22	MG	H	201	1/1	0.84	0.22	83,83,83,83	0
22	MG	A	1758	1/1	0.84	1.46	139,139,139,139	0
22	MG	A	1716	1/1	0.85	0.25	497,497,497,497	0
22	MG	A	1643	1/1	0.85	0.19	245,245,245,245	0
22	MG	F	201	1/1	0.87	0.26	127,127,127,127	0
22	MG	A	1652	1/1	0.87	0.39	127,127,127,127	0
22	MG	A	1746	1/1	0.88	0.07	185,185,185,185	0
22	MG	A	1681	1/1	0.88	0.70	107,107,107,107	0
22	MG	A	1615	1/1	0.88	0.54	92,92,92,92	0
22	MG	A	1661	1/1	0.88	0.14	105,105,105,105	0
22	MG	A	1676	1/1	0.88	0.21	153,153,153,153	0
22	MG	A	1679	1/1	0.88	0.52	140,140,140,140	0
22	MG	A	1761	1/1	0.88	0.10	148,148,148,148	0
22	MG	A	1731	1/1	0.89	1.36	185,185,185,185	0
22	MG	A	1659	1/1	0.89	0.17	100,100,100,100	0
22	MG	A	1703	1/1	0.89	0.37	475,475,475,475	0
22	MG	A	1745	1/1	0.89	1.41	107,107,107,107	0
22	MG	A	1705	1/1	0.89	0.10	310,310,310,310	0
22	MG	A	1726	1/1	0.89	0.15	127,127,127,127	0
22	MG	A	1678	1/1	0.89	0.99	79,79,79,79	0
22	MG	A	1639	1/1	0.89	0.13	133,133,133,133	0
22	MG	A	1727	1/1	0.90	0.29	92,92,92,92	0
22	MG	A	1631	1/1	0.90	0.11	277,277,277,277	0
22	MG	A	1695	1/1	0.90	0.08	184,184,184,184	0
22	MG	A	1730	1/1	0.90	0.22	181,181,181,181	0
22	MG	K	202	1/1	0.90	0.07	110,110,110,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	MG	A	1685	1/1	0.90	0.18	136,136,136,136	0
22	MG	A	1607	1/1	0.91	0.11	134,134,134,134	0
22	MG	A	1671	1/1	0.91	0.83	108,108,108,108	0
22	MG	A	1694	1/1	0.91	0.09	244,244,244,244	0
22	MG	A	1710	1/1	0.91	0.07	470,470,470,470	0
22	MG	A	1649	1/1	0.91	0.28	102,102,102,102	0
22	MG	A	1644	1/1	0.91	0.20	279,279,279,279	0
22	MG	A	1720	1/1	0.91	0.06	324,324,324,324	0
22	MG	A	1660	1/1	0.91	0.45	107,107,107,107	0
22	MG	A	1683	1/1	0.91	0.06	264,264,264,264	0
22	MG	A	1696	1/1	0.92	0.19	390,390,390,390	0
22	MG	A	1629	1/1	0.92	0.13	192,192,192,192	0
22	MG	A	1635	1/1	0.92	0.06	129,129,129,129	0
22	MG	A	1693	1/1	0.92	0.81	94,94,94,94	0
22	MG	A	1658	1/1	0.92	0.26	130,130,130,130	0
22	MG	K	201	1/1	0.92	0.44	93,93,93,93	0
22	MG	A	1633	1/1	0.92	0.17	171,171,171,171	0
22	MG	A	1763	1/1	0.92	0.20	148,148,148,148	0
22	MG	A	1621	1/1	0.93	0.21	107,107,107,107	0
22	MG	A	1669	1/1	0.93	0.80	89,89,89,89	0
22	MG	A	1759	1/1	0.93	1.00	132,132,132,132	0
22	MG	A	1691	1/1	0.94	0.08	109,109,109,109	0
22	MG	A	1665	1/1	0.94	0.21	102,102,102,102	0
22	MG	A	1708	1/1	0.94	0.09	262,262,262,262	0
22	MG	A	1657	1/1	0.94	0.26	95,95,95,95	0
22	MG	A	1711	1/1	0.94	0.13	398,398,398,398	0
22	MG	A	1609	1/1	0.94	0.21	140,140,140,140	0
22	MG	A	1603	1/1	0.94	0.09	184,184,184,184	0
22	MG	A	1642	1/1	0.94	0.08	191,191,191,191	0
22	MG	A	1721	1/1	0.94	0.12	259,259,259,259	0
22	MG	A	1684	1/1	0.94	0.66	128,128,128,128	0
22	MG	A	1740	1/1	0.94	0.19	130,130,130,130	0
22	MG	A	1647	1/1	0.94	0.97	141,141,141,141	0
22	MG	A	1662	1/1	0.94	0.24	110,110,110,110	0
22	MG	A	1733	1/1	0.95	0.14	143,143,143,143	0
22	MG	A	1743	1/1	0.95	0.35	104,104,104,104	0
22	MG	A	1692	1/1	0.95	0.12	126,126,126,126	0
22	MG	D	302	1/1	0.95	0.19	130,130,130,130	0
22	MG	A	1702	1/1	0.95	0.08	259,259,259,259	0
22	MG	A	1610	1/1	0.95	0.27	87,87,87,87	0
22	MG	A	1757	1/1	0.95	0.93	121,121,121,121	0
22	MG	A	1623	1/1	0.95	0.41	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	MG	A	1611	1/1	0.95	0.19	153,153,153,153	0
22	MG	A	1690	1/1	0.95	0.42	96,96,96,96	0
22	MG	A	1663	1/1	0.95	0.41	122,122,122,122	0
22	MG	A	1624	1/1	0.96	0.10	114,114,114,114	0
22	MG	A	1651	1/1	0.96	0.27	95,95,95,95	0
22	MG	A	1713	1/1	0.96	0.12	192,192,192,192	0
22	MG	A	1714	1/1	0.96	0.13	200,200,200,200	0
22	MG	A	1666	1/1	0.96	0.32	97,97,97,97	0
22	MG	A	1667	1/1	0.96	0.51	93,93,93,93	0
22	MG	A	1668	1/1	0.96	0.21	115,115,115,115	0
22	MG	A	1654	1/1	0.96	0.09	105,105,105,105	0
22	MG	A	1670	1/1	0.96	0.94	111,111,111,111	0
22	MG	A	1687	1/1	0.97	0.31	157,157,157,157	0
22	MG	A	1699	1/1	0.97	0.09	426,426,426,426	0
22	MG	A	1620	1/1	0.97	0.15	114,114,114,114	0
22	MG	A	1748	1/1	0.97	1.41	97,97,97,97	0
22	MG	A	1677	1/1	0.97	0.79	89,89,89,89	0
22	MG	A	1640	1/1	0.97	0.35	141,141,141,141	0
22	MG	A	1704	1/1	0.97	0.08	436,436,436,436	0
22	MG	A	1664	1/1	0.97	0.12	101,101,101,101	0
22	MG	A	1724	1/1	0.97	0.11	290,290,290,290	0
22	MG	A	1608	1/1	0.97	0.11	143,143,143,143	0
22	MG	A	1626	1/1	0.97	0.14	108,108,108,108	0
22	MG	A	1637	1/1	0.97	0.17	235,235,235,235	0
22	MG	A	1616	1/1	0.97	0.21	127,127,127,127	0
22	MG	A	1697	1/1	0.97	0.09	411,411,411,411	0
22	MG	A	1719	1/1	0.98	0.09	320,320,320,320	0
22	MG	A	1618	1/1	0.98	0.18	147,147,147,147	0
22	MG	A	1739	1/1	0.98	0.46	96,96,96,96	0
22	MG	A	1686	1/1	0.98	0.12	118,118,118,118	0
22	MG	A	1636	1/1	0.98	0.59	186,186,186,186	0
22	MG	A	1680	1/1	0.98	0.13	134,134,134,134	0
22	MG	A	1655	1/1	0.98	0.14	96,96,96,96	0
22	MG	A	1656	1/1	0.98	0.14	68,68,68,68	0
22	MG	A	1625	1/1	0.98	0.30	123,123,123,123	0
22	MG	A	1712	1/1	0.99	0.65	376,376,376,376	0
22	MG	A	1641	1/1	0.99	0.27	96,96,96,96	0
22	MG	A	1604	1/1	0.99	0.11	90,90,90,90	0
22	MG	A	1627	1/1	0.99	0.23	121,121,121,121	0
22	MG	A	1602	1/1	0.99	0.13	114,114,114,114	0
22	MG	A	1717	1/1	0.99	0.19	254,254,254,254	0
22	MG	A	1645	1/1	0.99	0.17	141,141,141,141	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	MG	A	1612	1/1	0.99	0.20	104,104,104,104	0
22	MG	A	1688	1/1	0.99	0.37	84,84,84,84	0
22	MG	A	1606	1/1	0.99	0.28	154,154,154,154	0
22	MG	A	1723	1/1	0.99	0.10	181,181,181,181	0
22	MG	A	1709	1/1	0.99	0.08	354,354,354,354	0
22	MG	A	1725	1/1	0.99	0.24	114,114,114,114	0
22	MG	A	1648	1/1	0.99	0.30	227,227,227,227	0
22	MG	A	1700	1/1	0.99	0.18	129,129,129,129	0
23	ZN	D	301	1/1	0.99	0.23	136,136,136,136	0
22	MG	A	1718	1/1	1.00	0.18	111,111,111,111	0
22	MG	A	1682	1/1	1.00	0.40	126,126,126,126	0
23	ZN	N	101	1/1	1.00	0.20	148,148,148,148	0

6.5 Other polymers (i)

There are no such residues in this entry.